ABSTRACT BOOK

International research
and practice conference:

NANOTECHNOLOGY AND NANOMATERIALS (NANO-2022)

25-27 August 2022
Lviv, Ukraine

INTERNATIONAL RESEARCH AND PRACTICE CONFERENCE “NANOTECHNOLOGY AND NANOMATERIALS”

(The NANO-2022 Conference is dedicated
to the International Year of Basic Sciences
for Sustainable Development)

25-27 of August 2022

Lviv, UKRAINE

Abstract book

УДК 536:669

The International research and practice conference “Nanotechnology and nanomaterials” (NANO-2022). Abstract Book of participants of the International research and practice conference, 25–27 August 2022, Lviv. Edited by Dr. Olena Fesenko. – Kyiv: LLC APF POLYGRAPH SERVICE, 2022. – P. 542.

This book contains the abstracts of contributions presented at the International research and practice conference “Nanotechnology and Nanomaterials” (NANO-2022).

The NANO-2022 Conference was organized by the Institute of Physics of NAS of Ukraine with the participation of the University of Tartu (Estonia), the Lviv Polytechnic National University, University of Turin (Italy) and Pierre and Marie Curie University – Paris 6 (France).

NANO-2021 was the ninth conference in the series of NANO-conferences initiated by the Institute of Physics of NAS of Ukraine in 2012 in the framework of FP7 Nanotwining project. From year to year, they attract more attention and participants. In 2012, the first meeting was held in the format of International Summer School for young scientists «Nanotechnology: from fundamental research to innovations». The 2013 and 2014 conferences were organized in conjunction with the International Summer Schools for young scientists under the same title. In 2013, this event was attended by more than 300 scientists, in 2014-2017, 450 scientists took part and in 2018 it gathered above 650 participants. In 2021 conference was attended by more than 700 scientists from Ukraine, Poland, Italy, Estonia, France, Austria, Germany, Greece, Turkey, USA, Romania, Moldova, Czech Republic, Taiwan, Lithuania, Egypt, Iran, India, Algeria, Indonesia and other countries. In 2021 the Organizer Committee has received more than 800 application forms from about 25 countries of the world.

The NANO-2022 conference brought together leading scientists and young researchers from many countries of the world. This year its topics were as follows: Nanobiotechnology for health-care; Nanochemistry and biotechnology; Nanocomposites and nanomaterials; Nanoobjects microscopy; Nanooptics and photonics; Nanoplasmonics and surface enhanced spectroscopy; Nanoscale physics; Nanostructured surfaces; Physico-chemical nanomaterials science.

Website of the Nano-2022 conference: http://nano-conference.iop.kiev.ua

In order to support the formation of the communications between the scientific and

innovation communities the EEN-Ukraine consortium together with EEN partners in Germany organized STARTUP2022 competition for selection 10 the best Ukrainian startups for participation in the Start-up BW Summit, Germany.

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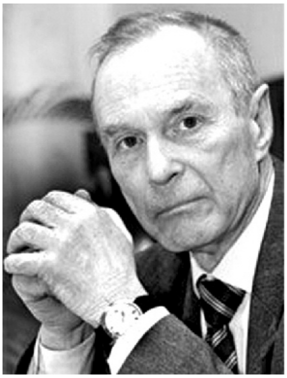
Welcome to International Conference «NANOTECHNOLOGY AND NANOMATERIALS»!



It gives me a great pleasure to welcome you all at the International Conference “Nanotechnology and nanomaterials” (NANO-2022) that will be held in Lviv from August 25 to 27, 2022. Its aim is to promote scientific contacts and discussions between researchers representing various fields.

Previous NANO Conferences, held in Ukraine in 2013-2021, allowed the participants, including young scientists, to familiarize with current research and application problems in this area and thus forward implementation of nanotechnologies into innovations meeting public needs. The events also gave the opportunity to young and early-career researchers to attend lectures of internationally recognized experts and roundtable discussions on the emerging fields in nanosciences and nanotechnologies.

Our previous International Conferences and Summer Schools received positive feedback from international experts and from the media. Now we are holding the 10th such meeting, for which we are deeply grateful to its indefatigable initiator and organizer, Dr. Olena Fesenko and all her assistants, as well as to the universities and institutes that hospitably welcome the participants.

This year above 600 registration forms have been received from scientists representing more than 30 countries. We especially appreciate the participation in the conference of our foreign colleagues, both those who attend here and those who communicate their works remotely.

The fruitful cooperation of scientists is highly important not only to science itself. It helps us to overcome political and war conflicts and misunderstandings and to find our just peaceful future, which is now vitally important not only to Ukraine but also to other countries.

I wish the participants of the Conference to successfully share and broaden their knowledge in nanoscience and nanotechnologies, to advance the networking and launch new contacts between academia and research players in this area and thus to create a good basis for further practical contributions.

May good health serve us and promote creative success in our research!

Academician of NAS of Ukraine,
Professor **Anton G. Naumovets**

Group photo of participants of the 1st International Summer School for young scientists "NANOTECHNOLOGY: from fundamental research to innovations" (Bukovel 2012)

Interview with Prof. Dr. Thomas A. Klar, Director of the Institute of Applied Physics, Johannes Kepler University of Linz, Austria

At the lecture during the 1st International Summer School

Summer school participants on the background of the monument, which is a symbol of the geographical center of Europe (Rakhiv district)

Closing ceremony of the 1st International Summer School for young scientists "NANOTECHNOLOGY: from fundamental research to innovations"

Group photo of the 2nd International Summer School participants
(Bukovel 2013)

Summer School participant
PhD. Vorokhta M. (Czech Republic)
tries to play trembita

Plenary Session

The organizing committee
working hard

PhD. Lyashchova A.G.
(Ukraine)

Group photo of 1st International NANO–2013 Conference participants
(Bukovel 2013)

Opening speech by Dr. habil. Emmanuelle Lacaze (France)

Online presentation of the Springer book with selected proceedings of the 1st International Summer School

Head of the Local organizing committee Dr. O.Fesenko

Excursion to the city of Lviv

Group photo of 3rd International Summer School participants (Yaremche 2014)

Discussion with speaker

Hiking the path of Dovbush, Carpathians

Director of Institute of Physics of NAS of Ukraine Prof. Leonid Yatsenko awards prizes to the winners of competition

Interview with Prof. Leonid Chernozatonskiy from Prokhorov Institute of general physics (Russia)

Group photo of the 3rd International NANO-2014 Conference participants (Lviv, 2014)

Choir of Lviv National Ivan Franko University performsthe national anthem of Ukraine

Opening speech of Rector of Ivan Franko National University of Lviv, Prof. Volodymyr Melnyk

Report of Prof. Francesco Bonaccorso, leading specialist in graphene investigations

Scientific discussion with the audience

Group photo of the 3rd International NANO-2015 Conference participants (Lviv 2015)

Scientific discussion with the audience

Report of Prof. Dr. Thomas A. Klar, Director of the Institute of Applied Physics, Johannes Kepler University of Linz, Austria

Ivan Franko National University of Lviv violin ensemble performans

"Cheremosh" folk song and dance ensemble during the Conference opening ceremony

Group photo of the 4th International NANO-2016 Conference participants (Lviv 2016)

Scientific discussion with the audience

Report of Prof.Dr S. S. Choi (South Korea)

Registration of participants

Excursion to the Museum of Folk Culture and Rural Life in Lviv

Group photo of 5th International Summer School participants
(Bukovel 2017)

Scientific reporting

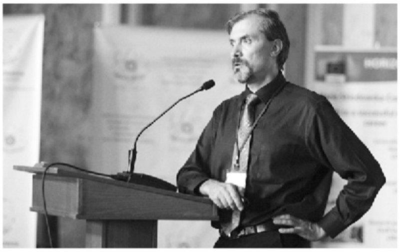
Report of Prof. Dr Stefano Bellucci

Tourist complex Mygovo

Don’t forget for dinner barbeque

Group photo of the 5th International NANO-2017 Conference participants (Chernivtsi 2017)

Report of heads of conference



Report of Prof. Dr. Vadym Mochalin (USA)

Registration of participants

Symphonic orchestra of Chernivtsi

Group photo of the 6th International NANO-2018
Conference participants (Kyiv 2018)

Registration of participants

Report of Dr. Hanna Morozovska
(Ukraine)

Discussion during the poster session

Organizing committee
of NANO-2018

Presentation of Philippe Mariani, CEO of Sophia Antipolis Foundation

Interview for a media

Experts in innovative ecosystem

Discussion with the audience

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choooseosses the best startups

Presentation of Philippe Mariani, CEO of Sophia Antipolis Foundation

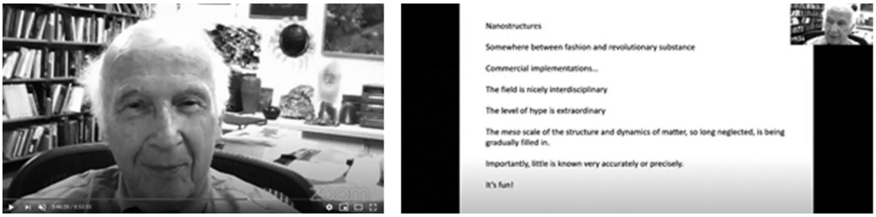
Registration of the participants

Report of Prof. Andzey Suchocki (Austria)

Mr. Jastin Taruska, member of the Innovation start-ups competition jury

Awarding the winners of the Innovation start-up competition

A collective photo of the participants of the NANO-2020 conference
on the stairs of the Lviv House of Scientists



Nanostructures

Somewhere between fashion and revolutionary substance

Commercial implementations...

The field is nicely interdisciplinary

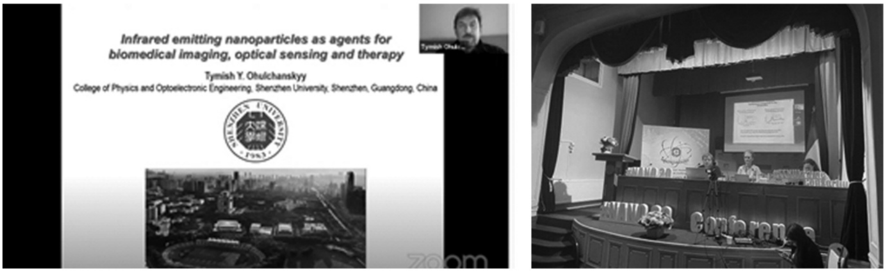
The level of hype is extraordinary

The meso scale of the structure and dynamics of matter, so long neglected, is being gradually filled in.

Importantly, little is known very accurately or precisely.

It's fun!

Online speech by Nobel laureate Roald Goffman

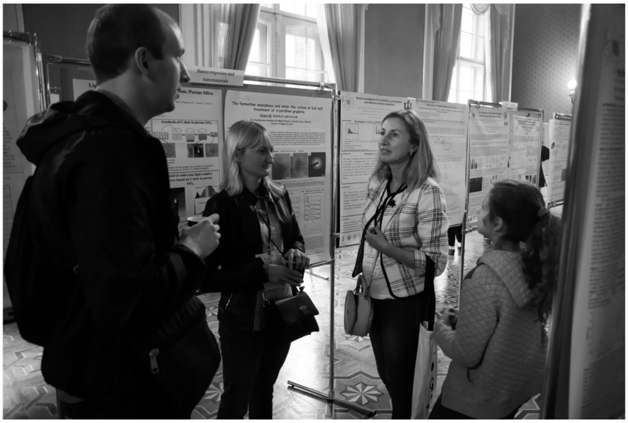


Infrared emitting nanoparticles as agents for biomedical imaging, optical sensing and therapy

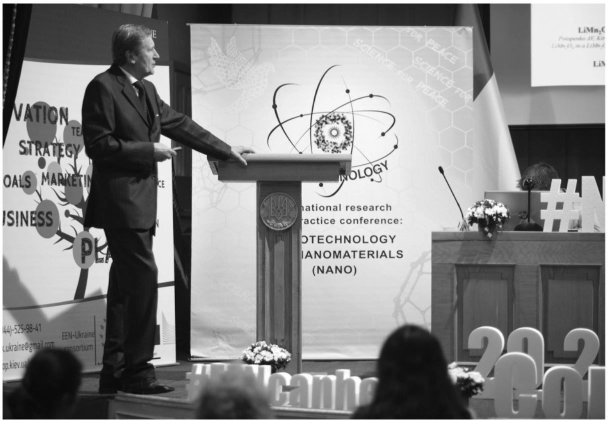
Tymish Y. Ohulchanskyy

College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, Guangdong, China

Online and offline speech by Prof. Tymish Y. Ohulchanskyy
and Dr. Sergey Kolotilov respectively



A participant of the NANO-2021 conference presents his poster to colleagues



Participant of the NANO-2021 conference presents his oral report

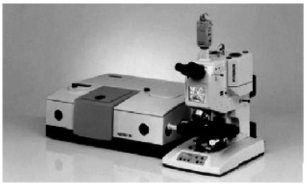
General photo of NANO-2021 conference participants after all official events

INTERNATIONAL LABORATORY "SURFACE ENHANCED SPECTROSCOPY"

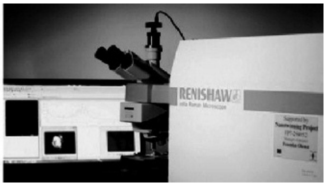
The International "Surface enhanced spectroscopy (SES)" laboratory was created at the International Research and Innovation Cooperation, Technology Transfer Department of the Institute of Physics NAS of Ukraine in the framework of implementation of Nanotwinning Project. This laboratory has a close cooperation with its Partners: Institute of Physics of the University of Tartu (Estonia), Pierre and Marie Curie University (France) and University of Turin (Italy).

Main activity: Study of mechanisms and effects of the enhancement of optical signals from bioorganic molecules near metal and non-metal (carbon, graphene) surfaces using IR and Raman spectroscopy, creation of a new type of substrates for spectroscopy, applications of Surface enhanced Infrared absorption (SEIRA) and Surface enhanced Raman scattering (SERS) spectroscopy.

Equipments: FTIR Spectrometer VERTEX 70 equipped with FTIR microscope HYPERION 1000 (Bruker, Germany), inVia micro-Raman spectrometer (Renishaw, England), UV-260 spectrophotometer (Shimadzu, Japan) with diffuse reflectance attachment and all needed equipment for sample preparation.



FTIR Spectrometer VERTEX 70 (Bruker, Germany)



InVia micro-Raman spectrometer with lasers λ = 786 and 633 nm (Renishaw, England)

The International Laboratory Team has many years' experience in preparation, implementation and management of International Projects.

Laboratory's Projects:

– STCU Project "Rose";
– FP7-PEOPLE-2013-IRSES, Marie Curie actions;
– FP7 Nanotwinning project No 294952;
– NATO "Science for Peace" Project NUKR.SFPP 984702;
– Horizon2020_COS-EEN Project for 2016–2020 years.

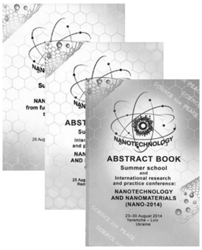
We are interested in cooperation in the field of development of scientific and infrastructural International projects in the frame of Horizon2020 and others Programs.

Head of Laboratory
Dr. Olena Fesenko

Tel: +38 044 525 98 41; mob. +380674076798

E-mail: fesenko@iop.kiev.ua

Our publications



Abstracts Book of the 1st International Summer School (2012)

Abstracts Book of the 1st International Summer School and International Conference NANO 2013

Abstracts Book of the 2nd International Summer School and International Conference NANO 2014

Abstracts Book of the 3nd International Conference NANO-2015

Abstracts Book of the 4nd International Conference NANO-2016

Abstracts Book of the 5nd International Conference NANO-2017

Abstracts Book of the 6nd International Conference NANO-2018

O. Fesenko, L.Yatsenko and M. Brodin et al. (eds.), Nanomaterials, Imaging techniques, Surface Studies, and Applications, Springer Proceedings in Physics 146, DOI: 10.1007/978-1-4614-7675-7, ©Springer Science+Business, Media, New York 2013

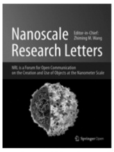
O. Fesenko, L. Yatsenko (eds.), Nanocomposites, Nanophotonics, Nanobiotechnology, and Applications, Springer Proceedings in Physics 156, DOI: 10.1007/978-3-319-0661-0, ©Springer International Publishing, Switzerland 2014

O. Fesenko, L. Yatsenko, Nanoplasmonics, Nano-Optics, Nanocomposites, and Surface Studies 167, DOI: 10.1007/978-3-319-18543-9, ©Springer International Publishing, Switzerland 2015

O. Fesenko, L. Yatsenko, Nanophysics, Nanophotonics, Surface Studies, and Applications 183, DOI: 10.1007/978-3-319-30737-4, ©Springer International Publishing, Switzerland 2016

O. Fesenko, L. Yatsenko, Nanocomposites, Nanostructures, and Their Applications 221, DOI: 10.1007/978-3-030-17759-1, ©Springer International Publishing, Switzerland 2019

O. Fesenko, L. Yatsenko, Nanophotonics, Nanooptics, Nanobiotechnology, and Their Applications 222, DOI: 10.1007/978-3-030-17755-3, ©Springer International Publishing, Switzerland 2019



Participants of International Summer Schools and International NANO Conferences - published their articles in Special Issue of Springer Open Journal “Nanoscale Research Letters” (in 2013, 2014 and 2015) dedicated to NANO Conferences. Impact Factor of Journal - 2.779.

In 2016-2018 it was also possible to publish an articles for participants of the NANO conference in Applied Nanoscience Journal, The European Physical Journal Plus (EPJ Plus) and Applied Sciences Journal (SN).

www.springer.com/materials/nanotechnology/journal/11671

Also, since 2017 year it was possible to publish the articles for participants of NANO Conference in the Molecular Crystals and Liquid Crystals Journal

https://www.tandfonline.com

Our Partners:

The Enterprise Europe Network helps businesses innovate and grow on an international scale. EEN-Ukraine Consortium can help you to find investors, international partner and promote your innovation products. Our contacts:

Website of Consortium: http://www.iop.kiev.ua/~een/

E-mail: een.network.ukraine@gmail.com

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EEN-Ukraine consortium
enterprise europe network
Business Support on Your Doorstep
European Commission

The Enterprise Europe Network (EEN) is a service that provides support for Small and Medium-sized Enterprises (SMEs) with international ambitions. Co-funded by the European Union's COSME and Horizon 2020 programmes, the Network's aim is to help businesses innovate and grow internationally.

The Enterprise Europe Network was launched on 7 February 2008 by former EU Commissioner Günter Verheugen. The Enterprise Europe Network combines the previous Euro Info Centres and the Innovation Relay Centres. From 2008 to 2014, the Network was co-financed by the EU's Competitiveness and Innovation Framework Programme (CIP), in cooperation with institutions at national and regional levels. From 2015-2020, the Network is co-financed under the European Union's programme for the competitiveness of SMEs (COSME) and Horizon 2020.

Under the responsibility of the European Commission's Directorate-General for Internal Market, Industry, Entrepreneurship and SMEs, the Enterprise Europe Network is managed by the Executive Agency for Small and Medium-sized Enterprises (EASME).

The Network is active in more than 70 countries worldwide. It brings together 6,000 experts from more than 600 member organisations, including:

- chambers of commerce and industry
- technology poles
- innovation support organisations
- universities and research institutes
- regional development organisations

Enterprise Europe Network innovation support services are available based on an assessment of the needs and development phase of the business.

At an entry level, Network services include:

- information on innovation-related policies, legislation and support programmes
- links with local innovation stakeholders
- information about access to local sources of funding/support

Network experts can provide one-to-one services to support innovation capacity building. Services include innovation audits, advice on intellectual property, marketing and access to finance.

Finally, the Network provides key account management services to businesses benefitting from the Horizon 2020 SME instrument programme, part of the European Innovation Council (EIC) pilot.

In 2017, Ukraine joined the European Enterprise Network (EEN) within the framework of the COSME program, which promotes the competitiveness and innovative development of SMEs, innovation organizations and institutes/universities. For this purpose in Ukraine was created a Consortium EEN-Ukraine, which included representatives of business and government agencies, as well as scientific organizations. The Coordinator of the EEN-Ukraine Consortium is Institute of Physics of NAS of Ukraine.

To contact EEN-Ukraine please follow the website
http://www.iop.kiev.ua/~een/index-en.html
E-mail: een.network.ukraine@gmail.com
Телефон: +380 44 525 9841

Session 1

Nanocomposites and Nanomaterials

Effect of annealing temperature on the crystal structure of bismuth ferrites

Dolgoshey V.B.

NTUU "KPI named after Igor Sikorsky"
Ukraine,03056, Kyiv, 37, Peremohy Ave.
E-mail: vdolgoshey@ukr.net

The work is devoted to the study of nanocomposites of bismuth ferrites (BFO) and bismuth lanthanum ferrites (BLFO).

The effect of the substitution of the cations Bi to the cations La on the crystalline structure and thermodynamic properties of the ferrites bithmuth were studied [1]. These composites are obtained by the modern method of sol-gel synthesis.

Using scanning electron microscope method it was established that the morphology of BFO and BLFO is the similar.

All samples have a granular microstructure with granule sizes from 20 to 100 nm. This means that on a scale above 200 nm, all samples are morphologically indistinguishable and structural features occurs on smaller scale levels.

The X-ray diffraction study the discovered the crystallinity of bismuth ferrite at a scale level of less than one nanometer. It was found that the formation of nanocomposites based on bismuth ferrite occurs according to the nucleation mechanism of non-isothermal crystallization [2]. Upon cooling of the BFO sample, a three-component material. As a result of the substitution of La cations for Bi cations, a more homogeneous – two-component structure BLFO is formed, which consists of $BiLaFeO_3$ crystallites and $Bi_2Fe_4O_9$ crystallites with approximately equal dimensions (about 0.400 nm^3) [3].

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1. W. Ge, A. Rahman, H. Cheng, M. Zhang, J. Liu, Z. Zhang, B. Ye Probing the role of cation vacancies on the ferromagnetism of La-doped $BiFeO_3$ ceramics // Journal of Magnetism and Magnetic Materials 449, 401 (2018).

2. V. Gerbaud, N. Shcherbakova, S. Da Cunha A nonequilibrium thermodynamics perspective on nature-inspired chemical engineering processes // Chemical Engineering Research and Design 154, 316 (2020).

3. O.Kratky, I.Pilz, P.J.Schmitz Absolute intensity measurement of small angle x-ray scattering by means of a standard sample // J. Colloid Interface Sci. 21(1), 24 (1966).

Improved photodegradation of anionic dyes using a complex graphitic carbon nitride and iron-based metal-organic framework material

Huan V. Doan[1]***, Hoa Thi Nguyen***[2]***, Valeska P. Ting***[3]***, Xuan Nui Pham***[2]

[1] School of Chemistry, University of Bristol, United Kingdom
E-mail: huan.v.doan@bath.edu

[2] Department of Chemical Engineering, Hanoi University of Mining and Geology, Vietnam

[3] Department of Mechanical Engineering, University of Bristol, United Kingdom

Introducing heterostructure to graphitic carbon nitrides (g-C_3N_4) can improve the activity of visible-light-driven catalysts for efficient treatment of multiple toxic pollutants in water [1,2]. Here we report for the first time that a complex material can be constructed from oxygen-doped g-C_3N_4 and MIL-53(Fe) metal-organic framework using a facile hydrothermal synthesis and recycled polyethylene terephthalate from plastic waste. The novel multi-walled nanotube structure with unique interfacial charge transfer at the heterojunction in O-g-C_3N_4/MIL-53(Fe) composite showed an obvious enhancement in separation efficiency of the photochemical electron-hole pairs, resulting in narrow bandgap energy (2.30 eV compared to 2.55 eV in O-g-C_3N_4), high photocurrent intensity (0.17 mA cm^{-2} compared to 0.12 mA cm^{-2} and 0.09 mA cm^{-2} in MIL-53(Fe) and O-g-C_3N_4, respectively), and excellent catalytic performance in the photodegradation of anionic azo dyes (95.1% RR-195 and 99.8% RY-145 degraded after 4 h, and only a minor change in the efficiency observed after four consecutive tests). These results demonstrate the development of new catalysts made from waste feedstocks, high stability and ease of fabrication, which can operate in natural light for environmental remediation.

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*1. Pham X. N., Nguyen B. M., Ngo H. S., Doan H. V., Highly efficient photocatalytic oxidative desulfurization of dibenzothiophene with sunlight irradiation using green catalyst of Ag@AgBr/Al-SBA-15 derived from natural halloysite // J Ind Eng Chem.-2020.-**90**(25).-P. 358-370.*

*2. Pham X. N., Nguyen T. H., Pham T. N., Nguyen T.-Thanh-Bao, Nguyen B. M., Tran Van Thi-T., Doan H. V., Green synthesis of H–ZSM-5 zeolite-anchored O-doped g–C3N4 for photodegradation of Reactive Red 195 (RR 195) under solar light // J Taiwan Inst Chem Eng.-2020.-**114**.-P. 91-102.*

The anticorrosion performances of the zeolite/$Zn(H_2PO_4)_2$ pigment for aluminium alloy

***Danyliak M.-O.M.*, Khlopyk O.P., Zin I.M., Korniy S.A.**

Karpenko Physico-Mechanical Institute of NAS of Ukraine.
Naukova str., 5, Lviv-79060, Ukraine.
E-mail: danyliak-olena@ukr.net

One of the common methods of protecting metal structures from corrosion is paint coatings, which must have high durability in corrosive environments and at the same time be environmentally friendly. Inhibiting pigments are used to increase their anti-corrosion properties [1]. The aim of this work was to study the corrosion inhibition of aluminium alloy by zeolite/$Zn(H_2PO_4)_2$ pigment. The corrosion resistance of the aluminium alloy in 0.1% NaCl solution with the addition of pigment was studied by the potentiodynamic polarization method, using a saturated Ag/AgCl reference electrode and a counter platinum electrode. Inhibiting effectiveness of the mechanochemically obtained zeolite/phosphate pigment at different components ratios was evaluated (fig. 1). The corrosion resistance of the alloy is significantly increased in the solution with the pigment extract compared to the non-inhibited solution. The greatest anti-corrosion effect is established for zeolite/$Zn(H_2PO_4)_2$ pigment with a concentration of 1 g/l at a 1:1 components ratio, probably due to optimal solubility of its phosphate phase.

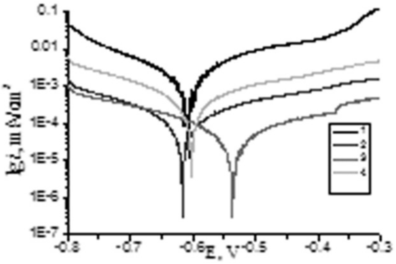

Fig. 1. *Polarization curves of D16T alloy after 96 h exposure in:*
1 - 0.1% NaCl solution and with the addition of the pigment (1 g/l) at different zeolite/$Zn(H_2PO_4)_2$ ratios: 2 - 3:1; 3 - 1:1; 4 - 1:3

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*1. Zin I.M., Korniy S.A., Danyliak M.-O.M., Khlopyk O.P., Holovchuk M.Ya. Anti-corrosion protection of aluminium alloy by zeolite doped with zinc, calcium and manganese cations // Int. J. Corros. Scale Inhib.-2021.-**10**, N 4.-P. 1715-1728.*

The work was performed within the project № 2020.02/0063 "Synthesis and properties of new complex anti-corrosion pigments for paint coatings based on aluminosilicate nanocontainers" of the National Research Foundation of Ukraine.

Transport properties of surface modified single-walled carbon nanotubes

Shpylka D.O.[1]***, Ovsiienko I.V.***[1]***, Len T.A.***[1]***, Matzui L.Yu.***[1]***,***
Prylutskyy Yu.I.[2]***, Tsaregradskaya T.L.***[1]***, Mirzoiev I.G***[3]

[1] *Taras Shevchenko National University of Kyiv, Department of Physics*[1] *and Biophysics*[2]*, 01601, Volodymyrska st. 64/13, Kyiv, Ukraine*

[3] *B. Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, 61103, Nauky Ave. 47, Kharkiv, Ukraine*
E-mail: denys8600@ukr.net

In the work the results of complex investigations of electrical and magnetic conductivity of bulk specimens of as prepared and surface modified single-walled carbon nanotubes (SWCNTs) are presented. As prepared SWCNTs have been produced by acetylene decomposition method with use nickel as catalysts. These SWCNTs have been modified on surface by cobalt-containing complexes according to several schemes with different sequence of main stages, such as cutting of tubes along defects, removal of metal catalyst and particles of disordered carbon, forming of complicated cobalt-containing complexes at SWCNTs surface. For investigation of electrical and magnetic resistivity, the bulk specimens from as prepared and modified SWCNTs powders have been made by cold compacting without binder. The resistance has been measured in the temperature interval from 4.2 K to 293 K and in the magnetic fields up to 2.5 T.

Figure 1 presents the temperature (a) and magnetic field (b) dependences of resistivity ρ for bulk specimens of as prepared and modified SWCNTs.

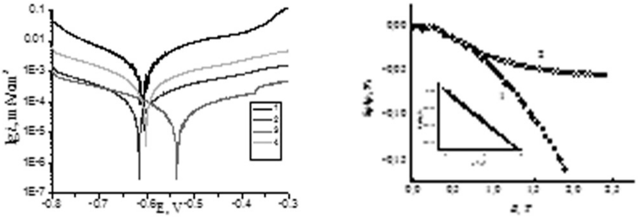

Fig 1. *Dependences of resistivity ρ(T)(a) and magnetoresistance δρ/ρ(B)(b) for bulk specimens of as prepared (1) and modified (2) SWCNTs. Inset: dependence δρ/ρ(B^2) for as prepared SWCNTs, T = 77 K*

It is found that for as prepared SWCNTs, the main mechanism of conductivity is 3D hopping with the variable hopping length. Surface modification of SWCNTs with cobalt -containing complexes leads to the creation on the surface of SWCNT small localized negative charge. For modified SWCNTs the bulk specimens' conductivity is described in the terms of power temperature law, that is typical for individual SWCNTs.

Transverse resistivity of acceptor graphite intercalation compounds

Ovsiienko I.V.[1], Len T.A.[1], Matzui L.Yu.[1], Shpylka D.O.[1], Naumova D.D.[2]

Taras Shevchenko National University of Kyiv, Departments of Physics[1] and Chemistry[2], 01601, Volodymyrska st. 64/13, Kyiv, Ukraine
E-mail: iaryna2002@gmail.com

The work presents the results of investigations of transverse resistivity (resistivity perpendicular to graphite layers) for acceptor graphite intercalation compounds (GICs) based both high oriented pyrolitic graphite (HOPG, distance between graphite layers $d_{002} = 0.335$ nm, crystalline size $L = 500$ nm, anisotropic parameter $\eta = 10^4$) and fine crystalline anisotropic pyrolytic graphite (FAPG, $d_{002} = 0.340$ nm, $L = 30$ nm, $\eta = 10^3$). Intercalation compounds with aluminum, iodine and antimony chlorides have been obtained by gas-phase two-temperature method. The transverse resistivity temperature dependence ($\rho_c(T)$) has been measured by standard four-probe methods in temperature interval from 4.2 K up to 300 K.

Figure 1 presents the dependences $\rho_c(T)$) for GICs of different stages with $SbCl_5$ based on HOPG (a) and FAPG) (b).

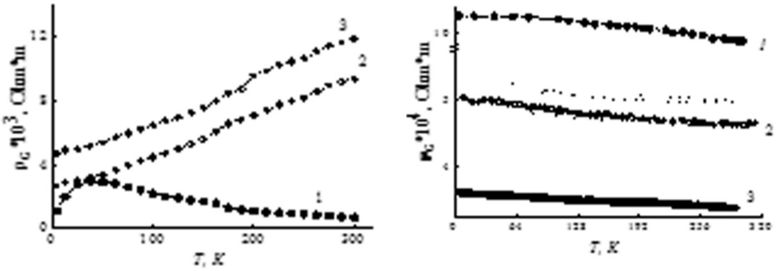

***Fig 1**. Dependences ρc(T) for GICs with SbCl5 based on HOPG (a) and FAPG) (b): 1 – host graphite, 2 - S = 2, 3 - S = 3.*

As can be seen from the Figure, the value of resistivity for GICs of different stages, as well as the character of the temperature dependence $\rho_c(T)$ significantly depend on the structure of the host graphite. Experimental and theoretical studies have shown that transverse conductivity is determined by a combination of two mechanisms. These mechanisms are diffusion motion along the graphite planes and jumping conductivity between adjacent graphite layers. Differences in the temperature dependence of the resistivity for GICs based on structurally different forms of graphite can be described in terms of proposed model and are related primarily to the difference in the crystallites size in the host graphites.

Prediction of Substitution Limits and Thermodynamic Stability for $Y_{1-x}Ln^{x}F_3$ (Ln = Sm–Lu) Nanosized Materials

***Get'man E.I.*[1]*, Oleksii Yu.A.*[1]*, Ardanova L.I.*[2,*]*, Radio S.V.*[1,*]**

[1] Vasyl' Stus Donetsk National University, Vinnytsia, 21027 Ukraine
[2] Minnesota State University, Mankato, Minnesota, 56001 USA
** e-mail: radio@donnu.edu.ua, lyudmyla.stackpool@mnsu.edu*

Recently the trifluorides of rare-earth elements (REE) attract more attention from researchers in various fields of science and technology, such as optoelectronic devices, phosphors, lasers, and others. The studies on their application in the form of nanomaterials in medicine as optical 3D devices, probes for visualization of biological objects, for intracellular labels or measurements, and immunoassays have become relevant. In many cases, not individual compounds but solid solutions whose properties can be controlled based on the composition are being used.

However, the physicochemical foundations for the synthesis of solid solutions such as state diagrams and the solubility regions are much less studied than the dependencies of the composition-physical properties. There are practically no data on substitution limits and stability regions of solid solutions.

Using V. Urusov's crystal-chemical model, in the approximation of regular solutions, the mixing energies (interaction parameters), critical temperatures of decomposition (stability), and substitution limits were calculated for 10 systems $Y_{1-x}Ln_xF_3$ solid solutions, where Ln = Sm–Lu. It was established that the mixing energies and critical decomposition temperatures of solid solutions first decrease in the series of Sm–Er, then increase in the series Er–Lu trifluoride systems as the REE atomic number increases. It was shown that the total mixing energy is determined mainly by the difference in the sizes of the substituting structural units and to a lesser extent by the difference in the degrees of ionicity of the chemical bond of the systems' components. The presented diagram of thermodynamic stability for systems $Y_{1-x}Ln_xF_3$, Ln = Sm–Lu makes it possible to visually evaluate not only the thermodynamic stability, instability, and metastability of the solid solutions in a wide range of compositions and temperatures but also the substitution limits for limited series of solid solutions for a given decomposition temperature, or the temperature of their decomposition according to the given substitution limit.

Using the Becker equation, the decomposition temperatures (T_d) of solid solutions in the $Y_{1-x}Ln_xF_3$, Ln = Sm–Lu systems were calculated for the composition range $1.0 > x > 0$ with a step size, $x = 0.05$. According to calculations, the T_d of solid solutions of the YF_3–LnF_3, Ln = Sm–Lu systems are in the interval 51 K–685 K.

XRD studies of the precursor thermal decomposition in the production of nanopowders $LaLuO_3$:Yb^{3+} with a perovskite type structure

***Shyrokov O.V.*[1], *Lobunets T.F.*[1], *Chudinovych O.V.*[1,2], *Ragulya A.V.*[1,2]**

[1] Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine.
Krzhizhanivskoho Str., 3, Kyiv-03142, Ukraine.
E-mail: shyrokovav@gmail.com

[2] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute". Prospect Peremohy, 37, Kyiv-03056, Ukraine.

Since the invention of the first laser with a polycrystalline active medium in 1964 [1], scientists have been constantly searching for ways to improve its performance, requiring the development and research of new materials with given properties.

The process of structure formation evolution during thermal decomposition of the precursor synthesized by precipitation in obtaining complex perovskite type oxide phases in La_2O_3-Lu_2O_3-Yb_2O_3 system was observed by X-ray diffraction using the powder method. Two main steps were found. The first one is related to the amorphous structure: the decomposition of the complex chemical compound formed after the precipitation and its internal rearrangement, and the second one to the formation and accumulation of the perovskite crystalline phase.

X-ray spectra of the samples obtained at temperatures up to 700°C at the first stage of the decomposition contain two broad diffuse peaks (halo) at 22-38° and 38-70°. In the interval of precursor's thermal decomposition temperatures from 120 to 700°C the processes of complex compound decomposition and internal rearrangement take place. An amorphous powder is formed with a gradual increase in the atomic ordering, evidenced by a decrease and a qualitative change in the background. Possibly ordered domains typical for REE carbides, hydrides or carbohydrides are formed in the amorphous matrix.

With further increase in temperature the second main stage of decomposition begins. The process of formation and accumulation of the perovskite crystal phase is not uniform. At 750-780 °C the size of crystallites of the perovskite type phase $LaLuO_3$:Yb^{3+} rapidly increases, after which the growth slows down.

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Ex-situ vs. in-situ fabrication routes for luminescent nanocomposites C-dots/porous silica

Rudko G.Yu.[1,2], Isaieva O.F[1,2], Vasin A.V. [1,3], Kysil D.V.[1],
Gule E.G.[1], Nazarov A.N.[1,3], Capoen B.[4],
Bouazaoui M.[4], Hamzaoui H. El.[4], Sevostianov S.V.[5]

[1] *V. Lashkaryov Institute of Semiconductor Physics of National Academy of Sciences of Ukraine, 45, Pr. Nauky, Kiev, 03028, Ukraine.*
E-mail: oksana.isaieva@isp.kiev.ua

[2] *National University "Kyiv-Mohyla Academy",*
Skovorody, 2, Kiev, 04070, Ukraine.

[3] *National Technical University Igor Sikorsky Kyiv Polytechnic Institute", Kyiv 03056, Ukraine*

[4] *Univ-Lille, CNRS, UMR8523 – Physique des Lasers AtomesetMolequles, CERLA/IRCICA, F-59000, Lille, France.*

[5] *Chuiko Institute of Surface Chemistry of NASU, Kyiv, Ukraine.*

It is known that carbon nanodots are effective light emitters. Colloidal solutions of carbon nanodots demonstrate quantum yield 90 % and above. Thus, they are promising candidates for the fabrication of light-emitting devices as well as for bio-medical applications, such as disease diagnostics. Among the advantages of these nano-objects one must mention their comparative cheapness, environmentally friendly fabrication routes, ability to control their color properties of emission. Therefore, carbon nanoobjects attract a lot of research attention nowadays.

Recently a new method of carbon nanostructures synthesis using a porous SiO_2 matrix has been advanced [1]. Carbon nanoparticles were synthesized within the pores of SiO_2 matrix. The silica sample was soaked in the solution of sucrose ($C_{12}H_{22}O_{11}$) that served as a carbon source, diluted in dimethyl sulfoxide (DMSO, $(CH_3)_2SO$). Synthesis of carbon nanoparticles was performed by thermolysis of the solution at temperature 170-180 °C. Thus, the pores restricted the size of the synthesized nanoparticles and the nanodots. This method is the *in-situ* growth.

In the present study we used both the above *in-situ* method and the alternative *ex-situ* method of carbon nano-objects fabrication. The latter method implies the growth of carbon nanoobjects by more standard colloidal route (using the same organic source of carbon and solvent). The first step was the thermolysis of sucrose/DMSO solution that resulted in the formation of concentrated colloid of luminescent carbon nanoparticles. Then the porous silica matrix has been infiltrated by this colloidal solution. Obviously, the sizes of the ready nanoparticles, that were incorporated into the porous silica were limited by the sizes of the pores. To compare the properties of nanoparticles grown by these two routes we washed out the nanoparticles from the porous silica/nanoparticles solid composites obtained either by in-situ or ex-situ methods, and studied the optical properties of the solutions obtained. The photoluminescence excitation and emission spectra of these colloidal solutions of carbon nanoparticles synthesized by two methods were studied. It is shown that the synthesis method does not significantly affect the spectral characteristics of the obtained nanoparticle solutions. In particular, when the porous SiO_2 matrix with a pore size of 7 nm was used, the spectral characteristics of nanoparticles synthesized by both methods completely coincide. When the porous SiO_2 matrix with a pore size of 40 nm was used, the position of the PL spectrum maximum for nanoparticles synthesized by the *in situ* method is slightly shifted to the long-wavelength region. Thus, both methods provide nanoparticles with almost the same properties.

When porous SiO_2 with a larger pore size is used, emission spectrum of carbon nanoparticles is characterized by larger half-bandwidth and the position of the maximum is red-shifted as compared with the spectrum of nanoparticles obtained using a matrix with the smaller pore size. Both features point to the formation of nanoparticles of larger sizes and larger dispersion of nanoparticles sizes.

In summary, the luminescent properties of the nanoparticles obtained depend rather on the size of pores in SiO_2 than on synthesis route. Both methods demonstrated the effect of the size of carbon nanoparticles on emission spectra, i.e. broadening and noticeable blue shift of emission band in larger nanoparticles.

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Preparation, characterization of C-doped TiO_2 nanostructures and their photocatalytic activity in visible-light induced decomposition of hydrazine

***Romanovska N.I.*, Manoryk P.A., Shulzhenko O.V.**

Physico-inorganic chemistry Department, L.V. Pysarzhevskii Institute of Physical Chemistry of the NAS of Ukraine.
Prospect Nauki, 31, Kyiv-03039, Ukraine.
E-mail: nat.romanovska@gmail.com

TiO_2 nanostructures are widely investigated as photocatalytic materials in ecological photocatalysis, conductive films for solar cells and Li-ion batteries etc. But, TiO_2 can photogenerate e-/h^+ pairs only under UV-light irradiation, whose share is only 4-5% of solar radiation. That why, nonmetal doping of TiO_2 was investigated as one of an effective instruments for the band gap narrowing and sensitization in the visible-light region. Carbon containing compounds are widely used as carbon precursors in C-doped TiO_2 synthesis, but influence of C-doping on phase composition, morphology, texture were investigated not enough.

The aim of this work was the investigation of phase composition, crystallites size, morphology, texture characteristics of C-TiO_2, obtained by hydrothermal sol-gel method, and testing of their photocatalytic activity in hydrazine photodecomposition processes. The C-TiO_2 were characterized by XRD, SEM, TEM, N_2-ad/desorption, UV-Vis and FTIR-spectroscopy.

It was shown, that carboxylic acids induce anatase phase formation with crystallites size near to 10 nm. The particles size and shape of C-TiO_2 doesn't change significantly with carbon content increasing. The texture characteristics are extremely dependent on dopant content and the maximal SBET and dmeso were 205 m^2/g and 5.5 nm respectively. The C-TiO_2 nanostructures characterized by band gap narrowing to 3,0 eV and wide adsorption band in the visible light range of UV-Vis spectra. The photocatalytic activity of C-TiO_2 was investigated in photocatalytic degradation of hydrazine under UV- and visible light irradiation. The conversion degree of hydrazine on C-TiO_2 is practically independent on dopant amount under UV-light irradiation, but extremely changes under visible light irradiation. The high conversion degree of hydrazine on C-TiO_2 may be induced by synergetic effect of carbon doping and high surface area with small mesopore diameter. It could be concluded, that C-TiO_2 nanostructures obtained by hydrothermal sol-gel method have a small anatase crystallites size, are characterized by high surface area values and demonstrate photocatalytic activity in hydrazine decomposition process under visible light irradiation.

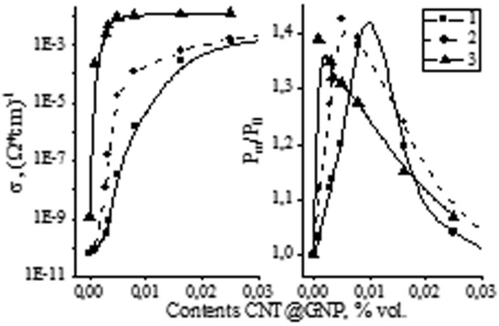
Electrophysical and strength characteristics of polychlortricfluoroethylene filled with carbon nanotubes dispersed in graphene suspensions

Makhno S.M.[1,2]***, Lisova O.M.***[2]***, Mazurenko R.V.***[2]***,***
Gorbyk P.P.[2]***, Kartel M.T.***[1,2]***, Sementsov Yu.I.***[1,2]

[1] Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute,
Kechuang building, N777 Zhongguan road, Ningbo, 315211, China
E-mail: ysementsov@ukr.net

[2] O. Chuiko Institute of Surface Chemistry, NAS of Ukraine,
17 General Naumov Str., Kyiv, 03164, Ukraine.

It is proved that one of the decisive factors that determines the effectiveness of the use of carbon nanotubes (CNT) for the reinforcement of polymeric matrices is their uniform distribution. In this case, it is shown, for example [1], that the flow threshold determined by electrical conductivity data shifts to the region of lower values with a more uniform distribution of CNT and correlates with the structural and strength characteristics of filled polymers. In this study, pre-deagglomeration of CNT was performed by ultrasound treatment in graphene nanoparticle dispersion (GNP). Three water systems with CNT content of 0.5 (1), 0.25 (2) and 0.125 (3) % wt. were dispersed. The GNP content was 0.1 m. h. to CNT. That is, the mass ratio of GNP to CNTs did not change for all systems. As can be seen from the figures, which show the dependences of the relative flexural strength (P_m/P_0) and electrical conductivity (σ) of PCTFE-CNT systems on the content of CNT@GNP, for the sample with the most homogeneous distribution of CNT, which was achieved at minimum CNT content during dispergation (0.125% wt. CNT) there is the lowest percolation threshold, which correlates with the maximum of strength limit.



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Complex Method of forming Composite nanostructures of coatings

Stetsko A.E.

Faculty of computer engineering printing,
Ukrainian Academy of Printing.
Pidgolosko Str., 19, Lviv-79020, Ukraine.
E-mail: andrew73@ukr.net

Structure and properties of surface layers make it an important influence on the performance of products in general. One of the main ways of strengthening steel products are surface diffusion saturation surfaces. Its use is economically more profitable than obtaining alloyed steel with similar properties. Chemical-thermal treatment products can provide a range of performance properties, the achievement of which surround by doping is impossible or economically inefficient.

For machine parts, perspective is a combination of two or more methods of diffusion saturation. Such treatment including special modes enables diffusion hardened surface layers of great hardness and low brittleness that work well in harsh operating conditions [1, 2].

Chemical precipitation is carried out in solutions with the presence of Nickel, which has a very good effect on the morphological features of the reinforced layer. Diffusion saturation is carried out in retorts with a fusible gate according to special thermal regimes. The obtained hardened layer on the surfaces of machine parts after the Complex hardening method has a large thickness up to 500 μm and substantive hardness (20,000 MPa and above) and wear resistance. The integrated method does not require expensive equipment and highly qualified personnel, which makes it extremely competitive.

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Effect of Ar^+ treatment on thermal stability and micromechanical properties of $Fe_{75}Mo_5Si_6B_{14}$ amorphous alloy

Tsaregradskaya T.L.**, **Kozachenko V.V, Ovsiienko I.V., Saenko G.V., Kuryliuk A.M., Turkov O.V., Maidanyk B.O.

Taras Shevchenko National University of Kyiv, Department of Physics
01601, Volodymyrska st. 64/13, Kyiv, Ukraine
E-mail: tsar_grd@ukr.net

Amorphous alloys, or metallic glasses, are materials with homogenous and isotropic structure, lacking long-distance order in atom arrangement. Such structure leads to a specific combination of mechanical and functional properties which makes them ideal for various applications. Amorphous alloys are kinetically and thermodynamically metastable and can exist in a certain range of certain parameters such as temperature, pressure, etc. Outside these ranges, they tend to stabilize through crystallization, usually resulting in a loss of favorable functional properties. Extending the ranges of amorphous alloys existing and controlling their mechanical properties is an important task. We tried solving this problem by amorphous alloy surface treating with Ar^+ ions.

Experimental studies were performed to determine the effect of Ar^+ treatment on the parameters of thermal stability and micromechanical properties of $Fe_{75}Mo_5Si_6B_{14}$ amorphous alloy. The amorphous alloy treatment with argon ions was performed at the following parameters: the voltage at the anode was of 1 kV, the current through the sample was of 1 mA. The morphology study of the surface of the amorphous alloy were performed using LensSEI SEM. The parameters of thermal stability of the amorphous alloy were determined using a highly sensitive dilatometric technique. It is shown, that after Ar^+ treatment of the amorphous alloy for (5-25) minutes, the thermal stability interval expanded by (30-120) K, respectively. When treating an amorphous alloy by Ar^+ for (5-15) minutes, the relative change in microhardness is (2.5-4)%, ie is within the experimental error (5%). When treating $Fe_{75}Mo_5Si_6B_{14}$ amorphous alloy for 25 minutes, the microhardness decreases by 13%, ie the effect of plasticization is observed. The effects of expanding the interval of thermal stability and plasticization of the amorphous alloy can be explained by the dissolution of frozen crystallization centers. This fact is confirmed by studies of the morphology of the amorphous alloy surface. The surface of the amorphous alloy changes dramatically after Ar^+ treatment: small grains disappear, which indicates that frozen crystallization centers dissolve in the amorphous matrix due to action of argon ions flux.

Optimization of photoelectric converters

Beliak Ie.V., Kryuchyn A.A., Manko D.Yu.

Institute for Information Recording of the NAS of Ukraine.
M. Shpak, str 2, Kyiv-03113, Ukraine.
E-mail: beliak1312@gmail.com

The improvement of the efficiency of photovoltaic converters (Power Electronic Transformer, PET) which absorbs solar radiation in the visible and near infrared ranges of the spectrum is relevant for the creation of a new generation of solar photovoltaic systems and optical channels energy transmission optoelectronic systems [1-2]. It should be also noticed that optimization of the characteristics of optoelectronic systems is one of the most important areas in the field of organization of optical monitoring and data transmissions systems. Compact camera units, which today are actively included in the composition of general-purpose electronic devices and, in particular, mobile devices due to the simplification of the optical photo-registration system are characterized by relatively low photosensitivity and imbalance of color rendering scheme. The concept of the luminescent solar concentrator has emerged as an efficient approach to harvesting sunlight economically, able to overcome the factors that limit the conversion efficiency of photovoltaic systems. LSCs (luminescent solar concentrator) consist of a layer containing optically active centers applied to a transparent substrate, which, when exposed to light, converts part of the absorbing radiation corresponding to the short-wave visible and ultraviolet part of the solar spectrum into radiation of a certain wavelength corresponding to the PET absorption spectrum. While part of the emitted signal will be lost at the surface (through the so-called exit cone), the rest will be trapped inside the layer and substrate and directed towards the edges (through total internal reflection) where it can be collected by the photovoltaic cell. Various optically active centers have been tested in LSC, including organic dyes, quantum dots, and trivalent lanthanide ions [3].

An effective way to optimize the characteristics of PET can be the application of photoluminescent layers based on nanostructured photoluminescent dyes with fixed Stokes shear and photoluminescence range, selected according to the absorption spectra of photovoltaic components of triad and tetrads of the photoelectric transducers. Conventional dyes often suffer from a low photoluminescence quantum yield, insufficient photostability, and a insufficient Stokes shift. In other hand the use of organic dye nanoparticles provides efficient luminescence's resonance energy transfer with markedly improved imaging performance. Currently, the most widely used organic dyes, which are usually encapsulated in various nanoparticles to overcome the internal limitations of conventional dyes, including poor hydrophilicity, low photostability, low quantum yield. Compared to pure dyes, organic dye nanoparticles have an almost 50-fold increased quantum yield, large Stokes shifts (~250 nm), and significantly increased photostability [3]. The general principle of optimizing the photoelectric conversion process by applying a photoluminescent layer to the elements of the photo matrix is to transfer radiation to the absorption region of the photoelectric converter — thus, the Stocks shift of the photoluminescent dye should be equal to the difference between the main peak of solar spectrum and the photoelectric converter absorption spectrum.

Obtaining the characteristics of the luminescent converter determined as a result of mathematical modeling is carried out through the use of the procedure of nanostructuring the organic photoluminescent dyes with zeolite pores, laser annealing, and the inclusion of impurities of polymeric materials (polymethyl methacrylate, polystyrene and others). Based on the study, the effectiveness of improving the photosensitivity and color rendering of photodetection systems by expanding the absorption spectrum of photocells was proved and the value of Stokes shift of photoluminescent materials of the coating layer for color channels was calculated.

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Structurally dependent electroconductivity properties of ultrafine composites α-FeOOH/α-Fe_2O_3

Hrubiak A.B.[1], Moklyak M.G.[2], Chelyadyn V.L.[1]

[1]G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,
36 Academician Vernadsky Boulevard, 03142 Kyiv, Ukraine

[2] Joint Educational and Scientific Laboratory of the Physics of Magnetic Films, G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine and Vasyl Stefanyk Precarpathian National University,
Ivano-Frankivsk, 76018, Ukraine
E-mail: mariamoklyak@gmail.com

The method of hydrothermal synthesis of ultrafine composite material defective α-FeOOH/defective α-Fe_2O_3 is implemented and the mechanism of its phase for¬mation is analyzed. It is revealed that due to the control of synthesis time and tem¬perature the processes of high-temperature hydrolysis are initiated with the subse¬quent nucleation of iron hydroxide nuclei and the formation of a defective three- dimensional xerogel network. The influence of material post-processing temperature on phase transformations, change of magnetic microstructure and electrically con¬ductive properties is traced. Two temperature ranges of phase and structural stability of the composite were revealed. Up to a temperature of 150°C there is a preservation of two components of the composite defective α-FeOOH and defective α-Fe_2O_3, which are in a magnetically ordered state and there is a partial recrystallization of ultrafine composite. At a temperature of 250°C completes the phase transition α-FeOOH→α-Fe_2O_3, which is reflected in the change in the mag¬netic microstructure of the material: the magnetically ordered component is repre-sented by only Zeeman sextets corresponding to crystalline and defect crystal structures α-Fe_2O_3.

The influence of phase and structural transformations of the formed ultra-dispersed composites on the manifestation of their electrically conductive properties is established. In particular, the structural organization of the ultrafine defective composite α-FeOOH/α-Fe_2O_3 provides the implementation of the proton conduction mechanism. Conduction in the polymer chains of the hydroxide phase is due to surface percolation of the charge, the initialization of which occurs immediately at low frequencies. Conductivity within hematite agglomerates is realized by capacitive and resistive mechanisms due to free charge carriers. Increasing the frequency of the external electric field causes the formation of free charge carriers within the polymer hydroxide network, as a result of which the conductivity at direct current is realized through both components of the composite.

Thermoelectric Nb doped $SrTiO_3$ with reduced graphene oxide

Okhay O.[1]***, Hortiguela-Gallo M.***[1]***, Otero-Irurueta G.***[1]***, Zlotnik S.***[2]***,***
Orlinski K.[2]***, Pawlak D.A.***[2]***, Xie W.***[3]***, Weidenkaff A.***[3]***, Tkach A.***[4]

[1] *TEMA, Department of Mechanical Engineering, University of Aveiro, 3810-193, Aveiro, Portugal.*
E-mail: olena@ua.pt

[2] *Institute of Electronic Materials Technology (ITME), Warsaw, Poland.*

[3] *Institute for Materials Science, University of Stuttgart, 70569 Stuttgart, Germany.*

[4] *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193, Aveiro, Portugal.*

New power generation strategies are needed for clean and sustainable energy sources due to exponentially rising energy demands of the word. Thermoelectric *(TE)* conversion of widely distributed waste heat was proposed as an alternative route to convert thermal or solar energy into electric power economically. Oxide materials are of current interest as high-temperature TEs in the energy-harvesting sectors due to high chemical robustness, low toxicity and low cost although their *TE* figure of merit *ZT* is lower than that of chalcogenides or skutterudites [1]. Driven by a need to improve *TE* performance of *n*-type oxides, ceramics and composites based on donor-doped $SrTiO_3$ are considered as a promising material.

Within this context, Nb-doped $SrTiO_3$ is mixed with graphene oxide (GO) and conventionally sintered in atmosphere of H_2/N_2 to reduce both Nb-doped $SrTiO_3$ and GO. Addition of reduced GO (rGO) in combination with introduction of Sr vacancies provides a synergistic effect of fastening charge transport and thereby increasing electrical conductivity and suppressing the thermal conductivity. These factors, together with a moderate Seebeck coefficient, result in a high power factor *PF* ~1.98 mW/(K^2m) and *ZT* up to 0.29 [2]. Such findings offer further prospects for seeking high performance $SrTiO_3$-based TEs by modification with rGO. Deep comparison with other thermoelectric composites with rGO is done.

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Synthesis and study of diatomite/alginate/Fe_3O_4 composite polymer material

***Frolova L.**, Pasenko O.*

Department of Technology Inorganic Materials and Ecology,
Ukrainian State University of Chemical Technology, ave Gagarina, 8,
Dnipro-49005, Ukraine.
Email: 19kozak83@gmail.com

The synthesis of deposited composite granules of diatomite-alginate and diatomite-alginate-Fe_3O_4 composite granules is proposed. Technological approaches to the use of diatomaceous earth as a raw material for the creation of composite adsorbents for wastewater treatment of cations and anions are analyzed. It is shown that the developed surface of diatomaceous earth can be used to create a granular adsorbent, and iron (II, III) oxide is an environmentally friendly, cheap, economically feasible modifier.

The influence of synthesis conditions (initial concentration of sodium alginate, nozzle diameter, solid phase content) and granulation of alginate-diatomite-magnetite composite adsorbent on its physicochemical properties is established. The process of applying the active magnetic phase of the adsorbent is studied. Granular composite adsorbents (alginate-bentonite-Fe_3O_4) were characterized by scanning microscopy, SEM-EDX elemental analysis, FTIR spectroscopy, X-ray phase analysis, UV spectroscopy, derivatography.

The conditions for the formation of spherical diatomite granules in the presence of sodium alginate C [$CaCl_2$] = 0.024 mol / L, ω (diatomite) = 5 - 20% were established.

Spherical granules of adsorbents using Fe_3O_4 as the active adsorption layer were obtained. It is established that the static strength of the obtained adsorbent granules is 17 - 25 kPa. The dependence of the static strength of granules on the solid phase content (17 - 25 kPa) is established. The thermal stability of the samples was studied, it was found that increasing the solid phase content improves the thermal stability. Polymeric granular adsorbents are obtained from diatomaceous earth and calcium alginate.

Structural and morphological properties of ultrasonic-modified $NiMoO_4$ hydrate

Khemii M.M., Budzulyak I.M.,
Popovych O.M., Spodarenko R.H.

Vasyl Stefanyk Precarpathian National University,
57 Shevchenko St. Ivano-Frankivsk-76018, Ukraine
E-mail: maryahemiy@gmail.com

Ultrasonic modification is a promising method of controlled change in the particle size and the surface area of nanomaterials. We analyzed the crystal structure and morphology of nickel molybdate ($NiMoO_4$) hydrate obtained by hydrothermal method and modified by ultrasound (the operating frequency is 22 kHz) for 15, 60 and 90 minutes.

According to the results of X-ray diffraction analysis, the average crystallites size, calculated by the Scherrer equation, was 17 nm for the initial nickel molybdate and for all modified samples. The morphological properties were investigated by the low-temperature nitrogen absorption / desorption porosimetry. IV hysteresis is observed for all materials (according to UIPAC classification) in the range P/P_0 0.5–1.0. The specific surface area of the initial nickel molybdate was 31 m^2/g and does not change for the modified materials (28-31 m^2/g). The pore size distribution spectra determined by the Barrett – Joyner – Halenda method indicate the mesoporous structure of nickel molybdates and an increase in the average pore diameter from 17 nm for the initial nickel molybdate to 28.8 nm for material modified by ultrasound for 90 min. DFT (density functional theory) histograms indicate a wide pore size distribution in the range of 2-26 nm and an increase in total mesopores volume from 0.135 cm^3/g to 0.223 cm^3/g with prolonged ultrasonic dispersion.

Thus, ultrasonic modification does not change the crystallite size of $NiMoO_4$ hydrate, however, in modified materials there is a redistribution of pores in size, namely, the volume of mesopores with a diameter of 20-28 nm increases. This is due to the fact that at ultrasonic frequencies from 20 kHz to 50 kHz, the most common are physical effects, including shock waves, which accelerate solid particles suspended in the liquid, causing changes in the morphology of materials.

Novel method for synthesis and characterization of Ni–Zn ferrite nanoparticles

Plutenko M.O.[1], Plutenko T.O.[2], Fedorchuk O.P.[2]

*[1] Faculty of Chemistry, Taras Shevchenko National University of Kyiv.
Lva Tolstoho Street, 12, Kyiv-01033, Ukraine.*

*[2] Solid State Chemistry Department Faculty of Chemistry,
V.I. Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine. Akad. Palladin ave, 32/34, Kyiv-03142, Ukraine.
E-mail: taplutenko@gmail.com*

Nanoparticles of the $Ni_{1-x}Zn_xFe_2O_4$ system (where $0 \leq x \leq 1$), were synthesized using urea and microwave radiation. The obtained samples were characterized by TGA and DTA. Then heat treatment was carried out at 500 °C for 4 hours in an air atmosphere. The obtained nanoparticles were characterized by XRD, FESEM-EDS, TEM, and FTIR methods. Magnetic characteristics were measured using a vibrating magnetometer LDJ-9500 and samples were compressed into tablets, at the temperature of 20 °C and a magnetic field of 3.98 kA/m. Mossbauer spectra were obtained using a dynamic type spectrometer operating in the mode of constant acceleration. 57Co in the Cr matrix was used as a source of γ-quanta. Measurements were performed at the temperature of 20 °C.

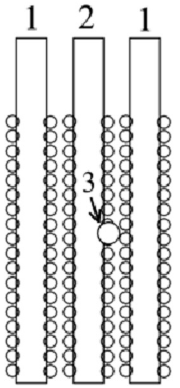
X-ray powder diffraction analysis showed the formation of a single-phase cubic structure of Ni-Zn ferrite spinel. Structural parameters such as lattice constant, crystallite size were estimated using XRD data. Characteristic bands for tetrahedral and octahedral regions of spinel were observed in the FTIR spectra. FESEM image analysis for Ni-Zn ferrite nanoparticles showed spherical geometry, fine size distribution, and agglomeration of nanoparticles. Analysis of EDX spectra showed good consistency of the calculated and experimentally obtained elemental composition. In addition, particle size determination and morphology studies were performed by the TEM method. The obtained particle size was about 27-34 nm for $Ni_{0.5}Zn_{0.5}Fe_2O_4$, which also confirms the nanocrystalline nature of the prepared nanoparticles of Ni-Zn spinel system. Zinc content leads to an increase in the size of nanoparticles and crystal cell volume. The magnetic properties change with increasing Zn concentration. The highest value of magnetic saturation is observed for ferrite $Ni_{0.5}Zn_{0.5}Fe_2O_4$. In the Mossbauer spectrum at room temperature for the $Ni_{0.5}Zn_{0.5}Fe_2O_4$ sample, two sextets are observed, which are associated with the presence of two different local structures in the material.

Photoluminescence of Eu³⁺ ions in thin-film opals and resonator structures based on them with spatial localized feedback

Moiseienko V.N., Gavrilyak V.R., Derhachov M.P., Ohiienko O.V.

Physics, Electronics and Computer Systems Department, Oles Honchar Dnipro National University. Prospect Gagarina, 72, Dnipro-49010, Ukraine.
E-mail: vnmois@ukr.net

Resonatorless generation of light in an active scattering medium under the condition k L = 1 (k is wave vector of light, L is photon mean free path) is of both scientific and practical interest [1, 2].



The photoluminescence spectra of the $C_6H_9EuO_6xH_2O$ salt in the pores of thin-film opals on a glass substrate, as well as in the pores of resonator structures based on them (see figure: 1 - D = 301 nm. 2 - D = 294 nm. 3 - salt-impregnated region) were measured.

The excitation of the samples was carried out in the "reflection" geometry from the (111) plane by the radiation of semiconductor laser with λ_{ex}= 405 nm. The spectra were measured using a DFS-12 double monochromator and a recording system in the photon counting mode with accumulation.

In the measured spectra the radiative transitions in the energy spectrum of Eu^{3+} $^5D_0 \rightarrow {}^7F_0$, $^5D_0 \rightarrow {}^7F_1$, and $^5D_0 \rightarrow {}^7F_2$ were observed at wavelength 580 nm, 592 nm and 617 nm respectively. The dependence of the intensities and splitting of the bands in the luminescence spectrum on the position of the stop-band and additional impregnation of the samples with glycerol has been established. An increase in the luminescence intensity (by a factor of 5) was observed for the bands located at the boundary of the stop band. The appearance of a narrow intense line in the photoluminescence spectra of the resonator structure in the region of 610 – 612 nm is revealed. It may be associated with the appearance of stimulated emission due to the formation of closed light trajectories during scattering of the exciting radiation in the globular structure of the film opal (random generation).

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Combined Polymer Nanostructures for Selective Gas Sensors

Tsizh B.[1,2], **Aksimentyeva O.**[3], **Horbenko Y.**[3], **Holyaka R.**[4]

[1] *Kazimierz Wielki University in Bydgoszcz,*
30, J.K. Chodkiewicza St., 85-064 Bydgoszcz, Poland
E-mail: tsizhb@ukr.net

[2] *Stepan Gzytskyi National University of Veterinary Medicine*
and Biotechnologies Lviv, 50, Pekarska St., Lviv 79010, Ukraine.

[3] *Ivan Franko National University of Lviv,*
6 Kyryla-Mefodia St., Lviv 79005, Ukraine

[4] *National University «Lvivska politehnika»,*
12, Bandery St., Lviv 79013, Ukraine

In recent years, significant progress has been made in the development of sensors for ammonia, hydrogen, chlorine, oxides of carbon and nitrogen, hydrogen sulfide, volatile organic compounds and other gases and volatile components. Gas-sensitive elements in such sensors are nanocomposite heterostructures based on polyaniline, polyacetylene, polypyrrole, polythiophene and other conducting polymers [1,2]. However, despite a large number of studies, today these structures have a relatively low selectivity, reproducibility and stability, which does not allow them to be used effectively in practice.

It is shown that optical gas sensors have additional possibilities to ensure their selectivity in comparison with electrical sensors by comparing changes in optical properties at different wavelengths under the action of gases. The features of changes in optical absorption of combined thin-film nanostructures polymeric active elements based on a mixture of polyorthotoluidine and polyorthoanisidine, which allow to selectively identify the presence of ammonia, hydrogen sulfide and carbon dioxide, have been established. A method of selective detection of the analyte by an optical gas sensor on optoelectronic pairs with a mobile matrix of LEDs and photodiodes and the possibility of simultaneous registration of independent signals of parallel optocouplers is proposed.

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Radiation resistance of steel T91 after deformation in different structural states

Rostova H.Yu., Tolstolutskaya G.D., Tikhonovsky M.A., Kalchenko A.S.

National Science Center "Kharkiv Institute of Physics and Technology".
1, Akademicheskaya St., Kharkiv, 61108, Ukraine
E-mail: veg-annie@ukr.net

Ferritic-martensitic steels are considered as promising structural materials for future generations of reactors. Their undoubted advantage is their high sensitivity to the conditions of thermal and thermomechanical treatment (TMT), which makes it possible to modernize their structure, mechanical characteristics and increase radiation tolerance.

In this work, as a TMT, we used the multi-cycle “upsetting-extrusion” (MUE) method developed at the NSC KIPT, which has proven itself in the production of ultrafine-grained materials, both in laboratory and industrial conditions [1].

MUE of T91 steel was carried out in two temperature ranges: in the austenitic region and with a sequential decrease in the deformation temperature in the ferrite region. Subsequent heat treatment was carried out at temperatures of 730 ... 550 °C for 1 ... 50 h to stabilize the structure and precipitate carbide phases. Irradiation was carried out with Ar ions with energy of 1.4 MeV up to a dose of 120 dpa.

It was found by optical and transmission electron microscopy that the average grain size of T91 steel as a result of MUE decreases from 20 μm in the initial state to 140 nm after 5 cycles of MUE, which led to the achievement of record values for this steel of the yield strength (1279 MPa at 25 °C and 502 MPa at 600 °C) and strength (1340 MPa at 25 °C and 511 MPa at 600 °C). With an increase in the number of cycles and a decrease in the "upsetting-extrusion" temperature, simultaneously with a decrease in the average grain size, an increase in the degree of uniformity of their size distribution occurs. The creation of a high density of traps for the recombination of radiation defects (grain boundaries, nanosized carbides) during such processing led to a decrease in swelling by a factor of 1.3.

A study of the development of void structure after irradiation of steel T91 in various structural states was carried out. It was shown that after irradiation with Ar ions with an energy 1.4 MeV to a dose 120 dpa at T = 460 °C, the swelling in the ultrafine-grained ferritic structure is 0.65% compared with 0.26% for the initial martensitic structure, which confirms the influence of structural-phase state of steel T91 on its swelling. For comparing, the swelling of steel with an austenitic structure is ~ 15.6%, which is 24 times more than the level of swelling of steel with a ferritic structure.

Argon stabilizes cavity formation by a pressure effect. Numerous prior studies have shown that when the argon concentration is low, the cavity swelling initially increases with increasing Ar concentration. For moderate to high Ar concentrations, relatively small pressurized bubbles and relatively large underpressurized voids lead to bimodal cavity size distributions. The observed cavity swelling temperature regime for MeV Ar ion irradiated T91 steel is much broader than values suggested by ion irradiation studies using low ion energies. This is attributed to several well-known artifacts for ion irradiation research: cavity denuded zones with an adjacent enhanced swelling region and diffusional broadening of injected ions can reduce the breadth of the temperature regime for cavity swelling, and generally shift the cavity swelling regime to higher temperatures with increasing dose rate.

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Structural and magnetic properties of lanthanum-strontium manganite nanopowder

Liedienov N.A.[1,2], Polynchuk P.Yu.[3],
Pashchenko A.V.[1,2,3], Dzhezherya Yu.I.[3], Levchenko G.G.[1,2]

[1] State Key Laboratory of Superhard Materials, International Centre of Future Science, Jilin University.
Qianjin Street, 2699, Changchun-130012, China.

[2] Donetsk Institute for Physics and Engineering named after O. O. Galkin, NAS of Ukraine. Prospect Nauki,46, Kyiv-03028, Ukraine.

[3] Institute of Magnetism, NAS of Ukraine and MES of Ukraine. Vernadsky Blvd., 36, Kyiv-03142, Ukraine. E-mail: phenix77310@gmail.com

Manganites with a perovskite structure belong to the multifunctional materials owing to their rich variety of phase diagrams and multiplicity of magnetic ground states [1]. All of this makes them a promising material for a wide application and deep investigation in different areas of science and technology [2].

Here, we have synthesized the $La_{0.6}Sr_{0.4}MnO_3$ (LSMO) nanopowder using the sol-gel method with a post-annealing at t_{ann} = 700–900 °C (each cycle 10 h). As the tann increases the impurity of $SrCO_3$ reduces and vanishes at 850 and 900 °C, whereas the specific surface area decreases and the average crystallite size grows from 16 to 30 nm. According to the magnetic data, the LSMO-800 nanopowder shows two critical temperatures T_{C1} = 328 K and T_{C2} = 362 K which are related to the particle size effect. As turned out the main part of the LSMO-800 nanoparticles is in the single-domain state, whereas others are in the superparamagnetic and multi-domain states. Such size dispersion leads to broadening the magnetocaloric effect with the maximum value $-\Delta S^{max}$ = 1.818 J/(kg·K) at 5 T near T_{C1}. The obtained results exhibit perspectives on the practical use of manganite nanomaterials in physics, chemistry, materials science, and nanotechnology.

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Structural properties of iron-formate under high pressure

Wei Ziyu[1], Liedienov N.A.[1,2], Yu Hanlin[1],
Gaspar A.B.[3], Real J.A.[3], Levchenko G.G.[1,2]

[1] *State Key Laboratory of Superhard Materials, International Centre of Future Science, Jilin University.*
Qianjin Street, 2699, Changchun-130012, China.
E-mail: nikita.ledenev.ssp@gmail.com

[2] *Donetsk Institute for Physics and Engineering named after O. O. Galkin, NAS of Ukraine. Prospect Nauki, 46, Kyiv-03028, Ukraine.*

[3] *Institut de Ciència Molecular/Departament de Química Inorgànica, Universitat de València. Catedràtric Beltrán 2,*
E-46980 Paterna València, Spain.

Hybrid organic-inorganic perovskites (HOIPs) have attracted a lot of recent research attention due to the diverse range of their physical and chemical properties including photovoltaic, optoelectronic, dielectric, ferroelectric, magnetic, ferroelastic, and multiferroic properties [1]. Among HOIP materials, the hybrid formate $[(CH_3)_2NH_2]M(HCOO)_3$ (M = Mn, Fe, Co, Ni) perovskites can exhibit both magnetic order and ferroelectricity at low temperature, as well as a possibility of magnetoelectric coupling in these compounds, which expands the prospect of their technical application [2].

It is well known that the functional properties of HOIPs change significantly with temperature. As another important thermodynamic parameter, pressure can also significantly vary the properties of these materials, especially the structural characteristics. Here, we performed *in situ* high-pressure X-ray diffraction and Raman spectroscopy studies of the $[(CH_3)_2NH_2]Fe(HCOO)_3$ formate using the diamond anvil cell (DAC) technique up to 10 GPa. The experimental results show that at about 6 GPa, the sample undergoes obvious structural transformation, and the characteristic peak positions of Raman spectra also shift significantly. The pronounced changes for the modes corresponding to the dimethylammonium cation and formate ion may indicate an order-disorder phase transition and the distortion of the metal-formate framework under high pressure, respectively.

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Bulk and supported nanocatalysts for hydrogenation of CO_2: improvement or degradation?

Dyachenko A.G.[2,3]***, Ischenko O.V.***[1]***, Lisnyak V.V.***[1]***,***
Goncharuk O.V.[2]***, Borysenko M.V.***[2]

[1] *Taras Shevchenko National University of Kyiv,*
64/13 Volodymyrs'ka Str, Kyiv, 01601, Ukraine

[2] *O.O. Chuiko Institute of Surface Chemistry National Academy of Science of Ukraine, 17 General Naumov Str, Kyiv, 03164, Ukraine*

[3] *Institute of Physical Chemistry of Polish Academy of Sciences, 44/52 Kaspzaka, 01-224 Warsaw, Poland.*
E-mail: dyachenko.alla@yahoo.com

The highly effective heterometallic catalysts were investigated in the reaction of CO_2 hydrogenation. The bulk NiCo, NiFe and CoFe catalysts synthesized by the coprecipitation method demonstrate high catalytic efficiency in the methane production by the reaction of $CO_2 + H_2$ compared with monometallic ones. The optimal ratio of the components of the presented bimetallic compositions is obtained for achieving maximum and selective conversion of CO_2 to methane.

The most effective bimetallic compositions were applied onto the surface of different carriers (carbon nanotubes, ultradispersed nanodiamonds, graphite nanoplatelets and inert oxides such as silica and alumina) by the method of wet impregnation with inorganic salt solutions of the appropriate metals. The amount of applied actives was 5-20 wt%. The activity of nanocomposite catalysts compared to their bulk counterparts varied depending on the composition of the active mass. Obviously, the application of NiFe and NiCo on the carrier leads to an increase in catalytic activity, and for CoFe the opposite effect of the carrier influence on the efficiency of bimetallic nanoparticles was found.

The data of CO_2 conversion **(X (CO_2))** and CH_4 yield **(Y (CH_4))** at the 300 °C over the bulk and some deposited catalysts are presented in the table below.

Catalyst	**X (CO_2), %**	**Y (CH_4), %**	**Catalyst**	**X (CO_2), %**	**Y (CH_4), %**
Ni	40	34	Co(80)Ni(20)/Al_2O_3	100	100
Co	55	52	Co(80)Ni(20)/SiO_2	90	64
Fe	10	0	Ni(80)Fe(20)/Al_2O_3	100	100
Co(80)Ni(20)	62	60	Ni(80)Fe(20)/SiO_2	95	68
Ni(80)Fe(20)	67	64	Co(93)Fe(07)/Al_2O_3	90	69
Co(93)Fe(07)	100	100	Co(93)Fe(07)/SiO_2	70	49

‘Green’ synthesis and characterization of silver nanoparticles using Artemisia vulgaris ‘hairy’ root extracts as reducing agents

Kobylinska N.G.[1]***, Kharchuk M.***[2]***, Duplij V.P.***[3]***, Matvieieva N.A.***[3]

[1] A.V. Dumansky Institute of Colloid Chemistry and Water Chemistry NAS of Ukraine, Ak. Vernadsky blvd. 42, Kyiv, 03142, Ukraine

[2] Institute of Microbiology and Virology, NAS of Ukraine,
152 Ak . Zabolotny Str., Kyiv, 03143, Ukraine

[3] Institute of Cell Biology and Genetic Engineering, NAS of Ukraine,
148 Ak. Zabolotny Str., Kyiv, 03143, Ukraine
E-mail: joyna@ukr.net

Unique combination of antibacterial, optical, electrical, and catalytic properties of nanoparticles (NPs) stimulates research on study of design and functionalization for various applications. Progress is currently made in the technologies for the various syntheses of silver nanoparticles (AgNPs).

In this work, we compared the peculiarities of the formation of AgNPs using aqueous and ethanolic (70%) extracts from *Artemisia vulgaris* control and transgenic ("hairy") roots. The content of flavonoids and reducing activity of extracts from the control roots were lower than the corresponding parameters of "hairy" root extracts. The content of flavonoids and reducing power in all ethanolic (70%) extracts were greater than in aqueous one.

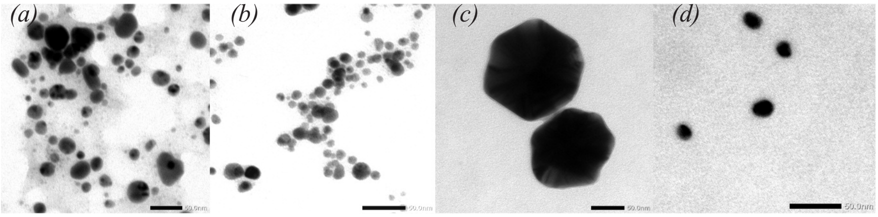

Fig. 1. *TEM images of obtained AgNPs using aqueous (a,c) and ethanolic (b,d) extracts of control (c,d) and ‘hairy’ (a,b) roots.*

The resulting colloidal solutions of all obtained AgNPs were stable during 6 month. AgNPs obtained using aqueous extracts were larger than those obtained by ethanolic extracts according TEM data *(Fig. 1)*. NPs obtained by aqueous extracts from the control roots were polyhedral, while the "hairy" root extracts produced oval shape NPs. Thus, the extracts properties depended on extraction solvents, root samples, etc. play a key role on the morphology and size of resulted AgNPs.

Investigation of the rate of resorption hydroxyapatite-based composites modified by magnetite and chitosan for medical application

Sych O.[1], Synytsia A.[1], Babutina T.[1]

[1] Department of Functional Materials for Medical Application, Frantsevich Institute for Problems of Materials Science of NAS of Ukraine.
Krzhyzhanovsky Str., 3, Kyiv-03142, Ukraine.
E-mail: synytsia.ann@gmail.com

Biogenic hydroxyapatite (BHA) and composite materials based on it are used in orthopedics and traumatology to replace bone defects of various origins due to its biocompatibility and chemical proximity to the mineral component of natural bone. In addition, materials based on BHA are bioresorption, ie in the process of "dissolution" of the implant is the mineralization of newly formed tissues. One of the most important parameters that *in vitro* allows to predict the behavior of the material in the body is the study of its behavior in the model physiological environment.

BHA / magnetite / chitosan composite powders based on magnetite obtained by chemical precipitation for 5 minutes and thermolysis in a nitrogen medium with different ratios of components (wt. % BHA / magnetite: 99/1, 95/5, 75/25 and 50/50 at a chitosan content of 0.1%) were used as test materials.

According to the results of the study of the resorption rate of the obtained BHA/magnetite/chitosan composites under thermostatic conditions in physiological isotonic solution, it was found that not only the content but also the type of magnetite used significantly affects the resorption rate in physiological saline. The increase in the content of magnetite leads to an increase in the resorption of composites, and the use of magnetite obtained by chemical precipitation allows achieving a resorption rate of 2.5-5.3 wt. % / day, which is 3.5-7.5 times higher than "pure" biogenic hydroxyapatite and 1.2-2 times higher than composites based on magnetite obtained by thermolysis in nitrogen.

The obtained results are fully consistent and confirmed by the results of chemical analysis of physiological solutions after contact with composites for 2 days. The presence of such chemical elements as calcium, phosphorus and iron was detected in the filtrates. The presence of calcium and phosphorus is due to the resorption of hydroxyapatite, and iron - magnetite, which are part of the composites. The content of elements in physiological solution is directly related to the ratio of components in the materials of BHA / magnetite / chitosan.

Enhanced magnetic anisotropy in small-sized elliptical synthetic-antiferromagnets

Borynskyi V.Yu.[1]***, Polishchuk D.M.***[2]***, Melnyk A.K.***[3]***,***
Kravets A.F.[1]***, Tovstolytkin A.I.***[1]***, Korenivski V.***[2]

[1] *Institute of Magnetism of the NAS of Ukraine and MES of Ukraine. Akad. Vernadsky blvd., 36-b, Kyiv-03142, Ukraine.*
E-mail: vladislav.borinskiy@gmail.com

[2] *Nanostructure Physics, Royal Institute of Technology. Hannes Alfvénsväg, 12, Stockholm-10691, Sweden.*

[3] *Institute for Sorption and Problems of Endoecology of the NAS of Ukraine. Naumov str., 13, Kyiv-03164, Ukraine.*

Our recent research has shown how both geometry and multilayered structure of synthetic-antiferromagnet (SAF) nanodisks can effectively modify the dynamics of standing spin waves inherent to such systems [1]. In the present work, we want to emphasize the importance of nanomagnet shape considering arrays of elliptical SAF nanostructures, which possess the average major-axis length of 75 nm.

Using the ferromagnetic resonance technique, we obtained a set of spectra for different directions of external magnetic field applied in the plane of the fabricated array. Despite common multi-mode spin-wave resonance, generally governed by magnetostatic interactions within ferromagnetic nanoelements, each spectrum revealed only one resonance line. This behavior originates from the exchange energy contribution that prevails in small-sized elements [2].

In addition, the resonance field of the single mode shifts up by 700 Oe for the 90° magnetization direction, implying strong influence of the individual SAF's shape. However, analytical calculations evidence that corresponding unidirectional anisotropy is rather enhanced by the SAF-specific spin excitation type.

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Formation of a conducting phase in Porous Glasses

Doycho I.[1], Lepikh Ya.[1], Filevska L.[1], Rysiakiewicz-Pasek E.[2], Grinevych V.[2]

[1] *Odessa I.I. Mechnikov National University, Dvoryanska str., 2, Odesa 65082, Ukraine. E-mail: lfilevska@gmail.com*

[2] *Department of Experimental Physics, Wrocław University of Science and Technology, Poland*

Porous silicate glasses may be used as matrices for the formation of nanoparticles' ensembles for sensors due to the peculiarities of their structure. At the same time, rather considerable intrinsic electrical resistance of such systems, causes their usage mainly for luminescent-type sensors. At the present work it is suggested to form inside the pores the nanoparticles' ensemble of a conducting substance for significant reduce of the sample resistance. This attitude will make it applicable as an active element in resistive type sensors. Such substance is a carbon, which in the form of graphite exhibits excellent conductive properties. To create a carbon conductive phase, the porous glass of any type should be saturated with aqueous solution of glucose. At the consequent heating to 150 ºC, it is easily reduced directly in the matrix cavities to carbon in the form of highly dispersed graphite with the release of water. This process, described by the equation

$$C_6H_{12}O_6 \xrightarrow{(t)} 6C+6H_2O,$$

lasts about 24 hours. Its completion can be fixed visually by sample blackening. After this treatment, the initial resistance of standard size samples $1\times0.5\times0.1$ cm^3, having several teraOhms is reduced by several orders of magnitude.Water vapor, always present in the atmosphere, saturates the pores to a certain extent thus reducing the electrical resistance of the system. This makes it possible to use porous glass as an active element of a resistive type humidity sensor. The presence of a wide range of pore sizes (from about 10 to 100 nm in different types of glasses) corresponds to the hydrophilicity of the system in a wide range of humidity. A significant decrease in the intrinsic resistance of the samples after carbon treatment, due to the conductive properties of graphite, eliminates the initial disadvantage, since it makes the fluctuations in the resistance of the system due to changes in humidity noticeable. This treatment also significantly reduces the sample cellularity at the ends, making it possible to create sufficiently reliable contacts to such a system using silicone or indium-gallium paste. Humidity sensors constructed according to this principle remain operational at any temperatures at which the system is not destroyed, including negative ones.

Such partial carbon treatment of the sample's ends using specially designed holders will allow the formation of ohmic contacts at the ends of an arbitrary porous system for further applications, such as possible correlation studies between luminescent and electrical properties.

Low-energy synthesis of magnetite nanoparticles from weakly magnetic hematite using biomass

Antonenko T.S., Dudchenko N.O., Ovsienko V.V., Cherevko Yu.I.

M.P. Semenenko Institute of Geochemistry, Mineralogy and Ore Formation of Natl. Acad. of Sci. of Ukraine, Palladina prosp, 34, Kyiv-03142, Ukraine.
E-mail: tetyana_savchenko@ukr.net

The aim of this work was to synthesize highly magnetic magnetite particles using weakly magnetic iron oxides (hematite) and biomass (starch) under the heating at the definite temperature.

For magnetite synthesis, the sample of weakly magnetic hematite was thoroughly mixed with 4% starch. The resulting mixture was placed in a quartz mini-reactor with limited oxygen access and kept for 30 minutes at 650°C. Heating and cooling of the sample was carried out using the device for analysis of the magnetization of magnetic materials and ores. The Curie temperature was also determined using this device for the samples, obtained during the transformation process.

Phase composition of initial and obtained samples was determined by X-ray diffraction (X-Ray diffractometer DRON-3M). Facility for express measurement of magnetization of ores and magnetic materials was used for determination of the specific saturation magnetization. The X-ray diffraction method showed that the initial samples consisted mainly of hematite (d-spacing of hematite (Å) 3,68 Å, 2,70 Å, 2,52 Å, 1,84 Å, 1,69 Å, 1,66 Å, 1,60 Å, 1,48) and quartz (d-spacing of quartz (Å) 4,25 Å, 3,34 Å, 2,46 Å, 2,28 Å, 2,24 Å, 2,21 Å, 2,13 Å, 1,82 Å, 1,72 Å, 1,67 Å, 1,54 Å, 1,46 Å). Specific saturation magnetization for initial samples was ~ 1 $A\cdot m^2$/кg. After the addition of starch and exposure to heating, the obtained samples consisted of magnetite, quartz and traces of hematite (d-spacing of magnetite (Å) 4,87 Å, 2,97 Å, 2,54 Å, 2,43 Å, 2,10 Å, 1,71 Å, 1,61 Å, 1,48 Å). Specific saturation magnetization of obtained samples was around 45 $A\cdot m^2$/кg. Therefore, we could conclude that the specific saturation magnetization of samples increased due to magnetic minerals (magnetite) formation. Curie temperature, determined by cooling curve of obtained samples, was ~583 °C that is close to Curie temperature of pure magnetite (580 °C). We can assume, by the Curie temperature (583 °C), that the obtained samples contain magnetite or isomorphically substituted magnetite.

The results could be used to solve the fundamental problems related to the synthesis of magnetic nanoparticles under the energy-consuming conditions.

Antimicrobial activity of transcarpathian clinoptilolite modified with salts of transition metals

Gromyko O.M.[1], Vasylechko V.O.[1,2], Gryshchouk G.V.[1], Roman I,I.[1], Kalychak Ya.M.[1], Fedorenko V.O.[1], Bagday S.R.[1]

[1] Department of Genetic and Biotechnology, Department of Analytical Chemistry Ivan Franko National University of Lviv.
1 Universytetska Str., 4, 79000 Lviv, Ukraine.
E-mail: vasylechko@ukr.net

[2] Department of Food Technology, Lviv University of Trade and Economics, 9 Samchuka Str., 79011 Lviv, Ukraine

The antimicrobial properties of highly dispersed (particle size ≤ 100 μm) Ukrainian transcarpathian clinoptilolite (CL) compositions with transition metal ions such as Mn^{2+} (Mn-CL), Cu^{2+} (Cu-CL) and Co^{2+} (Co-CL) were studied. The concentration of metal ions in the compositions: Mn^{2+} - 560 μg/g, Cu^{2+} - 670 μg/g, Co^{2+} - 1800 μg/g.

Bacterial and yeast strains including *Escherichia coli* ATCC 25922, *Staphylococcus aureus* ATCC 25923, and *Candida albicans* ATCC 885-653 were used as indicator pathogens. Antibacterial activity was evaluated by incubation of indicator pathogens ($1\text{-}2 \times 10^5$ cells per 1 ml of solution) for 2 min in the presence of suitable compositions in concentrations 0.1, 0.5, and 1.0 mg/ml. In fact, CL has a very weak antimicrobial effect. Cu-CL in increasing concentrations delayed the growth of *S. aureus* from 50 to 35%, *E. coli* - from 17 to 3%, *C. albicans* - from 11 to 1%. Co-CL and Mn-CL had a stronger antimicrobial effect. In particular, at a maximum concentration (1.0 mg/ml), these compositions reduced the survival of *S. aureus* to 10-11%, *E. coli* - to 0.3-0.5%, *C. albicans* – 0.1-0.2%. Although the action of these compositions is weaker than the action of Ag-CL that was described earlier [1], they can be considered as a basis for the development of antimicrobial drugs for the treatment of skin lesions, in particular, due to their lower cost.

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Influence of ratio of silicon complex and hydrolyser agent on silicon dioxide characteristics

Kamenskyh D.S.[1], Tkachenko T.V.[1], Tecer L.H.[2], Sheludko Y.V.[1], Povazhny V.A.[1], Jafarov M.A.[3], Yevdokymenko V.O.[1]

[1] *V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of the NAS of Ukraine, Murmanskaya str, 1, Kyiv-94, 02094, Ukraine.*
E-mail: ttv13ttv@gmail.com

[2] *Namık Kemal Üniversitesi, Namık Kemal Mahallesi Kampüs Caddesi No:1 Süleymanpaşa, 59030, Tekirdağ, Turkey*

[3] *Baku State University, Akademik Zahid Xəlilov küçəsi-23, Baku, AZ1148, Republic of Azerbaijan*

It is known that the physicochemical characteristics of amorphous SiO_2 are influenced by the raw material, process temperature, pH of the reaction medium, the ratio of reagents and many other indicators. Previously, a waste-free technology for the production of biogenic silicon dioxide was described. However, there was a question of the ability to control the size of the final product. Therefore, the aim of our work was to study the effect of the ratio of mass concentrations of silicon-containing solution (5:100; 5:500; 5:1000) and hydrolyzing agent on the physicochemical properties of the final product.

The obtained samples of silicon dioxide were studied by various physicochemical methods: low-temperature nitrogen sorption-desorption, XRD, XRF, FTIR-ATR, AFM, TGA and DSC. XRD pattern of the obtained silica showed that the 2-theta region between 5° to 45° at long collection times indicates no crystalline peaks. The FT-IR spectrum of the whole silica samples show typical functional groups correspond to pure silicon dioxide at 1074, 982, 800 and 457 cm^{-1}. There are two distinct mass loss steps in termograms (TGA). The first step (less than 130 °C) is abrupt (1.5-24 % depending on samples) and is most probably due to the removal of physisorbed water from the silica surface. The second step (1.2-3 % depending on samples) is border and is considered to correspond to slow condensation of silanols. It was established that obtained samples had a specific surface area 86.8, 318.3 and 310.2 m^2/g and pore size 3.3, 13.8 and 9.2 nm depending on concentration (100, 500 and 1000). The AFM method established that the obtained silica has a relief consisting of spherical particles (80.3 nm) and densely packed rod formations (1.5x160.6 nm). After reducing the SiO_2 concentration by 5 times, the presence of individual particles and folded aggregates (ridges) is characteristic. Characteristically, the 3D image clearly shows the pointed vertices of SiO_2 tetrahedral after a 10-fold decrease in SiO_2 concentration.

Features of dispersion of dimensional and magnetic parameters in spinel ferrite nanoparticles

Zamorskyi V.O.[1], Solopan S.O.[2], Belous A.G.[2], Tovstolytkin A.I.[1]

[1] *Institute of Magnetism of the NAS of Ukraine and MES of Ukraine,*
36b Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine
E-mail: 0vl0ad0@gmail.com

[2] *V.I. Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine, 32/34 Academician Palladin Ave., UA-03142 Kyiv, Ukraine*

Magnetic nanoparticles (MNPs) have been used in many important technological applications such as ultra-high density magnetic recording and data storage, highly sensitive magnetic sensors, permanent magnets and various biomedical applications, which are of a great interest nowadays [1]. Here, we suggest the ways to account for the dispersion of size and magnetic parameters, and adequately predict the behavior of MNP ensembles under various conditions.

AFe_2O_4 (A = Ni, Zn, Co) MNPs were synthesized by precipitation from non-aqueous solutions as described in [2]. Unfortunately, the synthesized NMPs do not have a uniform size distribution, and this may significantly affect their widespread use, since obtaining monodispersed nanoparticles requires a complicated additional step, which increases production cost. Thus, it is of a paramount importance to develop a relatively simple approach to predict the behavior of such NMPs under different external factors.

The analysis of the magnetization curves of nanopowders displaying superparamagnetic-like behavior has been performed. The distribution functions of MNPs in terms of magnetic moment and size have been determined. It is shown that the size distribution function obtained from the magnetic characteristics makes it possible to adequately describe the behavior of an ensemble of nanoparticles containing weakly magnetic or nonmagnetic shells. As concluded, the proposed approach is effective for analyzing the dispersion of the dimensional and magnetic parameters of nanoparticle ensembles and for predicting their behavior under the influence of electro-magnetic fields.

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Influence of vacuum annealing on the dispersion of thin double niobium-palladium films deposited onto oxide ceramic materials

Stetsyuk T.V.[1], Fesenko O.M.[2], Shakhnin D.B.[3], Gab A.I.[3]

[1] *Frantsevich Institute for Materials Science Problems of NAS of Ukraine,*
3 Krzhyzhanovskogo st., Kyiv, 03142, Ukraine.
E-mail: tvst@ukr.net

[2] *Transfer Technology Department, Institute of Physics of the NAS of*
Ukraine. Prospect Nauki, 46, Kyiv-03039, Ukraine.

[3] *University "Ukraine", 23 L'vivska st., Kyiv, 03115, Ukraine.*

Permanent vacuum-tight precision ceramic joints with an ultra-thin seam can be made by brazing or pressure welding of metallized ceramic parts. This purpose can be achieved by application onto ceramic surfaces of double metal films, one part of which is 100–200 nm thick and consists of an adhesion-active metal (e.g. Hf, Nb etc.), and the other layer is slightly thicker (1–3 μm) and serves as a solder (e.g. Pd, Ag, Ni etc.) ensuring joining of metallized ceramic materials during brazing or pressure welding with a fine brazed seam (2–4 μm thickness). In this work, specimens made of leucosapphire, alumina and dioxide-zirconium ceramics were used metallized with a 150 nm Nb nanofilm and then by 1,5 μm Pd film atop serving as a soldering metal for ceramic samples joining.

As a result of annealing at 1000 °C for 5 min, the films remained almost unchanged; after 10 min, the number of defects in the film on all oxides increased, the film began to swell and even crack; and after 20 min, the number of defects in the film on all oxides increased even more. With annealing temperature up to 1100 °C, the film underwent significant changes after 5 min of exposure; after 20 min, the number of defects on all oxides increased. Annealing at 1200 °C accelerated sharply the dispersion of the film which began to deteriorate significantly after 10 min of exposure; 20 min of annealing led not only to significant decay of the film, but also to the interaction of Pd with Nb, with film residues still covering 70-80% of the substrate surface area, which made it possible to use double Nb-Pd films to join oxide ceramics at temperatures up to 1200 °C.

According to our study results, kinetic curves of the investigated thin double metallic films decomposition have been built, from which the basic process parameters (temperature and exposition time at this temperature) for brazing or pressure welding of ceramic materials can be determined. Using the data obtained, process regimes for joining by brazing and pressure welding were selected. According to these regimes, joints' prototypes with seams up to 2 μm thick were made, which strength reached 150 MPa.

Thermally reduced graphene oxide (TRGO): study of thermal defunctionalization

Basnukaeva R.M.*[1], *Barabashko M.S.*[1], *Dolbin A.V.*[1],
Drozd M.*[2], *Vinnikov N.A.*[1]

[1] B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 47 Nauky Ave., Kharkiv 61103, Ukraine
E-mail: msbarabashko@gmail.com

[2] Institite for Low Temperatures and Structure Research Polish Academy of Sciences, ul. Okólna 2, Wrocław 50-422, Poland.

The thermal stability and the kinetics of thermal decomposition of the thermally reduced graphene oxide (TRGO) have been studied. Modified Hummers method was used for obtaining the initial graphite oxide (GO) from graphite powders. The thermal exfoliation of the graphene oxide powder has been performed in the vacuum conditions when heated with the temperature rate of 5–7 degrees per minute to a temperature of 300°C for obtain the TRGO. The samples of TRGO were treated by a pulsed high-frequency discharge in a hydrogen atmosphere before measurements. Pulsed high-frequency discharge in a hydrogen atmosphere of TRGO lead for partial graphene hydrogenation (chemical addition of atomic hydrogen) that leads to structural changes in the carbon planes and the formation of C-H sp3 bonds. The TGA measurements of TRGO samples for study the mass loss have been carried from room to 1000°C in a nitrogen atmosphere with a nitrogen flow and different heating rates. The Kissinger's multiple heating rate method has been used to determine activation energy for decomposing substances. Activation energies have been compared with the energies of the activation of thermal defunctionalization of multi-walled carbon nanotubes. Obtained experimental results are useful for practical application of TRGO, such as hydrogen energy and high temperature sintering of new promising composite materials with its additives.

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Influence of the additives of multi-walled carbon nanotubes to the porosity of hydroxyapatite composite

Barabashko M.S.[1]***, Basnukaeva R.M.***[1]***, Tkachenko M.V.***[2]

[1] *B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 47 Nauky Ave., Kharkiv 61103, Ukraine*
E-mail: msbarabashko@gmail.com

[2] *V.N. Karazin Kharkiv National University, 4 Maidan Svobody, Kharkiv, 61077, Ukraine*

Hydroxyapatite (HA) powder was synthesized by the reaction between calcium carbonate and orthophosphoric acid. Calcination of the obtained HA powder was carried out at 900°C for 1 h. The cylindrical compacts were obtained from calcined powder under a pressure 120 MPa. Composite ceramics based on hydroxyapatite (HA) with additives of multi-walled carbon nanotubes (MWCNTs) have been sintered in the Ar atmosphere. The concentration of nanotubes was varied in the range 0 - 0.5 wt%. HA is a bioactive matrix, while MWCNTs additives can improve the mechanical properties of ceramics. In particular, the additives of MWCNTs lead to the unique electrical, thermal, and mechanical properties of composite materials.

X-ray, IR, and TEM have been studied. In addition, the increase of the density and decrease of the porosity have been observed. The obtained results are discussed. It was found that HA ceramics has higher macrostresses than in the case of HA ceramics with the additives of MWCNTs. HA ceramics have low thermal diffusivity and the temperature gradients occur during heterogeneous heating/cooling of different parts of ceramics at sintering. The additives of MWCNTs allow to increase the thermal diffusivity and reduce internal residual macrostresses in the HA-MWCNTs ceramics.

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Thermodynamic and kinetic compatibility of nanoscale nonmetallic particles with metallic materials in casting and welding technologies

Korzhyk V.M., Shcheretskyi V.O., Strohonov D.V.,
Demianov O.I., Konoreva O.V.

E.O. Paton Electric Welding Institute the NAS of Ukraine, 1 Kazymyr Malevych St., Kyiv 03150 Ukraine.

The study reveals the effect of non-metallic microstructure modifiers (ZrO_2, TiC, WC, TiB_2, etc.) on the microstructure and mechanical and functional properties of metallic alloys on the base of aluminum copper and iron.

The usage of non-metallic nano-scale particles is expedient for effect at the crystallization of a metal melt, within processes of foundry and welding technologies, and formation of protective and functional coatings. The approach includes the usage of mutual theoretical thermodynamic CALPHAD calculations and experimental studies (microstructure and thermal analyzes, mechanical and functional testing) to discover features (atmosphere, time-temperature range, secondary phases, distribution) of nano-scale particles addition effect on the mechanical and functional properties of cast items, metallic coatings, and welded joints.The important thing is discovering the conditions of chemical compatibility of the components of such composite structure, including thermodynamic and kinetic compatibility because of heterogeneity of such material.

The study provides data to predict impact and discover subject of nanoscale particles usage by metallic base and particles type. There is discovered impact of nano-scale additions in cast alloys (aluminum alloys) [1], welding processes (aluminum, steels) [2], protective and functional (frictional) layers (copper alloy layer on a steel base) [3].

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Adsorption and protolytic properties of nanocryptomelane and its activity in ozone decomposition reaction

Rakitskaya T.L., Truba A.S., Sokolova Z.V., Slobodianyk I.O.

Faculty of Chemistry and Pharmacy, Odesa I.I. Mechnikov National University,2, St. Dvoryanska, 65082, Odesa, Ukraine.
E-mail: email.of corresponding truba@onu.edu.ua

Activity of polymorphic nanooxide forms of manganese(IV) in ozone decomposition reaction significantly depends on relative humidity of ozone–air mixture and residual content of hydrogen ions on the samples' surface. The influence of these two factors on the catalytic properties of manganese nanooxides is practically not discussed in the literature. Cryptomelane samples were synthesized by different methods: reflux method **(I)**, melting together **(II)**, sol-gel method **(III)**, solid-phase reaction **(IV)**. All the samples were characterized by XRD method, SEM, FT-IR spectroscopy. We studied the protolytic (pH_s) and adsorption properties of these samples in relation to water vapor. Based on isotherms of water vapor adsorption by above cryptomelane samples at a constant adsorption value a = 2.0 mmol/g the thermodynamic activity of adsorbed water a_{H2O} = P/Ps and pH values were determined. These values depend significantly on the origin of cryptomelane (method of synthesis). So the pH_s values increases in a row **I** < **II** < **III** < **IV**, and corresponding a_{H2O} values are in the range of 0.76-0.92. The activity of these samples in ozone decomposition reaction was characterized using two parameters: τ_{MPC} (time of protective action) and Q_{sp} (specific amount of ozone, which decomposed into half-life of ozone). The combined effect of the activity of water and hydrogen ions on the τ_{MPC} and Q_{sp} values was estimated using the values of the GTP = $\lg a_{H2O}/a_{H3O^+}$ (table). It was found that sample **II** with GTP = 5.40 is characterized by the maximum values of τ_{MPC} and Q_{sp}.

Characteristics of nanocryptomelan samples and their activity in ozone decomposition reaction

Sample	**I**	**II**	**III**	**IV**
GTP	2.87	5.40	7.10	11.50
Q_{sp}·103, moles of O_3/g	2.20	4.86	1.73	0.22
τ_{MPC}, min	30	1055	1	1

Investigation of Ni Doping on the Structural, Luminescence, Optical and Electronic Properties of ZnO Nanopowders

Amari R.[1,2]***, Benrzgua E.***[1,3]***, Deghfel B.***[1,4]***, Boukhari A.***[1,5]***, Allali D.***[4,6]

[1] Laboratory of Materials and Renewable Energy, Faculty of Sciences, University of M'sila, Algeria.
[2] Department of Civil Engineering, Faculty of Technology, University of M'sila, Algeria.
E-mail address: rabie.amari@univ-msila.dz
[3] Department of natural and life sciences, Faculty of Sciences, University of M'sila, Algeria.
[4] Department of Physics, Faculty of Sciences, University of M'sila, Algeria.
[5] Department of Mechanical Engineering, Faculty of Technology, University of M'sila, Algeria.
[6] Physics and Chemistry of Materials Lab, Department of Physics, University of M'sila, 28000, M'sila, Algeria.

In this Study, pure and Ni-doped ZnO nanoparticles (NPs) with concentration of Ni (3.12%) were successfully prepared by using co-precipitation method [1]. Among TM, nickel is very significant element which has a similar ionic radius as that of Zn. Literature studies show that Ni doping into ZnO matrix can enhance its various properties [2, 3]. Zinc acetate dihydrate [Zn $(CH_3COO)_2$ $2H_2O$], nickel acetate dihydrate [Ni $(CH_3COO)_2$ $2H_2O$] and sodium hydroxide solution [NaOH] were used as precursors. For getting homogeneous solution, stoichiometric amount of zinc and nickel acetate were dissolved in methanol, after stirred continuously on a magnetic stirrer at room temperature. For raising the pH of the obtained solution to ~9, small amount of sodium hydroxide solution [NaOH] was added drop by drop. The precursor solution is then stirred again until the liquid solution turns into a gel. After gel formation, the beaker was transferred on the hot plate at 500°C for 1h. The obtained sample yield in the form of loose powder was then finely grounded by agate mortar and pestle. The prepared samples in powder form were characterized by X-ray diffraction spectroscopy (XRD), Scanning Electron Microscopy (SEM), Ultraviolet–visible spectroscopy (UV-Vis), Photoluminescence (PL) and Fourier transform infrared spectroscopy (FTIR). The obtained results have been discussed and compared with those from other sources whatever possible.

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Adsorption properties of nanoporous carbon materials obtained from waste coffee grounds

***Sklepova S-V.S.*, Gasyuk I.M., Ivanichok N.Ya., Soltys A.M., Klymkovych S.M., Lisovskiy R.P., Rachiy B.I.**

The Department of Material Science and New Technology, Vasyl Stefanyk Precarpathian National University. 57 Shevchenko Str., Ivano-Frankivsk, Ukraine.
E-mail: sonja93sklepova@gmail.com

Nanoporous carbon materials (NCM) are used to prepare supercapacitor (SC) electrodes. The high specific energy characteristics of SC are closely related to the physicochemical characteristics of NCM. NCM with a highly developed surface area and controlled pore size distribution can be obtained by chemical and thermal activation of carbon containing precursors. In our work we propose a method of obtaining NCM with a high specific surface area. The NCM is obtained by thermochemical activation of potassium hydroxide waste coffee grounds (WCG). The WCG, from commercial beverage manufacturers, was dried at 65-85 °C for 48 h. The dried WCG was mixed at a weight ratio of 1:0.5:1 with KOH and distilled water. The resulting mixture was stirred thoroughly for 1-2 hours; after which it was dried at a temperature of 90 ºC. The dry material was placed in an autoclave and heated to a given temperature and kept at this temperature for 30 min. After cooling, the resulting material was washed to neutral pH and dried at 90 ºC. The series of samples (S400 ÷ S900) were numbered according to the thermochemical activation temperature. For example, S900 is a material activated at 900 ºC. The table shows the characteristics of the porous structure of NCM.

The parameters of the porous structure of the NCM

Sample	S400	S500	S550	S600	S700	S800	S900
S_{BET}, m^2/g	31	172	246	374	446	703	1056
S_{DFT}, m^2/g	23	193	218	309	478	632	1170
S_{meso}, m^2/g	30	44	30	27	27	22	45
S_{micro}, m^2/g	-	80	175	319	402	671	996
V_{total}, cm^3/g	0.092	0.161	0.176	0.228	0.237	0.331	0.507
V_{micro}, cm^3/g	-	0.038	0.071	0.132	0.162	0.272	0.398

The specifications of porous structure (it means surface area and general volume) of NCM were determined on the basis of analysis of adsorption/desorption isotherms of nitrogen. A number of complementary methods BET, DFT, BJH and t-method were used.

Comparative analysis of nanostructures formed by the chemical route in the iron-lanthanum-containing systems

Lavrynenko O.M., Pavlenko O.Yu., Olifan O.I.

I. Frantsevich Institute for Problems in Material Science, NAS of Ukraine.
Krzhizhanovsky Str., 3, Kyiv-03142, Ukraine alena.lavrynenko@gmail.com

At present, interest in the preparation and practical application of lanthanum-containing materials is closely related to their high oxidative-catalytic and electrocatalytic activity [1]. At the same time, the combination of the catalytic properties of lanthanum oxides with the magnetic properties of iron oxides and the formation of mixed structures such as perovskite makes it possible to form magnetoelectric and multiferroic materials [2]. In addition, nanocomposites based on rare-earth orthoferrites and iron oxides are recognized as promising materials for use in biomedicine, for example, for magnetic hyperthermia [3].

The aim of the present work is the comparative study of the structure, phase and chemical composition of nanostructures formed via co-precipitation of ferric / ferrous and lanthanum water salt solution in low alkaline medium. The iron-lanthanum-containing precipitates were subjected to thermal treatment in the temperature range from 160 to 1100 °C and were analyzed by X-ray phase analysis, scanning electron microscopy, and energy-dispersive spectroscopy.

The results of the study made it possible to determine the effect of the chemical composition of the initial metal's salts on the characteristics of the final reaction products and to find the optimal conditions to obtain homogenous nanosized structures of lanthanum-containing orthoferrite with the perovskite-type structure. Nanostructures, received during the study, are planned to be analyzed for the presence of catalytic activity in the neutralization of a number of organic dyes and magnetic susceptibility to ensure the magnetic separation of spent particles.

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Hong-Ou-Mandel quantum effect on “polymer - multiwall CNT” composites

Karachevtseva L.A.[1], Kartel M.T.[2],
Lytvynenko O.O.[1], Sementsov Yu.I.[2]

[1] Laboratory of Photonic Semiconductor Structures, V. Lashkaryov Institute of Semiconductor Physics, NASU, Prsp. Nauki, 41, Kiev-03028, Ukraine.
E-mail: lytvole@gmail.com

[2] Department of Nanoporous and Nanosized Carbon Materials, O. Chuiko Institute of Surface Chemistry, NASU,
17 General Naymov Street, Kyiv 03164 Ukraine.

The possibilities to enhance the properties of nanostructured surfaces are evaluated on “polymer-multiwall carbon nanotube” composites. Influence of sp3 hybridization bonds is investigated in composites derived from polypropylene, polyamide-6, polyamide-12 and polyvinyl chloride after adding CNTs to polymers. IR absorption of “polymer- CNTs" films exceeds that of polymer by 10-103 times in the entire measured spectral range. In addition, two-polar IR absorption are measured on composites with negative components at spectral positions of “D-band” and “2D-band” of sp^3 hybridization. In this case, the greater oscillation amplitudes of C-C, CH_2 and CH_3 bonds correspond to a higher absorption at the oscillation frequencies $\gamma_\omega(CH)$ and $\gamma_\omega(CH_2)$. Frequencies of 2D-band correspond to the second order frequencies of D-band. The intensity of 2D band increases with an increase in the concentration of defects. The absorption of light increases when the frequencies of local oscillations of surface bonds in carbon nanotubes correspond to the frequencies of slotted modes along the boundary of the "nanotube polymer" (surface polaritons). Two-polar oscillations have an ultra-small half width 0.4-0.6 cm^{-1}, which indicates a strong interaction of surface polaritons with photons. Vertically polarized light along carbon nanotubes and horizontally polarized light of D and 2D bands resulted in light beams splitting, two-photon interference and realization of the quantum Hong-Ou-Mandel effect.

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Ab initio study of the piezoelectric effects of the 2D semiconductors of IV group monochalcogenides (GeSe, GeS)

Balabai R.M., Zadorozhnii V.M.

Kryvyi Rih State Pedagogical University,
54 Gagarina Ave., Kryvyi Rih, 50086, Ukraine.
E-mail: balabai@i.ua , vitaliy_zadorozhniy@ukr.net

The piezoelectric effect in nanostructured semiconductor attracts attentions in recent years. Since Zhong Lin Wang group observed piezoelectric generation in a ZnO nanowire and coined a new term in 2006, which is piezotronics [1]. The piezotronics takes advantage of the coupling properties of piezoelectric effect and semiconductor characteristic. The rapid development of piezoelectric applications, including wearable electronics and human–machine interfacing, put forward a new requirement for piezoelectric materials, which must be highly flexible and atomically thin. However, conventional piezoelectric materials, such as piezoelectric ceramics and piezoelectric semiconductors suffer from fragile and bulk characteristics; therefore, 2D materials with atomic layer thickness and mechanical flexibility have been regarded as a new generation of piezoelectric materials. Existing 2D materials are piezoelectric if they fulfill two criteria: they must have a non-symmetric crystal structure and they must be non-metallic [2]. The family of 2D semiconductors, group IV monochalcogenides is non piezoelectric in the bulk form as they are centro-symmetric. However, their inversion centers disappear in mono-layers, resulting in piezoelectricity [3]. The strong in-plane covalent bonding and weak interlayer van der Waals interaction in these 2D materials provides high in-plane stability allowing to produce it freestanding in nature.

In this paper the piezoelectric effects of the 2D semiconductors of IV group monochalcogenides (GeS, GeSe) are studied by methods of the density functional theory and first-principles pseudopotential based on own program code. The spatial distribution of valence electron density, density of states, and Coulomb potential along transverse direction are calculated. The redistribution of the valence electrons in films with an even number of mono-layers (centro-symmetric) and with an odd number (non centro-symmetric) under mechanical action are discussed.

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Electrochemical properties of carbon material obtained from walnuts

Ivanichok O.M.**, **Ivanichok N.Ya., Ivaniv I.I.,
Kolkovskyi P.I., Rachiy B.I.

Vasyl Stefanyk Precarparhian National University,
Shevchenko Street, 57, Ivano-Frankivsk-76018, Ukraine.
E-mail: iomm@ukr.net

Nanoporous carbon (NPC) is a promising material for perfectly polarized electrodes of electrochemical energy sources. In this work, carbon materials were obtained by the method of thermal carbonization of walnut shells at a temperature of 800 ºC. In the process of obtaining the raw material with a fraction of 5-15 mm was poured into an autoclave, placed in an oven and heated to a given temperature at a rate of 5 ºC/min [1].

The dependence of the specific capacitance of the obtained NPC on the value of the charge / discharge current in 33% KOH was studied by the method of galvanostatic cycling. Moreover, the discharge specific capacity and internal resistance of the NPC were determined based on the obtained chronopotentiograms. It is determined that the primary carbonization of plant biomass at a temperature of 800 ºC makes it possible to obtain NPC with a specific capacity of up to 97-121 F/g in the range of operating currents of 5-100 mA at a maximum charge / discharge voltage of 1 V. A sharp drop in voltage at a charge / discharge current indicates the presence of ohmic resistance in the NPC / electrolyte electrochemical system. The maximum operating discharge current is up to 100 mA for all samples, since with its further increase, the voltage drop during discharge exceeds 20% of the maximum voltage [2]. However, it should be noted that the value of the charge/discharge current has practically no effect on the internal resistance of the electrochemical system, the value of which is 1-1.5 Ω .

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Effect of alternative treatments methods on the electronic structure of ZrO_2-TiO_2

Zaika V.V.[1], Sachuk O.V.[2], Karbivskii V.L.[1]

[1] *G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine,*
36 Academician Vernadsky Boulevard, UA 03142 Kyiv, Ukraine.
E-mail:zaikavladimir228@gmail.com

[2] *Institute of Sorption and Problems of Endoecology N.A.S. of Ukraine,*
13 General Naumov street, UA-03164 13,Kiev, Ukraine.

In recent years, materials based on ZrO_2-TiO_2 have attracted the attention of researchers as hydrophobic, hydrophilic, corrosion-resistant coatings, solar converter elements, and moisture sensors.

A significant part of the materials based on ZrO_2-TiO_2 is obtained by sol-gel method, which is an energy-intensive process. In this work, the initial composite was obtained by mixing TiO_2 and ZrO_2 powder in a 1:1 ratio, after which the effect of mechanochemical and ultrasonic treatment on the electronic structure was investigated. It was shown that when analyzing the atomic composition of the surface, the most corrosion-resistant is the sample after mechanical treatment.

In the paper [1] it was shown that the energy shift of the X-ray photoelectron spectra peaks can be caused by the different sizes of nanoparticles. This effect was established for the investigated nanoparticles.

It is indicated that the area of titanium oxide nanoparticles has a difference of 2.5 times, and for zirconium oxide a difference of 1.8 times in comparison with the original sample.

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Structure of the Composites Based on Bacterial Cellulose and Multi Walled Carbon Nanotubes

Polishchuk E.V.[1], ***Shevchenko V.B.***[1], ***Nizhelska O.I.***[2], ***Voychuk S.***[1,3]

[1] *Faculty of Physics, Taras Shevchenko National University of Kyiv,*
Prospect Glushkova, 2, Kyiv- 03022, Ukraine
E-mail: shevchenko@univ.kiev.ua

[2] *Laboratory 36 Composite Materials for Nuclear-Hydrogen Energy,*
Institute of Applied Physics of NASU (Sumy), room 606, building 3,
Prospect Nauki, 46, Kyiv - 03028, Ukraine.

[3] *Department of Physiology of Industrial Microorganisms, D. K. Zabolotny*
Institute of Microbiology and Virology of NASU,
Zabolotny Str., 154, Kyiv - 03143, Ukraine.

Bacterial cellulose (BC), consisting of a 3-D network of oriented cellulose 2-8 nm diameter fibrils, which combine into nanofibers, can be a promising substance to produce electrically conductive composite materials with biodegradable properties. Biocompatible composite films containing carbon nanotubes (CNTs) due to their electrical conductivity can serve as sensors for communication between living tissues in the body and biomedical instruments or neuroelectronic prostheses.

The aim of our work was to create a composite material based on BC, synthesized by bacteria of the genus *Gluconacetobacter sp.*, and multi walled CNTs, and studying the effect of the method of its preparation on the composite structure.

The samples of composite materials were formed with wet gel films and dried films of BC and CNTs with different degrees of dispersion. Optical microscopy and scanning electron microscopy shown that the BC network acts as a matrix, containing dispersed CNTs and aggregated CNTs. Composites formed with wet BC gel and dispersed CNTs contained a continuous branched network of carbon components showing an ability for current conduction that contrasted with composites synthesized by other methods.

X-ray diffraction analysis showed that the structure of pure BC and cellulose, which was a matrix of BC composite with CNTs have some differences. Namely, for the composite made with wet cellulose gel and dispersed CNTs, a decrease in the size of the crystallites in the cellulose and a decrease of the degree of its crystallinity were observed.

Catalyst containing natural nanosilica, palladium(II) and copper(II) salts in oxidation of carbon monoxide with oxygen

Rakitskaya T.L., Nazar A.P., Kiose T.O.

Faculty of Chemistry and Pharmacy, Odesa I.I.
Mechnikov National University,2, St. Dvoryanska, 65082, Odesa, Ukraine.
E-mail: email.of. corresponding annnzr1401@gmail.com

The search for readily available and cheap carriers for the basic components (K_2PdCl_4 and $Cu(NO_3)_2$) of a catalyst for low-temperature oxidation of carbon monoxide in the development of new functional nanomaterials is very important and actual. Phlogopite (Phl) concentrate is one of polyphase natural materials, which contains diopside, tremolite, and clinochlore phases in addition to the main phase. This work presents the results of the study of an influence of acid modification conditions on the phase and chemical composition of phlogopite concentrate. The samples were modified with 8M nitric acid at room temperature, the treatment time was 1; 24; 48; 72 hours. Samples 8H-Phl-1, 8H-Phl-24, 8H-Phl-48 and 8H-Phl-72 ($\overline{S}$) were characterized by XRD, SEM, FT-IR spectroscopy, and pH-metry. The samples were used for the synthesis of catalysts with the composition Pd(II)-Cu(II)/$\overline{S}$. It is shown that in above row of indicated carriers the following trends are observed: the content of the Phl phase decreases, the content of the clinochlore phase increases, the content of diopside and tremolite phases changes irregularly; the content of silicon increases to 92 wt% of SiO_2. The data of fig. demonstrate a decrease in the final concentration of CO in stationary mode with an increase in the duration of treatment of a carrier. In case of $\overline{S}$= 8H-Phl-72, the catalyst provides air purification from CO below MPC = 20 mg/m³.

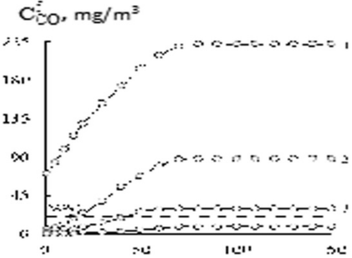

Fig. *Time dependence of the final concentration of CO during its oxidation in the presence of Pd(II)-Cu(II)/$\overline{S}$ catalyst $\overline{S}$: 1 – 8H -Phl-1; 2 – 8H -Phl-24; 3 – 8H -Phl-48; 4 – 8 -Phl-72*

Quantum chemical study on the structure and transformations of hydrated forms of tin dioxide

Filonenko O.V., Grebenyuk A.G., Lobanov V.V.

Chuiko Institute of Surface Chemistry, NAS of Ukraine,
17 General Naumov Str., Kyiv 03164, Ukraine
E-mail: oksana.filonenko@isc.gov.ua

Nanoscale materials based on SnO_2 in the form of nanoparticles, nanospheres, nanotubes, nanowires, nanobands are of great interest due to the combination of a number of their unique optical and electrophysical properties.

One of the most common methods of obtaining nanostructured forms of SnO_2 is hydrothermal synthesis. Precursors in the production of nanoparticles of tin dioxide are its hydroxides and oxide hydroxides (so-called stannic acids), which are obtained by the action of an aqueous solution of ammonia on tin tetrachloride:

$$SnCl_4 + 4\ NH_4OH \rightarrow SnO_2{\cdot}nH_2O\downarrow + 4\ NH_4Cl + (2 - n)\ H_2O.$$

As a rule, there are two individual forms: α- and β-stannatic acids, which differ in composition, acidity and solubility. First, α-stannatic acid $SnO_2{\cdot}nH_2O$ ($1 < n \leq 2$) precipitates from solutions of tin (IV) salts due to action of alkalis. Over time, the precipitate of α-stannatic acid is gradually converted to β-stannatic acid $SnO_2{\cdot}nH_2O$ ($n < 1$), losing water. Subsequent drying of the precipitate produces nanoparticles of SnO_2. There is no unambiguous idea on the relationship between the structure and properties of these acids. The mechanisms of growth of the nanostructured forms of tin dioxide are not completely studied.

To find the regularities of the formation of these species, a systematic quantum chemical study was been carried out on the spatial structures and energy characteristics of the cluster models for nanoparticles of tin dioxide hydrated forms. The mechanisms of formation were studied of the simplest nanostructures containing up to four tin atoms from $Sn(OH)_4$ units. Calculations of the properties of reagents, transition states, intermediates and reaction products were performed by the density functional method with exchange-correlation functional B3LYP and basis set 3-21G (d) using PC GAMESS software (FireFly 8.2.0).

It has been shown that $Sn(OH)_4$ molecules tend to form two types of associates: hydrogen-bonded and stronger coordination; transitions between them lead to the formation of Sn-O-Sn and Sn-OH-Sn bridges. Structures with water molecules coordinated to Sn atoms can lose them quite easily, as evidenced by small values of activation energy and bonding energy (several kJ/mol), so forming intermediates with pentacoordinated Sn atoms; their further transformations lead to denser structures that have signs of crystallinity inherent in solid SnO_2.

Functional nanomaterials based on zinc oxide

***Hutsul K.R.*, Ivanenlo I.M.**

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 4 build, 37, Prosp. Peremohy, Kyiv 03056, Ukraine
E-mail: x_gucul1997@ukr.net, irinaivanenko@hotmail.com

Nowadays, nanomaterials (whose internal structure or surface structure is in the range of ~1 nm to 100 nm) attract a lot of attention from researchers due to a unique set of properties that can be adjusted by changing the size and morphology of the particles. This approach has led to the widespread use of nanomaterials in many areas of human activity, including industry [1].

Oxides of transition metals are representatives of the class of nanomaterials that are also being actively studied. These oxides are of particular interest due to the different ratios of metal and oxygen content, a large number of possible phases with different structures, variable properties, and wide application. Zinc oxide, which belongs to the oxides of transition metals, is one of the most widely studied oxides due to its availability, low cost, chemical stability, biocompatibility, and a unique combination of chemical, electronic, and optical and optoelectronic properties. All this leads to the use of zinc oxide in various fields, such as catalysis, medicine, electronic sensors, hygiene products, solar cells, electronics, etc. [2-4].

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Structural, elastic and thermodynamic properties of Ag-based oxides XAgO (X = Li and Na): An *ab initio* study

***Allali D.*[1,2,*], *Amari R.*[3], *Deghfel B.*[4], *Boukhari A.*[3]**

[1] *Physics and Chemistry of Materials Lab, Department of Physics, University of M'sila, 28000, M'sila, Algeria.*

[2] *University of M'sila, Faculty of Technology, B.P. 166 Ichbilia, 28000, M'sila, Algeria.*
Email: djamel.allali@univ-msila.dz

[3] *Laboratory of Materials and Renewable Energy, Faculty of Sciences, Mohamed Boudiaf University of M'sila, 28000, M'sila, Algeria.*

[4] *University of M'sila, Faculty of Science, Department of Physics, 28000, M'sila, Algeria.*

Structural parameters, elastic constants and thermodynamic properties of the tetragonal ternary Ag-based oxides LiAgO and NaAgO are investigated theoretically for the first time using the plane-wave ultra-soft pseudopotential method [1] based on the density functional theory [2,3]. The optimized lattice parameters and atomic positions agree well with the available theoretical and experimental counterparts. Pressure dependence of the structural parameters is also explored. Pressure dependences of the single-crystal elastic constants *Cij* for LiAgO and NaAgO are explored. The elastic wave velocities propagating along the principal crystallographic directions are numerically estimated. The elastic anisotropy is estimated and further illustrated by 3D-direction-dependent of the Young's modulus. A set of some macroscopic elastic moduli, including the bulk, Young's and shear moduli, Poisson's coefficient, average elastic wave velocities and Debye temperature, were calculated for polycrystalline LiAgO and NaAgO from the *Cij via* the Voigt-Reuss-Hill approximations [4–6]. Through the quasiharmonic Debye model [7], which takes into account the phonon effects, the temperature and pressure dependencies of the bulk modulus, unit cell volume, volume thermal expansion coefficient, Debye temperature and volume constant and pressure constant heat capacities of LiAgO and NaAgO are explored systematically in the ranges of 0–20 GPa and 0–1200 K.

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Fibrous polymer sorbents modified with nanoparticles of hydrated tin (IV) oxide for removal of anionic U(VI) compounds from aqueous solutions

Perlova O.V.[1], Dzyazko Yu.S.[2], Rodyvylova R.A.[1], Palchik A.V.[2]

[1] Odesa I.I. Mechnikov National University,
2 Dvoryanska Str., 65082 Odesa, Ukraine
E-mail: Rodyvylova@ukr.net

[2] V.I. Vernadskii Institute of General and Inorganic Chemistry of the NAS of Ukraine, 32/34 Palladin ave., 03142 Kyiv, Ukraine

Fibrous polymer anion-exchanger FIBAN A-6 was modified with nanoparticles of hydrated tin(IV) oxide (HTO). Thermodynamical approach was applied to deposition of particles inside polymer matrix: it takes into consideration solubility of the inorganic modifier in under and oversaturated solutions, temperature, ion exchange capacity of polymer and other parameters. If no special conditions are applied to the modifier deposition, for instance, additions of complex forming agent, tin oxide was estimated to be precipitated as nanoparticles. It was a criterion for choice of this modifier. HTO was deposited in a form of non-aggregated nanoparticles. As known, namely this morphological feature provides fast sorption as well as high sorption capacity. The composites were investigated by means of SEM, TEM and porometric methods. Chemical composition of the modifier was identified by means of FTIR spectroscopy.

The main kinetic characteristics of the sorption process were calculated using pseudo-first and pseudo-second order models, Weber-Morris and Yelovich approaches. The half-time of exchange is 10 min. (pristine fibers) and 6 min. (modified fibers). U(VI) ions are removed completely after 40 and 25 min respectively. Uranium sorption isotherms have been obtained, their modeling is carried out using Henry, Langmuir, Freundlich, Dubinin-Radushkevich, Frumkin models, constants of these equations and thermodynamic sorption parameters have been calculated. As found, sorption of carbonate forms of uranium by the studied sorbent is a spontaneous endothermic process, which is accompanied by an increase in entropy. The possibility to use the modified fibrous anion exchange resin FIBAN A-6 for extraction of small amounts of uranium from model solutions that simulated technological solutions has been established. It is interesting that increase in U(VI) concentration from 1 to 4 mg dm-3 improves the recovery of these ions (%) from 58 to 95 (pristine polymer) and from 68 to 100 (composite).

Observation of spin-selective collective excitations of the condensates relative phase in proximitized singlet superconductor – half-metallic manganite nanostructures

***Krivoruchko V.N.*, Tarenkov V.Yu.**

Donetsk Institute for Physics and Engineering of the NAS of Ukraine,
Prospect Nauki, 46, Kyiv-03028, Ukraine.
E-mail: krivoruc@gmail.com

Proximitized materials based on conventional superconductor/half-metallic ferromagnet (SC/hmF) heterostructures are promising materials with spin-triplet superconductivity. Their multi-band superconducting state is characterized by the superposition of singlet and triplet Cooper pairs condensates. In a multi-band SC, collective excitations of a relative phase of the condensates (Leggett modes) are allowed. Thus, the question about possible connection of Leggett-like collective excitations in SC/hmF proximity materials with the spin conservation law is a burning question.

In this report, we present the results of experimental investigations by the point-contact (Andreev) spectroscopy of the Leggett modes in proximity induced three-band superconducting state of the s-wave SC/hmF nanocomposite, $MgB_2/(La,Sr)MnO_3$. Two types of point contacts (PC) have been used: the nanocomposite - hmF and the nanocomposite - nonmagnetic metal PCs. Small amplitude spin-dependent equidistant oscillations against the background of the gap structure were observed in the conductance characteristics of both types of high-quality Andreev junctions. The distinctive feature between the PCs conductance is the period of oscillations, it is doubled for contacts with a nonmagnetic metal in comparison to the nanocomposite - hmF PCs. We attribute the spin-selective conductance oscillations to an emission/absorption of nonequilibrium *spin-selective* Leggett excitations – the collective fluctuation of phase difference between Cooper pair condensates. To our best knowledge, the obtained experimental data are the first observation of Leggett excitations in proximity induced mixture of *s*- and *p*- Cooper pair condensates.

Influence of iron content on magnetic properties of EB-PVD-condensates of Fe-NaCl with magnetite nanoparticles

***Lytvyn S.Ye.*, Kurapov Yu.A., Didikin G.G.**

E. O. Paton Electric Welding Institute of the NAS of Ukraine,
Kazymyr Malevych, 11, Kyiv- 03150, Ukraine
E-mail: lytvynse@hotmail.com

Iron nanoparticles in condensates of the system 10…43 wt. % Fe-NaCl obtained by electron beam evaporation and co-condensation in vacuum of molecular beams of Fe and NaCl (EB-PVD method) were studied. After depressurization of the vacuum chamber, small nanoparticles of iron in the porous structure of NaCl are oxidized in air to Fe_3O_4, and larger ones do not have time to fully oxidize and have a nucleus of pure iron inside. The structure and size of nanoparticles in Fe-NaCl condensates, their phase and chemical composition, and magnetic properties were studied using transmission electron microscopy (TEM), X-ray diffraction (XRD), dynamic light scattering (DLS), and vibration magnetometers. The size of Fe_3O_4 nanoparticles in condensates depending on the temperature of their synthesis and the size of nanoparticle crystallites depending on the concentration of iron in condensates were determined. The influence of the amount of iron in the condensates on the crystallite size of nanoparticles is shown. According to XRD analysis, the size of Fe_3O_4 crystallites in the concentration range 2…15 at. % Fe is in the range of 3…14 nm, and in the range of 20…30 at. % Fe - 17…22 nm. The average size of Fe_3O_4 crystallites (8…15 nm) obtained at a substrate temperature of 45 °C increases as the substrate temperature increases to 25…40 nm (410 °C). It should be noted that in nanoparticles the phase of pure iron is detected when the iron content in the condensate is more than 20 at. % Fe. It is proved that the condensation temperature can be considered as a reliable factor for regulating the size of nanoparticles in the technological process. A study of the distribution of the hydrodynamic size of aggregates of Fe_3O_4 nanoparticles in aqueous colloids with dextran was performed. An increase in the saturation magnetization and coercive force of Fe-NaCl condensates with magnetite nanoparticles with increasing iron content was revealed.

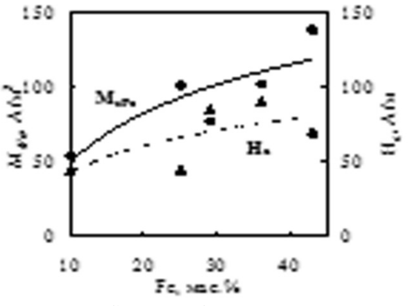

***Fig. 1.** Influence of Fe content on MsFe saturation magnetization and Hc coercive force in EB-PVD condensates of Fe-NaCl.*

Theoretical prerequisites for the use of preparations based on metallic nanoparticles

Lopatko S., Vinrchuk K., Lopatko K., Aftandilyants Y., Chaika V.

National University of Life and Environmental Sciences of Ukraine, 15, Heroyiv Oborony Str., Kiev, 03041, lopatko_konst@hotmail.com

The nutrition of the biological injection of nanomaterials, their toxicity and the ability to positively contribute to the metabolic processes and the physiological state of the organism as a whole, is becoming the key to the fundamental interactions of nanoparticles with the biological medium.

Because the basic properties of nanomaterials are formed at the stage of their formation, the issues of biological efficiency are closely related to the kinetics of processes occurring in the reaction zone. There are prerequisites for obtaining materials with a sharply unbalanced structure, which means with an increased level of free energy and, therefore, increased ability to interact with the environment. The size of nanoparticles significantly affects the expected result of their application, but this is not the only important parameter of their state. The presence of other factors, such as structural-phase composition, particle shape, surface charge, preparative form of nanomaterial, acidity of the environment, processes that characterize the functionality of a particular system, directly affect the efficiency of nanomaterials.

Phase and chemical composition of nanoparticles, crystal lattice parameters and dimensions of coherent scattering regions in the state of production are given in table.

Characteristics of Fe-containing phases in iron nanoparticles	**Type of crystalline phase**			
	α–Fe	**g–Fe**	**FeO**	**Fe_3O_4**
Max value of the phase content, %	15,4	54,5	7,2	77,4
a, nм	0,2864	0,3624	0,4301	0,8372
DCSR, nм	53	24	3,2	1

Nanocomposites NiFe(CoFe)/Silica(Alumina) for the catalytic hydrogenation of CO_2

Dyachenko A.[2,3]***, Ischenko O.***[1]***, Prygunova O.***[1]***,***
Borysenko M.[2]***, Bonarowska M.***[3]

[1]*Taras Shevchenko National University of Kyiv, 64/13 Volodymyrs'ka Str, Kyiv, 01601, Ukraine*

[2] *O.O. Chuiko Institute of Surface Chemistry National Academy of Science of Ukraine, 17 General Naumov Str, Kyiv, 03164, Ukraine*

[3] *Institute of Physical Chemistry of Polish Academy of Sciences, 44/52 Kaspzaka, 01-224 Warsaw, Poland.*
E-mail: dyachenko.alla@yahoo.com

Nanocomposite materials on the base of Silica or Alumina with NiFe or CoFe bimetallic nanoparticles localized on the surface of them have a high potential for the use as catalysts in the process of CO_2 hydrogenation. It was observed that a high specific surface area of the carrier (200-300 m^2/g) causes an uneven distribution of active mass components on the carrier surface and does not contribute to the formation of catalytically active sites and as a consequence the efficient conversion of CO_2 to methane [1,2].

The aim of this study was to determine the catalytic activity of nanocomposites with a specific surface area of about 80 m^2/g. The fumed oxides (SiO_2 and Al_2O_3) were used for the synthesis of NCs as the carriers, and catalytically active bimetallic compositions (NiFe and CoFe) were applied on the surface by the method of solvatostimulated modification with subsequent processes of thermal degradation and reduction.

The long-time catalytic test demonstrates the high stability of the catalyst during 5 weeks of exposure to the reaction mixture. Catalytic reactor worked in the next mode: 8 hours of working in the methanation process at temperature range 350-450 °C then the catalyst was kept under reaction mixture at room temperature for 1 week. This cycle was repeated 3 times for each catalyst. The yield of methane was decreased on 11-15% after a long time test.

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Hydrogen sorption/desorption kinetics in the Mg-C system

Lakhnik A.M., Kirian I.M., Rud A.D.

G.V. Kurdyumov Institute for Metal Physics of N.A.S. of Ukraine
36 Academician Vernadsky Boulevard Kyiv 03142, Ukraine
E-mail: kiryan.inna@gmail.com

Magnesium occupies a special place among metals due to its high hydrogen capacity of 7.67%. But its use as a hydrogen storage medium is limited by several factors: high operating temperatures, slow kinetics of interaction with hydrogen and low cyclic stability. A wide range of methods has been proposed to overcome these shortcomings. Mechanical activation of magnesium with various additives occupies a special place as it allows controlling the synthesis of nanoscale systems, which are characterized by more "soft" modes of sorption/desorption of hydrogen.

Samples Mg-10 wt% C (C – graphite with different specific surface areas) were prepared by ball milling under a hydrogen atmosphere at 400 rpm for 30 h. Initial hydrogen pressure in the milling vial was ~1 MPa. Every one hour the grinding process was stopped and a new portion of hydrogen gas was added. This technique allowed the control of the hydrogen absorption process. During grinding, the mixture exhibited high activity of interaction with hydrogen. This approach allowed obtaining highly active powder mixtures, which are characterized by fast kinetics of interaction with hydrogen and high capacity.

The sorption properties of the composite Mg-10 wt% C after reactive ball milling have been tested by Sieverts technique. The sorption/desorption kinetics of hydrogen was studied both under conditions of linear heating at a constant rate and under isothermal conditions. A systematic study of the composite Mg-10 wt. % C showed that its ability to sorption/desorption hydrogen and kinetics depend on the BET surface area of graphite. The addition of graphite with a BET surface area of 8.135 m^2g-1 showed the best catalytic effect on the kinetics of the interaction of H2 with Mg. After activation sample can relies 4.24 wt.% H_2 within 18 min at 270 °C, 4.48 wt.% for 14 min at 280 °C, 4.66 wt.% for 9 min at 300 °C, and 5.19 wt.% for 8 min at 320 °C. The activation energy of the hydrogen desorption/sorption process was determined by the Kissinger method. Desorption activation energies Ea determined for the sample before and after activation are 165 and 78 kJ/mol, respectively. The analysis of hydrogen sorption curves obtained under isothermal conditions at a temperature of 175, 200, 225, 250, and 300 °C was performed. It was found that at a minimum temperature of 175 °C the sample absorbed 2.8 wt.% H_2 for 34 min, and at a temperature of 300 °C the composite absorbed 4.56 wt.% H_2 for 14 min. The sorption activation energy Ea for composite is 111 kJ/mol.

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Diffusion and diffusion-driven local ordering in Co-Pt thin films

Pedan R.[1]***, Makushko P.***[1,2]***, Dubikovskyi O.***[1,3]***,***
Bodnaruk A.[1,4]***, Burmak A.***[1]***, Makarov D.***[2]***, Vladymyrskyi I.***[1]

[1] Igor Sikorsky Kyiv Polytechnic Institute,
Prospect Peremogy 37, Kyiv 03056, Ukraine.
E-mail: roman1pedan@gmail.com

[2] Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research,
Bautzner Landstrasse 400, 01328 Dresden, Germany.

[3] V. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, Prospect Nauky 41, Kyiv 03680, Ukraine.

[4] Institute of Physics, National Academy of Sciences of Ukraine,
Prospect Nauky 46, Kyiv 03028, Ukraine.

Co-Pt based alloys are perspective materials for spintronics and data storage applications [1]. Thus, investigation of diffusion and diffusion-controlled formation of the ordered magnetic phases in Co/Pt-based thin films is of practical relevance [2].

In this work, magnetron deposited layered stacks of Pt(14 nm)/Co(13 nm)/Ta(3 nm) were annealed in high vacuum in the temperature range of 200 °C – 550 °C. The structure, chemical composition and magnetic properties of the post-annealed stacks were analyzed by chemical depth profiling, X-ray spectroscopy, scanning transmission electron microscopy, x-ray diffraction, and VSM magnetometry.

We demonstrate that although the formation of a long-range chemical order in the CoPt film was not achieved, heat treatment leads to an increase in the coercive field and the formation of local anisotropy in the Co-Pt alloy.

The results of our work show the relevance of further studies of diffusion processes and the formation of hard magnetic phases via diffusion induced grain boundary migration mechanism in Co-Pt thin films during low-temperature annealing.

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Formation of ordered L10 FePt phase in Pt/Ag(Au)/Fe and Fe/Ag(Au)/Pt trilayers

Makushko P.V.*[1]*, Schmidt N.Yu.*[2]*, Verbytska T.I.*[1]*, Katona G.*[3]*,
***Beke D.*[3]*, Albrecht M.2, Makogon Iu.M.*[1]**

[1] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prospect Peremogy 37, Kiev 03056, Ukraine.
E-mail: email.of. corresponding_verbitska@kpm.kpi.ua

[2] Institute of Physics, University of Augsburg,
Universitätstrasse 1, 86135 Augsburg, Germany.

[3] Department of Solid State Physics, Faculty of Sciences and Technology,
University of Debrecen, P.O. Box 400, H-4002 Debrecen, Hungary.

In HAMR (Heat Assisted Magnetic Recording) technology at the manufacture of a medium for magnetic recording it is important to create layers with different magnetic hardness. The intermediate layers are necessary in recording media design because they induce textured growth in the recording layer and improve the exchange decoupling between the magnetic grains.

In this work the diffusion formation of an ordered $L1_0$ FePt phase in Pt(15 nm)/Ag(Au)/Fe(15 nm) and Fe(15 nm)/Ag(Au)/Pt(15 nm) trilayers with Ag(Au) interlayer thickness of 10 nm is studied.

The films were prepared by magnetron sputtering on SiO_2/Si(001) substrate. Isothermal annealing of the tri-layered samples were carried out in a vacuum of $1{,}3 \cdot 10^{-3}$ Pa at temperature of 700 °C for 30 s, 2 min, 5 min, 15 min and 30 min. The structural properties of the as-deposited and annealed films were characterized by X-ray diffraction. Depth profiles of the films were investigated by secondary neutral mass spectrometry. The magnetic properties were determined by a superconducting quantum interference device (SQUID).

It was found that by changing the sequence of Fe or Pt layers deposition it is possible to form the soft magnetic and hard magnetic layers due to directed Ag(Au) diffusion, creating a heterogeneity of the chemical composition along the film thickness.

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Synthesis of thermally stable ultrasmall metallic Ni nanoparticles confined in microporous carbon

Boychuk V.M.[1], Kotsyubynsky V.O.[1], Rachiy B.I.[1], Solonets D.M[1],
Zapukhlyak R.M.[1], Turovska L.V.[2]

[1] *Vasyl Stefanyk Precarpathian National University, 57 Shevchenko Str.,*
Ivano-Frankivsk, 76018, Ukraine.
E-mail: kotsuybynsky@gmail.com

[2] *Ivano-Frankivsk National Medical University, 2 Halytska Str.,*
Ivano-Frankivsk, 76018, Ukraine

The search for highly efficient, inexpensive, and durable non-noble-metal electrocatalysts for hydrogen evolution reaction in an acidic environment is crucially important for the further progress of a clean sustainable economy. The present study reports on the synthesis and characterization of hybrid materials formed by ultrafine Ni nanoparticles and microporous carbon. A hemp fiber derived carbon template was prepared using the stages of carbonization (800 °C) and chemical activation (KOH as an agent) (labeled as AC materials). Additionally, AC was treated with HNO_3 as a source of nitrogen at 70 °C in an N_2 atmosphere to form N-containing surface functional groups and increase wettability with an aqueous electrolyte (labeled as ACN materials). The carbon templates were degassed in a vacuum (200 °C, 12 h) and transferred at low pressure to a quartz chamber with vapors of sublimated nickelocene ($Ni(Cp)_2$). After adsorption of $Ni(Cp)_2$, for its dissociation, the obtained materials were irradiated with UV light (27 W, main wavelength of 365 nm) with continuous stirring for 5 days (labeled as Ni:AC and Ni:ACN materials, respectively). According to XRF data (Exper-3L analyzer), Ni load was 4-5 wt %. Thermal treatment of both AC and ACN was carried out in an inert atmosphere (argon flow) at a temperature of 400 °C for 1 hour. XRD patterns (XRD-7000, Shimadzu) of AC and ACN templates show broad peaks (002) and (10l) indicating turbostratic ordering of carbon matrices. There are no changes in the XRD patterns of as-synthesized and annealed at $T \leq 400$ °C Ni:AC and Ni:ACN samples. A distinct presence of the Ni metal phase was observed for Ni:AC-700 and Ni:ACN-600 materials. Nitrogen adsorption–desorption isotherms (Autosorb Nova 2200e, Quantachrome) of all Ni:AC and Ni:ACN samples are a mixture of types II and IV. As-prepared and annealed samples had micropores (NLDFT model) with a size of 1.35 nm. The presence of Ni particles leads to the filling of some of these micropores and a decrease in the BET surface area from 1200 to 1000 m^2/g. Annealing leads to the growth of micropore-confined Ni particles and causes its migration to the surface of carbon grains, which manifests itself in the gradual restoration of the initial pore size distribution and BET surface area.

Mechanical properties of SiGe core-shell nanowires: molecular dynamics simulations

***Semchuk S.S.*, Kuryiluk V.V.**

Faculty of Physics, Taras Shevchenko National University of Kyiv.
64/13, Volodymyrska Street, City of Kyiv, Ukraine, 01601.
E-mail: cavej85@gmail.com, kuryliuk@knu.ua

Recently, Si/Ge core–shell nanowires (NWs) have been studied extensively, both experimentally and theoretically for their promising use in the current [1] and, potentially, the next generation of nanodevices [2,3]. In current planar technology essentially all high-performance Si-based microprocessors incorporate strain to enhance their performance. Core-shell structure offers a unique opportunity to control Young's modulus of the NW since it allows to rearrange Si and Ge atoms without compromising the electric properties of the NW.

This work focuses on the study of the mechanical properties of Si/Ge and Ge/Si core-shell NWs using molecular dynamics method. Young's modulus and failure mechanism of the NWs is determined by calculating stress-strain dependencies. We first apply and test two different interatomic potentials, Tersoff and MEAM, to define the one that represents the mechanical properties of Si and Ge NW most accurately. Testing Tersoff and MEAM potentials for stress-strain dependence of Si and Ge NWs show that Tersoff potential fails to represent mechanical properties of Si and Ge nanowires in a way that would correspond to experimental data, while MEAM potential accurately displays both Young's modulus and failure mechanisms of the NWs.

Further study of mechanical properties of Si/Ge core-shell NWs shows that with the increase of Si to Ge ratio Young's modulus increases while staying within the limits of Young's modulus of Si and Ge respectively. Meanwhile, the ultimate strength of the NWs can exceed the corresponding value for pristine Si and Ge NWs. These results have a mirrored effect with Ge/Si core-shell NWs.

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Evaluation of the degree of solid solution hardening of multielement metal composite material's diborides

Zakarian D.*[*], *Khachatrian A., Kartuzov V.

Frantzevich Institute for Problems of Materials Science,
Krzhizhanovsky str., 3, 03142, Kyiv-142, Ukraine

A method has been developed with the help of which the degree of solid solution hardening of multielement metal composite material's diborides (HEA'S diborides) having an AlB2 type structure is estimated. The method makes it possible to estimate the hardness of both nanosized structures and bulk materials.

To describe the random distribution of metal atoms over the nodes of the crystal lattice, the concept of a characteristic volume is introduced, as a volume where the distribution of atoms of all metals, included in the composition of the alloy, is realized. In this volume, all possible neighborhoods of atoms in the crystal lattice are taken into account. The characteristic volume is a necessary building element, which can be used to construct the HEA'S structure of diborides by its translation. The volume of the characteristic region depends both on the number of possible pair interactions of atoms and on the type of the crystal lattice of the alloy, which are determined from first principles (pseudopotential method) [1].

One of the fundamental properties of multi-element composite HEA'S materials is that the lattice structure of the solid solution is strongly distorted and this creates an obstacle to the free movement of dislocations. To describe hardening, the main emphasis in research is on taking into account the difference in the radii of the atoms present in the alloy.

The main characteristics of alloys that correlate with mechanical properties are the number of various metal elements, the mismatch parameter, which represents the maximum difference in the atomic radii of the elements in the alloy, and the average crystal lattice parameter of the alloy. The increase in hardness depends on the ratio of the values of the mismatch parameter and the lattice parameter of the alloy. If the first factor is associated with the difference in the atomic radii of the elements (the degree of distortion of the crystal lattice of the alloy), then the second is indirectly related to the potentials of different elements, as well as their interaction.

The calculation was carried out for diborides of multielement metal composite materials ($Zr_{0.5}Hf_{0.5}B_2$; $Ti_{1/3}Zr_{1/3}Hf_{1/3}B_2$; $Ti_{0.25}Zr_{0.25}Hf_{0.25}Cr_{0.25}B_2$; $Ti_{0.2}Zr_{0.2}Hf_{0.2}Cr_{0.2}Ta_{0.2}B_2$). It has been found that an increase in the number of types of metal atoms in a composite material leads to an increase in hardness, even if the difference in atomic radii is small.

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Electro-transport properties of CNT decorated by FeNi nanoparticles

Syvolozhskyi O.A.[1]***, Matzui L.Yu.***[1]***, Ovsiienko I.V.***[1]***,***
Len T.A.[1]***, Vovchenko L.L.***[1]

[1]Taras Shevchenko National University of Kyiv, 01601, Kyiv,
Volodymyrska st. 64/13, Department of Physics
E-mail: mail.olexiy@gmail.com

This work presents the study of segregated polymer composites based on ultra-high-molecular-weight polyethylene (UHMWPE) filed with hybrid filler - carbon nanotubes (CNTs) decorated by NiFe nanoparticles.

The main objective is to ascertain the influence of hybrid filler in segregated polyethylene composites on their electrical properties.

Electrical conductivity of the investigated composites was measured by standard two-probe method in DC mode at room temperature

The electrical conductivity σDC of CNTs/UHMPE and (CNTs- NiFe)/UHMPE composites with segregated filler distribution was studied as function of fillers volume content φ; results are shown in Fig. 1

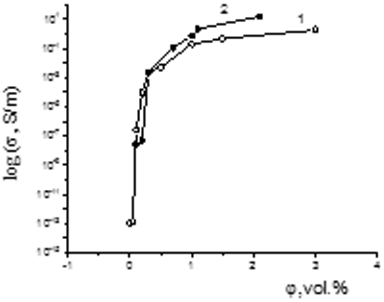

Fig. 1. *Concentration dependences of conductivity for the segregated UHMPE-based composites filled with, CNTs(1) and CNTs-NiFe.(2)*

As one can see from the Fig. 1, the use of CNTs- NiFe as a filler leads to increase in conductivity at higher concentrations. The effect of decoration on the electrical transport properties of composites at low concentrations was not detected

The electrical conductivity of both systems demonstrates percolation behavior with a sharp magnitude increase when the percolation threshold is reached.

Hydrogen production through catalytic hydrolysis of borohydrides

Lesik S.M., Ivanenko I.M.

Department of Inorganic Substances Technology, Water Treatment and General Chemical Engineering, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",
Ukraine, Kyiv, 03056, 37 pr. Peremohy, 4 building,
luckystrike191012@gmail.com

The invention of internal combustion engines shows that traditional sources of energy from fossil fuels are unviable in the long run because they have obvious limitations due to raw materials. At the same time, the rate of use of fossil resources is thousands of times higher than the rate of formation of new ones. One of the advanced systems for obtaining energy from alternative raw materials is systems that use hydrogen as an energy source. The use of hydrogen as an energy resource was first published in an article in 1972 [1]. Already today, several automakers produce hydrogen cars, namely: Honda, Toyota, Hyundai, etc. [2]. Since the energy density of hydrogen is one of the highest, it is $1.4 \cdot 10^8$ J/kg, hydrogen cannot be a source of energy for portable devices such as mobile phones and laptops, but can meet the needs of industry [3].

The key problem of storing and transporting hydrogen due to explosiveness can be solved in several ways, one of which is the use of sodium borohydride with its subsequent hydrolysis. $NaBH_4$ is a non-combustible and environmentally friendly compound in both dry and dissolved states, with a high ratio of energy density to mass, which is an excellent material for storing hydrogen, the content of which is ~ 10.8% of the mass. The hydrolysis reaction of sodium borohydride is a liquid-phase catalytic heterogeneous process with heat release, and the decomposition product, sodium metaborate, can be used further as hydrogen storage. According to the literature [4], the rate of decomposition of sodium borohydride is virtually independent of rising temperatures above 40°C, and complete decomposition occurs within about an hour. It is essential that the

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decomposition rate can be significantly adjusted using a suitable catalyst. It should be noted that currently there are two methods of industrial production of sodium borohydride, which increase the prospects for the use of this carrier: the Brown-Schlesinger process (sodium hydride reaction with trimethylborate) [5] and the Bayer process (borosilicate glass reaction with sodium and hydrogen) [6].

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Kinetic and equilibrium studies for the sorption of benzene and phenol from water on functional MCM-41 silicas

***Trofymchuk I.M.*, Roik N.V., Belyakova L.O.**

Chuiko Institute of Surface Chemistry of NAS of Ukraine,
17 General Naumov Str., 03164 Kyiv, Ukraine.
E-mail: trofymchuk_iryna@ukr.net

Mobile crystalline materials (MCM-41) are ordered silicas synthesized via liquid crystal templating mechanism by subsequent removal of the organic template using calcination or acid dissolution [1]. High surface area, regular channel type structures, large pore volume and diameter, excellent hydrothermal, thermal and hydrolytic stabilities, active silanol groups on the surface of MCM-41 silicas make them an interesting alternative to the usage of popular available sorbents (carbon and polymeric materials) for aromatic compounds removal. Moreover, to increase the efficiency of sorption on MCM-41 in water treatment processes it is possible to modify the surface of silica with highly active and/or selective groups.

In the present work, supramolecular approach of the synthesis of MCM-41 silicas with oligosaccharide units was used for obtaining nanoporous materials with high affinity to aromatic compounds in aqueous solutions. Here, the unique ability of β-cyclodextrin (β-CD) to form inclusion complexes with different compounds, combined with hexagonally ordered mesoporous structure of silicas, offers attractive opportunities. MCM-41 silicas with different content of β-CD-containing functional groups were synthesized by sol-gel co-condensation of silane precursors in the presence of ionic surfactant as template. To elucidate the contribution of oligosaccharide units as supramolecular centers into the properties of synthesized materials, the removal of benzene and phenol from aqueous solutions by pristine MCM-41, amino- and β-CD-functionalized MCM-41 silicas was conducted. Multibatch sorption tests were carried out at room temperature to examine the efficiency of synthesized silicas toward aromatics' uptake from water depending on time and equilibrium concentration. Typical kinetic and isotherm adsorption models were used to analyze the sorption processes on synthesized silicas. Prepared MCM-41 silicas demonstrate stronger affinity towards benzene than to phenol that could be very promising for selective removing of hazardous compounds in water treatment processes.

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Influence of carbon nanotubes content on the thermal-structural properties of high-density polyethylene

***<u>Khelil S.</u>*[1], *Barama N.*[1], *Dorbani T.*[1], *Naoui Y.*[1],**
***Boulakleb M.C.*[1], *Nedilko S.G.*[2], *Revo S.*[2], *Hamamda S.*[1]**

[1] *LTTSM, Mentouri Brothers Constantine 1 University, Algeria.*
E-mail: shamamda@yahoo.com

[2] *Taras Shevchenko National University of Kyiv, Institute of High Technologies, Volodymyrska St. 64/13, Kyiv 01601, Ukraine.*

This note aims at characterizing polyethylene-based nanocomposites containing different amounts of multiwall carbon nanotubes. The elaborated nanocomposites samples contained of 0, 0.1, 0.25, 0.5, 1.0, 2.5 and 5% MWCNTs. The studied materials were prepared using a high energy ball mill with a centrifugal force up to 50g. Several modern techniques such as dilatometry, calorimetry, mass loss, X-ray diffraction, infrared and Raman spectroscopy were used for investigation of the samples.

The calorific values of the studied samples changed with concentrations, thus, the PE+0.25%MWCNTS sample has the highest heating value. On the other hand, PE+0.1%MWCNTs was of the least intense.

The content of the introduced MWCNTs plays a significant role in the mass loss of the samples. Their thermogravimetric curve changes little. This suggests that the insertion of the MWCNTs in the high-density polyethylene is the cause of the nanocomposites stability.

The dilatometric measurements were made both in the radial and longitudinal directions. the longitudinal direction, they contain an anomaly around 50 – 55 °C and the curves overlap after 60 °C. In the radial direction, the expansion of PE+2.5%MWCNTs is higher than that of all other samples. It contains an intense anomaly located near 97 °C. The dilatometric curves of the other nanocomposites show very low expansion coefficients of the same order of magnitude.

The Raman spectra of all samples have almost the same shapes. The D peaks are observable but the G peaks are undetectable. The infrared spectra change shape from one sample to another and the relative intensities of the peaks depend strongly on the concentration.

X-ray diffraction showed that the crystallites size are concentration dependent. On the other hand, there was a refinement of all the structures concerning that of the matrix.

Study of aluminium containing multiwall carbon nanotubes

Barama N.[1], Khelil S.[1], Boulakleb M.C.[1], Dorbani T.[1], Naoui Y.[1], Nedilko S.G.[2], Revo S.[2], Hamamda S.[1]

[1] LTTSM, Mentouri Brothers Constantine 1 University, Algeria.
E-mail: shamamda@yahoo.com

[2] Taras Shevchenko National University of Kyiv, Volodymyrska St. 64/13,
Kyiv 01601, Ukraine.

This abstract focuses on the dilatometric and structural variations of aluminium containing different concentrations of multiwall carbon nanotubes.

The use of planetary ball mill has allowed obtaining aluminium-based nanocomposites containing 0.1, 0.25, 1.0 and 1.5%MWCNTs, respectively. Their characterization was done using different experimental techniques such as differential scanning calorimetry, thermogravimetry, dilatometry, X-ray diffraction and IR and Raman spectroscopies.

The dilatometry measurements showed that the coefficient of thermal expansion measured along the perpendicular direction of the rolling plane of the different samples decreases drastically. It becomes of the order of the dilatation of the nanotubes themselves. On the other hand, in the directions perpendicular and parallel to the rolling direction, it is very significant. It is two to three times larger than the previous one. Thus, it is strongly anisotropic. This situation is certainly related to the dispersion of the MWCNTs.

As for calorimetry, it displays similar graphs. They have the same shape but their intensity depends strongly on the MWCNTs concentration. The differences are very strong. The intensities of the extreme heat capacities of the two samples Al+1.5%MWCNTs and Al+0.25%MWCNTs are equal to 0.5 mW/mg and 14.5mW/mg respectively. The rest ones are included in this range. Concerning the two other nanomaterials, the calorific value of Al+1.0%MWCNTs is 1/5 before that of Al+0.1%MWCNTs. The calorific value decreases with the concentration.

The thermogravimetry of the samples is relatively comparable. The sample containing 1%MWCNTs appeared to be the most stable. The oxidation is very low. The infrared spectra are almost identical. They contain the same anomalies with relative intensities depending on the concentration.

The Raman technique displays spectra having the shapes each containing two characteristic peaks of carbon. The D and G peaks are more or less intense depending on the concentration of multiwall carbon nanotubes.

Polymer and inorganic glass-ceramics nanocomposites filled with luminescent oxides

Nedilko S.G.

Taras Shevchenko National University of Kyiv,
Volodymyrska St. 64/13, Kyiv 01601, Ukraine.

It is known that intermediate regions are formed between the initial phases of the composites and structure of such interphase regions does not correspond to the composition and structure of the initial phases. The contribution of the interphase to the properties of the material and the interaction between the matrix and the initial phases, may be clarified by the difference in characteristics of simple "filled matrix" and "composite based on that matrix".

The role of the interphases in determining characteristics of hybrid nanocomposite materials is discussed in the contribution. Suitable literature data and the results of our own experimental and computer simulation studies were used for this discussion.

The main direction of interphase behaviour in composite material study is a determination of the relationships between the properties of the material, on the one hand, and the atomic and energy structure, composition of the object, the size of its components - on the other hand. Although the mechanisms of interaction between any possible components of the composite, in principle, are predictable, nevertheless, their role and contribution in the case of a particular type, especially - nanoscale composite material (nanocomposite) containing oxides fillers needs to be clarified.

These features are discussed here on the base of results obtained for nanocomposites of three types where nanocrystalline dielectric oxides fillers were embedded into: 1) the glass oxide dielectric matrices; 2) the polymer matrices, particularly, microcrystalline cellulose and nanocellulose; 3) carbon nanoforms (nanotubes, graphene and graphene oxide. Optical, electron and atomic force scanning microscopy methods as well as XRD, diffuse optical reflectance and photoluminescence methods were used for study mechanisms of phase interactions and interfaces in noted nanostructured composites and the impact of these mechanisms on optical and luminescent macro-characteristics of materials under study. This work is aimed not only to clarify and explain the role of interphases/interfaces, but also to identify the ways to develop materials with properties that can be used as basic for studied composites practical application.

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RF plasma modification of MoS_2 2D material

Slobodian O.[1], Okholin P.[1], Nikolenko A.[1],
Lytvyn P.[1] and Nazarov Al.[1,2*]

[1] Lashkaryov Institute of Semiconductor Physics of the NAS of Ukraine
Kyiv 03028, Ukraine
E-mail: nazarov51@lab15.kiev.ua

[2] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"
Kyiv 03056, Ukraine

Single and multy layer MoS_2 materials are intensively studied in last decade. Single layer MoS_2 material is 2D semiconductor with direct band gap of 1.8 eV which is very promising for next generation of nanoelectronic and optoelectronic devices. Control doping of such 2D layers is impontant point in these research. RF plasma treatment is low temperature methods which allows us to change effectively electrical parameters of the materials. In suggested research the RF plasma of forming gas ($10\%H_2+90\%N_2$) has been used to modificate and doping of the multilayer MoS_2 film.

The MoS_2 pristine flakes in ethanol/water solution were purcharsed from Graphene Supermarket Co (USA) and deposited on Au interdigitated electrode array (IDA) on SiO_2/Si by ultrasonic spray coating technique. The IDA used for electrical and AFM measurments. For Raman, FTIR and XPS experiments the MoS_2 flakes were deposited on Si wafer. The samples were treated by RF plasma (13.6 MHz) at room temperature during 30-90 sec at $0.5W/cm^2$ in forming gas.

It was shown that RF plasma treatment of the flakes results in decrease of differential resistance near zero volt in compare with initial structure, and when a time of the treatment reaches to 90 sec the reduction amounts factor of 100. Raman spectra show characteristic peaks for multilayer MoS_2 at 386, 406 and 454 cm^{-1}, which can be assigned to the E^1_{2g}, A_{1g} and longitudinal acoustic phonon modes, respectively. After RF plasma treatments the E^1_{2g} and A_{1g} lines are shifted in blue side that corresponds to additional hole doping of the MoS_2 flakes. XPS spectra demonstrate presence peaks at 228.5, 320 and 235 eV. Two first ones correspond to the Mo^{4+} $3d_{5/2}$ and Mo^{4+} $3d_{3/2}$ components in 2H-MoS_2, and last peak – to Mo^{6+} $3d_{5/2}$ and associated with MoO_3 oxide formation. It is known that oxygen incorporation into MoS_2 layer can result in additional hole doping. However the MoO3 is wide bandgap semiconductor which has high resistivity and its formation is unable to reduce resistance oft he material. Nitrogen incorporation in oxygen vacancy of the MoS_2 can also dope it with holes. Possibly nitrogen doping or formation of MoOX oxides, which can be low resistance, leads to reduction of electrical resistance of MoS_2 flakes.

Vacuum synthesis of high-temperature polymeric axially symmetric nanostructures

***Svavil'nyi M.Ye.*, Panarin V.Ye.**

G.V. Kurdyumov Institute for Metal Physics of the National Academy of Sciences of Ukraine, blvd. Acad. Vernadsky 36, Kyiv-03142, Ukraine.
E-mail: myksvavil@gmail.com

It follows from the well-known Ferrari-Robertson diagram [1] that, depending on the ratio between the components of the mixture of carbon elements with sp^2, sp^3 phases and hydrogen, various either carbon or polymer materials can be synthesized from this three-component mixture. Technological conditions for the implementation of possible synthesis options i.e. the specific type of material from this diagram does not follow. Vacuum synthesis of carbon nanotubes (CNTs) in a wide range of technological conditions has shown that in some modes, polymer structures are formed that are very similar to conventional CNTs. A typical view of such polymers is shown in Fig. 1a. With a relatively long exposure of individual sections of such polymers under an electron beam of a microscope (~ 20 sec), they increase their size, as can be seen in Fig. 1b, i.e. they melt under the action of an electron beam, although their synthesis was carried out at a temperature of ~700°C. At these temperatures, and even when the substrate was heated to 800°C, there was no noticeable destruction of the structures.

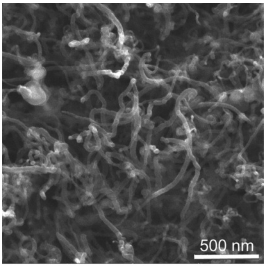

***Fig**.1a*

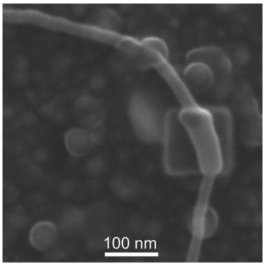

***Fig.**1в*

The technology of CNT synthesis processes, setup, and experimental conditions are described in detail earlier in [2].

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Optical Properties of Au-CuS Core-Shell Nanoparticles

Bulavinets T.O.[1]***, Yaremchuk I.Y.***[1]***, Volskyi R.R.***[1]***, Bobitski Y.V.***[1,2]

[1] *Department of Electronic Engineering,*
Lviv Polytechnic National University,
12, S. Bandera Str., Lviv 79013, Ukraine
E-mail: tetiana.o.bulavinets@lpnu.ua

[2] *University of Rzeszow, Pigonia Str.1, 35959 Rzeszow, Poland*

Localized surface plasmon resonance, as well as the efficiency of absorption and scattering of radiation is determined mainly by structural and geometric nanoshells parameters. The ratio of the core and the shell size has a significant effect on the nanoshells optical properties with a certain shape. Thus, in this work the Mi theory and the dipole equivalence method are used to analyze the optical properties of spherical and ellipsoidal (prolate and oblate) Au-CuS nanoshells. The combination of the metallic core (gold) ability to localized plasmon resonance [1] and the semiconductor shell (copper monosulfide) [2] provides a high concentration of electromagnetic field on the nanoshells surface and opens new prospects in understanding of plasmonic properties behavior.

This paper studies the nature of changes in extinction spectra when changing the core/shell size ratio in spherical and ellipsoidal (prolate and oblate) Au-CuS nanoshells. The obtained results are analyzed to establish the regularity of changes in the nanoshells extinction spectra, which can be used to develop devices based on them for different application. The plasmon properties of spherical and ellipsoidal Au -CuS nanoparticles with different sizes were determined. It is established that the intensity of the extinction cross section of spherical nanoshells strongly depends on the ratio between the thickness of the core and the shell. Ellipsoidal oblate and prolate core-shell nanoparticles are characterized by two maxima, which corresponds to the plasmon peak of gold and copper monosulfide nanoparticles, respectively. It is possible to configure the plasmon properties of oblate and prolate ellipsoidal core-shell nanoparticles by changing the core and shell thickness in both directions. Thus, the results of the study suggest that Au-CuS nanoparticles can be used as potential elements of various sensitive sensors.

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Nanocrystalline Y–TiO_2 thin-film electrodes for determination of Pb(II) and oxygen in aqueous medium

Medyk I.A.[1]***, Vorobets V.S.***[2]***, Fomanyuk S.S.***[2]***,***
Kolbasov G.Y.[2]***, Karpenko S.V.***[2]

[1] Department of Chemistry, National University of „Kyiv-Mohyla Academy". Skovoroda str., 2, Kyiv-04070, Ukraine.

[2] Department of electrochemistry and photoelectrochemistry of non-metallic systems, Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine. Acad. Palladin Str., 32/34, Kyiv-03142, Ukraine.
E-mail: vorobetsvs@i.ua

We present study results of possibility to use electrodes based on nanocrystalline Y-doped titanium oxide thin films to determine the concentration of Pb^{2+} ions and O_2 by anodic stripping voltammetry (ASV) method and inversion spectral photoelectrochemical (ISP) method. Lead by the ASV method was determined during anodic potential scanning, recording the current of electrodissolution of the reaction products formed on the surface of the indicator electrode after previous cathodic electroconcentration in an electrolyte solution containing lead ions. Oxygen was determined by the oxygen electroreduction current observed during the cathode potential scan. Solutions of 0.1 M hydrochloric acid, 0.4 M formic acid and acetate buffer (pH=5.5) were used as background electrolytes. It is determined that the value of analytical signal of lead in the studied electrolytes is proportional to the concentration of Pb (II) in solution, thus Y-TiO_2 electrodes can be used as indicator electrodes for determination of Pb^{2+} ions by ASV method. The optimum conditions of Pb^{2+} ions determination are: background solution based on 0.1M hydrochloric acid, electroconcentrating potential -1,4 V; time of electrolysis 120 s, scanning speed of potential 50 mV.s-1. The sensitivity of the ASV method to Pb^{2+} – 0.1 $mg \cdot l^{-1}$, to O_2 – $(3\text{-}6) \cdot 10^{-3}$ $mg \cdot l^{-1}$.

To increase the sensitivity of Y-doped TiO_2 electrodes to lead, an ISP method was used, which consists in concentrating of Pb^{2+} at the anode and comparing photoelectrochemical current before and after concentrating on different parts of spectral range. It has been shown that at concentrating potential of -1.4 V in acetate buffer, the deposition of metallic lead from the solution occurs. Metallic lead blocks the active centers of the surface, which results in significant decrease in the photocurrent value in the spectral range of 250-350 nm, which corresponds to light absorption by the TiO_2 film. The dependence of photocurrent quantum yield on Pb^{2+} is straight-line at $CPb^{2+} < 0.3$ $mg \cdot l^{-1}$. The sensitivity of ISP method to Pb^{2+}on Y-doped TiO_2 electrodes was 0.01 $mg \cdot l^{-1}$.

Influence of "pompom" graphene additive on characteristics of graphite electrodes for LIBs

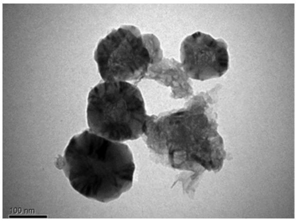
Dubinevycha S.[1], Zinin V.[1], Potapenko A.V. [2,3], Potapenko O.V.[2,3]

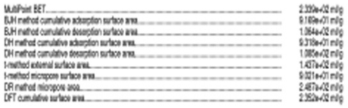
[1] LLC "MaxAh" K, Kiev, 01001, Ukraine
[2] Joint Department of Electrochemical Energy Systems NAS of Ukraine
E-mail: 1978hiking@gmail.com

[3] Faculty of Materials Metallurgy and Chemistry, Jiangxi University of Science and Technology, Ganzhou, Jiangxi, P.R. China

Graphene is a new generation material that finds potential and practical application in a variety of research areas. It has unsurpassed characteristics in terms of electronic conductivity and thermal conductivity, mechanical strength and large surface area, and its special structural and morphological characteristics have great prospects for use in energy storage devices and supercapacitors [1-2].

The use of "pompom" graphene developed by LLC MaxAh, Ukraine opens up possibility for improving the characteristics of materials for both existing LIBs and new systems being developed, such as "lithium-sulfur". Small additions of "pompom" graphene to graphite electrodes can significantly increase the electronic conductivity of the material, which in turn affects the increase in current loads in the battery. And the special morphology of “pompom” graphene, from our point of view, will make it possible to obtain outstanding characteristics of electrodes in terms of life cycle stability. Primary results obtained upon cycling of natural graphite (grade GAK - 1; 99.5%) with the addition of graphene show stable cycling of electrodes with a realized specific capacity of 307 mAh/g at the charge/discharge current density of 0.25C. The TEM image of "pompom" graphene particles and the characteristics of its specific surface, obtained using BET method, are presented below.





Surface Area Data

MultiPoint BET	2.339e+02 m^2/g
BJH method cumulative adsorption surface area	9.169e+01 m^2/g
BJH method cumulative desorption surface area	1.064e+02 m^2/g
DH method cumulative adsorption surface area	9.318e+01 m^2/g
DH method cumulative desorption surface area	1.085e+02 m^2/g
t-method external surface area	1.437e+02 m^2/g
t-method micropore surface area	9.321e+01 m^2/g
DR method micropore area	2.487e+02 m^2/g
DFT cumulative surface area	2.352e+02 m^2/g

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Nano-dispersed Zn-Al double hydroxide and oxides for photocatalytic application

Sydorchuk V.**, **Levytska S., Khalameida S., Kuznetsova L.

Institute for Sorption and Problems of Endoecology, NAS of Ukraine.
13 Naumova St., Kyiv-03164, Ukraine E-mail: bilychi@ukr.net

The layered double hydroxides LDHs and oxide compositions prepared from them are sorption and catalytically active materials used to purify polluted air and water, for example as photocatalysts. They should have certain physicochemical properties in order to be effective photocatalysts.

The hydrothermal and mechanochemical treatments (HTT and MChT) of coprecipitated Zn/Al hydroxide with Zn/Al ratio were used to regulate physicochemical parameters. These kinds of modification were performed in the form of wet gel and dried xerogel. Such approach has not previously been used to modification of Zn/Al hydroxide although was effective for other oxides

XRD, DTA-TG and FTIR measurements show that MChT in air results in partially decomposition of LDHs structure without formation of other phases while only modification of its structure takes place after milling in water. At the same time, elevation in HTT temperature leads to gradual decomposition of LDHs: if its structure is improved at a temperature of 150°C, then it is partially destroyed at 200°C, and zinc oxide is formed at 250°C. Crystal structure of ZnO is also improved after next calcination of all modified LDHs. Also, significant changes in porous structure occurs during MChT and HTT. It is important that formation of additional mesoporosity and corresponding increase in specific surface area take place. Thus, the samples after have value of mesopores up to 0.70-0.75 cm^3/g and specific surface area 50-67 m^2/g and the latter for samples milled in water reaches 106 m^2/g. The changes in crystal structure are accompanied by changing the electronic characteristics: the narrowing of band gap from 3.2 eV (initial sample) to 2.8-2.9 eV (hydrothermally treated samples) is observed.

All of these changes result in enhancement of the photocatalytic activity of modified samples under visible irradiation. Indeed, initial sample is practically non-active in process of photocatalytic degradation of safranin T (as model substrate) in aqueous medium under these conditions. At the same time, sample subjected to dry milling at 300 rpm which has the bang gap 3.1 eV becomes active: rate constant of degradation $K_d = 1.8\ 10^-5\ s^{-1}$. The sample, modified by HTT in the form of gel at 200°C, possesses the maximal activity ($K_d = 3.4\ 10^{-5}\ s^{-1}$) since it simultaneously has band gap 2.9 eV and high value of specific surface area - 67 m^2/g.

Electrochromic and gas-chromic properties of conjugated polymer films doped with nanoclusters on flexible substrates

Horbenko Yu.Yu.[1]***, Aksimentyeva O.I.***[1]***, Starykov H.O.***[1]***, Ivaniuk K.B.***[2]

[1] *Ivan Franko National University of Lviv,*
Kyryla &Mefodia str., 6/8, Lviv 79005, Ukraine.
E-mail: yuliia.horbenko@lnu.edu.ua

[2] *Lviv Polytechnic National University, Bandera str., 12, Lviv 79013, Ukraine.*

Due to the development of organic electronics, studies related to the production of thin polymer layers with different functions, such as electrical conductivity, sensory sensitivity, absorption or emitting light in a fixed optical range, become particularly relevant. Such coatings can be obtained by simple non-vacuum methods, including polymerization on solid surfaces. One of the main advantages of this approach is the ability to obtain functional materials directly on polymer substrates, which is important for the production of flexible screens, organic LEDs, and electrochromic devices [1, 2].

In this research, the methods of formation of conjugated polymers films – polyaniline, poly-ortho-anisidine (PoA), and poly-3,4-ethylenedioxythiophene, and their doping by nanoclusters of $K_3[Fe(CN)_6]$, graphene oxide, etc. were optimized. Samples were obtained by electrochemical deposition of polymers on transparent flexible substrates of polyethyleneterephthalate (PET) with a conductive layer of Indium tin oxide (ITO). The impact of the electric field on the changes in the optical absorption spectra of the polymer films and their electrochromic characteristics were studied. It was established that the most significant changes in the optical characteristics of PoA (76%) were observed in polymer electrolyte based on PVA and lithium perchlorate at $\lambda = 650$ nm when the potential switch from -0.2 to +0.6 V (Ag/AgCl). Moreover, the influence of gas vapors of various nature on the film's absorption spectra was investigated. The results will be the basis for further development of the method of functional polymer layer formation for flexible optoelectronic devices and optical sensors for the selective detection of harmful vapors in industry and the environment.

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Nanocomposites of polyaniline and polymethacrylic acid

***Dutka V.S.*, Kovalskyi Ya.P., Khamar O.O., Halechko H.M.**

Ivan Franko National University of Lviv,
6 Kyryla & Mefodia St., Lviv, 79005, Ukraine
e.mail: vdutka@ukr.net

Polymer-polymer composites (PPCs) based on electrical conductive polymer – polyaniline (PANI) and polymethacrylic acid (PMAA) have unique properties. Along with the electrical conductivity of the PPC can form films on different surfaces. Such composites can be successfully used for the design of chemosensors, protection of metals from corrosion, etc. Such PPC can be obtained by conducting oxidative polycondensation of aniline with peroxydisulfate of ammonium in the presence of PMAA. But this method does not allow you to control the exact relationship between the components. Another method of obtaining a PPC is a mechanical mixing of PMAA and PANI in a small amount of water and processing the resulting mixture by ultrasonic for 15 minutes. After drying the resulting composites, their physic-chemical properties were investigated.

The study of X -ray spectra of PANI and PMAA and composites on their basis showed that ligaments are formed between the components of the PPC. FTIR-spectroscopy and quantum-chemical calculations confirmed the possibility of forming hydrogen bonds between composite components. Different confirmation states of macromolecules of the PANI and PMAA lead to the formation of several types of hydrogen bonds, which are characterized by different energy and length.

The electrical conductivity of the resulting composites has been studied. The electrical conductivity depends on the ratio of the PANI and PMAA and is characterized by the maximum. The study of the dependence of electrical conductivity on the temperature allowed determining the energy of activation of charge transfer, which changes within quite wide limits.

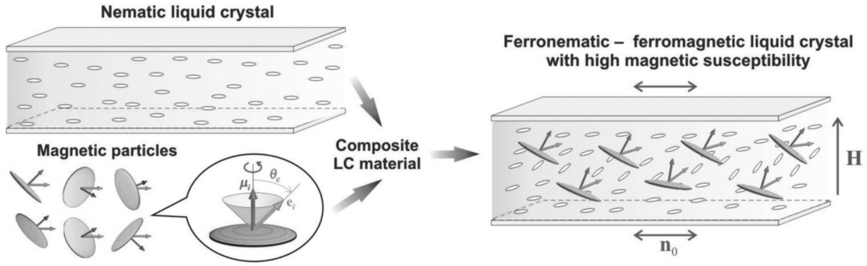
The study of thermal destruction of the PANI, PMAA and PPC was carried out by thermal gravimetry. The destruction of the PMAA is stepped: when heated at temperatures of about 100 °C PMAA cleaves the water molecules when the deep destruction runs through. Moreover, the mechanism of decomposition runs both on the mechanism of destruction and depolymerization. The destruction of PANI is also in several stages. The PPC destruction is also stepped, but at slightly higher temperatures. Therefore, the components of the PPC have one on the other stabilizing influence.

Magneto-orientational effects in ferronematics with conically degenerated anchoring at particles surfaces

***Burylov S.V.*, Skosar V.Yu., Burylova N.V.,**
Novikov V.F., Voroshilov O.C.

Institute of Transport Systems and Technologies of the NAS of Ukraine,
Pisargevskogo Str.,5,Dnipro -49005, Ukraine.
E-mail: S.Burylov@nas.gov.ua

We consider a new type of liquid crystal nanomaterials called ferronematic (FN). They refer to a nematic suspension doped with disk-shaped magnetic particles having specific conically degenerated anchoring of nematic molecules at particles surfaces [1].



We investigate the theoretical aspects of magnetically induced orientation transitions in a flat FN cell. We show that depending on the value of the conical anchoring angle and relations between the system material parameters, different FN behavior can be observed under the magnetic field action, including orientational phase transitions of the first and/or second order between uniform and non-uniform states as well as re-entrant transitions – "uniform phase – non-uniform phase – uniform phase – non-uniform phase". We have determined the conditions of these transitions, calculated and described in detail the orientation profiles of the nematic director and the particles magnetic moments, as well as the concentration distribution of the magnetic impurity in the cell. The magneto-optical response of the cell has also been found and analyzed.

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Functionalization of montmorillonite nanoparticles and synthesis of oligomer on their surface

Gonchar O.M.**, **Travinska T.V., Savelyev Yu.V.

Institute of Macromolecular Chemistry, NAS of Ukraine,
Kharkovskoe shosse,48, 02160 Kiev, Ukraine.
E-mail: lexgon@ukr.net

Organophilization of the surface of silicate nanoparticles is important for the production of polymeric organo/inorganic nanocomposites with montmorillonite (Mt) and other layered silicates based on polar polymers. This is achieved by modifying the surface of Mt nanoparticles with organic cations of different nature. Common modifiers used for organic modification of Mt are cations of Quaternary organic ammonium salts [1], cations of Quaternary salts of phosphonium [2], diamines and amino acids. Mt, modified with organic cations, is dispersed in the polymer matrix, where it acts as a strengthening agent, improving the properties of the polymeric material. In the case of polar polymers such as polyurethanes, polyamides, polyepoxides, Mt modified with aliphatic surfactants does not lead to delamination in the polymer matrix. This is due to the lack of sufficient quality interaction between the nanofiller and the polar polymer matrix [8-10]. In order to create organoclay with a functionalized surface for use as a nanofiller in the creation of organic/inorganic nanocomposites based on polar polymers, a method of modification of Mt with cationic oligourethane (oligourethanamine ammonium chloride (OUAAC)) was developed. Aromatic and aliphatic diisocyanate addition reactions, as well as sequential addition of aromatic diisocyanate, glycerol, and again diisocyanate, were performed in a suspension of amino-functionalized modified Mt. Thus, the possibility of synthesis on the surface of Mt nanoparticles of an organic layer with the required structural hierarchy is demonstrated. This method can also be used for matrix synthesis of the oligomer on Mt nanoparticles. he interlayer distance of all types of the obtained modified Mt was determined by the WAXS method, and the addition of diisocyanates corresponding to the content of amino groups was proved by thermogravimetric analysis.

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Stability and lifetime of carbyne chains in nanotubes

***<u>Timoshevskii A.</u>*[1], *Kotrechko S.*[1,2,3], *Kolyvoshko E.*[1], *Stetsenko N.*[1]**

[1] *G.V. Kurdyumov Institute for Metal Physics, National Academy of Sciences of Ukraine, 36, Academician Vernadsky Blvd., Kyiv-03680, Ukraine.*
E-mail: atimoshevskii@gmail.com

[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" 37, Peremohy Ave. UA-03056 Kyiv, Ukraine*

[3] *Taras Shevchenko Kyiv National University,*
60, Volodymyrska Str., Kyiv-01601, Ukraine.

Carbyne chains are rather unique research objects, but authors of [1,2] have managed to study their atomic structure, strength as well as the lifetime of carbyne-graphene nanoelements (CGNs) under thermomechanical loading by ab-initio modelling method. The study have shown that CGNs could be used for straintronic devices. Also, technology of the long carbyne chains production within the graphene nanotubes "cases" was recently developed. Thus, problem of stability and lifetime of carbyne chains in nanotubes at wide temperatures and stretching deformation is topical. To analyze atomic structure of graphene nanotube with a carbyne chain, the calculations were performed using the VASP [3] package]. Accuracy of the total energy calculation is 1meV/atom and 0.02 eV/Å for the structural optimization calculations. The lifetime of nanotube was estimated under the conditions of thermo-mechanical loading within the fluctuation model [2]. It has been ascertained that the lifetime of nanotube with a chain is governed by the waiting time for breaking the contact bond between the chain and the top of nanotube. It is the atomic structure of this connection that determines its strength and, ultimately, its lifetime. The strongest chain "fastenings" to nanotube are found. Within suggested fluctuation model, it is shown that the found "fastenings" provide sufficient lifetime for practical use of nanotubes with carbyne chains.

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Hydroxyl radicals scavenging by small oxide | nanocrystals with variable valence ions

Maksimchuk P.[1]***, Hubenko K.***[1]***, Seminko V.***[1]***,***
Onishchenko A.[2]***, Bespalova I.***[1]***, Klochkov V.***[1]***, Yefimova S.***[1]

[1] *Yu.V. Malyukin Nanostructured Materials Department, Institute for Scintillation Materials NAS of Ukraine,*
60 Nauky Ave., Kharkiv-61072, Ukraine.
E-mail: pavel.maksimchuk@gmail.com

[2] *Department of Physics, Kharkiv National University of Radio Electronics,*
14 Nauky Ave., Kharkiv-61166, Ukraine.

Reactive oxygen species (superoxide anions, hydrogen peroxide and hydroxyl radicals) are biologically active molecules which are formed inside the mitochondria of living cells during cellular respiration. Some of them play indispensable role in the metabolism of the cell. At the same time, an increase of the content of hydroxyl radicals (·OH) which are the strongest oxidants among all reactive oxygen species can trigger the number of pathological processes inside the cell from enhanced lipid peroxidation of cell membranes to DNA damage.

Hydroxyl radicals are formed at water radiolysis during X-ray or gamma-irradiation of the cell. Extremely high reactivity of ·OH radicals (average ·OH lifetime in the biological environment of only few nanoseconds) makes the task of its effective elimination by the internal systems of the living cell rather difficult. We propose three different types of small oxide nanocrystals with variable valence ions (CeO_2, $GdYVO_4$ and TiO_2) as promising materials for effective elimination of hydroxyl radicals.

CeO_2, $GdYVO_4$ and TiO_2 nanocrystals demonstrate high ROS scavenging activity against hydroxyl radicals formed during X-ray irradiation of water solutions. Hydroxyl radicals scavenging properties have been revealed to be directly related to the high content of reduced variable valence ions (Ce^{3+} for CeO_2, V^{4+} and V^{3+} for $GdYVO_4$, Ti^{3+} for TiO_2) which could donate electrons in hydroxyl radical neutralization reaction. A large amount of structural defects, such as oxygen vacancies, is a feature of small oxide nanocrystals. Formation of oxygen vacancies can be accompanied by the reduction of neighboring atoms, which were shown by XPS experiment for all types of nanocrystals.

The efficiency of hydroxyl radicals scavenging by small oxide nanocrystals with variable valence ions (CeO_2, $GdYVO_4$ and TiO_2) in water solutions allows suggesting such materials as effective antioxidants in living cells as well.

Intensification of the compaction process of diamond nanopowder under high pressure and high temperature

Bochechka O.O., Chernienko O.I., Kushch O.V., Venikov V.O., Havrylova V.S.

V. Bakul Institute for Superhard Materials, Natl. Acad. of Sci. of Ukraine.
Avtozavodska, 2, Kyiv-04074, Ukraine.
E-mail: obochechka@gmail.com

The influence of surface modification of particles of diamond nanopowder of static synthesis by carbon–tungsten bonds on the degree of compaction of diamond–tungsten carbide composite samples sintered from it at a pressure of 8 GPa has been studied. The process of W–C bonds formation on the surface of diamond particles is described in [1].

The ratio of the volume of the diamond component in the composite or polycrystal, V_d, to the volume of the sample, V, is taken as the compaction characteristic V_d/V.

It has been established that the compaction degree of diamond nanopowder increases by 8% (fig.) due to surface modification with carbon-tungsten binders in combination with degassing before sintering and the reaction interaction of diamond with tungsten. Thus, the modification of the surface intensifies the process of compaction of the diamond nanopowder of static synthesis under the action of high pressure and high temperature.

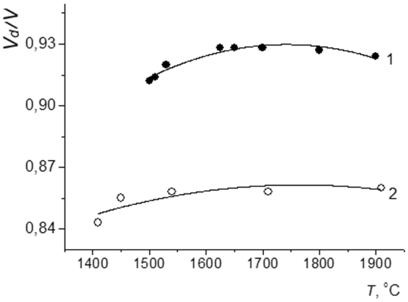

Fig. *Dependence of the V_d/V value of the diamond-tungsten carbide nanocomposite (1) sintered from the ACM5 0.1/0 diamond nanopowder modified with C–W bonds and a polycrystal from this powder without modification and degassing (2) on the sintering temperature: pressure 8 GPa, sintering time 20 s.*

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Catalytic properties of Zn-Mg(Zr)Si oxide nanosystems modified with alkali metals and rare-earth elements in the 1,3-butadiene production from ethanol

Larina O.V.**, **Zikrata O.V., Alekseenko L.M.,
Kyriienko P.I., Soloviev S.O.

L.V. Pisarzhevskii Institute of Physical Chemistry of the NAS of Ukraine,
Prospect Nauky, 31, Kyiv-03028, Ukraine.
E-mail: olga.larina@ukr.net

The processes for production of valuable chemicals and fuels based on bio-raw materials, in particular bioethanol, is an alternative to a number of petrochemical processes. Ethanol is considered as a universal precursor for the synthesis of such industrially important substances as ethene, propene, 1,3-butadiene, etc. hydrocarbons. Zeolite and silica-supported acid-base materials (e.g. Mg and Zr containing systems) doped with dehydrogenating components (ZnO, Ag, Cu, etc.) are promising catalysts for the ethanol-to-butadiene process.

In present work, the effect of alkali metal ions (Na^+, K^+) and rare-earth elements (Y, La, Ce) on acid–base and catalytic properties of Zn-Mg(Zr)Si oxide nanosystems in the process of obtaining 1,3-butadiene from ethanol was studied. It was found [1] that the modification of Zn-MgSi oxide systems with Na(K) leads to an increase in the 1,3-butadiene selectivity by reducing the formation of by-products. In the composition of Zn-ZrSi oxide systems, alkali metal additives lead to a decrease in the ethene and diethyl ether selectivity due to a decrease in the content of strong acid sites which catalyze ethanol dehydration reaction. Among the catalysts modified with rare-earth elements, higher indices of the ethanol-to-butadiene process are achieved in the presence of Mg-containing oxide catalysts, which are characterized by higher concentration of base and acid surface sites of medium strength. Among Zr-containing systems modified with rare-earth elements, Zn-Y-ZrSi sample is characterized by a higher number of Lewis acid sites of weak and medium strength, which accelerates the reaction of aldol condensation of acetaldehyde, a key step of the ethanol-to-butadiene process.

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Properties of the nanosized zinc pyrovanadate synthesized by mechanochemical, barothermal and ultrasonic methods

Diyuk N.V.[1], Diyuk O.A.[2], Keda T.Ye.[1], Zazhigalov V.O.[2]

[1] Taras Shevchenko National University of Kyiv
60 Volodymyrska Street, Kyiv 01033, Ukrain.
E-mail: nvdiyuk@gmail.com

[2] Institute for Sorption and Problems of Endoecology of NAS of Ukraine,
General Naumov Street, 13, Kyiv 03164, Ukraine
E-mail: diyukhelen@ukr.net

In recent years $Zn_3V_2O_8$ have attracted considerable attention as an effective catalyst for selective oxidation of glucose to galacturonic acid and as highly sensitive material for detecting acetone in air. $Zn_3V_2O_8$ is a promising rare-earth-free phosphor due to its high absorption and emission properties and low cost of raw materials. But traditional methods syntheses of zinc pyrovanadate have some efficiency problems and are not eco-friendly. Currently, zinc pyrovanadate is synthesized by two conventional methods: i) – co-precipitation of salts, ii) – solid state synthesis from salts or oxides. Both conventional syntheses were performed and compared with the alternative syntheses.

As raw materials for the implementation of alternative syntheses used ZnO and V_2O_5:

1) Mechanochemical synthesis was realized in a planetary ball mill in water medium during 20 min, rotation frequency – 500 rpm.

2) Barothermal synthesis was realized into a Teflon-lined steel autoclave in water medium at 150°C for 1 h.

3) Ultrasonic treatment was carried out in water medium for 20 min at room temperature.

$Zn_3V_2O_7(OH)_2\cdot 2(H_2O)$ phase was detected by XRD in all cases of alternative syntheses. DTA shows a loss of crystalline water up to 300°C with the formation of $Zn_3V_2O_8$ confirmed by XRD analysis. SEM and TEM images show that $Zn_3V_2O_7(OH)_2\cdot 2(H_2O)$ and $Zn_3V_2O_8$ obtained by alternative syntheses have the morphology of thin nanoplates with an average diameter about 1 nm. The sample synthesized by co-precipitation has a similar morphology.

SBET all samples synthesized by alternative methods and SBET of $Zn_3V_2O_8$ synthesized by the co-precipitation method were about 15 – 18 m^2/g, while SBET sample synthesized by solid-state method was 1 m^2/g.

The PL spectra of zinc pyrovanadate obtained by alternative syntheses have intense broadband emission from 400 nm to 700 nm.

Alternative syntheses allowed to obtain the $Zn_3V_2O_8$ with intense broadband emission by simple, fast method exclude pollution of environment by-products.

Polymer-Magnet Nanosystems

Aksimentyeva O.I., Horbenko Yu.Yu.

Ivan Franko National University of Lviv,
Kyryla &Mefodia str., 6/8, Lviv 79005, Ukraine.
E-mail: aksimen@ukr.net

Providing macroscopic magnetism in organic materials is a very complex but quite promising scientific problem [1]. The need to create an organic magnet is due to a number of expected advantages, such as lightness, transparency, flexibility, ability to switch under the influence of light (magneto-optics), sensitivity to external influences (sensors), creation of modern toners for digital printing, adsorbers of radiation, etc. Studying the state of a spin glass, biomagnetism, and the mechanism of action of paramagnetic probes in living tissues can help to understand the mechanism of biological processes, in particular, human thinking and DNA functioning [2].

In this report, we are considering the methods of synthesis, structure, magnetic and other properties of the new organic molecular magnetics based on organometallic complexes, conducting polymers doped with magnetic probes, and the polymers filled with transition metal oxides nanoclusters.

The dependences of the magnetic susceptibility of the polymer-magnet nanomaterials on the temperature in the range of 1.5-300 K, frequency and magnetic field strength were measured and analyzed. At low temperatures, the peculiarities of magnetic behavior characteristic of the state of spin glass are revealed for iron complexes with 1-nitroso-2-naphthol [2]. The temperature and frequency transformation in ESR spectra has been studied in model polymer-magnet nanostructures of conjugated polyarenes doped by magnetic clusters. For the first time, hybrid composites simultaneously with magnetic, luminescent and electrically conductive functions were obtained by surface modification of polymer-magnetic nanocapsules with luminescent nanocrystals and a conducting polymer shell.

The study of magnetic properties of polymer-magnet nanosystems can help to understand the nature of "organic magnetism" and identify new approaches to the creation of functional hybrid nanomaterials.

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Fast synthesis of Mg-Al-hydrotalcite derived nanosystems with enhanced catalytic performance in the Guerbet ethanol condensation

***Valihura K.V.*, Larina O.V., Soloviev S.O.**

L.V. Pisarzhevskii Institute of Physical Chemistry of the NAS of Ukraine.
Prospect Nauky, 31, Kyiv-03039, Ukraine.
E-mail: karina.valigura@ukr.net

During the last decades the conversion of biomass-derived ethanol into 1-butanol via Guerbet condensation has a high interest of researchers. This process consists in the carbon chain elongation and involves dehydrogenation, aldol condensation, dehydration and reduction steps [1]. The promising catalysts for the gas phase condensation of ethanol to 1-butanol are Mg-Al-oxide nanosystems, which textural, acid-base and catalytic properties could be regulated by preparation method [2].

A series of hydrotalcite derived Mg-Al oxide systems with Mg/Al atomic ratio of 2(3) were synthesized and marked as Mg-Al-2(3). In conventional method hydrotalcites were kept in mother liquor for 24 h, and in the “fast” method – only for 1 h. Based on the study of Mg-Al oxide catalysts, it was found that reducing the maturation time of the mother liquor after hydrotalcite coprecipitation from 24 to 1 h leads to a notable decrease in size of particles from 80−150 nm to 50−100 nm. Using a number of physicochemical methods, we noted that an implementation of the fast synthesis gave the increase in the volume of mesopores in 1.5 times and the surface concentration of the basic sites of medium strength in 1.6 times, which increases the activity of catalysts and the selectivity of the 1-butanol formation in the process of ethanol Guerbet condensation. The highest 1-buthanol selectivity 64% and yield 23.4% is achieved over sample Mg-Al-2-fast at 548 K. Also, Mg-Al-2-fast demonstrates the high 1-buthanol selectivity remaining on the same level during 12 h time on stream. The obtained catalyst is reusable and its activity is sustainable after at least six catalytic cycles.

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Silicon nanoparticles preparation and the formation of carbon-silicon hybrid nanoparticles for sensor applications

Mussabek G.[1,2], Zhylkybayeva N.[1,2], Zaderko A.N.[3], Baktygerey S.[1,2],
Yermukhamed D.[1,2], Taurbayev Ye.[1,2], Lisnyak V.V.[1,3]

[1] Institute of Information and Computational Technologies,
Pushkina Str., 125, 050010 Almaty, Kazakhstan.

[2] Al-Farabi Kazakh National University,
al-Farabi Ave., 71, 050040 Almaty, Kazakhstan

[3] Taras Shevchenko National University of Kyiv, Volodymyrska Str., 64/13,
01601 Kyiv, Ukraine. E-mail: lisnyak@univ.kiev.ua

Preparing silicon nanoparticles (Si NPs) is a problem that needs a nontrivial solution. For this aim, we performed by preparing Si NPs using different routes, including the reduction of silica NPs and silicon-organic compounds and mechanical grinding using porous silicon materials of various origins. Si NPs have developed inner surface and moderate chemical reactivity. The sensitive layer of Si NPs was modified with carbon adatoms by using chemical routs and by carbonization of organic compounds, including sugars, on the surface of Si NPs. We carried these modifications to regulate adsorptive properties for preparing advanced vapor sensors. Prepared by different processes, silicon nanomaterials, in the form of hybrids and composites, were briefly characterized by TEM and SEM methods. We carried out the modification of Si NPs and Si nanoscale filaments with nanocarbon and nanostructured carbon. The formation of hybrids of various types, including the desired ones, in which nanocarbon modifies the nanosilicon surface, occurs because of high-temperature structuring processes. They are passed during the carbonization of carbon-containing precursors. We have developed and successfully applied synthetic techniques for the experimental production of hybrids bound by a thin interface and surface-modified Si NPs. The sensor characteristics of some surface-modified Si NPs were examined with ammonia and alcohol vapors. The obtained nanohybrids with the carbon decorated surface at the interfacial boundaries and the edge defects/oxidized surface of Si NPs showed sensor response towards ammonia in the gas phase being indifferent to low molecular weight alcohols.

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Silicon-carbon hybrid nanoparticles for sensing applications

Mussabek G.[1,2]***, Zhylkybayeva N.***[1,2]***, Baktygerey S.***[1,2]***,***
Yermukhamed D.[1,2]***, Taurbayev Ye.***[1,2]***, Sadykov G.***[1]***,***
Zaderko A.N.[3]***, Lisnyak V.V.***[1,3]

[1] Institute of Information and Computational Technologies,
Pushkina Str., 125, 050010 Almaty, Kazakhstan.

[2] Al-Farabi Kazakh National University,
al-Farabi Ave., 71, 050040 Almaty, Kazakhstan

[3] Taras Shevchenko National University of Kyiv,
Volodymyrska Str., 64/13, 01601 Kyiv, Ukraine.
E-mail: lisnyak@univ.kiev.ua

Preparing advanced silicon nanomaterials (Si NMs) with given properties is the main task of fundamental and applied research. To date, nanostructured Si is used in modern optoelectronics and sensors. The nanostructured Si exhibits developed inner surface, variable surface chemical composition, and moderate chemical reactivity. The sensitive layer of Si NMs can be adjusted with adatoms and dopants in order to change adsorptive properties using chemical modification. This regulation is a promising method for the creation of advanced optoelectronics and organic vapor sensors. Besides, the modification of nanosilicon can stimulate the development of cardinal ways in the creation and integration of Si NMs in many devices and processes in the form of hybrids and composites. Here we report O, C-containing silicon nanoparticles ((O, C)-Si NPs) synthesized by the one-step method. In this work, the O, C-Si NPs were studied with TEM. Hybrid structures of (O, C)-Si NPs were produced after annealing of aged thermally oxidized Si NPs coated by carbon nanostructures (CNs). The surface chemistry was studied by different methods, and carboxyl and phenol groups were found. The room temperature electrical characteristics of sensors with and without NH_3 gas were measured in the cell. The results showed that the nature, specific surface area of (O, C)-Si NPs, and morphological structure of the CNs and Si NPs strongly affected the electrophysical characteristics. An enhancement in sensitivity, response, and recovery times of a gas sensor based on a hybrid structure was successfully realized due to the specific structure of the hybrid.

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Fenton processes for the treatment of pharmaceutical wastewater

Danyliuk N.V.[1]**, *Tatarchuk T.R.***[2]

[1] *Educational and Scientific Center of Material Science and Nanotechnology,*
Vasyl Stefanyk Precarpathian National University,
201 Galytska str., Ivano-Frankivsk 76018, Ukraine
E-mail: danyliuk.nazariy@gmail.com

[2] *Department of Chemistry, Vasyl Stefanyk Precarpathian National*
University, 57 Shevchenko str, Ivano-Frankivsk 76018, Ukraine

The Fenton and Fenton-based systems are very promising as oxidation processes, which can be used to reduce the amount of pharmaceutical contaminants in the wastewaters. Due to the spread of coronavirus infection, there is a sharp increase in the pharmaceuticals concentration in wastewaters, which need to be disposed. The presence of pharmaceutical contaminants in water mediums makes them unsuitable for domestic use. It is established that improved oxidation processes are an environmentally friendly processes of complex organic compounds degradation. However, one of the most effective is the Fenton process, as an advanced cleaning process for the removal of many hazardous pharmaceutical contaminants. The Fenton reaction is an advanced oxidation process that has been widely recognized for its effectiveness in removing pharmaceutical organic contaminants over a wide range of concentrations.

This work involves the critical review of some problems related to Fenton and Fenton-based processes. The mechanism of reactions with all possible side effects is considered. The overview of most used catalysts and their activity in hydrogen peroxide activation processes is presented. Iron-based catalysts are considered and the limitations affecting their environmental application are highlighted. However, future research should increase the stability of the process for wider operating conditions to avoid leaching of the metal into the solution and their negative impact on the environment. It is expected that combined methods based on heterogeneous Fenton systems will reduce the formation of secondary contaminants. A study of the progress of the Fenton processes has demonstrated their economic and commercial feasibility to treat wastewater from pharmaceuticals.

Low temperature magnetotransport properties in GaAs whiskers

Druzhinin A.A., Ostrovskii I.P., Khoverko Yu.M., Liakh-Kaguy N.S., Chemerys D.V.

Lviv Polytechnic National University.
Bandery st., 12, Lviv-79013, Ukraine.
E-mail: dmytro.v.chemerys@lpnu.ua

The nanostructures of A3B5 compound are investigated by researchers due to their wide application, especially compounds based on GaAs are used as photodiodes with high bandwidth [1]. Magnetotransport properties in $GaP_{0.4}As_{0.6}$ whiskers were studied in our previous work [2]. The negative magnetoresistance effect was revealed and explained due to size effect existence in studied whiskers. Therefore, magnetoresistance behaviour studies of GaAs whiskers at low temperatures and magnetic fields 0-14 T are the aim of the work.

GaAs whiskers were grown by chemical transport reactions method in closed bromide system with the diameter of 20-40 µm. The studied whiskers were doped to concentration in vicinity of the metal-insulated transition (~ 1017 cm^{-3}). The ohmic electrical contacts to GaAs whiskers with Au microwires were created due to the pulse welding method.

The magnetoresistance and temperature dependencies of resistance in GaAs whiskers were studied in the temperature range 4.2-77 K. Changes in the magnetoresistance behavior were found at different temperatures. Both positive and negative magnetoresistances in the field of magnetic fields 0-14 T was found. The nature of the detected positive and negative effects of magnetoresistance in GaAs whiskers and various possible reasons for explaining their behaviour were proposed. The practical application of GaAs whiskers was also proposed as result of the studied low temperature properties.

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Sensitive liquid crystal composites for optical sensors

Mykytyuk Z.M., Barylo G.I., Kremer I.P.,
Kachurak Y.M., Shymchyshyn O.Y., Ivakh M.S.

Department of Electronic Engineering, Institute of Telecommunications,
Radio Electronics and Electronic Engineering,
Lviv Polytechnic National University.
Mytropolyta Andreya str., 1, Lviv-79000, Ukraine.
E-mail: yurii.m.kachurak@lpnu.ua

In recent years, the use of liquid crystal mixtures as sensitive elements of optical sensors is of increasing interest [1-3].

The paper presents a comparative analysis of liquid crystal cholesteric-nematic mixtures for their use as sensitive elements of gas sensors. Liquid crystalline mixtures based on nematic E7 and cholesteric impurity CB15 are considered. To determine the optimal composition of the mixture, their spectral characteristics were studied. The main bandwidths for different concentrations of optically active impurities were determined. The temperature characteristics of liquid crystal composites were measured to determine the threshold values of their transition to the isotropic state and to establish stable temperature ranges for use in optical sensors.

The results of the research show that as a sensitive element of optical sensors it is advisable to use liquid crystal mixtures with CB15 impurity concentrations of 38% and 44%. Their main bandwidths are in the visible region of the spectrum of 500-600 nm. The first mixture has better temperature characteristics, but the second shows a higher sensitivity to vapors of organic matter.

Further study of mixtures can be carried out during the direct development of optical gas sensors.

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Optimization of multilayered electromagnetic shields using mesh adaptive direct search

***Vovchenko L.L.*, Lozitsky O.V., Matzui L.Yu., Zagorodnii V.V.**

Department of Physics, Taras Shevchenko National University of Kyiv.
64/13, Volodymyrska Street, Kyiv-01601, Ukraine.
E-mail: vovch@univ.kiev.ua

Multilayered composite structures have been proven to have superior shielding properties, compared to bulk composites if the layers' thickness and effective permittivity are set in a way to utilize electromagnetic interference between the layers at frequency ranges, where a specific transmission or absorption spectrum is required. This spectrum is essentially an objective function used in many mathematical optimization algorithms. In this work a modified mesh adaptive direct search algorithm [1] has been used to design 3-layered composite structures to obtain the highest absorption and to achieve frequency filtering of the EMR. This method does not require differentiability of the objective function, and thus is better suited for multilayered composites, where the required shielding spectra may have multiple local minimums in parameter space.

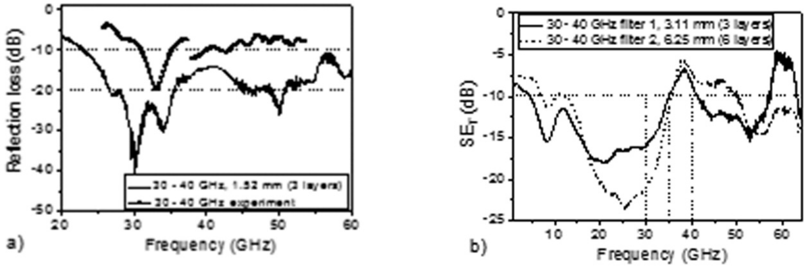

Figure 1. Optimized spectra of reflection loss (a) and shielding effectiveness (b) of multilayered samples.

A number of multilayered samples were optimized for achieving i) the lowest reflection loss in range 30-40 GHz (Fig. 1a) and ii) the filtering of microwave radiation (Fig. 1b). The results show the possibility of designing the composites with specific shielding spectra, however the inaccuracies in manufacture of the composite layers may lead to significant mismatch between measured and modeled spectra.

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Structure investigation of highly porous hydroxyapatite glass ceramics modified by graphene-like structures

Iatsenko A.P.[1], Sych O.E.[2], Nikolenko A.S.[3]

[1] Department of Chemical Technology of Ceramics and Glass, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",
37, Peremogy Ave., Kyiv 03056, Ukraine

[2] Department of Functional Materials for Medical Application, Frantsevich Institute for Problems of Materials Science of NAS of Ukraine.
3, Krzhyzhanovsky Str., Kyiv 03142, Ukraine
E-mail: lena_sych@ukr.net

[3] Laboratory of Optical Submicron Spectroscopy, Institute of Semiconductor Physics NAS of Ukraine, 45, Nauky Ave, Kyiv 03028, Ukraine

Graphene and graphene-like structures (such as graphene oxide) due to their unique structure and properties have found extensive application in medicine in recent years. It could be used as surface coatings for implants due to its ability to accelerate the growth, differentiation and proliferation of stromal stem cells, significantly improve biocompatibility, adsorption and antibacterial properties.

Highly porous glass ceramics samples (porosity more than 90 %) based on nanostructured biogenic hydroxyapatite (obtained by calcination of bovine bone at 900 °C) and sodium SiO_2-Na_2O-CaO (obtained by melting of glassforming components at 1150 °C) were prepared by foam replication method at 900 °C and used for modification by graphene-like structures by chemical vapor deposition method. For comparison, silicon single crystals were coated by graphene-like structures by the same method.

The microstructure of highly porous ceramics and silicon single crystals with and without coating was investigated by scanning electron microscopy using a Tescan Mira 3 LMU microscope (Tescan, Czech Republic). The micro-Raman measurements were performed in backscattering geometry at room temperature using Horiba Jobin Yvon T-64000 Raman spectrometer. Line of Ar-Kr ion laser with wavelength of 488 nm was used for excitation.

According to the obtained results it was established the formation of graphene-like structures on the surface of silicon single crystals samples and highly porous glass ceramics and confirmed the possibility of use chemical vapor deposition method for modification of bioceramics by graphene-like coating.

Influence of an external electric field on sub-structural nano-formations of domain walls in ferrite garnet films

***Koronovskyy V.E.*, Vakyla Y.A.**

Taras Shevchenko Kyiv National University, Faculty of Radiophysics,
Electronics and Computer Systems
4-g, Prospekt Glushkova Street, 03127 Kyiv, Ukraine
E-mail: koron@univ.kiev.ua

This paper reports on the investigation of the magneto-electric (ME) properties of domain walls and sub-structural magnetic nano-formations on domain walls in thin epitaxial films of ferrite garnets with using of the optical methods for investigation [1]. The investigated films were deposited on the (111) $Gd_3Ga_5O_{12}$ substrate with a thickness of about 600 μm. The thickness of the films were about 7 μm. The domain's magnetization was near to normal to the film plane and the external electric field (ω = 800 Hz) was oriented perpendicular to the plane of the film. We adapted the dark field optical microscopy method [2] to investigate the influence of an external electric field on the micromagnetic structural elements and inhomogeneities of the domain structure of thin magnetic films. We revealed the magneto-electric activity effect of vertical Bloch lines of investigated garnet films in external electric field which visually manifests itself as local distortion of their profile and broadening of the regions of their localization. This phenomena can be explained as the effect of additional amplification by the external electric field of the initially existing micro-slope of the domain wall region in the vicinity of the Bloch lines. These perturbations are significantly amplified in additional impact of the external magnetic field, oriented in the plane of the film along the domain walls profile. In particular, in the external AC electric field, we revealed visually observable displacement of the Bloch lines along the domain walls in the range of the DC magnetic field value approximately from 35 to 45 Oe. Reaction of the domain structure to influence of external AC electric field was caused by changing the magnetic anisotropy parameters of ferrite garnets in an external electric field.

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Deformability of nanodispersed titanium alloys under isothermal conditions

***Titov A.V.*[1]*, Balushok K.B.*[2]*, Shmeleva L.V.*[3]*, Suprun A.D.*[3]**

[1] *Educational and Research Institute of Mechanical Engineering of the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prospect Nauki, 37, Prosp.Peremohy, Solomyanskyi district, Kyiv, Ukraine, 03056.*

[2] *The Motor Sich Joint Stock Company,*
15, Motorobudivnikiv Avenue Zaporizhzhia, Ukraine, 69068

[3] *Department of Theoretical Physics, Faculty of Physics, Taras Shevchenko National University of Kyiv.*
Volodymyrska Street, 64/13, Kyiv, Ukraine, 01601
E-mail: lshmel@univ.kiev.ua

This investigation is devoted to the study of the possibility of creating processes of forming parts with thin-walled elements of titanium alloys and powder materials. The goal of the research is to increase the deformability of products in the conditions of viscoplastic flow at certain process parameters. The effect of short-term creep for difficult-to-deform titanium alloys and especially for powdered titanium materials, can be achieved only in a narrow temperature range. And the presence of this effect directly depends on the state of the source material, namely, the grain size of the source material and the distribution of components for multiphase materials. As a rule, in fine-grained alloys the grain size can vary in the range from tens of nanometers to tens of micrometers. Therefore, previously, the paper conducted a theoretical and experimental study to clarify the question of the prospects of deformability of the material depending on the grain size of the source material. The acquired knowledge will be the basis for choosing a nanostructured material more suitable for technological use.

Based on nanostructured titanium and powder materials, the model is constructed to study the elastic characteristics in a certain temperature range, in particular, the strains speeds. The influence of temperatures and strain rates on the plasticity of the base material is also investigated.

Influence of temperature fields on the process of plastic flow of eutectically strengthened fine-grained titanium alloys

Titov V.A.[1], Kondratiuk E.V.[2], Shmeleva L.V.[3], Titov A.V.[1], Suprun A.D.[3]

[1] Educational and Research Institute of Mechanical Engineering of the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prospect Nauki, 37, Prosp.Peremohy, Solomyanskyi district, Kyiv, Ukraine, 03056.

[2] Zaporizhzhia Machine-Building Design Bureau "Progress" State Enterprise named after Academician O.H.Ivchenko,
2, Ivanova str, Zaporizhzhia, Ukraine, 69068

[3] Department of Theoretical Physics, Faculty of Physics, Taras Shevchenko National University of Kyiv. Volodymyrska Street, 64/13, Kyiv, Ukraine, 01601
E-mail: lshmel@univ.kiev.ua

Creating the foundations of effective technology for the manufacture of accurate blanks with thin-walled elements from refractory titanium alloys and powder materials for the machine-building and aviation industries is an important technological problem.

The paper considers a promising direction of plastic forming of accurate workpieces based on eutectically strengthened titanium alloys and powder materials. The deformation properties of these materials, which are described by the viscoplastic model of the material, depend on the conditions of formation (temperature, strain rate, initial state of the material, etc.). Therefore, this research is devoted to theoretical analysis direct at predicting the conditions of practical tests for each type and condition of the material. The friction conditions are taken into account in the study, which are determined by the high, in relation to aluminum alloys, adhesive properties of titanium alloys.

The sustainability of the process of plastic flow of metal in the formation of details with thin-walled elements depends on the gradient of the temperature field. Therefore, special attention is given to gaining knowledge about the conditions of control of this temperature field. Such research is needed to reduce the cost of the technological process at the stage of creating non-standard equipment, namely, installations for isothermal shaping.

Insights into synthesis of nanosized Ni and Fe particles by chemical reduction method

Wodak I.[1]***, Yakymovych A.***[1]***, Khatibi G.***[1,2]

[1] Institute of Chemical Technologies and Analytics,
TU Wien, Vienna 1060, Austria

[2] Christian Doppler Laboratory for Lifetime and Reliability of Interfaces in
Complex Multi-Material Electronics,
TU Wien, Vienna 1060, Austria
E-mail: andriy.yakymovych @tuwien.ac.at

The synthesis of metal nanoparticles (NPs) by chemical reduction involves the reduction of metal ions of an inorganic soluble metal salt with a reducing agent [1]. This is the most common method to produce metal NPs due to its simple and reliable procedure.

In this study, two procedures have been used to produce Fe and Ni NPs. According to the first procedure, the reduction of the metal salt by hydrazine hydrate in an aqueous solution, while sodium hydroxide has been used as a stabilizing solvent as well as polyvinylpyrrolidone as a surface stabilizer and as a protective agent. A similar method has been used in our previous study [2]. The second procedure is the so-called polyol chemical reduction using ethylene glycol as a reduction agent, while chloroplatinic acid has been used as a heterogeneous nucleating agent.

The powder X-ray diffraction has been employed to determine the phases presented in the nano-sized metal powder. The scanning transmission electron microscopy (STEM) has provided images from which the shape, size, and size distribution of the produced nanoparticles have been determined.

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Structure and properties of CoCrFeNiMnBe high-entropy alloy films obtained by liquid quenching

Bashev V.F., Kushnerov O.I., Ryabtsev S.I.

Department of Experimental Physics, Oles Honchar Dnipro National
University. Gagarin ave., 72, Dnipro, 49010, Ukraine.
E-mail: kushnrv@gmail.com

In recent decades, a new class of metal compounds has been developed - the so-called high-entropy alloys (HEAs) with multiple principal elements. HEAs have received more and more attention due to their unique structure and excellent properties in hardness and wear resistance, exceptional high-temperature strength, good structural stability, radiation, and corrosion resistance. Each principal element in HEA should have a concentration between 5 and 35 at.%. Because of the high mixing entropy of HEAs (12-19 J/(K·mol)), they usually consist of some simple solid solutions, instead of complex phases.

In this study, a new nanostructured CoCrFeNiMnBe high-entropy alloy films were synthesized by the means of liquid quenching (LQ) technique, which consisted of rapid cooling of melt drops upon their collision with the internal heat-conducted surface of a rapidly rotating (~8000 RPM) hollow cylinder. The estimated cooling rate was ~10^6 K/s.

The analysis of the XRD patterns allowed us to establish that the investigated HEA in the as-cast state has a multiphase structure in which there is the FCC phase with lattice parameter a=0.3588 nm and the coherently scattering domain size (crystallite size) estimated by the Sherer formula L =20 nm, BCC phase (a=0.2872 nm, L =19 nm), and B_2 type intermetallic compounds BeNi(Co) (a=0.2616 nm, L=20 nm). At the same time, the LQ sample has a structure consisting of the FCC phase (a=0.3599 nm, L = 15 nm) and the BeNi(Co) phase (a=0.2610 nm, L = 18 nm). The microhardness in the as-cast state is Hμ=3400 MPa, while in the LQ state Hμ=5600 MPa. So, the addition of Be significantly improves the mechanical characteristics of the studied HEA as compared with the original Cantor alloy (CoCrFeNiMn). The fact that the LQ HEA of the Co-Cr-Fe-Ni-Mn-Be system is characterized by higher values of Hμ than as-cast alloys is not unexpected, since the microstructure and the phase composition of the as-cast alloy after decomposition are in a more equilibrium multiphase state, while LQ alloy yields a higher level of microstrains, dislocation density and smaller grain sizes.

The magnetic properties of the films were measured by a vibrating sample magnetometer. For the as-cast CoCrFeNiMnBe HEA the saturated magnetizations (Ms), and coercivity force (Hc) were 5.1 A·m^2/kg and 2800 A/m, while for the LQ films – 2.7 A·m^2/kg and 4000 A/m respectively.

Composites based on silicon and carbon nanostructures for ionizing radiation sensing

Olenych I.B.[1]***, Horbenko Yu.Yu.***[2]***, Monastyrskii L.S.***[1]***,***
Aksimentyeva O.I.[2]***, Dzendzeliuk O.S.***[1]***, Sokolovskii B.S.***[1]

[1] Electronics and Computer Technologies Department, Ivan Franko National University of Lviv, 50 Dragomanov Str., Lviv-79005, Ukraine
E-mail: iolenych@gmail.com

[2] Chemistry Department, Ivan Franko National University of Lviv,
6 Kyrylo and Mefodiy Str., Lviv-79005, Ukraine

The search for new functional materials with predictable properties is at the forefront of R&D in nanoelectronics. In particular, composite materials that are a collection of related to each other nanoparticles are actively studied. Particular attention is paid to nanosystems based on graphene and porous silicon nanostructures due to their unique properties. The significant specific area of the porous silicon, high carrier mobility and mechanical strength of the graphene, as well as significant sensitivity of electrical conductivity of silicon and carbon nanostructures to adsorbed molecules and local electric fields, make nanocomposites based on them strong candidates for sensor development [1, 2].

In this work, PS–graphene hybrid structures were created and their electrical properties in the AC regime under ionizing radiation from the 226Ra source were studied. A decrease in electrical resistance and capacitance of the PS–graphene structures with increasing frequency from 25 Hz to 1 MHz was established based on the measurement of frequency dependences of the impedance. We have found that the obtained hybrid structures show a decrease in resistance and an increase in capacitance due to the combined action of α-, β-, and γ-radiation. Radiation-induced charge in the PS causes a change in the local electric field and, as a consequence, a change in the electrical characteristics of graphene. A study of the ionizing radiation effect on electrical parameters of the PS–graphene nanocomposites opens the way to creating new types of ionizing radiation detectors.

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Electrical and photoelectric properties of hybrid structures based on reduced graphene oxide and doped porous silicon

Olenych I.B.[1]***, Horbenko Yu.Yu.***[2]

[1] *Electronics and Computer Technologies Department, Ivan Franko National University of Lviv, 50 Dragomanov Str., Lviv-79005, Ukraine*
E-mail: iolenych@gmail.com

[2] *Chemistry Department, Ivan Franko National University of Lviv, 6 Kyrylo and Mefodiy Str., Lviv-79005, Ukraine*

Useful properties of hybrid structures combining graphene and porous semiconductors, in particular, porous silicon (PS) have caused the emergence of potential applications, ranging from photoreceivers and chemical sensors to field-effect transistors and electrodes for power sources [1-3]. Graphene is effectively used as a transparent electrode in displays and photonic devices due to its outstanding optical properties. Besides, the conical shape of the electron spectrum of graphene determines the most unique properties of graphene as a gapless semiconductor. In particular, it is possible to easily control the electrical conductivity of graphene and inject carriers with a positive or negative charge by means of a local electric field. This feature of graphene can be used to create a new type of photodetectors.

In this work, the PS–reduced graphene oxide (rGO) hybrid structures were created and their electrical properties were studied in both DC and AC modes. Graphene field effect transistors in obtained structures were used as a light photon detector. The influence of back-gate voltage and doping of the PS layer with metals on the electrical and photoelectric properties of the PS–rGO structures has been studied. The electrical conductivity of the PS–rGO hybrid structures depends not only on the direct collection of charges but also on the change in the graphene conductivity due to the local electric field of photogenerated charge carriers.

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Conductivity of nanocomposite SiO_xN_y and $SiO_xN_yAl_z$ films

***Kizjak A.Yu.*[1], *Evtukh A.A.*[1,2], *Bratus' O.L.*[1], *Antonin S.V.*[1], *Muriy Ya.*[2]**

[1] V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine
41, Nauky ave., 03028 Kyiv, Ukraine.
E-mail: antoninsv@gmail.com

[2] Taras Shevchenko National University of Kyiv, Institute of High Technologies, 2 Glushkova avenue, Kiev, Ukraine.

Promising for the development of new types of turn-less inductors with controlled parameters that can be used in various integrated circuits are semiconductor-dielectric nanocomposite materials that fully fit into the principles of planar silicon technology. The purpose of this work is to study the mechanisms of conduction in planar semiconductor/SiO_xN_y nanostructures containing nanoparticles of Si (silicon) and oxidized metal (Al).

The films were deposited by ion-plasma sputtering, and the formation of structures and methods of their analysis are similar to those described in [1].

Based on the results of measurements, an analysis was carried out and the mechanisms of electrical conductivity of the obtained films were determined. Considerable attention is paid to a comparative analysis of the temperature dependence of the conductivity of SiO_xN_y and $SiO_xN_yAl_z$ films. For example, the temperature dependences of conductivity (Fig. 1) in the range of high voltages show that the type of annealing of SiO_xN_y films affects the character of conductivity, but not in $SiO_xN_yAl_z$ films.

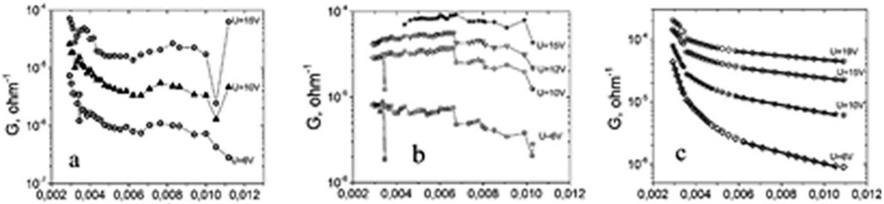

***Fig.1** Reciprocal temperature dependence of conductivity for thin films: a) SiO_xN_y annealed in nitrogen, b) SiO_xN_y annealed in argon and c) $SiO_xN_yAl_z$ annealed in nitrogen.*

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Thermal efficiency of nanoscale aluminum layer modified by ionic implantation

Honcharov V.V.[1]***, Zazhigalov V.A.***[1]***, Honcharova A.V.***[2]

[1] *Departmen of Heterogeneous Catalytic Oxidation Processes, Institute for Sorption and Problems of Endoecology NAS of Ukraine,*
General Naumov Str., 13, Kyiv-03164, Ukraine.

[2] *Junior Academy of Sciences of Ukraine,*
Mendeleev Str., 1, Rubizhne 93000, Ukraine.

Much attention is paid to the issue of modifying materials using high-energy technologies. In particular, studies of improving the thermal properties of materials through the use of ion implantation are promising [1, 2]. Among its advantages this technology has low consumption of active element and the formation of nanosized modified layers.

Therefore, the aim of this work was to study the thermophysical characteristics of aluminum modified with titanium ions, for further use as a material of the heat exchange device.

Ionic implantation is chosen as the modification technology.

Samples of aluminum foil were taken for research. Some of them were treated with titanium and nitrogen ions (simultaneously).

Temperatures were measured using an infrared thermometer "HoldPeak HP-1300" with a measuring range up to +1300 °C. The surface microstructure of the samples was studied using optical microscopy and computer simulation.

According to the results of the surface microstructure study, it was found that ion implantation changes the microgeometry and creates a nanoscale (about 30 nm) modified layer.

Studies have shown that the treated samples have higher thermal conductivity than the original.

The absorption capacity of infrared heat was 4% higher for implants as well.

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Graft copolymer-assisted synthesis of nickel nanoparticles in aqueous solutions

Zheltonozhskaya T.B.[1]***, Permyakova N.M.***[1]***, Kunitskaya L.R.***[1]***,***
Klepko V.V.[1]***, Grishchenko L.M.***[2]***, Klymchuk D.O.***[3]

[1] *Department of Polymer Physics, Institute of Macromolecular Science of the NAS of Ukraine, 48 Kharkivske Shosse, 02160 Kyiv, Ukraine.*
E-mail: zheltonozhskaya@ukr.net

[2] *Faculty of Chemistry, Taras Shevchenko National University of Kyiv, 60 Volodimirska St., 01033 Kyiv, Ukraine.*

[3] *Laboratory of Electron Microscopy, M.G. Kholodniy Institute of Botany of the NAS of Ukraine, 2 Tereshchenkivska St., 01601 Kyiv, Ukraine.*

A special hydrophilic graft copolymer with interacting poly(vinyl alcohol) backbone and grafted polyacrylamide chains (PVA-*g*-PAAm) was synthesized, characterized and used as a matrix for *in situ* synthesis of nickel nanoparticles (NiNPs) in aqueous media. The copolymer solutions contained individual macromolecules (monomolecular micelles) of ellipsoidal shape and length of ~18-64 nm, and their various fractal aggregates (Figure 1 a). To study the borohydride reduction of Ni^{2+}-ions in PVA-g-PAAm solutions and pure water, an original method for monitoring the kinetics of the formation of metal nanoparticles was proposed and implemented for the cases where there is no a surface plasmon resonance band in UV-Vis spectra. An increase in the initial rate of accumulation and yield of NiNPs with an increase in the concentration of Ni-salt and a decrease in both parameters in copolymer solutions in comparison with pure water was established. The complex role of matrix concentration was also shown.

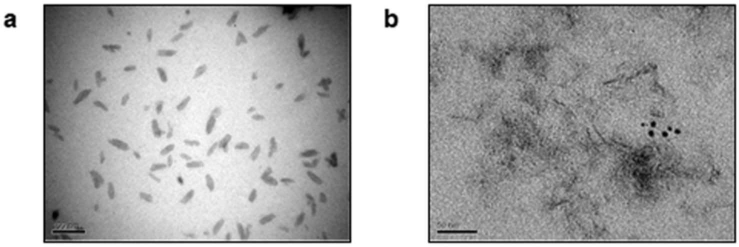

Figure 1. TEM images of (a) PVA-g-PAAm matrices and (b) their compositions with NiNPs.

In the final NiNPs/PVA-g-PAAm compositions (Figure 1 b), the emergence of new structures such as “hairy coils” and “hairy rods” with small individual spherical NiNPs and their chains was identified.

Impact of albumin sorption on the morphology of the dispersed phase of aqueous dispersions of phosphorus-containing polyesters

Stasiuk A.V.[1]***, Dron I.A.***[1]***, Pasetto P.***[2]***, Samaryk V.Y.***[1]

[1] *Department of Organic Chemistry, Lviv Polytechnic National University*
S.Bandera Str., 12, Lviv-79013, Ukraine
E-mail: anna.v.stasiuk@lpnu.ua

[2] *Institut des Molécules et Matériaux du Mans, UMR CNRS 6283,*
Le Mans Université, Avenue Olivier Messiaen 72085 Le Mans Cedex 9,
France.

Polyesters have been studied for biomedical application for several decades due to their biodegradability and biocompatibility. Significant in the research of this class of polymers is the creation of dispersed polymer systems for drug delivery. It is important that such drug delivery systems be able to reach their destination within a certain period of time. Therefore, polyesters for this purpose should have surfactant properties, be non-toxic, and form self-stabilized dispersions with a dispersed phase size in the range of 40-150 nm [1].

The synthesis of phosphorus-containing polyesters (PPE) based on N-steroylglutamic acid and dipolyethyleneglycol ethylphosphate by the irreversible polycondensation reaction was investigated, the structure was confirmed by IR and NMR spectroscopy, and their surface properties and solubilization capacity were investigated. The phosphate group introduced into the hydrophilic chain of polyoxyethylene glycol is able to provide chemisorption of a number of organic compounds due to the formation of an ionic bond. Based on PPE obtain stable dispersions with a particle size of the dispersed phase 60-100 nm, able to form dispersions with nanometer-sized particles at high concentrations of the dispersed phase. The influence of adsorption on the stability of the dispersion in the conditions of sorption of bovine serum albumin (BSA) on the particles of the dispersed phase of PPE was studied. It has been established that the effects associated with additional albumin stabilization of the particles of their dispersed phase, which is manifested in a decrease in the average diameter of the particles in the dispersions. Therefore, the properties of new phosphorus-containing polyesters allow us to consider them as potential systems for drug delivery.

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Peculiarities of the microstructure of gelatin hydrogel structured by bifunctional dioxirane crosslinkers

Maikovych O.V., Nosova N.G., Varvarenko S.M.

Organic Chemistry Department, Lviv Polytechnic National University.
12 Bandera str., Lviv-79013, Ukraine.
E-mail: olha.v.maikovych@lpnu.ua

In the treatment of wounds of various origins, hydrogel dressings are increasingly used, which combine a number of properties, for example, intensive absorption of wound exudate, the creation of a protective barrier that protects the wound from infection, prolonged and targeted release of therapeutics. Most of the properties are greatly influenced by the porosity of the hydrogel, which depends on the presence of cross-linking bonds.

We obtain gelatin hydrogels structured by bifunctional dioxirane crosslinkers based on polyethylene glycols of various molecular weights. Investigation of structure (SEM, TEM) showed a dependence of the pore size on the structuring agents and their concentration. Pores are irregularly shaped and of heterogeneous size. Table 1, for example, shows the results of studies of hydrogels based on a bifunctional dioxirane derivative of polyethylene glycol-400 (DOX-500) and type A gelatin (bloom 180). The results are given for unstructured gelatin and gelatin hydrogels with different content of the structuring agent.

Table 1

The pore size of Gelatin 15 % and cross-linked gelatin hydrogels

Sample	*Pore Size (μm)*
Gelatin 15 %	25 ± 10
DOX 500 3 %	7 ± 3
DOX 500 3.6 %	9 ± 3
DOX 500 4.5 %	12 ± 5
DOX 500 6 %	15 ± 7

Thus, we studied the structure of gelatin hydrogel materials depending on the synthesis conditions and the concentration of the structuring agent. The optimal conditions for their production are determined, making it possible to obtain hydrogels with satisfactory properties for using the obtained material as the basis of a specialized hydrogel dressing to treat chronic wounds.

Preparation and optical properties of phosphotungstate nanostructured glass-ceramics

Chornii V.P.[1,2]***, Boyko V.V.***[1]***, Nedilko S.G.***[2]***, Terebilenko K.V.***[2]***,***
Zozulia V.O.[2]***, Slobodyanik M.S.***[2]***, Sheludko V.I.***[3]***, Gomenyuk O.V.***[3]

[1] *National University of Life and Environmental Sciences of Ukraine.*
Geroiv Oborony st., 15, Kyiv-03041, Ukraine.
E-mail: vchornii@gmail.com, vchornii@nubip.edu.ua.

[2] *Taras Shevchenko National University of Kyiv,*
Volodymyrs'ka st., 60, Kyiv-01601, Ukraine.

[3] *Oleksandr Dovzhenko Hlukhiv National Pedagogical University,*
Kyjevo-Moskovs'ka st, 24, Hlukhiv-41400, Ukraine.

The luminescent glass-ceramics (GC), those are mostly the composites with crystalline phosphors inside of glass host, appear to be very promising materials for light emission sources [1]. Such materials can be obtained by co-sintering, sol-gel, glass crystallization or some other techniques. Among them, the advantage of glass crystallization technique is related with close composition of glass and crystalline components that decreases a light scattering in GC. The optical quality of GC depends strongly on composition of the glass host and size of crystalline grains. Phosphate-based glasses are known to be transparent in visible spectral range and can be considered as good host for GC elaboration. Depending on glass modifiers (Bi_2O_3, MoO_3, WO_3, etc) there are many oxide compounds which can be crystallized in such glass systems – phosphates, molybdates, tungstates and some other of mixed anion compounds.

In this work the glass-ceramics those consist of K_2O-P_2O_5-WO_3-V_2O_5 glass and $K_2Eu(PO_4)(WO_4)$ micro/nanocrystallites were prepared and studied. The samples of GC were characterized by means of powder X-ray diffraction, thermogravimetric analysis (DTA), scanning electron microscopy, energy dispersive X-ray analysis, infrared vibration, absorption and luminescence electron-vibration spectroscopy.

The results have showed that studied glass ceramics are perspective luminescent materials for white LED applications.

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Effect of optical vibrations on thermoluminescence of polysilane films and nanocomposites

Ostapenko N.I.[1]***, Ostapenko Yu.V.***[1]***, Chursanova M.V.***[2]

[1] *Institute of Physics, National Academy of Sciences of Ukraine,*
46 Prospect Nauky, Kyiv 03028, Ukraine
E-mail: nina.ostapenko@gmail.com

[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37 Prospect Peremohy, Kyiv 03056, Ukraine.*

A comparative study of low-temperature (5–120 K) thermoluminescence of silicon organic polymer poly(di-n-hexylsilane) within the linear and fractional heating regimes is carried out. Polymer films, nanocomposites with the polymer introduced into the nanopores of silica matrices with the pore diameter of 2.8 nm and 10 nm, as well as dilute polymer solutions (10^{-5} mol/l) are investigated. It is found that the maxima and half-widths of the thermoluminescence curves of nanocomposites significantly depend on the diameter of silica nanopores, which is consistent with the data from the study of the polymer solutions. Based on the data on the thermoluminescence of nanocomposites with different pore diameters, the possibility to controllably change the number of charge carrier traps and their energy distribution is established. It is determined that the energy spectrum of traps in the films and nanocomposites has discrete character, and the activation energies coincide with the energy of vibrational quanta found from the Raman spectra of the polymer. This indicates that charge carriers release from the traps occurs when a charge carrier absorbs a single quantum of optical vibration [1]. For the polymer film, it is found that there are six trap activation energies that coincide with the photon energy of both symmetric and deformational optical vibrations of the polymer chain (0.011, 0.018, 0.026, 0.032, 0.042, 0.046 eV). For the nanocomposite with the minimum nanopore diameter (2.8 nm), the number and depth of traps, as well as their distribution over energies, decrease significantly; only two activation energies (0.032, 0.046 eV) are observed, which coincide with the energies of quanta of symmetric optical vibrations of the polymer. The disappearance of some vibrations can be associated with the change in the processes of charge carriers' recombination as a result of different nature of their diffusion in the films and in the nanocomposites with small pore diameter.

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Carbon nanotubes as a base material for working electrodes increasing the sensitivity of determinations in striping voltammetry

Grabarczyk M.**, Adamczyk M., Wlazlowska E.

Department of Analytical Chemistry, Institute of Chemical Sciences,
Faculty of Chemistry, Maria Curie-Skłodowska University,
Maria Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland
**E-mail: malgorzata.grabarczyk@mail.umcs.pl*

Stripping voltammetry (SV) is a powerful technique for determination of low levels of metal ions. The key element in voltammetric procedures is the selection of the working electrode. The first procedures were developed using hanging mercury drop electrodes, however their major drawback was high toxicity. In recent years, the literature has described many different working electrodes which use the formation of metallic films, most often on a glassy carbon substrate [1,2]. In our research, we used nanotubes to modify the working electrode thanks to which the sensitivity of the determinations was increased compared to the procedures based on classic glassy carbon electrodes. The carbon nanotubes modified electrode was obtained by mixing carbon nanotubes and epoxy resin. The resulting paste was put under pressure in glass capillary of diameter 2 mm. Such composition turns out to be a very good basis for metal film formation. The use of this electrode has the additional advantage: the deoxygenating of the sample before measurement is unnecessary. It also simplifies the apparatus necessary to perform metal ions determination in field conditions. To confirm the applicability of nanotubes to modify the working electrode the stripping voltammetric determination of selected metal ions in nanoconcentrations in natural water samples was performed.

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Thermal properties of the POSS-containing nanocomposites based on PU/PHPMA semi-IPNs

Karabanova L.V., Honcharova L.A.

Institute of Macromolecular Chemistry of the NAS of Ukraine.
Kharkivs'ke shose 48, Kyiv-02160, Ukraine;
E-mail: lyudmyla_karaban@ukr.net

The nanocomposites based on crosslinked polyurethane (PU), linear poly (hydroxylpropyl methacrylate) (PHPMA) contained 1,2-propandiolisobutyl-POSS were created and the impact of different amount of POSS on the thermal properties and structure of the nanocomposites were investigated.

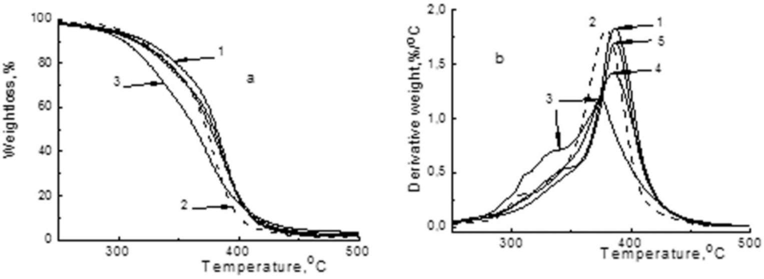

Fig. 1.*TGA (a,b) thermograms of the matrix semi-IPNs PU/PHPMA 85/15 (1) and nanocomposites with POSS content 1 (2), 3 (3), 5 (4) and 10 % (5) under inert atmosphere (N_2) at the heating rate of 20°C/min.*

Thermal properties of the nanocomposites were studied by using dynamic scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Introduction of POSS nanofiller into the matrix was found results in increased thermal stability of the created nanocomposites. From the DSC data the glass transition temperature (Tg) of the nanocomposite was found to be increased with increasing of POSS content.

The TGA curves (Fig.1) for all the samples displayed similar degradation profiles. For all the samples, degradation was observed in two steps, around 280-300°C and above 380°C, which is indicative of the soft and hard segments in polyurethane.

The structure of the nanocomposites were characterized by Fourier transform infrared (FTIR) spectroscopy. FTIR spectra showed the chemical bonding of the nanofiller 1,2-propandiolisobutyl-POSS and PU component of the matrix.

Overall, the results of thermal properties investigation of nanocomposite based on PU/POSS and semi-IPNs demonstrate that the obtained nanocomposites are significantly more thermally stable than the native PU network and native semi-IPN-15.

Copper-sensitive ion-selective electrode with solid contact based on copper oxide nanoparticles- multiwalled carbon nanotubes-nanopomposite

Wardak C.*, Pietrzak K.

Department of Analytical Chemistry, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University, Maria Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland
*E-mail: *cecylia.wardak@mail.umcs.pl*

Potentiometry with ion-selective electrodes (ISEs) allows to directly determine free ion concentration in aqueous samples. The main advantages of this technique are low costs, speed which samples can be analyzed with, device portability, no sample destruction and the requirement of minimum sample preparation. Among the various types of ISEs, those with solid contact are becoming increasingly popular. In comparison to conventional ISEs they are characterized by unquestionable advantages including small size, simple construction, lower cost of production, and ability to operate in high pressure environments. Moreover they can have various shapes, sizes and can work in any position. Unfortunately solid contact ion-selective electrodes (SCISEs) often exhibited big potential drift and poor reproducibility because of blocked interface between ion-selective membrane with ionic conductivity and electronic conductor.

This paper presents electrodes sensitive to copper (II) ions, in which copper (II) oxide nanoparticles-multi-walled carbon nanotubes (MWCNTs) composite was used as solid contact. In order to investigate the influence of modification of the electrode structure, the selected analytical parameters obtained by means of potentiometric measurements (slope, linearity range, detection limit, potential stability and reversibility) and electrochemical impedance spectroscopy and chronopotentiometry measurements (membrane resistance and charge transfer resistance as well as double layer capacitance) were compared. The use of both copper (II) oxide nanoparticles and their composite with MWCNTs as a solid contact had a positive effect on the operation of the obtained electrodes. Nanocomposite based electrode showed a lower detection limit, better potential stability and reproducibility. It was not sensitive to gases (O_2, CO_2) and light. In addition no redox response was observed.

Construction and characterization of polymer-coated CeO_2

Hubina A.V.[1]***, Lobko Ye. V.***[2]***, Tarasyuk O.P.***[1]***, Rogalsky S.P.***[1]

[1] *V.P.Kukhar Institute of Bioorganic Chemistry and Petrochemistry NAS of Ukraine, Kharkiske shose, 50, Kyiv-02160, Ukraine.*
E-mail: zurako@ukr.net

[2] *Charles University,*
V Holešovičkách 747/2, 18000 Praha 8, Czech Republic

CeO_2 nanoparticles (CeNP) exhibit outstanding antioxidant activity due to redox change between Ce^{3+} and Ce^{4+} in response to the conditions of the media. These properties allow nanoceria to demonstrate properties similar to such enzimes as superoxide dismutase, peroxidase, oxidase etc. The use of CeNP as enzyme-mimetic agents in biomedicine meets difficulties due to self-aggregation of NP and low stability of the suspension.

In this research we constructed polymer-coated CeNP with enhanced stability which demonstrate high level of antioxidant activity. The series of polymers including poly (acrylamide) (pAA), and poly (methacrylic acid) (pMA) were synthesised by means of controlled radical polymerization (CRP). pAA was synthesized via nitroxide-mediated polymerization while pMA was obtained using CRP in the presence of metal complexes.

The polymers obtained by both CRP methods showed narrow polydispersity in the range of 1,2- 1,4 according to GPC data. Hybrid polymer-CeO_2 nanoparticles were obtained via nanoprecipitation method. TGA results demonstrated that the ratio of inorganic and polymer was app. 75:25.

Antioxydant activity of polymer-coated CeNPs was determined using TMB assay (peroxidase activity) and SOD assay (superoxidase dismutase). Obtained results revealed that polymer-coating did not affect the peroxidase-mimic activity of CeNP but noticeably enhanced the superoxidase dismutase-like properties of nanoceria.

Effect of electrolysis conditions on the composition and structure of the Co-W(WO_2)-TiO_2 composite coatings

Yermolenko I.Yu.[1], Saray V.V.[1], Tur Yu.I.[1],
Sakhnenko N.D.[1], Karakurkchi H.V.[2]

[1] National Technical University «Kharkov Polytechnic Institute»,
2 Kyrpychova St., Kharkov-61002, Ukraine.
E-mail: kirilesha72@gmail.com

[2] National Defense University of Ukraine named after Ivan Cherniakhovskyi,
28, Povitroflotskyi Ave., Kyiv-03049, Ukraine

The results of studies of the influence of the electrolysis regimes and condition on the Co-W(WO_2)-TiO_2-coatings composition and structure are discusses.

The Co-W(WO_2)-TiO_2 coatings were formed onto a mild steel substrate from citrate electrolyte by direct current. The coatings composition was determined by EDS on an Oxford INCA Energy 350 electron probe microanalysis. The surface morphology and topography was examined by an atomic force microscopy.

Stirring allows provides the working solution in a suspension state and uniform distribution of the dispersed phase in the volume of the electrolyte, which provides an increase in the content of TiO_2 in the coating. It is shown that the best conditions for the incorporation of TiO_2 into the coating metal matrix, and tungsten in the form of variable valence oxides are created at a current density of 1.5 – 2.5 A/dm^2, temperature 45 – 50°C and at electrolyte stirring up to 100 rpm. More intensive mixing of the working solution causes a decrease in the tungsten content in the coating to 4 at.% due to the peculiarities of the co-deposition mechanism of tungsten with cobalt [1]. In addition, the deposition of dense matte coatings with a mass of up to 6 mg/cm^2 and a tungsten content of up to 10 at.% is provide by using an ultrasonic disperser during electrolysis and a current density of 3 A/dm^2.

The analyses results of the composition, surface morphology and topography of composites testify to its significant development compared substrate material and allow predicting the high electro catalytic properties of the obtained materials.

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Effect of low molecular weight arenes additives on the interphase layer structure of SAN-PS systems and dielectric behavior of such compositions

Anoshenko M.[1], **Bazylyuk T.**[1], **Iukhymenko N.**[1], **Budzinska V.**[2]

[1] *Faculty of Chemistry, Macromolecular Chemistry Department, Taras Shevchenko National University of Kyiv,*
Kyiv, 01033, 60 Volodymyrska Street, Ukraine.
E-mail: yukhimenko.n@gmail.com

[2] *Institute of Macromolecular Chemistry of National Academy of Sciences of Ukraine, 48 Kharkivske shouse, Kyiv 02155, Ukraine*

The aim of this work was to study the low molecular weight arenes (LMWA) influence on the dielectric behavior of binary system with limited compatibility between components based on styrene-acrylonitrile copolymers (SAN) – polystyrene (PS). It could be expected that the LMWA will enhance the interphase layer (IPL) due to the π-π electron conjugation of the phenyl groups of components and, respectively, intermolecular interaction (IMI) in the IPL.

The industrial thermoplastic polymers SAN of azeotropic composition and suspension PS were used in the work.

The benzene, toluene, styrene, benzonitrile (BN) were used as low molecular weight components. LMWA were incorporated into a polymer matrix by sorption of the corresponding liquid under saturated vapor (desiccator method). The amount of low molecular weight substances incorporated into polymers were ~ 0.5% wt. % relative to the polymer matrix.

The following dielectric parameters, such as the tangent of the dielectric loss angle (tg δ) and dielectric permittivity (ε'), were estimated. Conclusions about the basic mechanisms of intermolecular interaction changing in the IPL were made based on the FTIR spectroscopy data. IR spectroscopic investigations were carried out in the range 400-4000 cm^{-1}.

It was established that benzene interacts selectively with SAN and PS, blocking the polymer-polymer interaction in the IPL.

The IPL structure rearrangement in the presence of toluene, as well as the growth of the stabilization of lyophilic fluctuating network which forms the IPL was detected. Styrene can be used as a compatibilizer of investigated polymer-polymer system.

Benzonitrile causes a weakening of the intermolecular interaction in the IPL due to the selectivity (similarly to benzene), as well as the dipole-dipole interaction of the nitrile groups of copolymers and benzonitrile. The complex IPLs structure is formed by competing (lyophilic and lyophobic) fluctuation networks. It was concluded that the rigid lyophobic network formation possibility, as well as the connected with this process mixtures heterogeneity mixtures is controlled, in general, by the SAN content in the compositions.

Sorption properties of porous aluminosilicate minerals of Ukraine, *in situ* modified by poly [5- (p-nitrophenylazo) -8-methacryloxyquinoline] of toxic metal ions

***Savchenko*[1], *Yanovska E.*[1], *Sternik D.*[2], *Kychkyruk O.*[3]**

[1] *National Taras Shevchenko University of Kyiv,*
60, Volodymyrska str., 01601 Kyiv, Ukraine
E-mail: iras@univ.kiev.ua

[2] *Maria Curie-Skłodowska University,*
pl. Maria Curie-Skłodowskiej 3, 20 031 Lublin, Poland

[3] *Ivan Franko Zhytomyr State University,*
40 Velyka Berdychivska St., 10008 Zhytomyr, Ukraine

Porous aluminosilicate minerals of Ukraine are widely known for their adsorption properties against a number of toxic organic substances, ions of toxic metals, pathogenic bacteria, etc. However, their natural properties can be improved, in particular by fixing on their surface homo- or copolymers of different chemical nature, capable of participating in the processes of complexation or ion exchange, resulting in composite materials with valuable sorption properties.

The main methods of fixing polymers on the surface of porous inorganic carriers are physical and chemical fixation, sol-gel method and *in situ* immobilization, each of which has its advantages and disadvantages. We have previously found that *in situ* immobilization and adsorption of poly [8-oxyquinoline methacrylate] on the saponite surface of the Tashkiv deposit and clinoptilolite of the Sokyrnytsia deposit led to an increase in their sorption capacity for Pb (II), Cu (II) and Fe (III) ions.

This paper is devoted to the synthesis and study of sorption properties of ions of Pb (II), Cu (II) and Fe (III) composites based on saponite and clinoptilolite, *in situ* immobilized poly [5- (p-nitrophenylazo) -8-methacryloxyquinoline] (AzoQN). *In situ* immobilization of AzoQN on the surface of selected minerals was performed by initiated radical polymerization in the presence of mineral particles.

Immobilization of AzoQN on the surface of saponite and clinoptilolite was confirmed using IR spectroscopy and thermogravimetric analysis combined with mass spectroscopy. Using mass thermogravimetric analysis, the mass fractions of polymer in the synthesized composites were determined. And the forms of immobilized polymer on the surface of minerals were described based on the analysis of photographs of the surface of the synthesized composites obtained by scanning electron microscopy.

It was found that as a result of *in situ* immobilization of poly [5- (p-nitrophenylazo) -8-methacryloxyquinoline] on the saponite surface, the sorption capacity of the mineral relative to Pb (II) and Cu (II) ions increases more than 2 times. Thus, the sorption capacity of the synthesized composite relative to Pb (II) ions is 1.5 times higher than that for the saponite composite with *in situ* immobilized poly [8-oxyquinoline methacrylate].

An increase in the sorption capacity of the synthesized clinoptilolite-based composite relative to Cu (II) and Pb (II) ions compared to the original mineral was not recorded. However, its significant increase relative to Fe (III) ions was found to be 5.6 times. This value is 4 times higher than that for a clinoptilolite-based composite with *in situ* immobilized poly [8-oxyquinoline methacrylate] and three times higher than that for a clinoptilolite-based composite with adsorbed poly [8-oxyquinoline methacrylate].

The obtained results can be explained by the additional introduction of azo groups into the immobilized polymer.

Comparative characteristics of sorption properties of silica gels with *in situ* immobilized azopolymers for Cu (II), Pb (II) Cd (II) and Fe (III) ions

Savchenko[1], Yanovska E.[1], Sternik D.[2], Kychkyruk O.[3]

[1] National Taras Shevchenko University of Kyiv,
60, Volodymyrska str., 01601 Kyiv, Ukraine
E-mail: iras@univ.kiev.ua

[2] Maria Curie-Skłodowska University,
pl. Maria Curie-Skłodowskiej 3, 20 031 Lublin, Poland

[3] Ivan Franko Zhytomyr State University, 40 Velyka Berdychivska St., 10008 Zhytomyr, Ukraine

To increase the efficiency of sorbents against transition metal ions on the surface of porous inorganic carriers, it is advisable to fix polymers with complexing properties. Previously, we synthesized and investigated the sorption properties of a number of organo-mineral composites, by *in situ* immobilization on the surface of mesoporous silica gels and natural macroporous aluminosilicate minerals of Ukraine, in particular with such amino- and az-containing homopolymers as poly [4- (methacryloylaminophenyl) -2-methacrylate], poly [p- (4-carboxyphenyl) - methacrylamide, poly [4-methacryloyloxy- (4'carboxy) -azobenzene], poly [4-methacryloyloxy- (4'carboxy) -3-chloro) -azobenzene] and poly [4-methacryloyloxy- (4'carboxy-2-nitro-5-methyl) -azobenzene] and poly [8-methacroyloxy-quinoline].

Studies of the sorption properties of the synthesized composites on Cu (II), Pb (II), Mn (II), Fe (III), Cd (II) ions showed that all synthesized composites show better sorption properties on the microquantities of the studied toxic metal ions in neutral aqueous environment compared to the original carriers. It was found that the sorption capacity of Fe (III) ions among the synthesized composites based on silica gels with immobilized azo-containing polymers is higher than that of composites with immobilized amine-containing homopolymers.

This paper is devoted to the synthesis and study of sorption properties of Cu (II), Cd (II), Pb (II), Fe (III) ions of new organo-mineral composites obtained by *in situ* immobilization on the surface of mesoporous silica gel of poly [5- (p -nitrophenylazo) -8-methacryloxyquinoline] (SiO_2-AzoQN), poly [1-methacryl- [4 - ((E) - {4 - [(E) - (4-aminophenyl) diazenyl) -phenyl} -diazenyl) - phenyl] ethanone] (SiO_2-BazoN) and poly [1-4 - (E) - {4 - [(E) - (4-nitrophenyl) diazenyl] -phenyl} -diazenyl) -phenylamine] (SiO_2-BazoN).

Immobilization of the synthesized azopolymers on the surface of silica gels was confirmed using IR spectroscopy and thermogravimetric analysis combined with mass spectroscopy. Using thermogravimetric analysis, their mass fractions in the synthesized composites were determined. From the analysis of photographs of the surface of the synthesized composites obtained by scanning electron microscopy, it was found that the polymers on the surface of silica gels are in the form of agglomerates of various shapes, covering most of the surface of the carrier particles.

As a result of research and comparison of the sorption capacity of the synthesized composites with respect to Cu (II), Cd (II), Pb (II) and Fe (III) ions, it was found that none of them showed sorption activity against Cd (II) and Pb (II) ions. However, their sorption capacity in comparison with that for the original silica gel increases significantly relative to Fe (III) ions, in particular for SiO_2-AzoQN - 4.5 times, for SiO_2-BazoN - 4.2 times, for (SiO_2-BazoM) in - 6.4 times. In addition, in contrast to other synthesized composites, the chemical activity of SiO_2-AzoQN against Cu (II) ions was recorded with an increase in sorption capacity compared to the original carrier by 5.3 times.

Antiferromagnetic composites for spin electronics

Sohatsky V.P.

T. Shevchenko National University of Kyiv.
Volodymyrska Str., 60, Kyiv-01601, Ukraine.
E-mail: vso@univ.kiev.ua

Among the problems of spintronics, which has not yet found a comprehensive solution is remagnetization on the nanoscale and increasing the operating frequencies of the spintronic and/or photonic elements. Composite thin film structures for spintronics have an advantage over monofilms due to combination of several substantial properties that make it possible to remagnetize them not only by a conventional external magnetic field but also by applying mechanical stresses, electric fields or optical irradiation. Our previous studies of mechanically stressed ferrimagnetics of various compositions showed a possibility of changing shape of their hysteresis loops (otherwise operating characteristics of the spin valve sensors) from linear (in analog mode) to almost rectangular (in discrete mode) [1]. Further simulations of remagnetization were performed on the basis of energy balance equations taking into account growing stray fields with decreasing size and coercivity of the nanosized elements. Thus the remagnetization conditions were obtained up to the nanometer spatial elements.

Antiferromagnets (AF) have a significant advantage in remagnetization rate over any other magneto-optical materials due to some non-collinearity of their magnetizations in sublattices. The resulting precession of their magnetic moments leads to fast-changing of spatial orientation of magnetization. Such a remagnetization was studying in AF orthoferrites ($Y(Eu, Tm)FeO_3$) and in iron borate ($FeBO_3$) under applied magnetic field and mechanical stress. Both materials are relevant for magnetooptics in transmission mode, although they have significantly different hysteresis loops, coercivity value (e.g. approx. 10 Oe in YFO and close to 0 in FB). Modelling and experiments with the mentioned materials allowed to determine the nature of their piezomagnetization in a wide frequency range, as well as to measure the magnetic response to the impact of the femtosecond laser pulses. Despite a simplicity of the applied model, it allowed to predict the distribution of magnetization in studied materials with a sufficient accuracy for a lot of specified parameters.

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Guerbet condensation of ethanol and 1–butanol over hydroxyapatite nanocatalysts

***Zikrata O.V.*, Larina O.V., Valihura K.V., Kyriienko P.I., Soloviev S.O.**

L.V. Pisarzhevskii Institute of Physical Chemistry of the NAS of Ukraine.
Prospect Nauki, 31, Kyiv-03028, Ukraine.
E-mail: oksanazikrata@ukr.net

The development of processes for the synthesis of valuable chemicals and fuels from renewable raw materials is an important area of research in sustainable chemistry. The unsaturated hydrocarbons and C^{4+} oxygenates such as 2-ethyl-1-hexanol (2-EH) can be obtained by successive vapor-phase Guerbet condensation of ethanol (EtOH) and 1-butanol (BuOH). Mg-Al oxide systems, zeolites and hydroxyapatites (HAP) are active catalysts for the process due to its acid-base properties.

To regulate acid-base properties of Ca-containing HAP catalysts during the synthesis, a partial substitution of Ca^{2+} ions by Mg^{2+} and Sr^{2+} in the HAP crystal structure are used in present work. The samples were characterized by XRD, SEM, EDX, XPS, FTIR and NMR, and TPD of NH_3 and CO_2. It is established that the partial replacement of Ca^{2+} ions by Mg^{2+} and Sr^{2+} in the HAP structure leads to deformation of its crystal lattice and to change in the number and strength of the surface acid and base sites of the. The high selectivity values for BuOH and C^{4+} oxygenates (57 and 79 %) and for 2-EH (62 %) are achieved over 2.5Mg-HAP at 300 °C due to higher number of acid sites of the surface. It also revealed an advanced resistance to deactivation during time-on-stream. Thus, Ca(Mg)-HAP nanosystems are promising catalysts for sustainable production of industrially important higher linear and branched alcohols from reducing raw materials.

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Properties of natural heteropolysaccharide xanthan in aqueous solutions and its compositions with cobalt nanoparticles

Permyakova N.M.[1], ***Zheltonozhskaya T.B.***[1],
Klepko V.V.[1], ***Kozak N.V.***[1], ***Klymchuk D.O.***[2]

[1] *Department of Polymer Physics, Institute of Macromolecular Chemistry of the NAS of Ukraine. 48 Kharkivske Shosse, Kyiv-02160, Ukraine.*
E-mail: permyakova@ukr.net

[2] *Laboratory of Electron Microscopy, M.G. Kholodny Institute of Botany of the NAS of Ukraine, 2 Tereshchenkovska St., Kyiv-01601, Ukraine.*

Natural polysaccharides are well known for their biocompatibility, non-toxicity and biodegradability. Among them, the heteropolysaccharide xanthan of microbial origin plays an important role in food and non-food industries as a matrix for tablets, nano- and microparticles, hydrogels. Due to its structure, xanthan can generate various types of interactions with other small molecules and macromolecules, forming interesting nano- and microstructures. In the present work, a xanthan sample produced by the bacterium *Xanthomonas campestris* was characterized in detail and used as a template for the *in situ* synthesis of cobalt nanoparticles (CoNPs) in an aqueous medium.

The molecular weight of xanthan (1170 kDa) and its electrochemical properties, viscosity behavior and structure in aqueous and aqueous/Co-salt solutions were determined using viscometry, potentiometric titration, FTIR spectroscopy and TEM. A significant excess of carboxylate groups (10.24 $mol \cdot kg^{-1}$) compared to carboxylic groups (1.29 $mol \cdot kg^{-1}$) in xanthan macromolecules was established. The absence of a polyelectrolyte effect in aqueous solutions of xanthan in a wide range of concentrations was also revealed. In the presence of Co-salt, xanthan interacted with metal ions that led to the compaction of its macro coils.

The process and products of the borohydride reduction of Co-salt in xanthan solutions were studied depending on the concentration of matrix and metal salt (and reducing agent) using photography, FTIR spectroscopy and TEM. An increase in the stability of black cobalt nanoparticles in reaction mixtures was established with an increase in the concentration of the Co-salt from 0.08 to 0.32 $kg \cdot м^{-3}$ and the molar ratio of $NaBH_4$/Co-ions from 1 to 5. The influence of the concentration of xanthan matrices on the stability of CoNPs with respect to their aggregation and sedimentation, as well as on the yield of metal nanoparticles, is also shown. The resulting composition consisted of swollen xanthan coils ~47-97 nm in size containing small amorphous CoNPs ~1.3-9.8 nm in diameter.

The post-carbonisation stage of carbon materials synthesis as a factor influencing its thermal stability

***Povazhnyi V.A.*, Pertko O.P., Melnychuk O.V.**

Department of catalytic synthesis, V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of the NAS of Ukraine,
Murmanska st., 1, Kyiv-94, 02094, Ukraine.

E-mail: vladpovazhnyi@hotmail.com

Carbon materials are widely used as catalysts [1, 2] and catalyst supports with metal addition [3] in many industrially important processes. The combination of specific properties (resistance to abrasion, dimensional and thermal stability and specific adsorption properties etc.) makes synthetic carbon materials (SCM) attractive and competitive compared to activated carbons (AC) [4]. This encourages research into improving existing SCM and creating new ones.

The thermal stability of nanostructured SCM produced by template synthesis according to an improved method (with an additional post-carbonization stage) has been investigated. The comparison was carried out with natural AC as well as with and without metal addition.

It has been shown that an additional post-carbonisation step in SCM synthesis helps to reduce amount of defects and increase their thermal stability compered with AC. This makes them promising for replacing activated carbons in liquid-phase reactions. The presence of metal in the samples tested (irrespective of their nature) negatively affects their thermostability by catalysing oxidation. The dependence of thermal stability on the amount of metal applied is antibat.

Thus, the proposed method for the synthesis of carbon material makes it possible to increase the thermal stability of carbon catalysts or to correct it for metal-containing carbon catalysts.

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Formation of active interphase on the iron particles in C/PVDF media

Panteleymonov R.A.[1], Sherbatuk I.M.[2], Boychuk O.V.[1], Pershina K.D.[1,2]

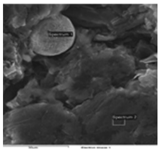
[1] *Vl.Vernadskii Institute of General and Inorganic Chemistry,*
Palladin Ave, 32/34, 03142, Kyiv, Ukraine,
e-mail:katherinepersh@gmail.com

[2] *Joint Department of Electrochemical Energy Systems*
Vernadsky Ave, 38, 03142, Kyiv, Ukraine

The use of catalyst support materials is essential for nanostructured catalytic systems for many energy-transformed devices. Ideal catalyst carrier should possess such properties: high conductivity, high surface area, low cost, electrochemical inertness, and stability. Carbon-based materials have been used as catalyst supports for a long time due to their unique properties such as, physical stability, excellent conductivity, and high surface area. That is why, the study of the formation of new interphases on the iron surface in the composite Fe/C/PVDF films and their impact on thermoelectric properties of composites are actual for the development of a new generation of energy storage. The aim of this work was, the study differences in the quantity of the elements and their ratio on the surface of iron particles and in the volume of the carbon phase. The micromorphological studies of composite samples and quantitative microanalysis of the surface were performed on a scanning electron microscope Tescan Mira 3 LMU, and on energy dispersed spectrometer Oxford Instruments X-Max 80 mm² SDD (table).

Table.

The composition of the surface of the composite film, wt.%

Zones film	C	O	Fe	F	Ratio (formula)	
Zone 1	23.21±2.1	48.83±0.3	26.23±0.5	0.77±0.5	FeC_4O_6	
Zone 2	96.44±2.1	2.79±0.3	26.23±0.5	0.77±0.5	$Fe_3O\ C_{48}$	

The difference in the oxygen content on the surface of iron particles and in the volume of graphite indicates the higher impact of the PVDF in the case of iron particles. It may be connected with the ability of Fe coated by Fe_3O_4 in the presence of graphite to induce the reduction of Fe^{3+} to Fe^{2+} with the generation of free high reactive oxygen [1]. High reactive oxygen is able to form -O–O- and C=O groups on PVDF mainly due to exchanging F in C-F [2]. So, on the surface of iron particles forms a new interface (with size 30 ÷ 80 nm) saturated by active oxygen compounds with high mobility. Confirmation of high mobility of oxygen species is the analysis of graphite in the volume, where at a distance of more than 30 μm the presence of oxygen was found, but in smaller quantities. Also, in this region was detected Fe. If the presence of Fe_2O_3 takes place, the probability of the formation Fe_3C increases in the graphite space. Thus, the simultaneous presence of proactive compounds of oxygen and iron carbide should significantly affect the formation of gradient phenomena and change the thermoelectric properties of the whole system.

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Electronic and optical properties of the $In_4/3P_2S_6$ crystal perspective for ferrielectric heterostructures

Babuka T.[1]***, Kharkhalis L.Yu.***[1]***, Glukhov K.E.***[1]***, Gomonnai O.O.***[2]

[1] *Institute for Physics and Chemistry of Solid State,*
Uzhhorod National University, 54 Voloshin St., 88000 Uzhhorod, Ukraine
E-mail: tanya.babuka@gmail.com

[2] *Uzhhorod National University,*
54 Voloshin St., 88000 Uzhhorod, Ukraine

Nowadays, considerable attention is devoted to the 2D functional materials based on the nonlinear dielectrics that exhibit a rich variety of ferroelectric, pyroelectric, high-κ, and piezoelectric functionalities [1]. In particular, the transition metal thio/selenophosphates (TPS) is a broad class of van der Waals layered solids in which metal cations are embedded into the lattice framework of thiophosphate $(P_2S_6)^{4-}$. Using the compositions of $M^{4+}[P_2X_6]^{4-}$ and $M^{1+}M^{3+}[P_2X_6]^{4}$_type gives a possibility to experimentally construct the excellent heterostructure $CuInP_2S_6/In_4/3P_2S_6$ [2]. While the $CuInP_2S_6$ crystal is investigated well it is very little information about the $In_{4/}3P_2S_6$. Therefore, it is of interest to study the peculiarities of the chemical bonds and the electron band structure of this crystal. It is known this compound is described by monoclinic (space group P21/c) at room temperature and rhombohedral (Rh3) at high temperatures (above 945 K28) and can be thought of as a parent matrix to $CuInP_2S_6$ and $AgInP_2S_6$ [1]. The presence of an ordered arrangement of unoccupied octahedral sites is the main peculiarity of the $In_4/3P_2S_6$ crystalline structure.

The main aim of the present report is to investigate the electronic and optical properties of the $In_4/3P_2S_6$ crystal. Using the DFT method we performed the calculations of the spatial distribution of electron density, band structures, and total and partial density of $In_4/3P_2S_6$ crystals. We obtained the refractive indices and extinction coefficients, real and imaginary parts of the dielectric function, and the absorption coefficient for different polarizations along crystal axes.

Additionally, the model of the $CuInP_2S_6/In_4/3P_2S_6$ heterostructure has been proposed and its parameters were determined.

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Visible light photocatalytic properties of nano-sized tin dioxide doped with iron.

Samsonenko M.[1], **Khalameida S.**[1], **Starchevskyy V.**[2], **Kotynska L.**[1]

[1] *Institute for Sorption and Problems of Endoecology, NAS of Ukraine.*
13, Naumova st., Kyiv 03164, Ukraine.
E-mail: mashuna.08@gmail.com

[2] *Institute of Chemistry and Chemical Technology, L'viv National Polytechnic University, 12 S. Bandera Str., 79013 L'viv, Ukraine.*

The application of nano-sized oxides for photocatalytic degradation is a promising method of wastewater treatment. The use of visible light simplifies and reduces the cost of this process. One of the promising photocatalysts is tin dioxide. To increase the efficiency of its use in photocatalytic processes under the action of visible light, can use its doping with transition metals. It is known that the use of iron as a doped additive to titanium dioxide can increase photocatalytic activity including through inhibition of electron/hole pairs recombination. For SnO_2, this approach has been little studied. Thus, the aim of this work is to study the effect of sonochemical doping on the photocatalytic properties of iron-doped tin dioxide.

Initial heterogeneous precipitation gel SnO_2 was subjected to doping with 5% Fe(III) by sonochemical treatment of wet gel and next thermal treatments at 300°C. Doping and thermal treatment of samples leads to more perfect crystalline structure and an increase in the size of the crystallites. Iron-doped samples of tin dioxide are characterized by high values of specific surface area (137 and 205 m^2/g), and mesoporous structure with pores with a diameter of about 4.7 nm. Changes in the electronic structure are manifested in an increase of absorption of visible light 3-4 times and decrease in the band gap E_g from 4.2 eV to 2.9 eV for initial and doped samples, respectively. These transformations of physico-chemical parameters contribute to the increase in photocatalytic activity of iron-doped tin dioxide in processes of the dyes degradation under visible light. The rate constant of rhodamine B and safranin T degradation for Fe-doped SnO_2 is increasing 2-3 times. In addition, in contrast to inactive initial tin dioxide, doped samples exhibit photocatalytic activity during the degradation of 4-chlorophenol under visible irradiation.

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Plasma-catalytic conversion of CO_2-CH_4 over metal-oxide catalysts

***Samoilenko D. E.*, Kyriienko P. I.**

L.V. Pisarzhevskii Institute of Physical Chemistry of the NAS of Ukraine.
Prospect Nauky, 31, Kyiv-03039, Ukraine.
E-mail: d.samoylenko96@gmail.com

Promising way to attract carbon dioxide into the production process may be combination of cold plasma and catalyst. Plasma will activate CO_2 at relatively low temperatures (about 373 K) and interaction of activated reagents with the formation of target products will occur on the surface of catalyst. Today use of plasma in the process of dry methane reforming was investigated [1]. The same plasma-catalytic approach is of high interest for valuable oxygenates production (alcohols, aldehydes and carboxylic acids) from CO_2-CH_4.

Plasma-catalytic conversion of a CO_2-CH_4 mixture at atmospheric pressure was performed on next metal-oxide catalysts: Al_2O_3, MgO, MgO-Al_2O_3, CuO-ZnO/Al_2O_3, ZnO/Al_2O_3, Ni-La/Al_2O_3. Samples are presented in ascending order of conversion, the maximum conversion was achieved over Ni-La/Al_2O_3 sample: 27% by CH_4 and 17% by CO_2. Catalyst electron structure defines conversion and yield of C-C coupling compounds (ethane, ethyl acetate, ethanol), which are increasing in the row dielectric-semiconductor-conductor. Selectivity of C-C coupling products is defined by acid-base catalyst characteristics. Maximum yield of ethanol (5%) was achieved over MgO-Al_2O_3 sample, which is characterized by the highest concentration of base sites (C_b=0.30 mmol CO_2/g).

Thus, the combination of cold plasma and the catalyst with specific acid-base characteristics and electron structure provides conversion of reagents into valuable C-C coupling products and syngas.

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Carbon nanospheres: synthesis and structure

Rud A.D.[1]***, Polunkin E.V.***[2]***, Boguslavskii L.Z.***[3]***,***
Vinnichenko D.P.[3]***,Kuskova N.I.***[3]***, Kirian I.M.***[1]***,***
Kornienko N.E.[4]***, Pilyavsky V.S.***[2]***, Haidai O.O.***[2]

[1] *G.V. Kurdyumov Institute for Metal Physics of N.A.S. of Ukraine,*
36 Academician Vernadsky Blvd., Kyiv 03142, Ukraine
E-mail: rud@imp.kiev.ua

[2] *V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of N.A.S. of Ukraine, 1 Murmanska str., Kyiv 02094, Ukraine*

[3] *Institute of Pulse Research and Engineering of N.A.S. of Ukraine,*
43A Bogoyavlenskiy Str., Mykolaiv 54018, Ukraine

[4] *Taras Shevchenko National University of Kyiv,*
60 Volodymyrska Str., Kyiv 01033, Ukraine

Electric discharge technologies (electric breakdown of organic liquids and high-frequency electric volume discharge in gaseous hydrocarbons) are elaborated for a large scale synthesis of carbon nanospheres (CNS) [1]. A destruction of hydrocarbon molecules into separate fragments occurs during such processing of organic media, what results in CNS formation in the process of ultra-fast cooling of the clusters. To investigate the influence of chemical nature of working media, organic liquids and gases from the class of arenes with sp^2-hybridisation of carbon atoms in molecule and alkanes with sp^3-hybridisation were used. Performed XRD, HRTEM and Raman studies showed that produced powders are typical amorphous materials with significant degree of disorder. But only in the case of electric breakdown of alkanes, carbon nanomaterials with developed surface (SBET= 150 g/cm^3) and complex core-shell structure were discovered. Individual particles of onion-like carbon consist of ~ 5 nm core surrounded by graphitic shell of 5-6 layers. Synthesized CNS are used as antifriction additives to industrial oils and fuels [2].

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Photocatalytic activity of nanosized TiO_2/Al_2O_3 and TiO_2/MgO composites synthesized by ultrasonic method in the decomposition of metronidazole

Zabolotnii Ye.V., Zazhigalov V.O., Kotynska L.Y., Tsyba M.M.

Institute for Sorption and Problems of Endoecology, National Academy of Sciences of Ukraine.
03164, Kyiv, General Naumov st., 13.
E-mail: evgeniy2019q@ukr.net

One of the promising methods of decomposition of drugs, especially antibiotics, such as metronidazole, which contaminate water sources, is the photocatalytic destruction of these substances on heterogeneous catalysts, among which TiO_2 is one of the most popular. However, this catalyst has a number of disadvantages, so the intensive search of the systems with improved characteristics on the base of complex oxides composition (including TiO_2) and the methods of their synthesis attracts the attention of the most scientific lab [1,2].

The ultrasonic synthesis (UST) of the samples TiO_2/Al_2O_3 and TiO_2/MgO with a molar ratio of 1: 1 in aqueous medium was realized in this study. Photocatalytic destruction of metronidazole (MNZ, C = 0.015 g/l) in aqueous solution was investigated under UV irradiation of the solution. The concentration of MNZ was determined at adsorption band with maximum at 320 nm. Concentration of the MNZ was determined after each hour of the reaction at maximum time of exposure equal to 5 hours.

It was shown that UST permits to obtain the samples with larger specific surface area and total pore volume than the initial oxides mixtures. It was established that the treated system $TiO_2/MgO = 1:1$ demonstrates there the significantly higher photocatalytic activity (K_d) and the degree of metronidazole photodegradation (G) under the action of UV light than the modified system $TiO_2/Al_2O_3 = 1: 1$.

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Novel Liquid Crystal System for Transdermal Drug Delivery

***Kravchenko I.A.*[1]*, Vashchenko O.V.*[2]*, Nesterkina M.V.*[1]*, Lisetski L.N.*[2]**

[1] Odessa International Medical University,
99 Kanatna Street, Odessa 65000 Ukraine.

[2] Institute for Scintillation Materials of NAS of Ukraine,
60 Nauky Ave. Kharkov 61072, Ukraine.
E-mail: olga_v@isma.kharkov.ua

Liquid crystal systems loaded with monocyclic terpenoids (menthone, carvone, verbenone or camphor) are under development as potential anticonvulsant and anti-inflammatory drugs with transdermal delivery path [1].

Maintenance of cholesteric liquid crystalline structure of the systems was proven in a wide temperature range (Fig. 2). Reliable drug deposition into the liquid crystal matrix was also shown. Model lipid membranes are used for biopharmaceutical studies of the drugs properties.

In a preliminary study, anticonvulsant activity was determined *in vivo* using the model of pentylenetetrazole-induced seizures after transdermal application of LC systems containing terpenoids. The obtained results indicate the high efficiency of the developed systems as transmembrane penetration enhancers possessing pharmacological action.

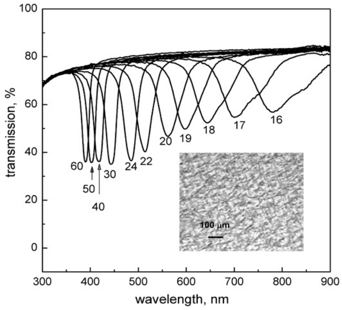

***Fig. 1**. A. Selective transmission spectra [2] of LC system loaded with menthone 5 % w/w. The numbers show the temperature (in °C). B: Microphotograph of the sample at 62 °C*

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Biocompatibility of γ-Fe_2O_3 nanoparticles with blood cells

Paryzhak S.Ya.[1]***, Dumych T.I.***[1]***, Zasońska B.A.***[2]***,***
Svoboda J.[2]***, Klyuchivska O.Yu.***[3]***, Skorokhyd N.R.***[3]***,***
Kozak Yu.S.[3]***, Horák D.***[2] ***& Stoika R.S.***[1,3]

[1] *Danylo Halytsky Lviv National Medical University,*
69 Pekarska Str., Lviv 79010, Ukraine
E-mail: sola.paryzhak@gmail.com

[2] *Institute of Macromolecular Chemistry, Czech Academy of Sciences,*
Heyrovského nám. 2, 162 06 Prague 6, Czech Republic

[3] *Institute of Cell Biology, National Academy of Sciences of Ukraine,*
14/16 Drahomanov St., Lviv 79005, Ukraine

The importance of nanotechnologies for industry, power engineering, IT, medicine and other fields is constantly growing. Because of their small size, nanoparticles (NPs) penetrate into systemic circulation, quickly spread throughout the body and overcome biological barriers [1]. Thus, blood cells are the first contacts for the NPs entering the organism [2].

Our research was aimed at interaction between γ-Fe_2O_3 NPs (~9 nm) and their poly(N,N-dimethylacrylamide) and SiO_2 coated derivatives and blood cells. By means of spectrophotometric measurements of released hemoglobin, it was found out that none of these three groups of NPs leads to erythrocytes damage. Incubation of NPs with isolated neutrophils resulted in slight granulocytes activation with the formation of neutrophil extracellular traps. Coating of γ-Fe_2O_3 with organic and inorganic shells decrease these effects. Besides, intravenous administration of NPs to laboratory animals did not manifest any toxic effect.

Studies involving animals were conducted in accordance with the established experimental protocols and requirements of Ethics committee of Institute of Cell Biology NAS of Ukraine, protocol № 3/07102020. This work was supported by the Czech Science Foundation (No. 20-02177J).

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Synthesis and structure of carbon nanospheres in liquid phase

Polunkin E.V.[1]***, Rud A.D.***[2]***, Haidai O.O.***[1]***, Vinnichenko D.P.***[3]

[1] *V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of N.A.S. of Ukraine, 1 Murmanska str., Kyiv 02094, Ukraine*
E-mail: polunkin@i.ua

[2] *G.V. Kurdyumov Institute for Metal Physics of N.A.S. of Ukraine,*
36 Academician Vernadsky Blvd., Kyiv 03142, Ukraine

[3] *Institute of Pulse Research and Engineering of N.A.S. of Ukraine,*
43A Bogoyavlenskiy Str., Mykolaiv 54018, Ukraine

For the first time, methods for the synthesis of carbon nanospheres from liquid aromatic and halogenated saturated hydrocarbons by high-frequency plasma-chemical method have been developed. To modify and change the properties of carbon nanospheres, the functionalization of these nanomaterials by adding organometallic and metal-complex compounds to the initial liquid raw material has been proposed and practically implemented. Using liquid hydrocarbons (hexane, heptane, isooctane, toluene, bromethane) laboratory samples of carbon nanospheres, as well as nanospheres with implanted metals were developed [1].

The structure and nature of chemical bonds in the obtained carbon nanospheres were studied by IR, NMR and Raman spectroscopy, SEM and HRTEM microscopy. It is confirmed that individual particles of onion-like carbon consist of a nucleus of ~ 5 nm, surrounded by a graphite shell of 5-6 layers [2].

Experimental batches of additives for automotive fuels were made on the basis of synthesized carbon nanospheres. Road-operational tests of influence of the created additives on energy efficiency of motor fuels at work of engines of cars in various modes are carried out, reduction of fuel consumption under the influence of additives by 10 -15% is established.

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Nanocomposite adsorbent based on natural zeolite for selective removal of ^{137}Cs from high salt solutions

***Bondar Yu.V.**, Kuzenko S.V., Olkhovyk Yu.O.*

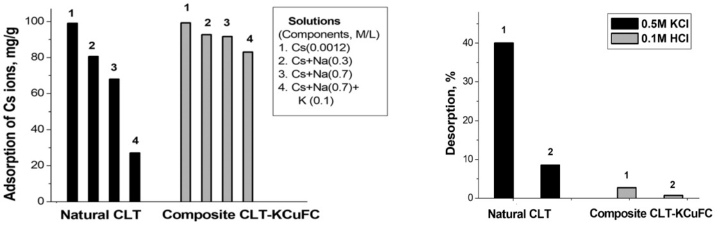
State Institution “The Institute of Environmental Geochemistry of National Academy of Sciences of Ukraine”, 34a Palladin ave., Kyiv 03142, Ukraine.
E-mail: juliavad_peremoga@ukr.net

The development of effective adsorbents for the selective removal of radionuclides from contaminated waters is a topical issue to reduce the amount of hazardous liquid radioactive waste and ensure radiation safety.

Synthesis of composite adsorbents based on natural zeolites with a sorption-active inorganic phase incorporated into their porous structure is considered a promising approach to the manufacture of low-cost adsorbents with high selectivity.

This study concerns the synthesis of a novel nanocomposite adsorbent based on clinoptilolite tuff of the Sokyrnytsia deposit (Ukraine) for selective removal of ^{137}Cs radionuclides. The composite adsorbent was fabricated by a two-stage synthesis: preliminary chemical treatment of the clinoptilolite tuff (CLT) grains with subsequent *in situ* formation of potassium copper ferrocyanide (KCuFC) nanoparticles within the CLT pores (Fig.1).

The efficiency of the synthesized adsorbent in selective removing cesium ions was evaluated under various experimental conditions. Unlike natural CLT samples, the composite ones (CLT-KCuFC) have been found to exhibit fast adsorption rate, high adsorption capacity over a wide pH range, and unique selectivity to Cs ions in model high salt solutions with sodium and potassium ions, as well as enhanced fixation of adsorbed cesium ions (Fig. 2). The synthesized adsorbent has a lot of advantages, such as its simplicity and low-cost fabrication process, chemical resistance, radiation and thermal stability, high selectivity to Cs ions in high salt solutions (for example, sea water).



Effect of the synthesis temperature on the electrophysical properties of zirconia nanoparticles

Shylo A.[1], Danilenko I.[1], Gorban O.[1], Lyubchyk A.[2,3]

[1] *Materials Science Department, Donetsk Institute for Physics and Engineering named after O.O. Galkin of the NAS of Ukraine, Nauki ave, 46, Kyiv-03028, Ukraine, e-mail:art.shylo@gmail.com*

[2] *NANOTECHCENTER ,Kyiv, Ukraine*

[3] *Lusófona University, Lisbon, Portugal*

The work is devoted to investigation of the evolution of an adsorbed water layer on the surface of zirconia nanoparticles with different synthesis temperatures and its effect on the electrophysical properties of compacted zirconia nanoparticles. The combination of methods used in this work allowed to analyze the structure of the hydrated shell of zirconia nanoparticles and to determine the relationship between the structure of the adsorbed layer on the surface of zirconia nanoparticles and the electrophysical properties of compacted hydrated zirconia nanoparticles with different synthesis temperatures.

Thus, the DSC method shows that the water in the adsorption layer has a different degree of connectivity, as indicated by several temperature ranges of water desorption on the surface of nanoparticles with different activation energies. It is shown that the activation energy of water desorption from the surface of zirconia nanoparticles increases by 25% for all temperature ranges with increasing nanoparticles synthesis temperature.

The distribution relaxation time was successfully demonstrated in the analysis of the impedance spectra of compacted zirconia nanoparticles. DRT was then applied to the spectra and polarization losses were separated based on their typical time constants. The EIS method shows that the electrophysical properties of compacted nanoparticles depend on their annealing temperature. This can be explained by the different type of ordering of some structural elements in the system of nanoparticles, the size of the nanoparticles and the structure of the adsorbed layer on their surface.

Acknowledgments

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The effect of interfaces number on solid state reactions in Ni-Ti thin films

Lozova A., Kruhlov I., Voloshko S., Orlov A.

Department of Physical Materials Science and Heat Treatment, National
Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"
Peremohy Ave 37, Kyiv, Ukraine, 03056
E-mail: anja.lozova@gmail.com

NiTi shape memory thin films are highly attractive materials for microelectromechanical systems (MEMS). The actuality of thin-film NiTi is attributed to its large recovery strain and high work output per unit, being useful for the fabrication of microactuators, microsensors, micropumps etc. The common pathway for NiTi fabrication is the film sputtering from the NiTi alloy target. However, the alternative approach is the deposition of layered stack with Ni and Ti individual layers, which is helpful in terms of more precise tuning of the chemical composition of the intermetallic compound. Upon the post-deposition annealing, the intermetallic compound is typically formed through the stages of amorphization and next crystallization [1]. However, in this case the number of the layers involved in the initial stack could drastically influe the solid-state reactions kinetics due to the crucial role of interfaces on the diffusion in thin films.

Present study is aimed to figure out the effect of interfaces number on the solid-state reactions taking place upon annealing in high vacuum (10^{-4} Pa) for 30 min of Ni(30 nm)/Ti(30 nm) and $[\mathrm{Ni(15\ nm)/Ti(15\ nm)}]_{2x}$ thin films prepared onto Si(001) substrate using rf magnetron sputtering at room temperature. Structural study performed using XRD technique revealed the difference in the amorphization behavior at the first stages of annealing of two- and four-layered stacks. It was found that the onset temperature of both amorphization and crystallization is about 100 °C lower in the film consisted of four layers compared to the bilayer system. The following rise of the temperature resulted in the similar recrystallization behavior with the formation of the NiTi intermetallic compounds observed for both films. The findings of this study can be useful for better understanding of the solid-state reactions taking place during the fabrication of application relevant NiTi thin films governed by the interfacial reactions between metal layers.

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Nanocrystalline $Li_{2-x}Na_xGe_4O_9$ solid solutions devitrified from glass

***Diachenko A.O.**, Trubitsyn M.P., Skrypnik Ye.V.*

Institute for Energy Efficient Technologies and Materials Sciences, Oles Honchar Dnipro National University, prosp. Gagarina 72, Dnipro-49005, Ukraine.E-mail: annadiachenko459@gmail.com

Lithium-sodium tetragermanate $LiNaGe_4O_9$ crystal undergoes a phase transition from the nonpolar phase (space symmetry group D_{2h}^8) to the ferroelectric one (group C_{2v}^5) on cooling below TC = 113 K [1]. Changing x from 1 to 0.2 in the series of $Li_{2-x}Na_xGe_4O_9$ crystalline solutions is accompanied by an increase in the phase transition temperature TC from 113 K ($x = 1$) to 330 K ($x = 0.2$). In addition, the typical values of electrical conductivity and the character of its anisotropy in $Li_{2-x}Na_xGe_4O_9$ change significantly [2]. In accord with the data in [2], charge transfer in $Li_{2-x}Na_xGe_4O_9$ crystals can be mainly associated with Li ions interstitials moving along the channels within the structural framework. In amorphous and nanocrystalline states, electrical conductivity of $LiNaGe_4O_9$ increases by approximately two and three orders of magnitude correspondingly as compared to the single crystal [3]. It is of interest to study the crystallization processes and ionic conductivity in glasses and nanocrystalline state of lithium-sodium tetragermanate solid solutions. Here we report the thermal analysis data on $Li_{2-x}Na_xGe_4O_9$ glasses ($x = 1, 0.6, 0.45, 0.2$) devitrification performed on heating. Also, we discuss electrical properties of $Li_{2-x}Na_xGe_4O_9$ in amorphous and partially crystallized nanocrystalline states.

The samples of $Li_{2-x}Na_xGe_4O_9$ glasses were obtained by rapid quenching the melt. The glasses were crystallized by heating the samples in the temperature range of 300 ÷ 1200 K. The heating and cooling rates were 10 and 20 K/min. Thermal analysis of devitrification processes was performed by differential scanning calorimetry (DSC). The phase states of amorphous and polycrystalline $Li_{2-x}Na_xGe_4O_9$ were controlled by X-ray diffraction analysis. Electrical properties were measured in the temperature interval 300 ÷ 930 K and frequency diapason 1 ÷ 500 kHz and 1 MHz.

For all studied compositions the DSC curves demonstrated presence of exothermic anomalies, which indicated softening and subsequent crystallization of the amorphous phase. The concentration dependences of the glass transition temperature $T_g(x)$, the crystallization temperatures $T_C(x)$, as well as the heat released on crystallization, were determined. The presence of a single intense exothermic peak on the DSC curves indicated a polymorphic mechanism of crystallization of the amorphous phase for all studied compositions $x = 1, 0.6, 0.45, 0.2$. A comprehensive analysis of DSC data and X-ray diffraction analysis was performed. The changes of ionic conductivity accompanying transitions from the glass to the nanometer and micrometer sized crystalline states were discussed.

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Magnetic and structural features of aged Cu-Al-Mn-Fe alloys

Demchenko L.[1,2]***, Titenko A.***[3]***, Bykanov T.***[1]***, Titenko O.***[1]***,***
Babanli M.[4]***, Troshchenkov Yu.3, Huseynov S.***[4]

[1] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37, Peremohy Ave., Kyiv 03056, Ukraine.*

[2] *Department of Materials and Environmental Chemistry,*
Stockholm University, Stockholm SE 106 91, Sweden
E-mail: lesyademch@gmail.com

[3] *Institute of Magnetism of the NAS and the MES of Ukraine,*
36-b, Vernadskoho Blvd., Kyiv 03142, Ukraine.

[4] *Azerbaijan State University of Oil and Industry,*
Azadliq Ave., 20, Baku, AZ1010, Azerbaijan

Cu-Al-Mn shape memory alloys (SMA), in addition to their good mechanical and functional properties (plasticity, superelasticity, shape memory effect, high damping capacity), have magnetic properties as well. Alloying with additional elements, as well as heat treatment are used to improve the mechanical properties and shape memory characteristics. Controlling the phase morphology, grain size, volume fractions, sizes, and distribution of precipitates, it is possible to an increase in alloy thermoelasticity associated with a decrease in the width of temperature hysteresis. It has been found that doping with Fe (~1%wt.) gives a good improvement in transformation temperature, ductility, and shape memory recovery.

The effect of aging at 100÷200°C for 0.5÷5 hrs on the ferromagnetic nanoparticles precipitation in a quenched Cu-Al-Mn-Fe alloy has been studied. The alloys structural feature is a rather large grain size of 5 mm and a martensitic state at room temperature. Using EPR spectroscopy, static magnetization, and low-field magnetic susceptibility, the interaction of precipitated ferromagnetic particles depending on their volume fraction and size was determined. Some anomalies in EPR spectra and a specific magnetization behavior, associated with the redistribution of magnetic carriers in Cu-Al-Mn-Fe alloy after annealing, which also differs compared to the Cu-Al-Mn alloy [1], were observed.

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Nano-engineered cement-based composites: Perspectives of advanced functional materials – a review

Sikora P.[1], Chougan M.[1]

[1] Faculty of Civil and Environmental Engineering, West Pomeranian University of Technology in Szczecin,
Al. Piastow 50a, 70-311 Szczecin, Poland
E-mail: pawel.sikora@zut.edu.pl

[2] Department of Civil and Environmental Engineering, Brunel University London, Uxbridge, UB8 3PH, United Kingdom

Over the years, nanomaterials were used to modify the fresh and hardened properties of cement-based composites. It was found that inclusion of tiny dosage of nanomaterials have substantial impact on the rheology and workability of fresh composites as well as significantly affects mechanical and durability performance of material. Besides modification of basic engineering properties it was found that incorporation of nanomaterials can endow the composites with various functional properties. Therefore, it is possible to produce so-called smart composites. This consists of self-sensing (e.g. sensing stress, strain, crack, damage, temperature, and smoke), self-heating and self-healing abilities.

This work is aimed to review the recent development in the field of nano-engineered cement-based composites. The impact of selected nanoparticles, including Fe_2O_3, Fe_3O_4, TiO_2 and carbon-based materials (carbon nanotubes, graphene oxide), on the physico-chemical properties of functional materials in cementitious composites are summarized. In addition, the effects of molecular hybrids (core-shell structures) is discussed. In the final part, technology potential, gaps and future perspectives are discussed.

Acknowledgement: This research was funded in part by the National Science Centre, Poland within Project No. 2020/39/D/ST8/00975 (SONATA-16).

Synthesis of Bi_2O_3-SiO_2 and Gd_2O_3-SiO_2 core-shell structures towards improvement of fresh and hardened properties of cement-based composites

***Sikora P.*, Cendrowski K., Federowicz K., Techman M.**

Faculty of Civil and Environmental Engineering, West Pomeranian
University of Technology in Szczecin,
Al. Piastow 50a, 70-311 Szczecin, Poland
E-mail: pawel.sikora@zut.edu.pl

Concrete is one of the most widely used materials for radiation shielding in radiation therapy facilities, hospitals, nuclear reactors as well as in military applications. In general, materials such as lead, with a high atomic number (High-Z), are preferred for absorbing ionizing radiation. Unfortunately, in the recent years serious concerns are raised regarding use of lead due to its potentially hazardous effects.

In recent years, special attention has been particularly paid to nanosized admixtures, which lead to far greater improvements in cementitious systems, in comparison to their micro-sized counterparts. Inclusion of high dosage of metal oxide nanoparticles results in decrement of heat of hydration as well as can negatively affect mechanical, microstructural and durability-related properties of cement-based composites. Therefore, methods towards improving the reactivity of metal oxide nanoparticles are required.

This study is devoted to synthesis of Bi_2O_3-SiO_2 and Gd_2O_3-SiO_2 core-shell structures towards improvement of fresh and hardened properties of cement-based composites. Hydration studies including isothermal calorimetry and thermogravimetric analysis were performed. In addition, rheological and mechanical properties were determined.

Study showed that cement can be effectively replaced with up to 10 wt% of nanoparticles without deteriorating substantially the properties of Portland cement paste. Therefore, inclusion of such nanoparticles into cementitious system can find its utilization in production of radiation shielding cement-based composites.

Acknowledgement: This research was funded in part by the National Science Centre, Poland within Project No. 2020/39/D/ST8/00975 (SONATA-16).

Mechanical properties of superionic ceramics based on $AG_7(SI_{1-X}GE_X)S_5I$ solid solutions

Shender I.O., Pogodin A.I., Filep M.J., Malakhovska T.O., Kokhan O.P., Suslikov L.M., Bilanych V.S., Pop M.M.

Uzhhorod National University,
Pidhirna St. 46, Uzhhorod, Ukraine
E-mail: iryna.shender@uzhnu.edu.ua.

Superionic conductors Ag_7SiS_{5I} and Ag_7GeS_{5I} belong to a wide family of compounds with an argyrodite structure [1]. Due to the high ionic conductivity of $Ag_7(Si_{1-x}Ge_x)S_5I$ crystals they are promising materials for creation an efficient electrode materials, photoanodes, supercapacitors, etc. [2]. Recently, increasing attention is observed to the preparation and investigation of superionic conductors in the form of ceramics due to their greater manufacturability.

Ceramic samples of $Ag_7(Si_{1-x}Ge_x)S_5I$ (x = 0.2, 0.4, 0.6, 0.8) solid solutions were made by sintering of pressed micro- and nanocrystalline powders. Nanocrystalline powders were obtained by grinding in a planetary ball mill PQ-N04 for 30 and 60 min, and microcrystalline powders were ground in an agate mortar. Annealing of the pressed samples was performed in evacuated quartz ampoules at 973 K for 36 h. Thus, ceramics were obtained in the form of disks with a diameter of 8 mm and a thickness of 3-4 mm. Measurements of microhardness was performed by indentation of the Vickers pyramid in the load range of 0.05-1.5 N. The depth of penetration of the indenter was 1-10 μm.

Established that the microhardness of $Ag_7(Si_{1-x}Ge_x)S_5I$-based ceramics decreases with increasing the depth of indentation. This is explained by the dimensional effect of indentation during microindentation of ceramics. The decrease in microhardness with decreasing Si content during the $Si^{4+} \rightarrow Ge^{4+}$ substitution is observed both for the studied ceramics and single crystals. The decrease in the values of microhardness for ceramic samples compared to the single crystals is established. This is due to the porosity and presence of intercrystalline areas (with a large number of structural defects) and, as a consequence, “free” volume in the ceramics.

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Study of mechanical characteristics of ceramic membrane supports

***Serhiienko A.O.*[1], *Pylypenko I.V.*[2], *Dontsova T.A.*[1]**

[1] *Department of Technology of Inorganic Substances, Water Treatment and General Chemical Technology,*

[2] *Department of Chemical Technology of Ceramics and Glass,*
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute". Peremohy avenue, 37, Kyiv-03056, Ukraine.
E-mail: allasergienko706@gmail.com

Interest in ceramic membranes as membrane water treatment methods is increasing every year due to their high strength, thermal stability, chemical resistance, resistance to abrasive particles, easy cleaning by back-flushing, and long service life. One of the main parts of ceramic membranes is the support layer, which determines the mechanical strength of the membrane.

The aim of the research is to investigate the effect of the sintering temperature and the different content of silicon carbide on the mechanical strength of ceramic membrane supports based on flexural strength.

By changing the silicon carbide content (0%, 10%, 20% and 30%, respectively) series of ceramic membrane supports were synthesised. The series of samples were prepared by dry pressing followed by sintering at different temperatures, such as 800 °C, 950 °C and 1100 °C.

The flexural strength was determined in accordance with ISO 14704:2006 Fine ceramics (advanced ceramics, technical ceramics).

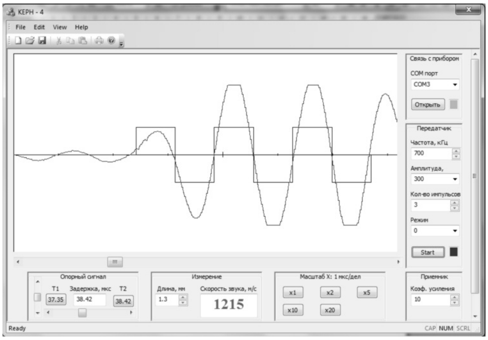
It was found that an increase in the sintering temperature from 800 °C to 1100 °C leads to a logical increase in the flexural strength. An increase in silicon carbide content also causes an increase in flexural strength for all the samples tested. The increase in strength, in this case, may be due to the formation of calcium silicate phases formed after the decomposition of silicon carbide and calcium carbonate. It is determined that the optimum silicon carbide content is 20% for sintering temperatures up to 950 °C. The results indicate an increase in the flexural strength when the sintering temperature is increased from 800 °C to 1100 °C. Established that the optimum sintering temperature for maximum strength values is in the range of 1000-1100 °C.

Mechanical spectroscopy of nanocomposites of multiwalled carbon nanotubes and polyamide, polyethylene, polyvinyl chloride, porous polystyrene

Onanko A.P.**, **Popruzhko V.M., Dmytrenko O.P., Kulish M.P.,
Onanko Y.A., Charnyi D.V., Pinchuk-Rugal T.M., Pavlenko O.L.
Busko T.O., Kurochka L.I., Gaponov A.M., Ilyin P.P.

Kyiv national university, Volodymyrs'ka str., 64, Kyiv-01601, Ukraine.
E-mail: onanko@i.ua

The influence of ultrasonic (US) deformation εUS was studed on inelastic internal friction (IF) Q^{-1} and elastic modulus E of nanocomposite polyamide-6 (PA-6) $(NH(CH_2)_5CO)_n$ + 1.7% methylene dye blue squaring (DBSQ) in Fig. 1 [1].



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Амплитуда,: 300
Кол-во импульсов: 3
Режим: 0
T1: 37.35
Задержка, мкс: 38.42
T2: 38.42
Длина, мм: 1.3
Скорость звука, м/с: 1215
Коэф. усиления: 10

***Fig. 1**. Illustration of the window for processing data of quasi-transversal elastic wave velocity measuring* $V^{\perp}$ *= 1215 m/sec in nanocomposite polyamide-6 (PA-6)* $(NH(CH_2)_5CO)_n$ *+ 1.7% methylene dye blue squaring*

Conclusions

1. The increase of the nanocomposite crystallinity degree at growth of multiwalled carbon nanotubes concentration filling with the methylene dye blue squaring of matrix results in the decline of content of organized phase.

Acknowledgements

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***DOI:** https://doi.org/10.21272/jnep.12(4).04026.*

Mechanochemical synthesis and characterization of $ZnMoO_4 \cdot 0,8H_2O$, and $ZnMoO_4$ nanostructures.

Diyuk N.V.[1]***, Diyuk O.A.***[2]***, Zazhigalov V.O.***[2]***, Shcherban N.D.***[3]

[1] *Taras Shevchenko National University of Kyiv,*
60 Volodymyrska Street, Kyiv 01033, Ukraine

[2] *Institute for Sorption and Problems of Endoecology of NAS of Ukraine,*
General Naumov Street, 13, Kyiv 03164, Ukraine
E-mail: diyukhelen@ukr.net

[3] *L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine,31 pr. Nauky, Kyiv 03028, Ukraine*

$ZnMoO_4$ is an industrial white pigment with anticorrosive and smoke-suppression properties. In addition, it has attracted more attention as a phosphor, catalyst for the partial oxidation of hydrocarbons, and anode material. At present, the traditional synthesis of $ZnMoO_4$ is either energy-consuming or leads to water pollution. It is worth noting that water pollution and global warming are among the top ten major environmental problems. Therefore, the development of a synthesis procedure does not require high temperatures and does not lead to environmental pollution is a very urgent task. Our goal is to develop a low-temperature synthesis of $ZnMoO_4$ without water pollution.

A mixture of ZnO and MoO_3 with a molar ratio of 1:1 was treated mechanochemically on a Pulverisette-6 planetary ball mill in an aqueous medium with rotation of 500rpm for 10, 20, and 60 min. Synthesized samples were characterized by XRD, BET, SEM, TEM, FTIR, TPR-H_2 and DTA. XRD data shows the formation of $ZnMoO_4 \cdot 0.8H_2O$ (JCPDS No. 00-025-1025) in all cases. SEM and TEM images of $ZnMoO_4 \cdot 0.8H_2O$ demonstrate the formation of flexible filament structures 20-100 nm wide and 200 μm long. These filament structures become entangled and form a secondary agglomerate web-like structure. Thermogravimetric measurements showed that $ZnMoO_4 \cdot 0.8H_2O$ has two forms of crystallized water: the first form desorbed up to 150°C, the second form desorbed in the temperature range of 150-280°C and at the same time $ZnMoO_4$ (JCPDS No 00-035-0765) is formed. The TEM and SEM images of $ZnMoO_4$ show that after the removal of the crystallization water, the flexible long structure was destroyed, and a structure of short needle-shaped particles was formed.

Mechanochemical treatment of a mixture of ZnO and MoO_3 in water medium makes it possible to synthesize nanostructured zinc molybdate at room temperature, avoiding environmental pollution.

Synthesis of nanocomposite materials based on TiO_2 for purification solutions

<u>Aleksyk A.I.</u>, Yanushevska O.I., Dontsova T.A.

National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute» Prospect Peremogy, 37/4, Kyiv-03056, Ukraine.
E-mail: aleksyk.al@gmail.com

Ceramic-based membranes have recently been increasingly used in water purification processes, including under extreme conditions, which requires high thermal, biological and chemical stability of ceramic membranes in a wide pH range and durability, their high hydrophilicity and permeability [1]. For manufacturing the selective layers of ceramic membranes oxides of aluminum, titanium, zirconium, copper, etc. are used. TiO_2 proved to be the most economical and highly effective material, which when covered with it the matrix of ceramic membrane demonstrates a high flow performance of treated water and can prevent bacterial fouling of the surface of ceramic membranes. TiO_2 for ceramic membranes was obtained by hydrothermal method. For this purpose, distilled water was added to an alcoholic solution of titanium isopropoxide under constant stirring. In this way two suspensions with different titanium content (in terms of titanium isopropoxide) were obtained, namely 2.8% and 28%. After stirring the suspension was kept in hydrothermal conditions for 12 hours at 170 °C. X-ray patterns of the obtained TiO_2 samples are shown in Figure, which shows that in both cases a predominantly anatase modification of titanium (IV) oxide (up to 95%) was obtained.

Curve 2 in Figure corresponds to 2.8% isopropoxide titanium in the sample, curve 1 in Figure corresponds to 28% isopropoxide titanium in the sample. Thus, the obtained suspensions were deposited on ceramic supports by spin-coating, then examined by scanning electron microscopy. SEM images show the morphology of the deposited selective layer characteristic of ultrafiltration and microfiltration membranes.

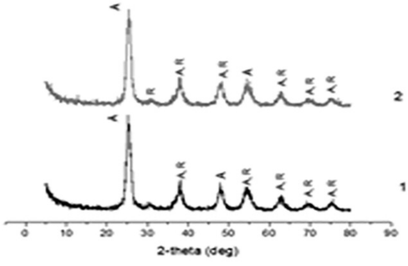

Figure – XRD analysis of TiO_2 samples

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Influence of heat treatment on the surface morphology of tin-doped silicon oxide films

Voitovych V.V.[1]***, Rudenko R.M.***[1]***, Poroshin V. M.***[1]***, Kras'ko M.M.***[1]***,***
Kolosiuk A.G.[1]***, Povarchuk V.Yu***[1]***, Voitovych M.V.***[2]

[1] *Department of Solid State Electronics, Institute of Physics of the NAS of Ukraine. Prospect Nauki, 46, Kyiv-03039, Ukraine. E-mail: vvoitovych@yahoo.com*

[2] *Laskarev Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, prosp. Nauki 41, Kyiv-03028, Ukraine*

The study was performed on thin non-stoichiometric films of silicon oxide (SiO_x, $x \approx 1.1$) with a high content of tin (Sn > 2.5 atomic %). In order to segregate SiO_x films into phases of silicon oxide (SiO_2) and silicon, and the effect of tin on these processes, the samples were subjected to heat treatment at 900 °C for 30 minutes in an argon atmosphere. After heat treatment of the samples, an image of their surface was obtained using an electron microscope. In addition to spherical silicon tin clusters [1], filamentous connections are also observed on the film surface. Using X-ray microanalysis, it was found that such filamentous inclusions consist of atoms: C (1.44 at.%), O (62.24 at.%), Si (29.79 at.%) та Sn (6.53 at.%). Some of the filamentous inclusions originate in large silicon-tin inclusions.

At a temperature of 900 °C, there is a final process of formation of amorphous nanoscale inclusions of silicon in the oxide matrix and the beginning of their crystallization, and the crystalline phase is very unstable [2]. In addition, in the process of thermally stimulated structural transformations, the films become denser. Such compaction of the film and its segregation leads to linear micro-concavities or convexities of the relief of its surface, and certain internal mechanical stresses. This compaction of the film and its separation leads to linear micro-concavities or convexities of the relief of its surface and certain internal mechanical stresses. Heat treatment of samples at a temperature of 1000 and 1100 °C renal inclusions were not observed.

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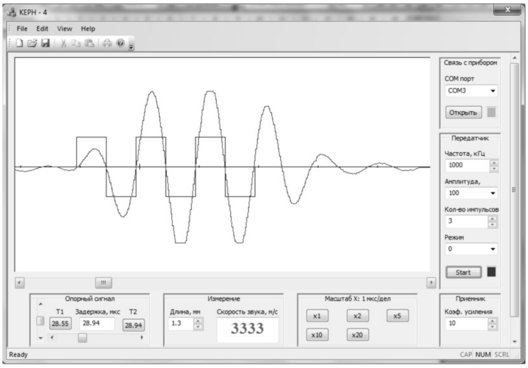
Characteristic mechanical spectroscopy of nanocomposites of multiwalled carbon nanotubes and polyamide, polyvinyl chloride, polyethylene, expanded polystyrene

Popruzhko V.M.*, Onanko A.P., Dmytrenko O.P., Kulish M.P., Onanko Y.A., Charnyi D.V., Yatsiuk M.V., Pinchuk-Rugal T.M., A.A. Kuzmych, Ilyin P.P.

Kyiv national university, Volodymyrs'ka str., 64, Kyiv-01601, Ukraine.
E-mail: onanko@i.ua

The quasi-longitudinal elastic wave ultrasound (US) velocity measuring $V\parallel = 3333 \pm 10$ m/sec, dynamical elastic modulus $E = \rho V\parallel^{2} = 13{,}719$ GPa, the quasi-transversal US velocity $V\perp = 1215 \pm 10$ m/sec, shear modulus $G = \rho V\perp^{2} = 1{,}823$ GPa of nanocomposite polyamide-6 (PA-6) $(NH(CH_2)_5CO)_n$ + 1.7% methylene dye blue squaring (DBSQ) were determined from the oscillogram in Fig. 1 [1].



COM порт: COM3
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Амплитуда,: 100
Кол-во импульсов: 3
Режим: 0
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Задержка, мкс: 28.94
T2: 28.94
Длина, мм: 1.3
Скорость звука, м/с: 3333
Коэф. усиления: 10

Conclusions

1. Mechanical studies have confirmed the strong interaction between polyamide-6 (PA-6) $(NH\ (CH_2)_5CO)_n$ and methylene blue dye.

Acknowledgements

This work has been supported by the Ministry of Education and Science of Ukraine: Grant of the Ministry of Education and Science of Ukraine for the prospective development of the scientific direction "Mathematical sciences and natural sciences" at Taras Shevchenko National University of Kyiv.

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DOI: https://doi.org/10.21272/jnep.13(5).05017.

Using gold nanoparticles for the development of a biosensor based on urease and potentiometric transducers

Marchenko S.V.[1]***, Rieznichenko L.S.***[2]***, Dybkova S.M.***[2]***,***
Dzyadevych S.V.[1]***, Soldatkin A.P.***[1]

[1] *Institute of Molecular Biology and Genetics, Natl.Acad. of Sci. of Ukraine,*
Zabolotnogo str., 150, Kiev, 03143, Ukraine.
E-mail: svmarchenko85@gmail.com

[2] *F.D. Ovcharenko Institute of Biocolloidal Chemistry, NAS of Ukraine,*
Kyiv 03142, Ukraine.

Gold nanoparticles (GNPs) can be widely used in biosensors based on enzymes. GNPs are highly conductive and biocompatible; they can form strong thiol bonds between organic substances (for example, cysteine residues of enzymes) [1]. Thus, nanoparticles form an appropriate microenvironment for the enzyme immobilization. Additionally, the activity of the immobilized enzyme can be preserved by immobilization on GNPs.

In this experimental work, we used the enzyme urease from soybeans and GNPs, 20 nm and 30 nm in size. Based on these elements and pH-sensitive field-effect transistors, working biosensors were developed, the parameters of which were studied in model solutions. In the course of research, the optimal ratio of gel components for co-immobilization was selected; different types of biosensors were developed, namely, without GNPs and with the addition of GNPs of different sizes and concentrations.

All types of the biosensors developed have been experimentally tested in model solutions; such characteristics as the response time, the magnitude of the signal to addition of the substrate in certain concentration have been studied; calibration curves have been plotted, the linear range has been established; the operational stability and reproducibility of biosensor preparation have been studied; a comparative analysis has been carried out.

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Computational investigation of atomic and electronic structures of phosphate-based crystal-glass composites

<u>Chornii V.</u>[1,2], Boyko V.[1], Nedilko S.G.[2], Borysiuk V.[2],
Hizhnyi Yu.[2], Zhydachevskyy Ya.[3]

[1] National University of Life and Environmental Sciences of Ukraine. Geroiv Oborony st., 15, Kyiv-03041, Ukraine.
E-mail: vchornii@gmail.com, vchornii@nubip.edu.ua.

[2] Taras Shevchenko National University of Kyiv,
Volodymyrs'ka st., 60, Kyiv-01601, Ukraine.

[3] Institute of Physics Polish Academy of Sciences,
al. Lotników, 32/46, Warsaw, Poland.

The interphase layers greatly determine the physical characteristics of composite materials, particularly, such as nanostructured glass-ceramics. These characteristics are difficult to predict using only general knowledge about atoms, ions or molecules interactions. At the same time, the mutual diffusion of component atoms can be effectively modeled in the molecular dynamics (MD) calculations. The further electronic structure calculations for the obtained atomic structures allow obtaining relevant micro and macro-characteristics of such layers.

In this work the computational studies of the atomic and electronic structures of glasses and crystal-glass interphases were carried out using Materials Studio 2019 software package [1]. Two types of composites were considered: a) $KBi(MoO_4)_2$ crystal - K_2O-P_2O_5-MoO_3-Bi_2O_3 glass; and b) $K_2Eu(PO_4)(WO_4)$ crystal - K_2O-P_2O_5-WO_3-V_2O_5 glass. The atomic structures of initial glasses and interphases were calculated by MD methods implemented in Amorphous Cell and Forcite programs. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method CASTEP for which the cells of smaller sizes were used. The key structure–properties relations in studied glasses and crystal-glass composites were clarified, in particular, dependence of the optical characteristics of composite materials on atomic and electronic structures of interphase layers. A possibility of "engineering" the physical properties of novel glass-ceramics was analyzed.

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Polymer coatings & brushes: electro-physical study and application

Izhyk O.[1]***, Balaban O.***[1]***, Mitina N.***[2]***, Zaichenko A.***[2]

[1] *Department of Applied Physics and Nanomaterials Science, Institute of Applied Mathematics and Fundamental Science, Lviv Polytechnic National University, St. Bandery st., 12, Lviv – 79013, Ukraine.*
E-mail: oksana.v.balaban@lpnu.ua

[2] *Department of Organic Chemistry, Institute of Chemistry and Chemical Technologies, Lviv Polytechnic National University,*
St. Bandery st., 12, Lviv – 79013, Ukraine.

Prospects for the use of polymeric materials are becoming increasingly evident. The natural reserves of substances are depleted every day, and the resource base for many applications is running out. That is why polymeric materials occupy vacated niches in various fields of application. Polymeric materials are popular due to the availability of synthesis, reproducibility of results, economy, and environmental friendliness. Recently, the production of coatings based on thin polymer films, which serve as a kind of barrier or protection from external influences, and the cultivation of polymer brushes on various surfaces have become popular. The last of them is developing more and more every day because it is variable. In particular, it is possible to control the thickness of the brush layer, its density, the purposeful inclusion of various nanoparticle impurities in the structure of the brushes, or grafting other brushes. All these features make brush polymer coatings widely functional and multifaceted in use. Special attention is paid to the performance of polymers in energy storage, conservation, and conversion devices. After all, as is well known, the requirements for the effective operation of these devices are expanding every day, but achieving the desired characteristics is becoming increasingly difficult. Many achievements have already been made along the way, as many works are dedicated to expanding the base of cathode materials for these devices. It is proposed to replace natural materials with artificial, and expensive materials with cheap, sometimes not even environmentally friendly ones. However, the desired result has not been obtained, so another way to solve this problem is to use functional polymer films that are stable in different conditions.

This paper presents a study of the accumulative properties of polymer brushes and suggests ways to use the synthesized materials.

Nitrogen-doped carbon for supercapacitors: synthesis, properties and applications

Maksymych V.*[1], Calus D.[2], Borysiuk A.[1], Chabecki P.[2], Ivashchyshyn F.[1,2]

[1] Department of Applied Physics and Nanomaterials Science, Lviv Polytechnic National University, S. Bandera st. 12, 79013 Lviv, Ukraine
E-mail: vitalii.m.maksymych@lpnu.ua

[2] Faculty of Electrical Engineering, Czestochowa University of Technology, J.H. Dąbrowskiego st., 69, 42-201 Częstochowa, Poland

The key to success in increasing the specific capacity of nanoporous carbons, which are used for the manufacture of supercapacitor electrodes, is to ensure the combination of optimal porous structure with the appropriate electronic structure of the material. This would ensure the release of the Helmholtz capacitance by the capacitance of the space charge region in the solid. Therefore, the aim of this work was to obtain nitrogen-doped environmentally safe nanoporous carbon material.

Nitrogen-containing carbon material was obtained by direct pyrolysis method. Glucose was used as a carbon source, sodium bicarbonate as an activator (porogen) and urea as a nitrogen source for carbon doping.

The resulting carbon material is characterized by high homogeneity as evidenced by the images taken on the Phenom ProX scanning electron microscope. The nitrogen content of the EDS analysis system ranged from 2.88% to 25.17 wt.%. According to the results of nitrogen adsorption-desorption received the maximum pore distribution in the radius corresponds to 1.42 nm, and the total surface area reaches 1247 m^2/g. The results of X-ray low-angle scattering confirm the obtained result of porometry, which indicates the openness of the pores and their availability to the electrolyte. Unexpectedly, in the process of studying the carbon material, its magnetization was revealed. The method of vibration magnetometry established that the specific saturation magnetization of carbon material in the magnetic field strength of 800 kA/m is $\sigma s = 1.4\ A \cdot m^2 \cdot kg^{-1}$, and the coercive force $H_c = 10$ kA/m. The method of impedance spectroscopy confirmed the relatively high electrical conductivity of carbon material. It was found that in a symmetrical supercapacitor with 30% water solution KOH electrolyte, the specific capacity of the obtained carbon material reaches 180 F/g, which is 80% higher compared to the existing on the market materials.

Influence of different polymers on photoluminescence of colloidal ZnO nanocrystals

***Isaieva O.F.*[1], *Dzhagan V.M.*[1], *Selyshchev O.*[2], *Toma M.*[3], *Gule E.G.*[1], *Yukhymchuk V.O.*[1], *Valakh M.Ya.*[1], *and Zahn D.R.T.*[2]**

[1] V. Lashkaryov Institute of Semiconductors Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine.
E-mail: dzhagan@isp.kiev.ua

[2] Semiconductor Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany.

[3] Babes-Bolyai University, Physics Faculty,
M. Kogalniceanu 1, 400084, Cluj-Napoca, Romania.

Embedding NCs in polymer matrices is a way to protect NCs from degradation and to tailor NC properties. Investigation of luminescent NCs in transparent polymers is important due to their perspective applications in photonics and bio-imaging, while NCs in conductive polymers can be promising for photovoltaics, electroluminescence, and photodetectors [1]. Here, we investigate the effects of embedding the ex-situ synthesized colloidal ZnO NCs [2] in different water-soluble polymers, such as polyvinyl alcohol (PVA), polyvinylpyrrolidone (PVP), polyethylene glycol (PEG), gelatine, and PEDOT:PSS. In addition to recording the spectral and intensity changes in the NC PL spectrum, caused by polymer, we infer possible recombination mechanisms of the NC PL and ways of the interaction between NCs and polymer. The common major effect of PVP, PEG, and PVA is suppression of defect- related PL band (DPL), although at low NC loading the effect of these polymers is more different from each other than at high loading. Gelatine caused unexpectedly quenching of both PL excitonic (EPL) and DPL. The effect of PEDOT:PSS is relatively weak, as for conductive polymer, although distinct indications of structural and electronic changes in the polymer are found in Raman and XPS spectra

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5-Alkyl-1,2,4-triazole-3-thiones as stabilizers in the synthesis of silver nanoparticles

Fizer M.M.[1]***, Hryhorka H.V.***[1]***, Slivka M.V.***[1]***,***
Fizer O.I.[1]***, Mariychuk R.T.***[2]

[1] *Organic Chemistry Department, Educational and Scientific Institute of Chemistry and Ecology, Uzhhorod National University,*
Pidhirna, 46, Uzhhorod-88000, Ukraine.
E-mail: mmfizer@gmail.com

[2] *Department of Ecology, Faculty of Humanity and Natural Sciences,*
University of Presov in Presov, 17th November,
1, Presov-08116, Slovak Republic.

Several novel 5-alkyl-4-methyl-1,2,4-triazole-3-thiones (alkyl can be pentyl, heptyl, pentadecyl, and heptadecyl) were synthesized from hydrazides of corresponding acids. Obtained triazoles exist in the form of thiolate anions in an alkaline medium, they are characterized by structural features of surfactants. The alkyl chain acts as a “hydrophobic tail,” while the more polar negatively charged fragment of 1,2,4-triazole-3-thiolate acts as a “hydrophilic head.”

It is known from the literature that structurally similar 4-amino-5-hexyl- 1,2,4-triazole-3-thione can be used as a flotation collector in the treatment of malachite [1]. The authors note that the surface activity is due to the interaction of sulfur and nitrogen atoms with the surface of malachite. Moreover, it was shown a strong binding of thiolate-containing stabilizers to silver nanoparticles [2].

Considering all the above, it was decided to investigate the possibility of using alkaline solutions of 5-alkyl-4-methyl-1,2,4-triazole-3-thiones as stabilizers in the chemical synthesis of silver nanoparticles. A series of solutions of silver nanoparticles of different concentrations were synthesized. It was found that triazoles with longer chains (5-pentadecyl, 5-heptadecyl) have a more significant stabilizing effect than triazoles with pentyl or heptyl groups.

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Application of nanoparticles of metal oxides In wooden building materials

***Lopatko L.S.*, Pinchevska O.O.**

National University of Life and Environmental Sciences of Ukraine Heroyiv
Oborony st., 15, Kyiv - 03041, Ukraine
E-mail:asp21-l.lopatko@it.nubip.edu.ua

Wood is a natural, environmentally friendly building material that accumulates carbon. Making products from it requires less energy. Despite its many benefits, wood is very sensitive to biological attacks and external factors. One of the ways to increase the service life of wood products is the use of nanoparticles, in particular alumina (Al_2O_3) and silica (SiO_2), etc. Recently, the use of nanoparticles in the construction sector has become significantly more widespread. Reuse of nanoparticle concrete has shown its durability advantage and enhanced mechanical properties compared to fresh concrete. There is experience in the use of Al_2O_3 nanoparticles in the production of medium density fiberboard (MDF) by adding them to synthetic adhesives, which has improved mechanical and physical properties. The efficiency of using Al_2O_3 nanoparticles as a sorbent for removing residual formaldehyde from urea-formaldehyde resin has been proved.

Nanoparticles of colloidal solutions obtained by electro-spark treatment of the corresponding metals have a positive effect. The thus obtained particles with a size of 20–100 nm have a competitive advantage over powder forms because they use water as a base. Because most metals are good conductors of heat, nanoparticles increase the conductivity of wood-based materials, which reduces time holding pressure.

High Pressure Laminate (HPL) panels, which are used for facing public buildings and private homes, have become very popular among wood composites. HPL consists of 5-50 layers of kraft paper (core) saturated with phenol-formaldehyde (PF) adhesive, the top layer is made of decorative paper and covered with a finish saturated with melamine-formaldehyde (MF) adhesive. After build-up, these layers become a single rigid laminated sheet under the influence of high literature and pressure, and PF and MF adhesives undergo a series of crosslinking reactions, thus creating strong irreversible bonds between the adhesive matrix and the impregnated layers of paper.

Laminate manufacturers are looking to develop HPLs that include new and combined features to gain a competitive edge in national and international markets. The use of metal nanoparticles in their production will make the panels more resistant to external factors, strengthen the internal structure, reduce toxicity by binding unreacted formaldehyde and reduce production time.

Influence of surfactants on adsorption and catalytic properties of Fenton-like catalysts

Makido O.Yu.[1], Khovanets' G.I.[1], Kurilets' O.G.[2], Diadenchuk A.V.[2]

[1] Department of PhChFF InPOCC NAS of Ukraine.
Naukova Str., 3a, Lviv-79060, Ukraine.
E-mail: khovanets_galyna@ukr.net

[2] Lviv Polytechnic National University.
S. Bandery str., 12, Lviv-79013, Ukraine.

Obtaining composite materials of a given composition, structure and physico-mechanical properties is one of the most important tasks of modern materials science. Advanced technological solutions in recent years, related to the creation of composites with catalytic and adsorption properties to solve the problem of wastewater treatment from organic pollutants, are based on the study of the relationship "composition - structure - properties". The use of surfactants in the synthesis of nanostructured magnetically sensitive Fenton-like catalysts improves their porosity. This requires additional study of the influence of the nature of surfactants (natural and synthetic origin) on the properties of the synthesized catalysts, which work simultaneously by two mechanisms: adsorption and destruction.

For this purpose, investigations of the catalytic and adsorption activity of pre-synthesized multilayer composites of the "core - shell" type based on CuO were carried out. The core of the composite is cobalt ferrite precipitated on amorphous SiO_2, which has magnetic properties. The presence of a magnetic core in the catalyst greatly simplifies its separation from the reaction volume by magnetic separation and allows reuse. To stabilize, the core is covered with a layer of porous SiO_2 with the addition of surfactants of various natures, on which clusters of copper oxide, which serve as catalytic centers, are precipitated. Investigations of the adsorption process were carried out by spectrophotometric method at a wavelength of 620 nm on a model solution of methylene blue (MB) with a volume of 5 ml and a concentration of $5 \cdot 10^{-5}$ mol/L in a static reactor at room temperature with stirring. Catalyst weight − 10 mg, surfactant − 500 mg.

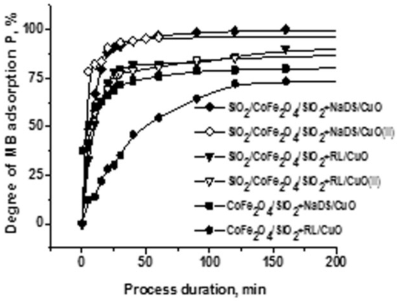

Fig. 1. *The dependence of the degree of MB adsorption on the structure of the synthesized catalysts in the dynamics of time: (II) − reuse of catalysts*

To investigation the influence of surfactants of different nature, we compared the $SiO_2/CoFe_2O_4/SiO_2/CuO$ composite with the addition of sodium dodecyl sulfate (NaDS) ($C_{12}H_{25}SO_4Na$) (sample 1) and rhamnolipid (RL) (Pseudomonas sp.) (sample 2). The influence of the nature of surfactants on the kinetic regularities of MB adsorption by the composite structure $CoFe_2O_4/SiO_2$+NaDS/CuO (sample 3) and $CoFe_2O_4/SiO_2$+RL/CuO (sample 4) was also investigated.

As shown by the results presented in Fig. 1, catalyst - sample 1 is characterized by high activity in the process of MB adsorption. Under optimal conditions, the MB adsorption for sample 1 reached 80.4% already after 15 min process, 91.8% − after 30 min, 96.4% − after 60 min. For sample 2 − 63.3%, 79.7% and 82.1%, respectively. For both samples, there is a sharp increase in the rate of MB adsorption from the beginning of the process for 20 min: P_1=89.1%, P_2=73.3%. Reuse of these catalysts after drying at 100°C showed their high efficiency. A significant difference is observed for the kinetic curves of MB adsorption for samples 3 and 4. Thus, the MB adsorption for sample 3 reached 63% already after 15 min process, 71.4% − after 30 min, 76.2% − after 60 min, and for sample 4 − 21.6%, 36.4% and 54.2%, respectively.

It has been determined that the nature of surfactants has a positive effect both on the structure of the synthesized catalysts and on their properties. As can be seen from the results of samples 1 and 3, despite the different synthesis technology, the addition of surfactants of synthetic origin (sodium dodecyl sulfate) has a greater influence on the porosity of the structure than surfactants of natural origin (rhamnolipid) and, accordingly, improves the adsorption properties of catalysts.

The effectiveness of practical use of the synthesized heterogeneous nanostructured magnetically separable catalyst $SiO_2/SiO_2/CoFe_2O_4/SiO_2$+NaDS/CuO in the Fenton system for fine post-treatment of dairy production wastewater has been established. This process does not require the addition of H_2O_2 to the system, because the supply of atmospheric oxygen to the reaction medium on the catalyst is the formation of peroxide compounds, which are involved in the oxidation of organic pollutants. This fact, together with the possibility of easy removal of the catalyst from the reaction medium by magnetic field and its reuse without loss of efficiency, makes this system economically viable and environmentally friendly.

Humidity sensor element based on oxidized porous silicon – reduced graphene oxide hybrid structures

Olenych I.B.[1], ***Horbenko Yu.Yu.***[2], ***Monastyrskii L.S.***[1],
Aksimentyeva O.I.[2], ***Boyko Ya.V.***[1]

[1] *Electronics and Computer Technologies Department, Ivan Franko National University of Lviv, 50 Dragomanov Str., Lviv-79005, Ukraine*
E-mail: iolenych@gmail.com

[2] *Chemistry Department, Ivan Franko National University of Lviv,*
6 Kyrylo and Mefodiy Str., Lviv-79005, Ukraine

Nanostructured semiconductors with an ultra-high specific surface are extremely promising in the field of sensor electronics. In particular, nanostructures of porous silicon (PS) are widely used as sensitive elements of gas sensors [1]. The combination of the PS with other nanoparticles can increase the sensitivity and selectivity of sensors. Given this, an up-and-coming technology is the deposition of graphene nanostructures on the PS layer [2, 3]. The local electric field of adsorbed gas molecules causes changes in the electrical conductivity of both PS nanostructures and graphene.

In this work, oxidized PS–reduced graphene oxide (rGO) hybrid structures were created to study their sensory properties. We have found that the obtained hybrid structures show a decrease in resistance and an increase in capacitance in AC mode with increasing relative humidity. Dependence of the sensing ability on relative humidity and kinetic characteristics of resistive and capacitive sensor elements were studied to evaluate the sensory properties of obtained structures. The obtained results demonstrate high potential applications of the oxidized PS–rGO hybrid structures in humidity sensors.

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Hierarchical zeolites as potential catalyst for Bayer-Villiger oxidations for cyclic ketones using H_2O_2

***Kurmach M.M.*, Yaremov P.S., Valihura K.V., Shvets O.V.**

Department of Porous Substances and Materials
L.V.Pisarzhevskiy Institute of Physical Chemistry of the NAS of Ukraine,
31, Nauky Ave., Kyiv 03028, Ukraine.
E-mail:mazinator3710@ukr.net

Bayer-Villiger oxidation process is well known industrial organic process with industrial use, especially, in production of naylone-666 using cyclohexanone as starting material. Although different homoheneous peroxyacids are used as industrial catalysts used, development of new heterogeneous catalysts for Bayer-Villiger oxidations still important role. It is known, that Sn-containing zeolites provide high efficiency in oxidation of some ketones [1], although their activity in process using bulk ketones decreases. Hierarchical zeolites are promising catalysts for a variety of catalytic process including bulk substrates due to their developed external surface and, consequently, high concentration of active sites available for them.

Fe-, Sn-, Zr- and Al-containing hierarchical zeolites were obtained using different Gemini-type surfactants as structure-directing agents (SDA) [2]. Significant decrease in particle size allow to increase values of external surface area and mesopore volume values of which achieved up to 400 $m^2 \cdot g^{-1}$ and 1,0 $cm^3 \cdot g^{-1}$, consequently. Zeolites possessed a high concentration of Brønsted (BAS) and Lewis acid sites (LAS) (50 – 200 $\mu mole \cdot g^{-1}$) available for bulk molecules.

Catalytic properties of Al-, Sn- and Zr-containing hierarchical zeolites were evaluated in oxidation of cyclic ketones with H_2O_2 as oxidant to ε-caprolactone. Zr-MTW and AlZr-BEA provide high conversion (up to 65%) of cyclohexanone as well as high selectivity towards desired ε-Caprolactone (up to 90%).

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Study of the adsorption of Immunoglobulinum humanum by functionalized - NH_2, - SH, - COOH groups on the surface of nanoscale magnetite

Kusyak N.V.[1], **Kusyak A.P.**[2]

[1] Nataliya Kusyak – Department of chemistry, Ivan Franko Zhytomyr State University, Zhytomyr, Ukraine, 40 Velyka Berdychivska St, 10008 Zhytomyr, Ukraine. E-mail: nkusyak@ukr.net,

[2] Chuiko Institute of Surface Chemistry of the NAS of Ukraine.
General Naumov Str., 17, Kyiv - 03164, Ukraine.

Nanomaterials as substrates for targeted delivery of therapeutic or diagnostic agents are widely used in modern medicine. However, it remains important to study their interaction with both transported drugs and components of the biological environment. Compliance with the principles of biocompatibility, adsorption activity, residence time in the biological environment and the target zone, hydrophilicity / hydrophobicity etc. - the main requirements for the physico-chemical parameters of these materials.

Increasing biocompatibility through surface functionalization ensures the activity of the target system, the selectivity of the binding of nanoparticles to certain chemicals or cells. Therefore, it is important to understand the process and mechanism of interaction of biological substances with surfaces of different nature, the impact on the conformation and functional ability of protein substances. This interaction will be determined by the chemical nature of the active centers of the surface: physicochemical (surface charge, reactive groups, pHIIP) and geometric (size, surface structure) properties of nanoparticles.

Since one of the forms of external stimulation of physical targeting of drug delivery to cells is the magnetic field, nanocomposites based on Fe_3O_4 with - NH_2, - SH, - COOH functional groups were synthesized for the study. Immunoglobulinum humanum (Ig), which has a wide range of opsonizing and neutralizing properties against bacteria, viruses and other pathogens, selected as a model protein. The main purpose of this work was to study the processes of adsorption immobilization of Ig on synthesized composites.

In vitro study of the bioactivity of sol-gel glass 60S doped with Y

Kusyak A.[1, 3], Dubok V.[2], Marcin Behunova D.[3], Chornyi V.[4], Burianov O.[4], Petranovska A.[2], Gorbyk P.[1]

[1] *Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine, 03164 Kyiv, Ukraine*
E-mail: a_kusyak@ukr.net

[2] *Frantsevich Institute of Problems of Materials Science, National Academy of Sciences of Ukraine, 03142, Kyiv, Ukraine*

[3] *Institute of Geotechnics, Slovak Academy of Sciences,*
45 Watsonova Str., 04001 Kosice, Slovakia

[4] *Bogomolets National Medical University,*
Taras Shevchenko Boulevard, 13, 02000 Kyiv, Ukraine

The high biocompatibility of these materials is due to the ability to form a layer of hydroxyapatite (HA) on the surface of bioglass in contact with biological fluids and the peculiarity of sol-gel synthesis allows the introduction of various biologically active components.

Apoptosis of cancer cells, decreased rate of bone resorption and bioceramics, selective immunomodulatory activity is the spectrum of therapeutic action of additives such as ions of rare earth elements. In addition, as a result of doping, the specific surface changes due to the reduction of the size of the primary crystals and active sorption centers are formed on the surface.

In this work, the synthesized and compared *in vitro* bioactivity nanostructured samples of sol-gel glass (60S), which have a composition (mol%) of 60% SiO_2, 36% CaO, 4% P_2O_5 and doped with Y - 60% SiO_2, 32% CaO, 4% P_2O_5, 4% Y_2O_3. The ability of the prepared glass to form apatite *in vitro*, after immersion in simulated body fluid (SBF), was assessed by Fourier Transform Infrared Spectroscopy (FTIR) and X-ray dispersion analysis (EDX). Changes in specific surface area, change in zeta potential and dispersion stability of nanoparticles were evaluated. The establishment of negative zeta potential, *in vitro* biological activity and nanometric particle size, make glass 60S doped with Y possible candidate for bone engineering.

Nanostructured adsorbents for arsenic compounds removal

Gusak A.[1]***, Litynska M.***[1]***, Krimets G.***[1]***, Dontsova T.***[1]

Department of Technology of Inorganic Substances, Water Treatment and General Chemical Technology of National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute".
Prospect Peremohy, 37, Kyiv-03056, Ukraine.
E-mail: m.litynska-2017@kpi.ua

Increasing of arsenic content in natural waters due to changes of groundwater level and acidic rains is the significant problem of drinking water treatment. Arsenic is one of the most dangerous elements in world. According to European Commission, the maximum allowable level of arsenic in drinking water is 10 µg/l. High arsenic concentration in natural water is typical for India, China, Bangladesh, Taiwan, Vietnam, Hungary, USA, Mexico, Chile, Argentina, Hungary, Ghana, Iran, etc. [1-3]. Chronic arsenic exposure provokes a lot of different health problems, including cancer of skin and internal organs, endocrine disorders, hyperkeratosis, melanosis, etc. [2,4].

We synthesized nanostructured iron oxyhydroxide and iron oxyhydroxide/activated carbon adsorbents by homogeneous precipitation. We used thermal hydrolysis of urea to precipitate iron oxyhydroxide from iron(III) chloride solution. Obtained nanostructured adsorbents could be used for arsenic removal from water phase due to significant efficiency (the best sample efficiency is about 70 mg As/g). Modifying of activated carbon by iron oxyhydroxide improved the arsenic removal more than twice. So, these sorption materials are perspective for drinking water treatment.

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Structure, optical properties and photocatalytic activity of undoped, Nd-doped ZnO nanocomposites

Myroniuk D. V.[1], ***Chudinovych O. V.***[1, 2], ***Shyrokov O. V.***[1], ***Myroniuk L. A.***[1], ***Danylenko I. M.***[3], ***Strelchuk V. V.***[3], ***Ievtushenko A. I.***[1, 2]

[1] *Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine,*
Krzhyzhanovsky Str., 3, Kyiv-03142, Ukraine.
E-mail: denysmyroniuk@gmail.com

[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Peremohy Av., 37, Kyiv-03056, Ukraine.*

[3] *Lashkaryov Institute of Semiconductor Physics of the NAS of Ukraine,*
Nauky Av., 41 Kyiv-03039, Ukraine.

ZnO is one of the promising photocatalytic materials. Its photocatalytic activity is determined by the sufficient size of its band gap (3.3 eV) and the appropriate position of its valence and conduction bands for oxidation reduction processes, with the generation of reactive oxygen species and the oxidation of organic pollutants. It is strongly depending on the defects and impurities. The Nd^{3+}, as the rare earth element dopant, reduces the band gap energy and enhances the possibility of the photodegradation of dyes under UV and visible light [1].

The undoped and Nd-doped ZnO nanoparticles were synthesized by means of chemically method from Zn^{2+} and Nd^{3+} nitrates solutions. The undoped ZnO nanoparticles are identified as a wurtzite structure ZnO. For all Nd-doped ZnO samples, the diffraction peaks are almost similar to undoped ZnO. It is possible for Nd^{3+} ions cooperate with the matrix of ZnO particles to form Nd-Zn-O solid solutions since the radius of Nd^{3+} is bigger than that of Zn^{2+} which confirms by Raman measurements. The influence of Nd doping on photocatalytic activity of ZnO will be presented and discusses in our report in detail.

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Synthesis and study of hybrid nanostructures based on nanoparticles of precious metals and magnetic nanoparticles

Kusyak A., Galaburda M., Gun'ko V.

Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine, 03164 Kyiv, Ukraine
E-mail: a_kusyak@ukr.net

The development of hybrid composite structures based on nanoparticles of precious metals and magnetic nanoparticles is currently one of the highest priorities in the development of nanomedicine. Such structures exhibit localized surface plasmon resonance, which makes them convenient in creating sensor materials for use in biomedical purposes.

Nanodispersed magnetite (Fe_3O_4), which was synthesized by the Elmore reaction, was used as a magnetically sensitive component of the synthesized nanocomposites. Both nanoparticles of the original Fe_3O_4 [1] and functionalized thiol groups [2] were used for the synthesis of composite nanoparticles consisting of gold and magnetic iron oxide (Fe_3O_4/Au).

The synthesized samples were examined by Fourier transform infrared spectroscopy (FTIR), thin-film X-ray diffraction and scanning electron microscopy (SEM), SBET surface area and pore size distribution (PSD) were also determined. Particles size-distributions were plotted based on photon cross-correlation spectroscopy (PCCS) analysis for water suspension materials. To indicate the stability of particle suspensions, the zeta potential of the particles was measured with a laser Doppler electrophoresis (LDE) instrument.

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Fabrication of magnetite-based core-shell nanoparticles with bifunctional amino-/mercapto- polysilsesquioxane layers

Muratova M.A.[1,2]***, Stolyarchuk N.V.***[2]***, Tomina V.V.***[2]***, Melnyk I.V.***[2,3]

[1] National University of Kyiv-Mohyla Academy,
2 Skovorody Str., Kyiv-04655, Ukraine,

[2] Chuiko Institute of Surface Chemistry, NAS of Ukraine,
17 General Naumov Str, Kyiv-03164, Ukraine,

[3] Institute of Geotechnics SAS,
45 Watsonova Str, Kosice-04001, Slovak Republic,
E-mail: melnyk@saske.sk

Magnetically controlled nanoparticles covered by silica shell with different groups are widely used and researched due to their obvious advantages, such as ease of extraction, high content of functional groups and well-developed shell porous structure [1]. Composite materials based on magnetite nanoparticles functionalized with mercaptopropyl [2] and aminopropyl groups [3] have been already applied as adsorbents for the removal of heavy and precious metal ions from aqueous solutions, sorption of organic dyes, and for the production of biocatalysts due to enzyme fixing.

The proposed research is focused on the developing of a one-step sol-gel method for obtaining magnetic nanoparticles with a bifunctional surface layer ($–(CH_2)_3$-SH and $–(CH_2)_3$-NH_2), using bridged silanes 1,2bis(triethoxysilyl)ethane and 1,4bis(triethoxysilyl)benzene as structuring agents. These bissilanes promote the formation of an outer shell with high porosity ($S_{BET} = 630 – 980$ m^2/g) and also organic bridges are expected to improve the access of target ions to the functional groups by increasing the distance between them. The combination of amino and mercapto groups has to create a specific environment for metals during their adsorption on the surface of such carriers, which may cause their different behavior on the surface. Creating clusters of a particular structure on the surface can promote the selective adsorption of certain metal cations, which was the purpose of the work.

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Chitosan-based nonwoven materials obtained by electrospinning

***Kuchynska D.A.*, Ishchenko O.V., Plavan V.P., Lyashok I.O.**

Kyiv National University of Technologies and Design
Nemyrovycha-Danchenka Street, 2, Kyiv-01011, Ukraine.
E-mail: email.of. e.ishchenko5@gmail.com

Chitosan-based nonwoven materials obtained by electrospinning are used to make bandages for the treatment of wounds of various origins. The use of such materials based on chitosan, which are biocompatible and biodegradable, accelerates skin regeneration [1-2].

The effect of the prescription composition of the PVA/chitosan composition (dissolved in aminocaproic acid) was investigated, in the ratios of the composition 1:1, 2:1, 3:1, 4:1, 5:1, 6:1. The use of a solution of chitosan in aminocaproic acid improves electrospinning, and aminocaproic acid has hemostatic properties. For PVA/chitosan compositions (1:1, 2:1) droplet formation was observed, leading to the impossibility of electrospinning. For PVA/chitosan compositions up to a ratio of 4:1, 5:1, 6:1 there was a slow electrospinning with the formation of droplets. Good results were observed for the PVA/chitosan composition in the ratio (3:1) and the distance between the electrodes of 10 cm. Nonwoven materials obtained from the PVA/chitosan compositions have fibers with a diameter in the range of 0.6-1.5 μm.

For samples of polymer compositions, the increase in the content of chitosan solution decreases the viscosity and surface tension. It is shown that the process of thermal stabilization of nonwoven materials based on ultrathin fibers for 1-3 hours allows you to adjust the water absorption from 250 % to 1250 % depending on the composition and duration of stabilization. In the study of NaCl sorption for PVA/chitosan-based films 3:1 and 5:1, respectively, the maximum absorption of physiological solution is observed from 200 % to 750 %, for samples 4:1 and 6:1 – from 150 % to 550 %.

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Synthesis of Barnsley fern-type silver nanostructures

Kytsya A. R.[1,2]***, Bazylyak L. I.***[1]***, Pilyuk Ya. V.***[1]***, Balashova I. Ye.***[1]

[1] *Department of Physical Chemistry of Fossil Fuels of the Institute of*
Physical Organic Chemistry and Coal Chemistry named after
L. M. Lytvynenko of the NAS of Ukraine,
3a Naukova Str., 79060, Lviv, Ukraine.
E-mail: andriy_kytsya@yahoo.com

[2] *Physico-Mechanical Institute named after G. V. Karpenko of the NAS of*
Ukraine, 5 Naukova Str., Lviv, 79060, Ukraine

The conditions of the formation of three-metal nanostructures by Ni–Co–Ag type were studied for the first time by the method of the galvanic replacement the silver with $Ni_{50}Co_{50}$ nanoparticles. The structure of the obtained Ni–Co–Ag nanostructures was confirmed by scanning electron microscopy (SEM), X-ray phase analysis (XRD) and energy-dispersive X-ray spectroscopy (EDS). It was determined that under the studied conditions it is possible to obtain the magnetoseparable trimetallic nanostructures of $Ni_{42}Co_{43}Ag_{15}$ composition; whereby the silver is crystallized in the form of a Barnsley fractal, the “petiole” of which “grows” from the agglomerates of $Ni_{50}Co_{50}$ nanoparticles (Figure).

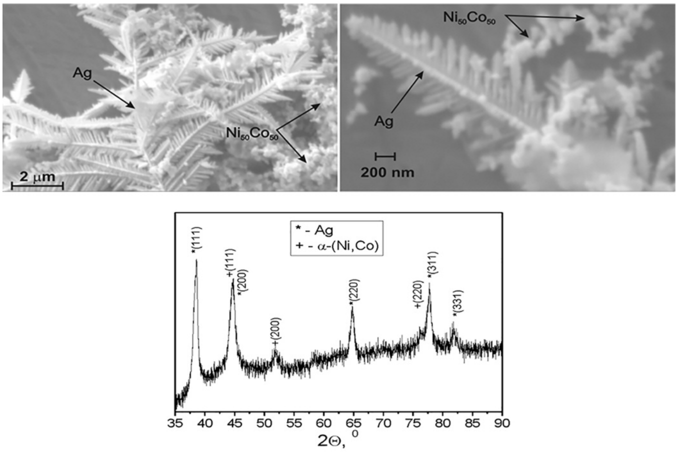

Fig. *SEM-image and XRD-pattern of the ternary nanostructures Ni–Co–A*

Fabrication of Cu-based-CNT composites via electroplating and powder metallurgy techniques

Shtablavyi I.[1], Popilovskyi N.[1], Kulyk Yu.[1], Serkiz R.[2], Tsizh B.[3,4], Mudry S.[1]

[1] *Metal Physics Department, Ivan Franko National University of Lviv,*
Kyrylo i Mephodiy 8, 79005 Lviv, Ukraine
E-mail: nazar.popilovskii@lnu.edu.ua

[2] *Solid State Physics Department, Ivan Franko National University of Lviv,*
79005 Lviv, Ukraine

[3] *Kazimierz Wielki University in Bydgoszcz,*
30 Chodkiewicza, Bydgoszcz, 85-064, Poland

[4] *Stepan Gzhytskyi National University of Veterinary Medicine and*
Biotechnologies Lviv, 50 Pekarska, Lviv, 79010, Ukraine

The creation of structural materials that would have satisfactory mechanical properties, and in particular at the same time high values of plasticity and strength, is always an urgent problem of modern materials science. The solution to this problem is possible by creating composite materials in which the matrix is a plastic metal with a high-strength filler. As a filler, the use of carbon nanotubes is promising.

It is known that when nanotubes are introduced into the metal, there are problems which are related with wetting the nanotubes by metal and dispersing them in the matrix. To solve these problems, several methods have been developed to obtain high-quality metal composites filled with carbon nanotubes. However, all of them do not allow achieving the values of mechanical properties provided by theory, so they need further improvement.

In this regard, the structure, morphology and microhardness of copper-based composites with carbon nanotubes were studied in this work. In order to obtain high-quality composites, the method of coating carbon nanotubes with metals was developed and the microstructure and results of X-ray structural studies of copper-coated nanotubes were presented.

Formation of nanoscale phases during rapid solidification of Al-Cu-Si alloys

Shtablavyi I.[1]***, Popilovskyi N.***[1]***, Kulyk Yu.***[1]***, Serkiz R.***[2]***, Tsizh B.***[3,4]***, Mudry S.***[1]

[1] *Metal Physics Department, Ivan Franko National University of Lviv,*
Kyrylo i Mephodiy 8, 79005 Lviv, Ukraine
E-mail: nazar.popilovskii@lnu.edu.ua

[2] *Solid State Physics Department, Ivan Franko National University of Lviv,*
79005 Lviv, Ukraine

[3] *Kazimierz Wielki University in Bydgoszcz, 30 Chodkiewicza, Bydgoszcz,*
85-064, Poland

[4] *Stepan Gzhytskyi National University of Veterinary Medicine and*
Biotechnologies Lviv, 50 Pekarska, Lviv, 79010, Ukraine

Ternary Al-Cu-Si system is the basis of wide range of lightweight high entropy alloys with unique properties. Their physical and chemical properties depend not only on the chemical composition of alloys but also on the morphology and distribution of phases. It is known that in the process of synthesis of high-entropy alloys, the ultimate goal is to obtain a material, consisting mainly of solid solutions of components. However, the presence of nanocrystalline phases in such alloys creates new opportunities to improve their mechanical properties. In this regard, the study of nanocrystallization processes in the formation of multicomponent alloys is an urgent task.

In this work, the formation of nanocrystalline phases in alloys of Al-Cu-Si system of near equiatomic composition is investigated. Alloys were obtained by crystallization from the liquid phase with different cooling rates. The phase composition of alloys was studied by X-ray diffraction method, and the microstructure as well as phase size were studied by electron microscopy. In order to study the crystallization process itself, the structure of these alloys was also studied in the liquid state.

Spectroscopic study of luminescent biphasic $La_{1-x}Yb_xVO_4$ nanoparticles

Chukova O.[1, 2]***, Nedilko S.A.***[1]***, Nedilko S.G.***[1, 2]***, Voitenko T.***[1]***,***
Rahimi Mosafer H.S.[2]***, Paszkowicz W.***[2]***, Stasiv V.***[2]***,***
Zhydachevskyy Y.[2]***, Suchocki A.***[2]

[1] Taras Shevchenko National University of Kyiv,
Volodymyrska Str., 64/13, Kyiv-01601, Ukraine.
E-mail: chukova@univ.kiev.ua

[2] Institute of Physics, Polish Academy of Sciences,
al. Lotnikow 32/46, Warsaw 02-668, Poland.

The $LaVO_4$ compound is widely used as a matrix for luminescent RE^{3+} ions and one of their various advantages is an opportunity to get crystal phases of different structure of lattice dependently on synthesis conditions and amount of dopants. The samples of biphasic crystal composition can also be formed.

The studied $La_{1-x}Yb_xVO_4$ ($x \leq 2$) nanoparticles were prepared by aqueous nitrate-citrate sol-gel synthesis. Phase compositions and crystal lattice parameters were determined using a Philips X'Pert Pro Alpha1 diffractometer operating with CuKα1 radiation. The XRD analysis has shown that all the synthesized samples are biphasic and they compose of monazite and zircon crystalline nanoparticles. The microstructure of the samples and chemical elements distributions were studied using SEM INCA X-max System from Oxford Instruments. Morphology of the nanoparticles depends on dopant concentration. Increase of the Yb^{3+} ions content leads to decrease of average sizes of nanoparticles from ~100 nm to 40 - 60 nm.

Luminescence properties of the synthesized samples were studied. They consist of spectral lines appeared in the 970 – 1040 nm range which are caused by the *f-f* electron transitions in the Yb^{3+} ions. Structure of the spectra depends on the Yb^{3+} concentration. The carried out analysis has revealed that Yb^{3+} ions form at least two different types of emission centers in the studied materials. Correlations between crystalline structure, morphology of the nanoparticles, reflection spectra and luminescence properties of the samples were analyzed and discussed. The assumption was made that changes of the samples morphology are caused by changes of nanoparticles crystal structure, as well as appearance of two types of emission centers are related with the Yb^{3+} ions located in the nanoparticles of different crystal structure.

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Evolution of low-frequency dispersion in solids with change of temperature

Fliunt O. Ye.

Faculty of Electronics and Computer Technologies, Ivan Franko National University of Lviv, Dragomanov Str., 50, Lviv-79005, Ukraine
E-mail: Orest.Fliunt@lnu.edu.ua

Strong by many orders of magnitude increasing of both dielectric constant and dielectric loss toward low frequencies is termed low-frequency dispersion (LFD) or quasi-DC conductivity. Frequency spectra of dielectric constant and loss in the region dominating by LFD obey power fractional law with small value of exponent n. In the time domain discharging current very weakly depends on time obeying power law t^{-n}. Many experimental works giving dielectric frequency spectra in low and infra-low regions confirm dominating of LFD on dielectric spectra in different class of dielectric and semiconducting materials, often even without direct indication. LFD represents partial case of universal fractional power law $(j\omega)^{-(1-n)}$, where j is imaginary unit and ω is circular frequency, with small side values of exponent from range $0<n<1$. In the case of LFD frequency dependence of dielectric loss is very close to frequency dependence of dielectric loss caused usual DC current, but with the important difference, that it is accompanied with accumulation of anomalously high amount of electrical charge.

In this work a model of temperature behavior of LFD or q-DC conductivity has been proposed. The model is based on distribution of relaxation times of effective dipoles, formed by elementary hopping charge localization over wide temporal range. The model gives possibility to explain revealed transition of LFD from low to high-temperature regime. In high temperature regime LFD shows thermally activated Arrhenius law shift with temperature independent shape in log-log scale. Calculated values of activation energy of LFD obtained from frequency shift of spectra with changing of temperature are close to experimental values. Drastic temperature change of exponent n from values above 0.4 to small values below 0.25 in narrow transition region of LFD has been explained. The low-resistivity GaSe layered crystals show high-temperature regime of LFD with $n= 0.19$ and activation energy $E\text{a}= 0.19$ eV, nevertheless dominating below 150 K temperature, that is in accordance with proposed model. Thereby, gap of experimental values of exponent n can be explained by thermally activated behavior of distributed effective dipoles under the condition of their continuous distribution according to power law.

Nanosized bimetallic oxide $CoTiO_3$ as anode material for lithium and sodium batteries

***Shmatok Yu.V.**, Globa N.I., Lisnycha T.V., Kirillov S.A.*

Joint Department of Electrochemical Energy Systems of the NAS of Ukraine.
Vernadsky blvd, 38a, Kyiv, 03680, Ukraine.
E-mail: yu.shmatok@gmail.com

Metal oxides are considered as possible candidates for use as anode materials for both lithium-ion and sodium-ion batteries. In view of this, a considerable attention is paid to various titanium oxides.

This work is focused on the synthesis, physico-chemical and electrochemical investigation of bimetallic oxide $CoTiO_3$ with the perovskite structure. Initially, binary mixture of titanium and cobalt oxides was precipitated by LiOH from $Co(NO_3)_2$ and $TiCl_4$ solution. Than previously washed and dried at 100 °C oxide mixture was annealed at 400-800 °C for 8 h. Obtained after annealing products were analyzed by the X-ray diffraction, scanning electron microscopy and porosimetry methods.

It was established by the X-ray diffraction analysis that the formation of crystalline oxides begins at a temperature of 500 °C and higher and the main product being $CoTiO_3$ with a perovskite structure. There are also impurities of individual titanium and cobalt oxides, which amount decreases with increasing annealing temperature. As a result of an increase in the annealing temperature, a growth in the average particle size from ~ 50 nm to ~ 150 nm is observed, as well as a significant decrease in the specific surface area from over 200 m^2/g to ~ 5 m^2/g.

The specific characteristics of the obtained $CoTiO_3$ samples in lithium and sodium cells were determined by galvanostatic cycling method. It is shown that the annealing temperature significantly affects the value of the specific capacity and its stability during cycling, both at low and high discharge current densities. The best specific characteristics were obtained after thermal annealing of the samples at the temperature of 700-800°C. In lithium cells $CoTiO_3$ demonstrate stable cyclability with specific capacity of ~ 200 mAh/g at the current density of 100 mA/g and good rate capability at the discharge currents up to 5 A/g. In a case of sodium cells, the specific capacity is stable too, but much lower being ~ 100 mAh/g at the current density of 100 mA/g, and discharge currents reach 1 A/g.

Zinc oxide nanotubes: An ab initio investigation of their structural and electronic properties

Tkach P.V., Kovalenko M.V., Bovgyra O.V.

Faculty of Physics, Ivan Franko National University of Lviv,
8a, Kyrylo and Mefodiy str., 79005 Lviv, Ukraine.
E-mail: mariya.kovalenko@lnu.edu.ua

One-dimensional nanomaterials including nanotubes, nanorods, and nanowires, have been attracting enormous interest due to their unique electronic, optical, and mechanical properties and big potential for nanotechnology applications compared to corresponding bulk materials. In particular, zinc oxide (ZnO) is a wide bandgap II−VI group semiconductor and is well known for its excellent performance in various application areas such as piezoelectrics, pyroelectrics, optoelectronics, and spintronics. At present, scientific research on ZnO nanostructure has made considerable progress. Research groups in the world have successfully synthesized ZnO nanomaterials with different structures, such as low-dimension ZnO nanowire, nanorod, nanotube, nanobelt, and other nanomaterials with unique structures, for example, ZnO nanodisk, and nanoflowers. The ZnO material research shows a potential application in nanometer optoelectronic systems, gas sensors, optoelectronic memory, catalysis, optical-electrical converter, laser, and transparent conductive film.

In this work, based on the density functional theory was performed the first-principles modeling of different chirality ZnO nanotube, particular, with armchair and zigzag structures. Structure optimization and band energy calculations were carried out using the generalized gradient approximation (GGA) in the PBEsol parameterization. We used the GGA+U approximation to more accurately describe the electronic structure of the ZnO nanotube. In our study, all nanotube structures were obtained by rolling up a graphitic ZnO single layer with subsequent structural optimization.

The calculations results show that after structure relaxation ZnO nanotubes have tubular structures in which zinc and oxygen atoms were slightly shifted inward and outward to the axis, forming homocentric cylinders with different diameters similar to carbon nanotubes. The electronic structure calculations show that all ZnO nanotubes are wide bandgap semiconductors with a bandgap bigger than wurtzite ZnO. It is established that the bandgaps of all investigated the ZnO nanotubes increase with their diameters. We hope that such a diameter dependence of the bandgap can perhaps be used to control the bandgap of the ZnO nanotubes by growing the ZnO nanotubes with a predefined diameter.

Aqueous dispersions based on the structured dextrins

Nahornyak M.[1], Fihurka N.[1], Bendoraitiene J.[2], Peciulyte L.[2], Rutkaite R.[2], Samaryk V.[1]

[1] Department of Organic Chemistry, Lviv Polytechnic National University.
S.Bandera Str. 12, Lviv -79013, Ukraine.
E-mail: figurka.nataliia@gmail.com

[2] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu Rd. 19, Kaunas 50254, Lithuania

Aqueous dispersions are widely used for various biomedical applications, in particular for drug delivery systems and immunological diagnostics. Such materials should meet several requirements; the most important are non-toxicity and biodegradability. Taking into consideration these requirements, systems based on natural polysaccharides are promising as a majority of natural polysaccharides are tolerant to the human body.

Polysaccharides able to form aqueous dispersions should be spatially structured. To the present day, structured polysaccharides have been widely used for chromatography of various types. Developed synthetic approaches to polysaccharide structuring use toxic substances, therefore, these approaches are not always suitable for the production of materials for medical purposes. Thus, the development of new methods for structuring polysaccharides leading to a product with specified characteristics is highly relevant.

In this work, a novel method for structuring dextrins with N-derivatives of glutamic acid via the Steglich reaction has been developed. Structurization of dextrin leads to the formation of two products: (1) cross-linked dextrin macromolecules able to form dispersions of microhydrogels in water medium and (2) branched macromolecules forming aqueous dispersions with nano-sized particles.

Obtained data allows establishing the dependence of polymer properties on the synthesis conditions; this, in turn, allows obtaining aqueous dispersions with the given properties. The dependence of the dispersed phase size and morphology on the synthesis conditions has been studied.

Biochemical and cytological studies confirmed the absence of toxic properties of the obtained products and products of their biochemical destruction, which allows considering them promising materials for biomedical applications.

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Li-containing$_{(1\text{-}x)}$BaTiO$_{3-x}$Li$_{0.5}$Bi$_{0.5}$TiO$_3$ solid solutions with colossal dielectric permittivity

Plutenko T.O.[1], V'yunov O.I.[1],
Fedorchuk O.P.[1], Ischenko M.V.[2], Plutenko M.O.[2]

[1] *Solid State Chemistry Department Faculty of Chemistry, V.I. Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine.*
Akad. Palladin ave, 32/34, Kyiv-03142, Ukraine.
E-mail: alex1377c9@gmail.com

[2] *Faculty of Chemistry, Taras Shevchenko National University of Kyiv.*
Lva Tolstoho Street, 12, Kyiv-01033, Ukraine.

To decrease the sintering and calcination temperatures of (1-x)BaTiO$_{3-x}$Li$_{0.5}$Bi$_{0.5}$TiO$_3$ solid solutions, barium titanate powders with particle sizes about 50 nm in diameter were pre-synthesized using a hydrothermal routine. In the first step nanocrystalline BaTiO$_3$ powders were prepared by a hydrothermal reaction of TiCl$_4$ and a BaCl$_2$ solution in an oxygen atmosphere. In the second step of the synthesis process, extra-pure Li$_2$CO$_3$, Bi$_2$O$_3$, and TiO$_2$ were added to BaTiO$_3$ to obtain (1-x)BaTiO$_{3-x}$Li$_{0.5}$Bi$_{0.5}$TiO$_3$ solid solutions. The powders were mixed by ball milling with ethanol for 4 h. The resultant mixtures were fired for 4 h at temperatures of 800 °C. After firing, the powders prepared by both methods were pressed into pellets, which were sintered in the air at a temperature range of 1100–1240 °C.

Obtained powders were characterized using TEM and X-ray powder diffraction spectroscopy. The dielectric parameters were measured as a function of temperature in the range of 20 to 500 °C. In impedance measurements, we used a Solartron Analytical 1260 impedance/gain phase analyzer in the range of 1 Hz to 1 MHz.

The effects of the amount of Li$_{0.5}$Bi$_{0.5}$TiO$_3$ on the structure and dielectric properties were examined. With an increase in Li and Bi concentration, the unit cell volume decreases due to lower values of lithium ionic radius compared with barium. It was shown that an increase in the lithium concentration leads to a blurring of the phase transition in barium titanate and makes it possible to significantly reduce the sintering temperature of barium titanate due to the formation of a liquid phase at the grain boundaries. It was shown that an increase in Li and Bi concentration leads to a decrease in sintering temperature from 1240 °C (at $x = 0.05$) to 1100 °C (at $x = 0.5$).

Structure and properties of antimicrobial nanocomposite materials filled with silver nanoparticles

Lysenkov E.A.[1]***, Polovenko L.S.***[1]***, Stryutsky O.V.***[2]

[1] *Laboratory of Nanocomposite Materials, Petro Mohyla Black Sea National University.*
68 Desantnykiv Str., 10, Mykolaiv-54003, Ukraine.
E-mail: ealysenkov@ukr.net

[2] *Department of Chemistry Mesh Polymers and Oligomers, Institute of Macromolecular Chemistry NAS of Ukraine.*
Kharkivske Sh., 48, Kyiv-02160, Ukraine.

The presence of antibacterial materials in biomedicine and related fields of science and technology has become essential. Among the functions more desirable for materials used in medicine antibacterial action occupies one of the first positions, because bacterial growth could be prevented on medical devices, prosthetic materials, catheters (urinary or venous catheters) and surgical masks. The development of stabilized polymer-silver nanocomposites containing nanoparticles is considered to be one of the most promising solutions. Here we show the novel approach for synthesis of stabilized silver nanoparticles and study of functional properties of antimicrobial polymeric nanocomposite materials based on oligotetrahydrofuranurethaneurea. Using the novel approach for synthesis we recieve silver nanoparticles with average size around 8-10 nm. We found that stabilized silver nanoparticles has a significant effect on thermophysical and dielectric properties of polymer matrix at relatively low concentrations of the nanofiller (~ 1-2%). Nanocomposite with 1 % of silver nanoparticles shows significant activity for Klebsiella (zone of inhibition is 16 mm) and material with 2 % of silver nanoparticles shows significant activity for Staphylococcus aureus (zone of inhibition is 20 mm). Our results demonstrate that synthesized stabilized nanoparticles have low tendency to aggregation in polymer matrix. We have developed new materials with high antimicrobial activity and improved physical properties. The novel approach for synthesis of stabilized silver nanoparticles open a new window of possibilities in the development of new antimicrobial materials, based on various polymer matrix: from thermoplastic to elastic. The developed materials with improved functional characteristics in the future can be used as antimicrobial coatings, antimicrobial films and creams, as well as construction products with the necessary functional characteristics and antimicrobial function.

Investigation of long-term oxidation resistance of titanium alloy with a Ti,Me-Al-C nanocomposite coating

Podhurska V.Ya.[1]***, Prikhna T.O.***[2]***, Ostash O.P.***[1]***, Sverdun V.B.***[2]***,***
Kuprin A.S.[3]***, Serbeniuk T.B.***[2]***, Bortnitskaya M.A.***[3]

[1] *Department of Hydrogen Technologies and Alternative Energy Materials,*
Karpenko Physico-Mechanical Institute of the NAS of Ukraine,
5 Naukova str., Lviv 79060, Ukraine.
E-mail: podhurskavika@gmail.com

[2] *Department of Sintering Technologies of Ceramics, Institute for Superhard*
Materials of the NAS of Ukraine, 2 Avtozavodska str., Kyiv 04074, Ukraine.

[3] *Laboratory of Ion-Plasma Processing of Materials, National Science*
Center Kharkiv Institute of Physics and Technology,
1 Akademicheskaya str., Kharkiv 61108, Ukraine.

Nowadays, solid oxide fuel cell (SOFC) interconnects are traditionally made of sheets of Crofer steels [1]. Interconnects made of titanium sheets with coatings based on MAX phases of the Ti–Al–C system can be more efficient [2]. The goal of this work is investigation of the long-term oxidation resistance of titanium alloy OT4-1 with a Ti,Me-Al-C nanocomposite coatings.

Ti,Me-Al-C nanocomposite coatings were deposited on polished samples of the titanium alloy OT4-1 by combine two methods DC magnetron sputtering of Ti_2AlC MAX phase target and cathodic arc evaporation of Me (Cr or Mo) cathode. It was shown that ~10 µm thick Ti,Cr-Al-C coatings coating has high mechanical properties (H=14 and E=240 GPa), oxidation resistance at 600 °C in air and provide high electrical conductivity ($6.8 \cdot 10^5$ Sm/m) after 1000 h oxidation. According to the obtained results, a OT4-1 alloy with a coatings can be used for the manufacture of the interconnects for intermediate-temperature fuel cells.

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Effects of the substrate bias voltage and gas pressure on electrical conductivity and microhardness of the nanostructured TiON coatings

Podhurska V.Ya.[1]***, Ostash O.P.***[1]***,***
Kyrysha A.A.[1]***, Kuprin A.S.***[2]***, Kovtun Yu.V.***[2]

[1] *Department of Hydrogen Technologies and Alternative Energy Materials,*
Karpenko Physico-Mechanical Institute of the NAS of Ukraine,
5 Naukova str., Lviv 79060, Ukraine.
E-mail: podhurskavika@gmail.com

[2] *National Science Center Kharkiv Institute of Physics and Technology,*
1 Akademicheskaya str., Kharkiv 61108, Ukraine.

Good mechanical properties, high resistance to corrosion and low density make titanium and its alloys the materials of choice for many applications in the aeronautical, marine and chemical industries. However, titanium displays poor tribological properties (highly unstable friction coefficients and low wear rate) which must be improved for some technological applications [1]. Titanium also is a widely used material for medical devices because of its inertness and high biocompatibility as compared to other metals, including stainless steel [2]. Transition metal oxynitride films represent a particular class of materials that possess the superior properties of oxides (chemical stability and biocompatibility) and nitrides (hardness and resistance).

The aim of this work was to study the effect of the steel substrate bias voltage and gas pressure on the microstructure, electrical conductivity, and microhardness of the TiON coatings. These coatings have been deposited on steel substrates in a "Bulat-3" cathodic arc system. Variable parameters of the deposition process were the negative potential on the substrate Ub = -50...-200 V. It is shown that TiON coatings represent nanostructure, high electrical conductivity, and microhardness depending on the magnitude of the bias potential on the substrate and gas pressure.

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Corrosion resistance of nanostructured titanium coatings deposited by cathodic arc evaporation

***Podhurska V.Ya.*[1], Ostash O.P.[1], Ivashkiv V.R.[1],**
Kuprin A.S.*[2], Rostova H.Yu.[2], Kovtun Yu.V.[2], Sayenko S.Yu.[2]

[1] Department of Hydrogen Technologies and Alternative Energy Materials,
Karpenko Physico-Mechanical Institute of the NAS of Ukraine,
5 Naukova str., Lviv 79060, Ukraine.
E-mail: podhurskavika@gmail.com

[2] National Science Center Kharkiv Institute of Physics and Technology,
1 Akademicheskaya str., Kharkiv 61108, Ukraine.

Hard chromium coatings are one of the most used anticorrosion coatings but are produced from chromic acid solutions containing chromium in the hexavalent state and several catalytic anions that are known to be carcinogenic [1]. The research into alternative processes to chromium plating is focused on finding new surface technologies based on more environmentally friendly processes. Cathodic arc evaporation PVD process has outstanding potential to deposit corrosion-resistant coatings with relatively dense structure [2]. Titanium and titanium alloys are widely used for corrosion protection because they offer high chemical resistance against various corrosive media due to a dense self-sealing oxide layer [3].

Titanium coatings have been deposited on steel substrates in a cathodic arc system. Variable parameters of the deposition process were the negative potential on the substrate Ub = -50...-200 V. The corrosion behaviours of coated samples were electrochemically characterized with voltamperometric measurements in 3% NaCl water solution. It is shown that titanium coatings represent nanostructure, high microhardness (4 GPa) and corrosion resistance depending on the magnitude of the bias potential on the substrate.

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Nonlinear optical response of ZnO-PMMA nanocomposites under picosecond laser excitation

Komarenko D.O.[1]***, Ronkovych A.V.***[1]***, Ovdenko V.M.***[1,2]***, Ilchenko S.G.***[1]***, Multian V.V.***[1]***, Pokutnyi S.I.***[1]***, Lisnyak V.V.***[2]***, Gayvoronsky V.Ya.***[1]

[1] *Advanced Materials Nonlinear Optical Diagnostics Lab., Institute of Physics of the NAS of Ukraine.*
pr. Nauki, 46, Kyiv 03028, Ukraine.
E-mail: vlad@iop.kiev.ua

[2] *Chemical Faculty, Taras Shevchenko National University of Kyiv,*
64 Volodymyrska Str., Kyiv 01033, Ukraine.
E-mail: lisnyak@univ.kiev.ua

In recent times, a remarkable interest has arisen in the development of organic-inorganic hybrid materials [1]. They are based on a polymer matrix with inorganic nanoparticles (NPs) used as solar cells, field-effect transistors, and optoelectronic and nonlinear optical (NLO) devices. Polymers can exhibit pronounced NLO properties or be optically inert matrices, but a composite with an inorganic component will give new synergetic or complementary behavior arising from the interaction of the polymer and NPs at the molecular level.

In the present study, we investigated the self-action effects in organic-inorganic PMMA–ZnO composites with 1 wt% of ZnO NPs embedded in PMMA films within the ps range of pulsed laser excitation at 1064 nm. We also examined their photoluminescence (PL) response in the UV-visible range. A set of small ZnO NPs with an efficient PL and quadratic NLO response was successfully prepared by the hydrolytic route in non-aqueous solvents [2]. A correlation was found between the $\mathrm{Im}(\chi^{(3)})$ and the PL band area at about 2.34–2.41 eV related to the contribution of oxygen vacancies in ZnO was revealed.

The highest efficiency of the refractive NLO response $|\mathrm{Re}(\chi^{(3)})| \sim 10^{-10}$ esu was observed for the composite with PL obtained from CH^3CN against 10^{-11} esu for that obtained from alcohol ethanol/isopropanol solutions on the background of the absorptive NLO response $|\mathrm{Im}(\chi^{(3)})| \sim 10^{-12}$ esu for the studied composites for the peak laser intensity excitation up to 1 GW/cm^2.

The results obtained are promising for developing organic-inorganic hybrid nanocomposite materials with effective NLO and PL responses.

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The influence of relative humidity on the ion (proton) conductivity of the intramolecular polycomplexes

***Kunitskaya L.**, Zheltonozhskaya T., Nesin S., Klepko V.*

Institute of Macromolecular Chemistry of the NAS of Ukraine.
48 Kharkivs'ke shosse St, Kyiv-02160, Ukraine.
E-mail: larisa_kunitskaya@ukr.net

The problem of the energy crisis is contributing to the increasingly active search for the alternative ways to obtain energy, including fuel cells. A solid polymer electrolytes (SPEs) with high ionic conductivity at room temperature has been an importance subject due to their interest in the all solid-state electrochemical devices development.

In the present study, block copolymers comprising chemically complementary poly(ethylene oxide)/polyacrylamide have been evaluated as proton conducting materials. With this aim in mind, two series of block copolymers PAAm-*b*-PEO (DBC) and PAAm-*b*-PEO-*b*-PAAm (TBC) with the variable PEO-block length and also their partially hydrolyzed derivatives (DBC_{hydr} and TBC_{hydr} respectively) were prepared by using a solution casting technique, and their ion (proton) conductivity was studied at the ambient temperature and at different relative humidity (RH).

The water absorption data show the rise of the absorbed water as the relative humidity grows in all the samples under study. It has been established that the conductivity of DBC and TBC membranes depends on the content of the adsorbed water and the PEO-block length. The rise in RH from 33% to 98% resulted in the increase in conductivity of DBC and TBC membranes up to 10^{-4} S·cm^{-1}. The study of the kinetics of the water absorption at 98% RH showed that the introduction of – COOH-groups into PAAm chains could accelerate the process of water absorption. The increase in conductivity of DBC and TBC membranes with the PEO-block lengthening has been noticed.

Thus, block copolymers comprising the interacting polymer components could be considered as potential solid polymer matrices for proton exchange membranes and they open the way for their application in fuel cells. They also demonstrate the possibility of using commercially available, nontoxic solid polymer electrolytes in electrochemical devices. Such polymer electrolytes could be produced at low cost and they are environmentally friendly.

Green synthesis of silver nanoparticles using grape pomace extract obtained by betaine-based deep eutectic solvent

***Vorobyova V.I.*[1]*, Vasyliev, G. S.*[1]*, Kotyk M.M.*[1]*, Skiba M.I.*[2]**

[1] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute". Prosp. Peremohy 37, Kyiv 03056, Ukraine.

[2] Ukrainian State University of Chemical Technology,
Gagarin Ave. 8, Dnipro 49005, Ukraine.
E-mail: g.vasyliev@kpi.ua

Green synthesis of silver nanoparticles is an emerging technique drawing more attention recently because of several advantages over the conventional chemical approaches. This study investigated the rapid and green synthesis of silver nanoparticles (AgNPs) using the grape pomace extract obtained by betaine-based deep eutectic solvent. New deep eutectic system (Betaine – Lactic acid) was prepared, its electrochemical properties were studied. The grape pomace extract was obtained by maceration and used as a reducing and capping agent in the synthesis of nanoparticles. The obtained nanoparticles were characterized with UV–Vis spectrometry that showed the SPR band at around 415 nm, which proves AgNP formation. SEM images verified the presence of spherical nanoparticles with no evidence of aggregations. Antimicrobial properties of AgNPs were tested and showed strong antibacterial activity against *E. coli.*

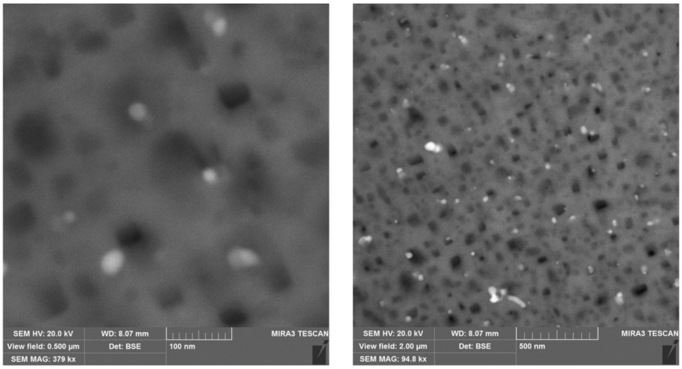

Fig. 1 *SEM microphotographs of AgNPs obtained with grape pomace extract in deep eutectic solvent*

Liquid crystalline substances doped with carbon nanotubes as a sensitive medium of the CO_2 sensor

Vistak M.V.[1], Diskovkyi I.S.[1], Kachurak Y.M.[2],
Kuchmiy G.L.[2], Horina O.M.[2]

[1] Danylo Halytsky Lviv National Medical University.
Pekarska str., 69, Lviv-79010, Ukraine.

[2] Lviv Polytechnic National University.
Stepana Bandery str., 12, Lviv-79000, Ukraine.
E-mail: yurii.m.kachurak@lpnu.ua

The creation of highly sensitive optical CO_2 in air sensors is an urgent problem, as it allows control of CO_2 content both indoors and in ambient air, where it's level usually 600… 1000 ppm.

We propose to use a liquid crystalline substance[1-3] (nemato-cholesterol mixture based on E7 with impurities of cholesterol), supplemented with multi-walled carbon nanotubes, as a sensitive element of the CO_2 sensor. The spectral characteristics of the liquid crystal mixture in the range of 400… 600 nm were studied. The content of carbon nanotubes varied in the range of 0.1… 0.5 wt.%. It is established that with increasing concentration in the range of 10… 100 mg/m^3 the minimum transmission shifts to the long-wavelength region of the spectrum. The maximum spectral sensitivity in this range is 6 $nm/mg/m^3$. The investigated material can be used as a sensitive element of the optical CO_2 sensor.

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Investigation of Nanodiamonds for NMR relaxometry sensors application

Milovanov Y.S.[1], Gavrilchenko I.V.[1], Ivanov I.I.[1],
Kozinetz O.V., Lysenko V.V.[2], Skryshevsky V.A.[1]

[1] Institute of High Technologies, Taras Shevchenko National University of
Kyiv, 01601 Volodymyrska str. 64, Kyiv, Ukraine.
E-mail: ir.gavril11@gmail.com

[2] Université Claude Bernard Lyon 1disabled, Villeurbanne, France.

Nanodiamonds (ND) are a separate class of nanoparticles in the carbon family. These nanoparticles are usually 1 to 100 nm in size and are produced by synthesis based on the detonation of a carbonaceous explosive. Different processing conditions, processing technologies and production methods create different surface properties, which leads to different types of ND, which differ in surface chemical composition, structure, shape and size.

The ND structure can be represented in a core-shell model in which the core (diamond carbon) is inert, while the surface shell is partially based on graphite, which allows to add various functional groups, such as carboxyl or hydroxyl, which will determine the properties of ND [1]. Therefore, they can be used as a delivery system for a huge range of drugs, antigens and antibodies. On the other hand, their spectroscopic properties make them ideal for in vivo imaging [1], especially for the diagnosis of specific target cells, increasing the sensitivity of the current therapeutic or diagnostic imaging. We used ND to alter the relaxation of nuclear spins, which is based on the NMR technique used to detect molecules. Nuclear magnetic resonance (NMR) is a powerful magnetic phenomenon that can be used toidentify, image, and detect molecules [2].The relaxation time in different alcohol solutions was measured. The results of the experiment show that the relaxation time T1 slightly (slightly) decreases with increasing concentration of water in alcohol. With the addition of nanodiamonds, the situation changes significantly, there is a sharp drop in relaxation time for all types of alcoholic beverages, depending on the concentration of water-spray solution.

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Influence of cavitation and non-cavitation ultrasonic treatment on the structure of nanoporous carbon materials

Ptashnyk V.[1]***, Bordun I.***[2,3]***, Maksymych V.***[3]***,***
Malovanyy M.[3]***, Calus D.***[2]***, Chabecki P.***[2]***, Szymczykiewicz E.***[2]

[1] Lviv National University of Nature Management,
1, Vol. Velykogo str., Dubliany, Lviv region, 80381, Ukraine.
E-mail: ptashnykproject@gmail.com

[2] Czestochowa University of Technology,
69, Dabrowskiego str., Czestochowa, 42-201, Poland.

[3] Lviv Polytechnik National University,
12, Bandera str., Lviv, 79013, Ukraine.

Activated carbon (AC) are the most common adsorbents and materials for the manufacture of electrodes of charge storage systems. This is due to the well-developed porous structure, good electrical conductivity, environmental friendliness and cheapness. However, traditional methods of obtaining AC do not give the desired quality material. Therefore, such carbon needs to be further modified, for example, using ultrasonic (US) technology.

For experimental studies the AC obtained by pyrolysis of birch wood was used. The process temperature was 800 ºC, activation time 90 min. AC was placed in the reactor of the ultrasonic unit BAKU-9050 to study the effect of US in cavitation mode. Non-cavitation treatment of the AC was performed in a spherical US reactor. The processing time was selected so that the energy of both types of exposure was the same. The parameters of the porous structure of AC were determined by isothermal adsorption/desorption of nitrogen an automated analyzer Quantachrome NOVAtouch LX2. X-ray diffraction curves of carbon materials and small-angle X-ray scattering (SAXS) spectra were obtained using a DRON-3 diffractometer.

The diffraction patterns of the samples show wide diffuse maxima localized in the vicinity of the diffraction angles $2\theta° \approx 23.90°$ and $2\theta° \approx 43.50°$, which are characteristic of the structure of amorphous carbon. Analysis of SAXS spectra and nitrogen adsorption/desorption isotherms showed that cavitation US treatment a decrease the specific surface area from 595 m^2/g to 530 m^2/g. More significant changes in the porous structure are observed after non-cavitation treatment. As a result, we have an increase in the specific surface area to 719 m^2/g. Thus, US in both cavitation and non-cavitation modes helps to change the porous structure of the nanostructured AC and can be used for controlled modification of the AC.

Proton conductive membranes for DMFC

***Zhyhailo M.M.*, Demchyna O.I.,**
Yevchuk I.Yu., Davydiuk N.M.

Department of Physico-Chemistry of Fossil Fuels, L.M. Lytvynenko Institute of Physico-Organic Chemistry and Coal Chemistry of the NAS of Ukraine.
Naukova Str., 3a, Lviv-79060, Ukraine.
E-mail: demchynaoksana@ukr.net

Direct methanol fuel cells (DMFCs) have recently gained much attention as perspective energy sources [1]. However, they have some shortcomings such as methanol crossover through membrane. Perfluorosulfonate ionomer membranes Nafion are currently used as PEMs in DMFCs. They have a serious methanol crossover problem.

We propose hybrid organic/inorganic cross-linked materials based on monomers acrylonitrile (AN), acrylic acid (AA), ethyleneglycole dimethacrylate (EGDMA), sodium styrene sulfonate (SSS) and sol-gel system of tetraethoxysilane (TEOS) and 3-methacyloxypropyltrimethoxysilane (MAPTMS) synthesized by UV-polymerization and sol-gel process *in situ*. Monomer ratio in feed composition was as follows: AN:AA:EGDMA:SSS = 44:20:20:14 wt. %. The amount of the added SGS was 3-5 wt. %.

The measured by impedance spectrometry proton conductivities of the prepared membranes at ambient temperature are high – 2.58 - 2.85 mSm/cm. The values of methanol uptake of the cross-linked composite membranes are within 9.5 - 8.3 wt. %, what is much lower than that of Nafion membrane.

Hence, the introduction of sol-gel precursor into monomer mixture leads to formation organic/inorganic network and greatly reduces methanol permeability of the membrane.

The proposed poly(AN-co-AA-co-EGDMA-co-SSS-co-MAPTMS)/SiO_2 may be considered as a potential candidate for DMFC application.

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Metal deposited nanoparticles as “bridge materials” for lead-free solder nanocomposites

Yakymovych A.[1]***, Plevachuk Yu.***[2]***, Švec Sr P.***[3]***,***
Švec P.[3,4]***, Sklyarchuk V.***[2]

[1]*Institute of Chemical Technologies and Analytics, TU Wien, Vienna, Austria*

[2] *Department of Metal Physics, Ivan Franko National University of Lviv, Lviv, Ukraine*

[3] *Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia*

[4] *Centre of Excellence for Advanced Materials Application, Slovak Academy of Sciences, Bratislava, Slovakia*
E-mail: yuriy.plevachuk@lnu.edu.ua

It is known that additions of metal or ceramic nanoparticles, as well as carbon nanotubes (CNTs) to the basic Sn-Ag-Cu matrix can improve significantly creep resistance and other important mechanical properties of lead-free solders as well as significantly decrease the total intermetallic thickness of solder-substrate joints.

In case of CNTs, it should be taken into account that practically all types of CNTs are completely not wettable by liquid metal alloys. This is the main reason that that inhibits the interaction betwen CNTs and the solder melt during the reflow process. In the course of soldering, most of carbides, oxides, and carbon-based ceramics can be pushed out of the molten solder during the reflowing process connected with the nonwettability, which is due to differences between some thermophysical properties such as, first of all, density and surface tension. To solve this problem, the surfaces of these carbon materials can be modified by the secondary metal phases to improve adoption with the solder matrixes before implementation.

The carbon nanotubes were added to the basic ternary metal Sn-Ag-Cu matrix. The conventional DC Diode Sputter Coater was used for the purpose of coating of CNTs by Ni and Co. Sputtered nanosized Ni and Co layers covered the surface of used nanoparticles, enhancing their uniform distribution in the matrix of the solder and forming a “bridge” substance, which reacts with the matrix of the SAC alloy and forms the layer of the intermetallic compounds in the course of the soldering procedure. The influence of different pure CNTs and CNTs coated by metals on structure and structure-sensitive properties of the Sn-Ag-Cu nanocomposite alloys was evaluated.

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Hybrid solder joints: the effect of nano-sized Ni and ceramic admixtures on morphology and shear strength of Sn-5.0Ag solder joints

Wodak I.[1], Yakymovych A.[1], Strutz P.[1], Wimmer C.[1], Yerbol S.1, Khatibi G.[1,2]

[1] *Institute of Chemical Technologies and Analytics, TU Wien, Vienna 1060, Austria*

[2] *Christian Doppler Laboratory for Lifetime and Reliability of Interfaces in Complex Multi-Material Electronics, TU Wien,*
Vienna 1060, Austria
E-mail: andriy.yakymovych@tuwien.ac.at

The concept of hybrid solder joints is a promising approach to improve the mechanical reliability of lead-free solder joints. For instance, the mechanical reliability of such solder/Cu joints has been improved by minor additions of nano-sized particles, while the morphology of the solder joints has been also enhanced [1].

The present research is the follow-up of our previous study of the hybrid Sn-3.0Ag-0.5Cu (SAC305) solder joints [2]. Furthermore, we have synthesized Ni nanoparticles (NPs) by the chemical reduction method. The Sn-5.0Ag foil has been used in this study to produce the solder joints, while the Ni NPs have been mixed into the commercial flux. As an alternative, the TiO_2 and ZrO_2 NPs have been used to produce the hybrid Sn-0.5Ag/Cu solder joints.

According to the SEM analysis, the morphology at the interface solder/Cu has been enhanced by the addition of nano-sized inclusions. The shear strength of the hybrid solder joints has been also improved compared to the undoped joint. The experimental results have been compared with the literature.

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Pseudospin modelling and mean field analysis of ferrielectricity in $CuInP_2S_6$ van der Waals crystals

***Vysochanskii Yu.*, Liubachko V., Yevych R., Hryts V., Medulych M., Kohutych A., Glukhov K.**

Institute for Solid State Physics and Chemistry, Uzhhorod University,
Pidgirna Str. 46, 88000 Uzhhorod, Ukraine
E-mail: vysochanskii@gmail.com

The $CuInP_2S_6$ ferroics are already involved into van der Waals heterostructures. Their functionality is determined by antiparallel polar ordering of Cu^+ and In^{3+} sublattices. For 2D $CuInP_2S_6$ crystals, the phase diagram and the spectrum of the spontaneous polarization fluctuations can be described in the quantum anharmonic oscillators (QAO) model that has already been applicated for ferroelectrics [1]. At this, the pseudospins s = +1/2, -1/2 are related to Cu^+ cations, that flip in two-well potential, and pseudospins S = +1, 0, -1 describe local dynamics of In^{3+} cations in three-well potential. Thermodynamics of such a system in the mixed Spin – 1/2 and Spin – 1 Ising model [2] demonstrates the evolution of temperature – pressure (composition) phase diagram topology at variation of the local crystal field anisotropy around In^{3+} cations: the tricritical point on the paraelectric phase stability boundary transforms into a triple point, that is joined by the first order phase transitions line with bicritical end point inside the ferrielectric phase. Such evolution can be realized by mechanical compression of $CuInP_2S_6$ crystals or at cooper by silver substitution in $(AgxCu_{1-x})InP_2S_6$ mixed crystals, and it is originated from the change of the In^{3+} cations local three-well potential. In the continuous mean-field approximation, with Landau – Devonshire thermodynamic functional containing invariants till eight order, has been predicted [3] a presence of a special point on temperature – pressure diagram of $CuInP_2S_6$ ferrielectrics, which can be related to the bicritical end point on temperature – electric field – pressure diagram.

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Pt-based catalysts: synthesis, structure, electrochemical activity and durability towards oxygen reduction reactions

***Lobko Y.V.*, Yakovlev Y.V., Darabut A.M., Veltruská K.,**
Gamón Rodríguez M., Kúš P., Nováková J., Matolínová I., Matolín V.

Department of Surface and Plasma Science, Charles University.
V Holešovičkách 2,180 00, Prague 8, Czech Republic.
E-mail: yevheniia.lobko@mff.cuni.cz

Nowadays, finding the more active catalysts for oxygen reduction reaction is one of the most important challenges of the hydrogen fuel cells industry. To date, platinum-based catalysts are the most active electrocatalyst in fuel cells. Though being uncompetitive in many regards there are still several challenges in the catalyst's development. The first one is the increase of the catalyst's electrochemical activity by maximizing the active surface area of the catalysts. Another one is an enhancement of the durability of the catalyst by finding and creating the electrochemically stable supports [1].

To increase the durability of the support such approaches as doping of the carbon-based materials with different atoms and carbonization of the N-doped polymers are employed [2].

Here, the carbon-based supports were decorated with platinum nanoparticles by hydrothermal method. The structure, electrochemical activity and durability of the catalysts nanoparticles were analyzed. The size of the platinum nanoparticles depends on the support structure and is in the range from 3 to 10 nm. For some supports the durability test demonstrates the partial degradation of the Pt catalyst during the electrochemical reaction. The platinum/polypyrrole nanotubes supported nanoparticles demonstrate the highest activity and support durability during a long continuous electrochemical reaction at the conditions of accelerated stress test. It is worth noting that the same parameters for undoped carbon materials are several times lower.

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Percolation behavior in electrical conductivity in epoxy resin/thermally expanded graphite nanocomposites

***Darabut A.M.*, Lobko Y., Yakovlev Y., Matolínová I., Matolín V.**

Charles University, Faculty of Mathematics and Physics,
Department of Surface and Plasma Science,
V Holešovičkách 747/2, 180 00 Prague 8, Prague, Czech Republic
E-mail: alinadarabut@gmail.com

Nowadays, alternative power energy sources play a crucial role in the energetic technology [1]. The polymer electrolyte membrane fuel cells are one of the key players on this field. For this reason, the creation of the polymer-based electrically conductive composites for fuel cell bipolar plates is important [2]. The balance between the high electrical conductivity, mechanical characteristics, and other properties of bipolar plates is very crucial for effective work of the fuel cells.

In this work, the polymer composites based on epoxy resin and different thermally expanded graphite (TEG) content were prepared by compression molding. The electrical properties of materials have been carried out by impedance spectroscopy. The results were compared to the electrical properties of polymer composites filled with commercial graphite of different particle size and carbon content.

The percolation behavior of the carbon fillers in the polymer matrix was analyzed. The percolation model used for the fitting of the different series is the statistical percolation model proposed by Kirkpatrick [3] and Zallen [4]. It was obtained that the percolation threshold of the epoxy resin/TEG composites is at 4 vol.%. The critical indexes t is equal 1.6 ± 0.12.

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Heat properties of PCTFE - TEG and PHTFE - TEG/SiO_2 nanocomposites

Rokytskyi M.O., Shut M.I., Sichkar T.G.,
Rokytska H.V., Shut A.M., Ursul K.V.

Faculty of Mathematics, Informatics and Physics, National Pedagogical Dragomanov University, Ministry of Education and Science of Ukraine.
Pyrohova Str., 9, Kyiv-01601, Ukraine.
E-mail: maksalrokitskiy@gmail.com

Based on research and comparative analysis of heat physical (specific heat capacity c_p, thermal coefficient of linear expansion α) properties of systems polychlorotrifluoroethylene (PCTFE) - nanodispersed thermally expanded graphite (TEG) and PCTFE - nanomodified silicon dioxide (SiO_2) TEG (30% SiO_2 for 70% TEG) the influence of the structural-morphological state of the components and their concentration, the level of interfacial interaction on the physical properties of nanocomposites has been studied.

It is established that the double effect of the modified nanofiller on the crystalline component of the matrix structure is that a more developed crystal structure is formed in the polymer-modified nanofiller interaction zones and, conversely, some amorphization in the peripheral zones. Depending on the nanofiller concentration, the structure of the matrix and the system as a whole shows a transformation in the size of the inhomogeneity of the system structure is associated with the transition from inhomogeneity as the size of crystallites, the growth of which is activated by nanofiller at low concentrations, through the percolation threshold, to inhomogeneities associated with coagulation of nanoparticles at concentrations exceeding the percolation threshold. Thus, the case of nanofillers, it is not advisable to use concentrations that significantly exceed the percolation threshold, as this leads to coagulation of the filler particles and the corresponding loosening of the matrix.

It is also shown that modification of the nanofiller (TRG/30%SiO_2) increases intermolecular interaction in the filler-matrix system. Depending on the concentration of the filler, the structure of the matrix and the system as a whole demonstrates dynamic transformations in the size of the heterogeneity of the structure. Also, research results show that modified nanofiller is more active against the polymer matrix than unmodified, which is a consequence of the fact of the double action of the modified nanofiller on the matrix structure is manifested, which consists in the formation of a strong crystalline structure in the zones of influence of the nanofiller and amorphization of the matrix in the peripheral zones.

Origin of band contrast on TEM and HRTEM images of nanoparticles obtained by pulsed electrical discharge

Monastyrsky G.E.

National Technical University of Ukraine “Igor Sikorsky Kyiv
Polytechnic Institute”, 37, Prosp. Peremohy, Kyiv, 03056, Ukraine.
E-mail: monastyrskygennady@gmail.com

The peculiarities of TEM and HRTEN contrast of nanosized particles of shape memory B2 alloys Ti-Ni [1], Ni-Al [2], Cu-Al-Ni [2] are considered and discussed. Powders were obtained by electrical pulse discharge method (or spark erosion method) in liquid argon. During this process particles with sizes less than 100 nm form a nano-fraction by condensation from the vapor phase gathering usually in agglomerates. Some of this particles demonstrate the specific band contrast as shown on Fig.1.

It was established that morphology of this banded contrast depends on the composition of alloy under consideration and to some extent on the particle size. In particular only in Ni-Al particles with the composition close to the composition of master alloy bands could be considered as twins associated with the martensitic transformation in nanosized particles. Bands in Ti-Ni, Cu-Al-Ni are rather structural twins.

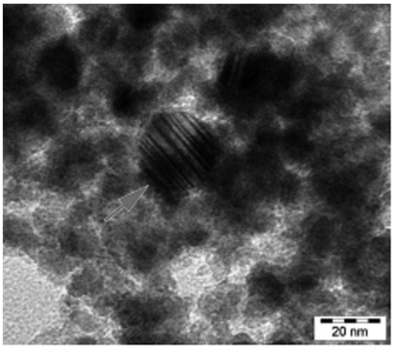

Fig.1 *Agglomerates of Ni-Al nanoparticles. Bright field TEM image with banded particle indicated by arrow*

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Color change of PVD zirconium-based oxycarbonitride coatings obtained at various deposition parameters

Taran A.V.[1], **Garkusha I.E.**[1], **Misiruk O.I.**[1],
Tymoshenko O.I.[1], **Romaniuk S.P.**[2]

[1] *National Science Center "Kharkiv Institute of Physics and Technology" (NSC KIPT) Institute of Plasma Physics*
Academicheskaya, 1, Kharkiv, Ukraine
E-mail: avtaran@ukr.net

[2] *The State Biotechnology University, Kharkiv, Ukraine*

The results of experiments on the application of decorative coatings based on Zr were investigated. Decorative coatings were synthesized by the method of vacuum-arc deposition on samples of stainless steel with dimensions of 20 × 20 × 2 mm [1-3]. Before coating, the samples were cleaned in an ultrasonic bath with isopropanol for 10 minutes.

The cathode was made of chemically pure zirconium (99.99%). The first step was to clean the samples by bombarding the surface with zirconium ions. This was achieved by applying a negative pulse bias with an amplitude of 1200 V at a frequency of 50 kHz from a high-voltage power supply. Then, to improve adhesion, before applying carbonitride and oxycarbonitride coatings, a thin buffer layer of zirconium with a thickness of 20 nm was applied. N_2, O_2 and CxHy (propane-butane) gas mixture in different proportions was used for decorative coatings. The coating time was 2 minutes. The structure and chemical composition of the coatings was investigated by SEM with EDS.

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Ti-Ni based nanocomposites produced by spark erosion method

***Gilchuk A.V.*, Monastyrsky G.E.**

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute". 37, Prosp. Peremohy, Kyiv, 03056, Ukraine.
E-mail: a.v.gilchuk@gmail.com

Interest to the nanocomposites based on well-known Ti-Ni shape memory alloy increases. For example, core-shell like structures Ni@Ti, Ni@TiO_2 and NiO@TiO_2 can occur during Ti-Ni nanopowder production [1]. Such nanocomposites can be used potentially as additional layers for solar cells efficiency increasement and as photocatalysts for H_2 generation.

A few types of nanoparticles can be formed during spark erosion of Ti-Ni-based alloys in cryogenic liquids [2,3]. The morphology and fine structure of the nanocomposites were investigated by transmission electron microscopy (TEM), high-resolution (HRTEM) and energy-filtered (EFTEM) transmission electron microscopy. The elemental composition was measured by energy-dispersive X-ray spectroscopy (EDX). The finest fraction (5-20 nm) consists on the mixture of TiO and NiO. At the same time, "core-shell" structures were observed in particles from tens to hundreds of nanometers in size. The core-shell nanocomposites have FCC structure. The core composition is close to the eutectic between the Ni and Ni_3Ti. The shell composition is almost TiO. The formation mechanism of the spark eroded Ti-Ni based nanocomposites, ways for output increasement and possible fields of application are discussed.

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Analysis of evolution of free volumes in the $BaGa_2O_4$ ceramics doped with Eu^{3+} ions

Klym H.[1]***, Ingram A.***[2]***, Kostiv Yu.***[1]***,***
Luchechko A.[1,3]***, Karbovnyk I.***[1,3]

[1] *Lviv Polytechnic National University,*
Bandery str., 12, Lviv-79013, Ukraine
E-mail: halyna.i.klym@lpnu.ua, klymha@yahoo.com

[2] *Opole University of Technology,*
Ozimska str., 75, Opole- 45370, Poland

[3] *Ivan Franko National University of Lviv,*
Tarnavskogo str., 107, Lviv-79017, Ukraine

The $BaGa_2O_4$ ceramics are considered as promising material for use as insulator in optoelectronic devices, as a secondary coating for plasma panels, etc. The doping of impurities in the form of rare-earth ions leads to the expansion of the functional properties of such ceramics. The goal of this work is to study the evolution of inner free volumes (extended defects and nanopores) in $BaGa_2O_4$ ceramics doped with different amounts of Eu^{3+} ions using positron annihilation lifetime spectroscopy (PAL) method.

The evolution of free-volume defects in the $BaGa_2O_4$ ceramics obtained by solid-phase synthesis from the initial $BaCO_3$ and Ga_2O_3 components with the addition of different amount of Eu_2O_3 content (1, 3 and 4 mol%) were investigated.

The ORTEC system with ^{22}Na isotope as positron source were used for PAL measurements. Investigation were performed at 22 °C and relative humidity of 35 % for two identical ceramic samples placed in a sandwich configuration. The measured PAL spectra were calculated using LT software at four-component fitting procedure as for spinel ceramics with branched porous structure.

For the $BaGa_2O_4$ ceramics two PAL channels are possible: capture of positrons by bulk defects as well as channel of decay of ortho-positronium atoms. The short-term component reflects the microstructural features of the main phase, the middle one is connected with defect-related voids near grain boundaries and the lifetimes of the third and fourth long-term components are estimated the transformation of nanopores. Additional phases in ceramics are mainly localized near the grain boundaries and create defective centers for positron capture studied by PAL spectroscopy. Analyzing the second component of PAL spectra for the undoped and Eu^{3+}-doped $BaGa_2O_4$ ceramics, it was shown that an increase of Eu^{3+} content from 1 to 3 mol% leads to agglomeration of free-volume defects near grain boundaries of ceramics. At the same time, nanopores in ceramics expand and their number increases. Further increase in the content of Eu^{3+} ions are accompanied with fragmentation of both free-volume defects and nanopores.

Ageing phenomena in temperature-sensitive thick-film nanostructures

Klym H.[1], Hadzaman I.[2], Kostiv Yu.[1]

[1] *Lviv Polytechnic National University,*
Bandery str., 12, Lviv-79013, Ukraine
E-mail: halyna.i.klym@lpnu.ua, klymha@yahoo.com

[2] *Ivan Franko Drohobych State Pedagogical University, I. Franko str., 24,*
Drohobych-82100, Ukraine

In this investigation of ageing processes in the single as well as two- and three-layered thick-film elements based on $NiMn_2O_4$-$CuMn_2O_4$-$MnCo_2O_4$ ceramics was performed.The ageing test was carried out at long-term isothermal treatment at 170 °C to study the thermal stability of the obtained thick films. General duration of ageing test was 250 h, measurements electrical resistance R was performed at 25 °C after 6, 12, 18, 24, 30, 48, 64, 104, 144, 208 and 250 hours.

It was established that all investigated temperature-sensitive have a characteristic linear dependence of electrical resistance on the temperature region from 298 K to 368 K in semilogarithmic scale. In the single-layered thick films change of electrical resistance at 250 h is ~ -7.5 % and -8.7 %. This behavior of relaxation kinetics occurs due to two independent processes: at first the rapid diffusion process of molecules in the surface layer is dominated and then organic components burn what is represented in diminishing of relative electric resistance over time of degradation test.

Kinetic dependences for studied single-layered thick-film elements show a typical suppressed-exponential dependence on time in accordance with the known relaxation function [1]. Such behavior is caused by burnout of organic compounds. This process is typical for structural-heterogeneous media such as thick-film ceramic structure. Typical increasing form of thermally-induced aging curve with relative saturation during prolongation of test is observed in two-layered thick-film structures in the first 50-150 hours. Maximum drift of electrical resistance is ~ 6 %. Ageing kinetics are described by extended exponential relaxation function. It should be noted that thermally-induced mechanism in these samples was complex including not only the cation redistribution, but also mass transfer processes.

Unfortunately, the two- and three-layered thick film structures are characterized by relatively high stability, the drift of electrical resistivity is 1.5 %. Such highly stable components are obtained at modification of paste compositions (for achieve the required viscosity) and preparation of thick-film layers based on different compositions of ceramics.

Structural properties and free volumes in the Y-doped $BaTiO_3$ ceramics

Klym H.[1], Karbovnyk I.[1,2], Kostiv Yu.[1]

[1] *Lviv Polytechnic National University,*
Bandery str., 12, Lviv-79013, Ukraine
E-mail: halyna.i.klym@lpnu.ua, klymha@yahoo.com

[2] *Ivan Franko National University of Lviv,*
Tarnavskogo str., 107, Lviv- 79017, Ukraine

In this work inner-structure properties in undoped and Y-doped $BaTiO_3$ ceramics were studied using combined methods. $BaTiO_3$ ceramics doped with 0.2, 0.4, 0.6 and 0.8 mol% of Y were sintered at 1250 °C. The positron annihilation lifetime (PAL) measurements were performed with an ORTEC spectrometer using ^{22}Na source placed between two sandwiched ceramic samples. The obtained data were treated with LT computer program, the best results were obtained to two-component fitting procedures.

In respect to SEM investigations, typical ceramic samples show grain-porous microstructure and assemblies of fractional grains. By accepting two-state positron trapping model, for polycrystalline ceramic materials the short lifetime of τ_1~0.16 ns is generally attributed to the free annihilation of positrons [1]. This value also correlated with theoretically calculated free positron lifetime in $BaTiO_3$. The obtained value is closed to $BaTiO_3$ single crystal. The presently observed values of τ_2~0.37 ns which is believed to come from the annihilation of positrons at vacancy complexes formed between the oxygen vacancies and the metal ion vacancies. It is shown that τ_2 decreases with rise of Y amount in $BaTiO_3$ ceramics from 0.2 to 0.6 mol% and increases in samples with 0.8 mol% of Y the intensity I_2 decreases from 20 to 15 %.

This indicates that doping of Y results in decreasing of the size of free-volume defects in ceramics and decreasing of their amount. So, process of so-called shrinking of defects is take place at posing of $BaTiO_3$ ceramics by Y in amount of 0.4 and 0.6 mol%, while future increasing the Y content to 0.8 mol% leads to weakly expressed agglomeration of free-volume defects.

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Multicomponent positron-positronium trapping models to study of internal nanovoids in ceramic solids

Klym H.[1]***, Ingram A.***[2]***, Hadzaman I.***[3]

[1] *Lviv Polytechnic National University,*
Bandery str., 12, Lviv-79013, Ukraine
E-mail: halyna..klym@lpnu.ua; klymha@yahoo.com

[2] *Opole University of Technology,*
Ozimska str., 75, Opole- 45370, Poland

[3] *Ivan Franko Drohobych State Pedagogical University,*
I. Franko str., 24, Drohobych-82100, Ukraine

Positron annihilation lifetime spectroscopy (PALS) is one of the most sensitive method to studying of internal nanovoids in solids. However, in relation to glassy and ceramic powder and fine-dispersed materials with functional properties, this method was rarely used due to complications in the interpretation of the obtained results and the absence of a model that would describe the annihilation processes in these materials. The aim of this work is study of free nanovolumes in humidity-sensitive ceramics using multicomponent positron-positronium trapping models.

It is shown that to humidity-sensitive ceramics the first component with parameters (τ_1, I_1) reflects the microstructural properties of material and the second one with parameters (τ_2, I_2) describes the volume defects near intergranular boundaries formed by additional phases. The second channel contained only one component with parameters (τ_3, I_3) and reflected the process of “pick-off” annihilation of ortho-positronium o-Ps in nanopores. After performance of PALS investigation in dry and wet modified MgO-Al_2O_3 ceramics using high-statistical measurements, it was possible to fix the schedule for the four components. Thus, the second channel contained two components with parameters (τ_3, I_3) and (τ_4, I_4) that reflected decay of o-Ps atoms in nanopores. The second o-Ps-related channel contains two components, the first of which with the parameters (τ_3, I_3) reflects the annihilation of o-Ps through the “pick-off process in nanopores with ~ 0.2-0.3 nm in size and in water by “bubble” mechanism, which leads to an increase in the intensity I_3. The second component of this channel with parameters (τ_4, I_4) describes the annihilation of o-Ps also through the “pick-off” process, but in an empty pore volume with radius of 1.8-2 nm. Water molecules are formed in layer on the walls of the pore.

Thus, multicomponent positron-positronium model is more acceptable to describe transformation of free volumes in materials with developed porous structure and study adsorption-desorption processes in such ceramics as MgO-Al_2O_3 spinel’s.

Peculiarities of preparing and characterization of thick-film nanostructures based on ceramics for sensors applications

Klym H.[1], ***Hadzaman I.***[2], ***Vasylchyshyn I.***[1]

[1] *Lviv Polytechnic National University,*
Bandery str., 12, Lviv-79013, Ukraine
E-mail: halyna..klym@lpnu.ua; klymha@yahoo.com

[2] *Ivan Franko Drohobych State Pedagogical University,*
I. Franko str., 24, Drohobych-82100, Ukraine

Thick-film performance of ceramics based on the mixed $NiMn_2O_4$-$CuMn_2O_4$-$MnCo_2O_4$ system has a number of advantages over other types of functional electroceramics, especially in combination with layers of humidity-sensitive nanostructured MgO-Al_2O_3 ceramics. The aim of this work is fabrication and characterization of structural properties of temperature- and humidity-sensitive thick-film nanostructures.

Thick-film temperature-sensitive elements and multilayered structures based on $Cu_{0,1}Ni_{0,8}Co_{0,2}Mn_{1,9}O_4$ with p-type electrical conductivity, $Cu_{0,1}Ni_{0,1}Co_{1,6}Mn_{1,2}O_4$ with p^+- type of electrical conductivity and dielectric MgO-Al_2O_3 (*i*-type) were investigated. The humidity-sensitive thick-film layer was applied to pre-formed temperature-sensitive layer. It should be noted that formation of p-p^+, p-p^+p, thick-film structures and integrated temperature-humidity-sensitive p-i-p+ structures was carried out within one technological cycle.

It is shown structure of humidity-sensitive thick films is especially expressly selected on a background of Al_2O_3 substrate with conductive Ag layer. Evidently, that material contains the far of shallow pores, which serve as ducting for the receipt of water to nanopores, where processes of capillary condensation takes place, and also macropores which provide the effective receipt of water in the inner structure of material from an environment.

In contrast to microstructure of humidity-sensitive MgO-Al_2O_3 thick films, $Cu_{0,1}Ni_{0,8}Co_{0,2}Mn_{1,9}O_4$ thick films contain a greater amount of macropores formed in clusters. A similar structure is also characteristic for bulk material of the same composition. Thus, the structural features of ceramics can be transformed into thick films of similar compositions.The use of ceramic with a spinel structure as the main output component for preparation of thick films provided the density of the multi-layer structure and the component for the production of thick films, provided the density of the multi-level structure and contact of their layers.

PEDOT:PSS polymer matrices reinforced with carbon nanotubes: electrical and structural properties

Zhydenko I.[1,2]***, Chalyy D.***[2]***, Karbovnyk I.***[1,3]***, Klym H.***[1]

[1] *Lviv Polytechnic National University,*
12, Bandera Str., Lviv-79013, Ukraine
E-mail: klymha@yahoo.com, halyna.i.klym@lpnu.ua

[2] *Lviv State University of Life Safety,*
35, Kleparivska Str., Lviv-79000, Ukraine

[3] *Department of Electronics and Computer Technologies,*
Ivan Franko National University of Lviv,
107, Tarnavskogo Str., Lviv-79000, Ukraine

In this of work we experimentally analyze structural features and electrical behavior of PEDOT:PSS polymer layers with inclusions of high-purity single-walled (SWCNTs) or multi-walled carbon nanotubes (MWCNTs) – two types of nanotubes that are characterized by high structural perfection.

All investigated samples show lowest impedance (highest conductivity) at room temperature and electrical conductivity decrease upon cooling. General trend is that Re(Z) slightly increases with frequency from 1 kHz to up to some threshold frequency and then drops rapidly. This threshold frequency for pure PEDOT:PSS and PEDOT:PSS/SWCNTs samples is about 100 kHz and is somewhat lower for composite layers with MWCNTs.

Most notable temperature effect on the real part of the impedance of fabricated polymer/CNTs composite layers is that Re (Z) increases drastically starting from certain temperature, which is different for samples with different composition. For pure polymer this occurs already at 80…90 K and below 60 K Re (Z) is almost out of the measurable range. For layers reinforced with SWCNTs, increase of impedance is more gradual and even more so for MWCNTs-reinforced composites. In the latter case, reliable measurements can be performed even at temperatures as low as 40K.

In samples with incorporated CNTs the conditions for residual water storage are potentially different due to structural changes introduced by specific nanofiller, so that time needed for complete water removal is different and the process is eventually finished at different temperature. This assumption is further supported by the fact that samples with MWCNTs show slower growth of real impedance with decreasing temperature and generally have higher conductivity at lowest measured temperatures.

Influence of frequency and temperature on electrical resistivity of polymer-based nanocomposites

Zhydenko I.[1,2]***, Karbovnyk I.***[1,3]***, Klym H.***[1]***, Chalyy D.***[2]

[1] Lviv Polytechnic National University,
12, Bandera Str., Lviv-79013, Ukraine
E-mail: klymha@yahoo.com, halyna.i.klym@lpnu.ua

[2] Lviv State University of Life Safety,
35, Kleparivska Str., Lviv-79000, Ukraine

[3] Department of Electronics and Computer Technologies, Ivan Franko
National University of Lviv, 107, Tarnavskogo Str., Lviv-79000, Ukraine

Low-temperature behavior of poly(3,4-ethylenedioxythiophene)-poly (styrenesulfonate) (PEDOT:PSS) thin layers reinforced with carbon nanotubes however, is much less analyzed. Different reliability issues and effects of nanofiller properties on the temperature dependence of con-ductivity in this range remain a rather open question.

In this work we report the results of the investigation of the influence of frequency and, most importantly, temperature on electrical resistivity of PEDOT:PSS micrometer thick films reinforced with multi-walled carbon nanotubes (MWCNT), prioritizing the temperature range from 10 to 300 K.

Cooling and heating modes of electrical measurements were realized by exploiting functions of Cryocon 32 temperature controller from Cryogenic Control Systems Inc., *ac* electrical measurements at different frequencies were done with the automated E7-20 RLC-meter from LLC “ZAPADPRIBOR” which allows registering active and reactive resistances in the range from 10–5 to 109 Ω. Standard 1 V sinewave was used as an *ac* excitation signal.

It is shown that two types of layers of conductive polymer PEDOT:PSS and polymer PEDOT:PSS with the addition of multilayer carbon nanotubes were prepared, with a thickness in the range of 30–50 μm. The electrical resistance of such layers was investigated depending on the temperature in the range of 10–300 K. The observed temperature behavior of PEDOT:PSS resistance is consistent line with one-dimensional variable hopping model, which speaks speaking in favor of possible partial contribution of tunneling conduction, as well as thermal activation mechanism and, possibly, Coulomb electron-electron interaction. The effect of adding nanotubes to the polymer matrix results also leads to the hysteresis of resistance measured in heating–cooling cycles, which is probably likely to be stimulated by the difference in thermal expansion coefficients of the matrix and the filler and by slow processes determined by these coefficients.

Catalytic activity of composites of nickel boride nanoparticles and anodic nanoporous alumina in hydrogenation reactions

***Lytvynenko A.S.**[1,2], Mishura A.M.[1], Kurmach M.M.[1], Brzózka A.[3], Zaraska L.[3]*

*[1] Porous Compounds and Materials Dept., L. V. Pisarzhevskii Institute
of Physical Chemistry of the NAS of Ukraine.
Prospect Nauky, 31, Kyiv, 03028, Ukraine.
E-mail: anton.s.lytvynenko@gmail.com*

*[2] Charles University, Faculty of Science, Department of Analytical
Chemistry, Albertov 6, 128 00 Prague 2, Czech Republic*

*[3] Jagiellonian University, Faculty of Chemistry,
Gronostajowa 2, 30-387 Kraków, Poland.*

Hydrogenation is an important process for organic synthesis leading to valuable chemicals for pharmaceutics and agrochemistry [1]. Ni-based nanoparticles (NPs) are promising substitutes for Pd catalysts typically employed for such reactions. Immobilization of NPs on a porous support improves their separation from the reaction mixture, mitigates their aggregation *etc*. The work aimed at assessment of the catalytic activity of Ni boride NPs immobilized on anodic nanoporous alumina (AAO) in hydrogenation of heteroaromatic compounds on an example of a substituted imidazo-[1,5-*a*]-pyridine **S** (Fig. 1).

The AAO samples were prepared by the two-step anodization of Al, as reported previously by us. Ni boride NPs were applied via treatment with $NiCl_2$ solution followed by reduction with $NaBH_4$. The hydrogenation of **S** was performed in CH_3OH by $NaBH_4$ or gaseous H_2 (1 atm). The keto-group of **S**, its pyridine ring or both groups could be affected. Both $NaBH_4$ and H_2 together with the obtained composites resulted in hydrogenation of both **S** groups, contrary to H_2 on Pd/C catalysts (yielding the mixture of all possible products). The composites exhibited notably higher activity than Ni boride without the support.

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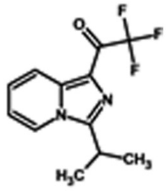

***Fig. 1**:*
*The compound **S***

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Sustainable-green synthesis of silver nanoparticles using waste extract obtained by deep eutectic solvent. Characterization, assessment of their electrochemical and antioxidant activities

Vorobyova V.I., Vasyliev, G. S., Skiba M.I., Goncharova A.

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute". Prosp. Peremohy-03056, 37, Kyiv, Ukraine.
E-mail: vorobyovavika1988@gmail.com

Nowadays, environmentally friendly methods such as green synthesis can be used, through the use of agri-food waste. The use of these wastes is a more sustainable method, because it reduces the environmental pollution, at the same time that silver nanoparticles are obtained. The current research is aimed at developing eco-friendly method for the synthesis of AgNPs using pomace extract obtained by ionic liquid and evaluation of the antibacterial, antiradical activity.

The analyses by TEM showed that the as-synthesized silver nanoparticles were uniform and spherical particles with an average diameter of 11.67 ± 14.7 nm and confirmed by SEM. The electron diffraction and TEM analyses showed the characteristic crystallinity of silver nanoparticles. The AgNPs were characterized by zeta-potential measurements and UV–Vis spectroscopy (absorption peak at 432 nm), scanning electron microscopy. The antimicrobial activity of AgNPs was tested against *Escherichia coli* using the agar diffusion method. DPPH and ABTS radicals scavenging activity were used to characterize antioxidant activity of the AgNPs.

Nanocatalyst for carbon monoxide oxidation based on palladium(II), copper(II) salts and carbon fiber material

Kiose T.O.[1,2]***, Rakitskaya T.L.***[1,2]***, Ennan A.A.-A.***[2]***, Truba A.S.***[1]

[1] Faculty of Chemistry and Pharmacy, Odesa I.I. Mechnikov National University,2, St. Dvoryanska, 65082, Odesa, Ukraine.

[2] Physico-Chemical Institute of Environment and Human' Protection, Preobrazhenska Str., 3, Odesa, 65082, Ukraine
E-mail: kiosetatyana@gmail.com

Carbon monoxide is dangerous for the environment and humans. It is known that carbon monoxide is oxidized to CO_2 only in the presence of catalysts. Analysis of research showed that Wacker-type metal-complex catalysts deposited on various carriers demonstrate stable protective properties and may be promising for the respiratory protective equipment use. The basic components of such catalysts are palladium(II) and copper(II) salts, as well as some additives supported on various carriers. Silica, alumina, activated carbons and carbon fiber materials (CFM), as well as natural minerals such as tripoli, clinoptilolite, mordenite, and bentonite are used as carriers. The carrier is not an inert support and affects the mechanisms of surface complexes formation, as well as the oxidation state of palladium in the case of carbon carriers. The phase composition, textural, protolytic properties, and activity of catalysts for the carbon monoxide low-temperature oxidation based on two series of non-woven carbon fiber material samples CFM-I and CFM-II, and K_2PdCl_4, $Cu(NO_3)_2$, KBr basic components were studied in this work. Catalysts and CFMs were studied by XRD, SEM, FT-IR spectroscopy, nitrogen ad/desorption, pH-metric, atomic absorption spectrophotometry metods. It has been found that the basic components K_2PdCl_4 and $Cu(NO_3)_2$ deposited on a microporous carbon surface undergo changes and form an X-ray amorphous Pd^0 phase and a paratacamite – $Cu_2(OH)_3Cl$ nanocrystalline phase. The catalysts were tested in the range of carbon monoxide initial concentrations from 50 to 300 mg/m^3 with an effective contact time of the catalyst with the gas-air mixture from 0.12 to 0.50 s. Catalysts provide air purification from CO to concentrations below MPCCO (20 mg/m^3) and can be used in respiratory devices.

Influence of anneal temperature on morphology, structure and chemical composition of zinc oxide films printed by 3D printer

Yermakov M.S., Dobrozhan O.A., Opanasyuk A.S.

Department of Electronics and Computer Technology, Sumy State University.
Rimsky-Korsakov str., 2, Sumy, UA-40007, Ukraine.
E-mail: m.yermakov@ekt.sumdu.edu.ua

Zinc oxide (ZnO) is of considerable interest to researchers due to its feasibility. This material has high radiation, chemical and thermal resistance and in the future can be widely used in the creation of elements of transparent electronics, gas sensors, ultraviolet detectors and more. Zinc oxide is a straight-band n-type semiconductor belonging to the group of compounds A_2B_6, its band gap at 300 K is ~ 3.27 eV. ZnO films can be used as elements of high-efficiency electronic auto emitters. a variety of optoelectronic devices, liquid crystal displays, photodiodes, window and conductive layers of solar panels and other electronic devices due to the high conductivity and transparency in the visible spectrum.

ZnO films were obtained on the cover glass by printing ink based on a suspension of nanocrystals synthesized by the polyol method. Because the ink contained organic substances as solvents, it was annealed for one hour in air and vacuum to remove uncontrolled impurities after film application. The annealing temperature was varied in the range from 200 °C to 400 °C.

As a result of research, it was established that the films were nanostructured, contained zinc and oxygen atoms, and the distribution of these elements by area was uniform. In addition to the main components of the material, the method of EDAX in the layers also recorded the carbon that is part of the developed ink. In some cases, because the applied films were thin, a peak of the Na element belonging to the glass substrate was observed. It was found that the concentration of carbon in the films decreased with increasing annealing temperature. However, the results of the study show that we failed to burn all the carbon that got into the organic films, so the time of their annealing in future work should be increased. It should be noted that during annealing the adhesion of the films to the glass substrate deteriorated sharply. This is due to the occurrence of large thermal deformations in the system, as the coefficients of linear expansion of materials differ significantly ($\alpha_{sl} = 5.9 \times 10^{-6}$ °C, $\alpha_{ZnO} = 29.0 \times 10^{-6}$ °C).

Thus, the annealing conditions of printed ZnO films are established, which allow to burn out impurities without disturbing the nanostructured state of the layers.

Stochastic nature of failure of carbyne-graphene nanoelements under thermomechanical loading

Kotrechko S.[1,2,3]***, Gianfranco P.***[4]***, Kolyvoshko E.***[1]***, Luigi T.***[4]***, Stetsenko N.***[1]

[1] *G.V. Kurdyumov Institute for Metal Physics, National Academy of Sciences of Ukraine, 36, Academician Vernadsky Blvd., Kyiv-03680, Ukraine.*
E-mail: serkotr@gmail.com

[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" 37, Peremohy Ave. UA-03056 Kyiv, Ukraine*

[3] *Taras Shevchenko Kyiv National University,*
60, Volodymyrska Str., Kyiv-01601, Ukraine.

[4] *Politecnico di Bary, 4, E. Orabona Str.,Bari-70125, Italy.*

Current trend of transition to practical use of nanoelements requires to study mechanisms that govern their lifetime under conditions of combined action of such factors as temperature and mechanical load. This is crucially important for straintronics elements, as they involve governing the functional properties of nanoelements by deforming them. Carbyne-graphene nanoelements (CGNs) are the most striking example of such nanoelements. They are graphene sheets connected by carbyne chains. Today they are considered as a key element of the all-carbon-based nanoelectronics of the future. When such nanoelements are stretched, the band gap changes significantly, so they can also be used, as the elements of nanoscale lasers and other optoelectronic devices with tunable wavelengths.

This study ascertained an atomistic mechanism that governs stability and lifetime of such nanoelements under thermomechanical loading. Based on the findings of molecular dynamics simulation of CGNs' stretching in a wide temperature range, it is shown that their lifetime is governed by the waiting time for critical fluctuations in the lengths of contact bonds (CB), resulting in their failure. It is ascertained that mechanism of CB break is stochastic in nature. Within the framework of the fluctuation model of CB break developed earlier [1], a statistical law was obtained for the lifetime of CGNs under thermomechanical loading. It is exhibited that the stochasticity inherent in the CB break process gives rise to a significant scatter in the lifetime value. The standard deviation of lifetime is equal to its average value. This means that in the practical utilisation of CGNs, not the average value of lifetime should be used, but the lower scatter limit with a given value of the probability of its realization.

Based on the findings obtained, the temperature-force conditions are found under which the practical use of CGNs is possible.

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Lightweight boron-based ceramic composites

***Barvitskyi P.P.**[1], **Prikhna T.O.**[1], **Karpets M.V.**[2], **Muratov V.B.**[2], **Moshchil` V.E.**[1], **Vasiliev O.O.**[2], **Lokatkina A.S.**[1], **Prysiazhna O.V.**[1]*

[1] Institute for Superhard Materials of the National Academy of Sciences of Ukraine, 2, Avtozavodska Str., Kyiv, 04074, Ukraine.
E-mail: barvitskp@gmail.com

[2] Institute for Problems in Material Science of the National Academy of Sciences of Ukraine, 3, Krzhizhanovsky Str., 03680, Kyiv, Ukraine.
E-mail: vasalexandr@gmail.com

The work is devoted to the study correlations between consolidation conditions, structures, mechanical, chemical and damping characteristics of α-AlB_{12}-, $AlB_{12}C2$-[1], B_4C-Al($AlB_{40}C_4$ [2]) - based lightweight, dense ceramics and composites synthesized or sintered under by hot pressing (at 30 MPa, 1500-2200 ° C) quasi-isostatic high pressures (at 2-4.5 GPa, 1100-1800 °C) conditions from the nanosized AlB_{12}~ powders with the additives of different amounts of C (carbon), TiC, SiC and AlN. Temperature, pressure, exposure time and composition of the starting powders were optimized to obtain sintered bodies with desired overall dimensions with high mechanical characteristics.

Relatively cheap nanopowders (50…150 nm, with a specific surface area of 21-15 m^2/g) α-AlB_{12} (three types with different content of amorphous carbon impurities from the graphite crucible during powder synthesis) and $AlB_{12}C_2$, synthesized by ph.Dr V.B. Muratov (IPM NAS of Ukraine) from h-BN, Al and C in graphite crucibles [3].

One of the best materials was a sample in which the additions of TiC to α-AlB_{12} resulted in the formation of 74 wt.% $AlB_{12}\tilde{C}_2$–22 wt.% $TiB_{\tilde{2}}$ wt.% Al_2O_3 composition (according x-ray) which contained $Al_{0.17}B_{4.55}C_2O_{0.04}N_{0.21}$, $TiB_{2.58}C_{0.8}Al_{0.02}$ and $Al_2O_{3.79}B_{2.04}C_{0.8}$ (according SEM EDX) havin Rcs=1143 MPa compression and Rbs=646 MPa bendin strengths, HV(49 N-load)=37.7 GPa hardness K_{1C}(49 N-load)=6.9 $MPa\cdot m^{0.5}$ fracture toughnes and ρ=3.2 g/m^3 density. The effect of TiC, SiC and C additions on the properties of the resultant composites and the particularities of the ceramics destruction under shock loading are discussed [4].

The use of source nanopowders allows to intensify consolidation processes, reduce synthesis and sintering temperatures, ie reduce the cost and simplify production technologies, as well as improve the mechanical properties of materials. Features of the structure of aluminum dodecaborides and decarbododecaborides (similar to boron carbide), namely the presence of the same structural elements - almost correct icosahedrons of boron atoms, high dispersion and reactivity allows to modify the structure and properties of such materials by adding additives. It was the reason for research in this area, aimed at creating new composites based on them, in particular, with improved damping and construction characteristics

The developed lightweight dodecaboride dicarbododecaboride -based ceramic composites hold great potential for a wide range of applications in extreme conditions: for the manufacture of abrasive nozzles, friction pairs for pumping oil and other aggressive liquids, constructional ceramics for nuclear power plants, as a personal protection or for armored defense of ground military equipment and vehicles, etc [5].

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Optimization of electronic properties of carbon nanostructures

Mykhailova H.Yu.**, **Shevchenko M.Ya.

G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine
36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine
E-mail: mihajlova.halina@gmail.com

The using of disordered carbon materials can open new perspectives in the creation of the thermoemission converter. The addition of the carbon nanostructures to the cathode material provides emission at lower temperatures [1]: they serve as electron emitters on the cathode surface. This makes it possible to determine the optimal technological conditions for the creation of new materials for alternative energy.

In this work, the electrophysical properties of nanocomposites containing carbon nanotubes and thermally expanded graphite were studied. The electrical conductivity of the sample was measured in a dielectric cylinder. The latter was filled with nanocomposite which were compressed when the piston was lowered. When the components of the sample come into contact and the circuit between the electrodes closes, the system (nanocomposite - air) passes into the electrically conductive state, which corresponds to transition of the dielectric - conductor. At the initial stage of compression, the initial increase in electrical conductivity and the achievement of the maximum value, followed by its fall for a pure sample of carbon nanotubes, increase or without changes for composite samples during subsequent compression. This is due to the increase in the total area between the outer shells of the components of the composite, which contributes to the increase in electrical conductivity and elastic deformation of CNTs, causing the opposite effect.

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Electrical conductivity features of metal-carbon nanocomposites

Mykhailova H.Yu., Yakymchuk M.M.

G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine
36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine
E-mail: mihajlova.halina@gmail.com

Carbon nanostructures have a unique anisotropic structure that determines their electronic properties. The electrical conductivity of individual particles of carbon nanostructures and the conductivity of a composite or material containing such structures differ.

For mass application of the thermoemission type of direct energy conversion in alternative sources it is necessary, with maintaining the parameters of electron emission from the cathodes of the thermoemission converter, to significantly reduce its operating temperature, which can be achieved by reducing the output.

The formation of metal- and carbon-containing composites opens the prospect of combining the advantages of both these types of materials, as well as the emergence of new characteristics in the created composites, which are not inherent in the original systems. Such features open up prospects for the creation of "cold" cathodes for thermophoto-emission energy converters based on composites of metal-carbon nanostructures.

The electromechanical properties of metal - carbon nanostructures were studied.

There is an increase in the maximum value of electrical conductivity up to 2 times compared to the original components, due to increasing contact area between the constituent particles of the composite, which increases the electrical conductivity due to increased free electrons in the carbon component during their transition from metal particles and deformation reduction.

Electrical conductivity features of metal-carbon nanocomposites

Mykhailova H.Yu., Yakymchuk M.M.

G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine
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The model of a giant magnetoresistance, built taking into account the bulk scattering of spins of conduction electrons

Politanskyi R.L.[1]***, Vistak M.V.***[2]

[1] Department of RadioEngeeniring and CyberSecurity ,
Yuriy Fedkovych Chernivtsi National University.
Kotsyubynsky, 2, Chernivtsi-58012, Ukraine.
E-mail:polrusl@i.ua

[2] Faculty of Pharmacy/Department of Biophysics, Danylo Halytsky
Lviv National University, Pekarska 69, Lviv-79010, Ukraine.

The properties of the "ferromagnetic" – "non-magnetic metal" heterojunction in the geometry of the current perpendicular to the plane of the heterojunction are modeled. Unlike the existing Motta two-channel conductivity model, the developed model takes into account spin scattering in the volume of the structure, which leads to the interaction between the conduction channels formed by electrons in the spin-up and spin-down states. The basis of this model is the equations of conductivity of electrons with spin-up and spin-down states, obtained by Firth-Valletta theory [1], which uses the semiclassical Boltzmann approach to determine the transport properties of electrons in the conduction band where spin degeneracy occurs. The general solutions of the problem obtained in the framework of the Firth-Valletta model are supplemented by boundary conditions on the heterojunction boundary to determine the constants of the general problem. The physical meaning of these boundary conditions is the preservation of the total number of electrons on the inner surface of the heterostructure that are reflected and pass through it [1]. The coefficients of reflection and transmission of electrons are derived without taking into account spin scattering on the surface of the heterostructure. Based on this model, the effect of the giant magnetic resistance for the three-layer structure "cobalt" – "copper" – "cobalt" is calculated. The results of the calculations are compared with the values of the giant magnetoresistance obtained based on the classical model of two-channel conductivity without channel interaction, which has been studied by us before [2].

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Session 2

Nanobiotechnology for healsth-care

Biofunctionalization of semiconductor nanocrystals for the development of impediometric DNA sensors for early diagnosis of genetic diseases

***Nesterenko E.O.*[1], *Grynko D.O.*[1,2]**

[1] *Institute of Molecular Biology and Genetics of the NAS of Ukraine*
Zabolotnogo str. 150, Kyiv-03143, Ukraine

[2] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine,*
41, prospect Nauky, Kyiv-03680, Ukraine,
E-mail: dgrynko@gmail.com

The aim of the paper is the development of oligonucleotides biofunctionalization techniques for nanostructured electrodes with an array of CdS nanocrystals on its surface. Optimization of the biofunctionalization procedure is necessary for the formation of bioselective sensor elements based on semiconductor nanocrystals, thiolated oligonucleotides and low molecular weight thiols for the detection of specific nucleic acid sequences.

Based on the analysis of the scientific literature on the methods of immobilization of oligonucleotides on the surface of semiconductor CdS nanocrystals we can draw a conclusion that the most promising method is the direct binding of thiolated oligonucleotides to CdS. Experimental studies of CdS nanocrystals arrays with using experimental methods such as electric impedance spectrometry, and piezoelectric nano-weighing were performed to identify thiol immobilization processes.

The fact of functionalization is proved and the optimal conditions for CdS nanocrystals are clarified. Electrochemical studies of the processes of formation of molecular shells of the modPh oligonucleotide on the surface of electrodes with different morphology are carried out. The fact of functionalization is proved and the optimal conditions for CdS nanocrystals are determined.

The process of hybridization of oligonucleotide P1, which is complementary to modPh, on the surface of nanocrystals with the immobilized modPh layer is demonstrated. Range of experimentally tested P1 concentrations was from 0.001 nM to 100 nM in SSC buffer solution. Peculiarities of interaction are investigated for immobilized probe oligonucleotide modPh with complementary (P1), partially complementary (BCRex14) and non-complementary (npt02) nucleic acid sequences.

Chip based plasmon-enhanced fluorescence sensor for highly-sensitive zearalenone analysis

Yarynka D.V.[1]***, Chegel V.I.***[2]***, Dubey I.Ya.***[1]***,***
Dubey L.V.[1]***, Stepanenko Ye.Yu.***[1]***, Brovko O.O.***[3]***, and Sergeyeva T.A.***[1]

[1] Institute of Molecular Biology and Genetics of the NAS of Ukraine.
Zabolotnogo str. 150, Kyiv-03143, Ukraine.
E-mail: d.v.yarinka@imbg.org.ua

[2] V.E. Lashkaryov Institute of Semiconductor Physics of the NAS of Ukraine,
Prospect Nauky, 41, Kyiv- 03680, Ukraine.

[3] Institute of Macromolecular Chemistry of the NAS of Ukraine.
Kharkivske Shosse, 48, Kyiv-02160, Ukraine.

The highly-sensitive chip-based plasmon-enhanced fluorescence (PEF) sensor system for fast and robust zearalenone analysis in grain foods was developed. Thin molecularly imprinted polymer (MIP) films with embedded *in situ*-synthesized Ag nanoparticles (AgNPs) immobilized on the surface of glass slides were used as sensing chips for the proposed PEF-based sensor system. The MIP films were synthesized according to a dummy template-based approach with cyclododecyl-2,4 dihydroxybenzoate as a template molecule and ethyleneglycol-methacrylatephosphate as a functional monomer. AgNPs were *in-situ* synthesized using reduction of $AgNO_3$ which was added to the monomer composition. Spherical AgNPs (30–70 nm in diameter) were formed in MIP films structure during the pre-heating step and further UV-initiated polymerization procedure on the surface of glass slides. To provide covalent immobilization of the MIP films, glass slides were treated with γ-methacryloxypropyltrimethoxysilane. Enhanced fluorescence of ZON selectively adsorbed on the surface of glass chips coated with thin MIP films was registered with the standard laboratory spectrofluorimeter. The transmission electron microscopy was used to investigate the morphology and size of AgNPs embedded in the MIP film structure. The influence of $AgNO_3$ concentration on the PEF phenomenon was also investigated. The LOD of ZON sensor chips was 5 ng/mL, and the linear detection range was 5-25 ng/mL. The developed AgNPs-containing MIP-based PEF sensor chips were successfully used for the analysis of ZON contamination in spiked and naturally contaminated grain samples.

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Genotoxicity of $GdVO_4:Eu^{3+}$ nanoparticles *in vitro:* an experimental assessment

Tkachenko A.S.[1]***, Prokopiuk V.Yu.***[1]***, Onishchenko A.I.***[1]***,***
Yefimova S.L.[2]***, Maksimchuk P.O.***[2]***, Klochkov V.K.***[2]

[1]*Research Institute of Experimental and Clinical Medicine,*
Kharkiv National Medical University. Nauki ave, 4, Kharkiv-61018, Ukraine.
E-mail: as.tkachenko@knmu.edu.ua

[2] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine).*
Nauki ave, 60, Kharkiv-61072, Ukraine.

Mutagenic properties are a major challenge to the application of drugs in clinical practice. Any potential drug is tested in the preclinical stage for genotoxicity. Novel nanomaterials, which are promising for use in oncology, infectology and implantology, should be tested for their harmfulness to genetic material.

The aim of this study was to evaluate the genotoxicity of gadolinium orthovanadate nanoparticles ($GdVO_4:Eu^{3+}$) *in vitro*.

Materials and methods. Genotoxicity studies were performed by the micronucleus assay. The skin fibroblasts of rat fetuses cultivated in DMEM medium with 10% fetal bovine serum in a CO_2 incubator were used after 3 passages. Following transplantation into a 24-well plate at a concentration of 50 000 cells per well, $GdVO_4:Eu^{3+}$ nanoparticles were added at concentrations of 0-30-65-130-260-520 μg / ml. The cells incubated for a short period of time with cisplatin were used as a positive control, while the intact cells were used as a negative control. After 72 hours, the cells were fixed with ethanol, stained according to Romanowsky – Giemsa. The number of cells with micronuclei was identified. Statistical data processing was performed by Kraskel-Wallis and Dunn's tests.

Results. In this study, the genotoxic effect of $GdVO_4:Eu^{3+}$ nanoparticles was evaluated by the micronucleus assay on the culture of fibroblasts and no damaging effect was revealed when using nanoparticles at concentrations of 30-65-130 μg / ml. The number of cells with micronuclei did not differ from the negative control. At high concentrations, it was technically impossible to perform micronucleus calculations due to loss of cell adhesion and lack of division. In cultures exposed to cisplatin, the number of cells with micronuclei was statistically significantly higher. The cell shape, shape and size of nuclei changed.

Conclusions. $GdVO_4:Eu^{3+}$ nanoparticles show no genotoxic effect on fibroblast cultures *in vitro*.

$LaVO_4:Eu^{3+}$ nanoparticles show no genotoxicity on fibroblast cultures

Prokopiuk V.Yu.[1]***, Tkachenko A.S.***[1]***, Onishchenko A.I.***[1]***,***
Yefimova S.L.[2]***, Maksimchuk P.O.***[2]***, Lazurenko V.V.***[3]***, Klochkov V.K.***[2]

[1] Research Institute of Experimental and Clinical Medicine,
Kharkiv National Medical University. Nauki ave, 4, Kharkiv-61018, Ukraine.
E-mail: v.yu.prokopiuk@gmail.com

[2] Institute for Scintillation Materials, NAS of Ukraine (Ukraine). Nauki ave,
60, Kharkiv-61072, Ukraine.

[3] Department of Obstetrics and Gynaecology No. 2, Kharkiv National
Medical University. Nauki ave, 4, Kharkiv-61018, Ukraine.

Therapeutic efficacy of any drug used in clinical medicine should prevail over its possible toxic effects. One of the manifestations of the negative impact of drugs on cells is genotoxicity, which has to be evaluated in screening of potential drugs, including nanomaterials.

The aim of this study was to assess the genotoxicity of lanthanum orthovanadate nanoparticles ($LaVO_4:Eu^{3+)}$ on fibroblast cultures.

Materials and methods. Genotoxicity was analyzed using the micronucleus assay. According to the protocol, dermal fibroblasts of rat fetuses were cultivated in DMEM enriched with 10% fetal bovine serum in a CO_2 incubator. The cells underwent 3 passages. The cells were transferred into a 24-well plate at 50 000 cells per well. Thereafter, $LaVO_4:Eu^{3+}$ nanoparticles were added (0-30-65-130-260-520 µg / ml). For a positive control, the cells were incubated with cisplatin. For a negative control, the intact cells were used. Following 72 hours, the fibroblasts were fixed using alcohol and stained (Romanowsky – Giemsa staining). The amount of fibroblasts with micronuclei was analyzed and compared. Statistical analysis was carried out by Kraskel-Wallis and Dunn's tests.

Results. When lanthanum orthovanadate nanoparticles ($LaVO_4:Eu^{3+}$) were added to fibroblast cell cultures at concentrations of 30-65-130 µg / ml, the number of cells with micronuclei did not differ statistically significantly from cultures without nanoparticles. Higher concentrations caused cell detachment from the surface and made it impossible to count the number of cells with micronuclei. Cisplatin in the positive control samples caused an increase in the number of cells from micronuclei and promoted changes in the shape of cells and nuclei.

Conclusions. $LaVO_4:Eu^{3+}$ nanoparticles demonstrate no genotoxicicty against fibroblast cultures *in vitro*.

Drug delivery with pH-sensitive star-like Dextran-Graft Polyacrylamide copolymer

***Ponomarenko S.*[1], *Grebinnyk A.*[2], *Prylutska S.*[3], *Grebinnyk S.*[2], *Chumachenko V.*[1], *Kutsevol N.*[1], *Prylutskyy Yu.*[1], *Frohme M.*[2]**

[1] *Taras Shevchenko National University of Kyiv,*
Volodymyrska Str., 64, 01601 Kyiv, Ukraine. E-mail: prylut@ukr.net

[2] *Technical University of Applied Sciences Wildau,*
Hochschulring 1, 15745 Wildau, Germany.

[3] *National University of Life and Environmental Science of Ukraine,*
Heroiv Oborony Str., 15, 03041 Kyiv, Ukraine.

Polymer nanoparticles represent one of the innovative non-invasive approaches for drug delivery applications in cancer therapy. In this study, the star-like dextran-graft-polyacrylamide (D-g-PAA) copolymer in anionic form (D-g-PAAan) was developed for the pH-triggered targeted drug delivery of the common chemotherapeutic drugs – Doxorubicin (Dox) and Cisplatin (Cis). The monodisperse size distribution of both Dox- and Cis-loaded polymeric nanoparticles was estimated at 80 nm. The acidification of the buffer from pH 7.4 to 5.0 promoted release of Dox and Cis on 26.0 and 32.5% at 48 h, respectively (Figure). D-g-PAAan nanoparticles increased toxic potential of the drugs against human and mouse lung carcinoma cells (A549 and LLC), but not against normal human lung cells (HEL299). The drug-loaded D-g-PAAan-nanoparticles promoted further oxidative stress and apoptosis induction in LLC cells by increasing intracellular ROS generation and activation of caspase 3/7. The data obtained indicate that the strategy of chemotherapeutic drugs encapsulation within the branched D-g-PAAan nanoparticle allows not only to realize pH-triggered drug release but also to potentiate its cytotoxic, prooxidant and proapoptotic effects against lung carcinoma cells *in vitro*.

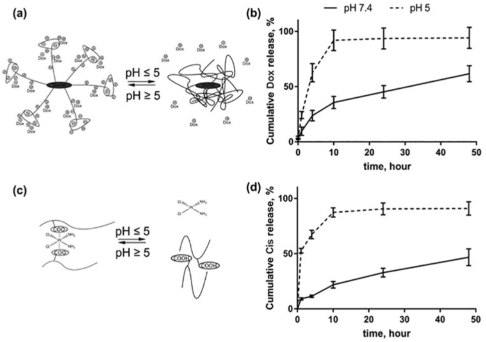

Fig. *Drug release from D-g-PAAan nanoparticles: schematic representation of Dox (a) and Cis (c) release; cumulative release of Dox (b) and Cis (d) during 48 h of incubation at pH 7.4 and 5.0.*

Toward development of new optical immunosensors based on nanostructured ZnO thin films

Tereshchenko A.

Odesa National I.I. Mechnikov University,
Pastera 42, 65023, Odesa, Ukraine.
E-mail: alla_teresc@onu.edu.ua

ZnO-based nanostructured thin films are broadly applied as a template for biosensors due to their fundamental physico-chemical properties such as the direct wide band gap semiconductor (Eg ~3.37eV) complemented by high surface to volume ratio of its nanostructures that has a high isoelectric point. Good biocompatibility and affinity towards biomaterials of ZnO along with its strong adsorption ability make it suitable for the immobilization of various protein-based immune complexes applied as biological recognition part in immunosensors. Excellent optical properties of ZnO, in particular, an intense room temperature photoluminescence (PL) open a great possibility to be used for optical biosensor applications [1]. Regarding to a progress in nanotechnology, the new methods have been developed to fabricate nanostructured ZnO templates with high surface area and advanced properties for biosensors, e.g. atomic layer deposition (ALD), metal organic chemical vapor deposition (MOCVD) and others. ALD is a relatively innovative technique, which allows the deposition of ultrathin metal oxide films with controlled thickness, grain size etc [2]. MOCVD is a well- known method for the formation of metal oxide thin films (as itself) and also can be used for the growth of nanorods of different size, shape and orientation on the substrate that can act as a resonator where whispering gallery modes (WGM) can be excited and utilized as a biosensor signal [3]. In this report, the influence of the immobilized proteins of an immune complex on the PL spectra of ZnO thin films formed by ALD and MOCVD will be demonstrated and discussed.

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Chitosan-based interpenetrating polymer network hydrogels

Nadtoka O.[1], **Virych P.**[1], **Vashchenko O.**[2], **Kutsevol N.**[1]

1Taras Shevchenko National University of Kyiv.
Volodymyrska Street, 64/13, Kyiv-01601, Ukraine

2 Institute for Scintillation Materials of NAS of Ukraine,
ave. Nauky, 60, Kharkiv, 61172, Ukraine
E-mail: oksananadtoka@ukr.net

The recent developments in polymeric science have led to many novel drug delivery systems. One of them are interpenetrating polymer networks (IPN) based on chitosan and PAA as bioactive materials for the pharmaceutical industry. These IPNs possess excellent properties because of their improved biocompatibility and good swelling properties. A synergistic effect can be produced using IPN technology by formulating an IPN between a natural and synthetic polymer, hence combining the properties of both polymers. In turn, it leads to interlacing between the different features and performances of the individual components of IPN [1]. Each network retains its individual properties so that synergistic improvements in properties like strength or toughness can be seen. In the present study, we have synthesized copolymer of acrylamide and chitosan with ceric ammonium nitrate as a redox system. The obtained copolymer was subjected to various analytical techniques such as FTIR, DSC, DTGA to confirm the copolymer formation. The swelling properties and absorption of bioactive Methylene Blue were also studied.

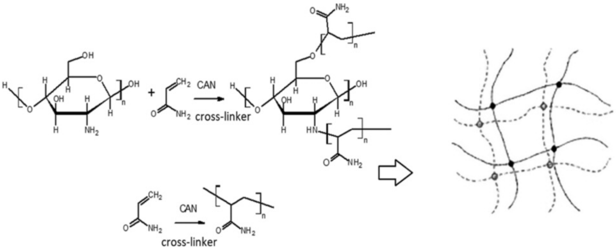

Fig 1. *Scheme of the possible reaction.*

Chitosan addition to polyacrylamide gel results in an increase in the total water content in the samples accompanied by a decrease in the fraction of bound water, which reflects partial dehydration of polyacrylamide. Coupled with the elevated thermostability of both polymers this may point to their strong interaction or grafted structure.

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Formation of a nanoporous coating on urea granules

***Yanovska G.O.*[1], *Vakal S.V.*[2], *Vakal V.S.*[2],**
***Artyukhov A.E.*[1], *Shkola V.Y.*[1], *Zelenskiy A.N.*[2]**

[1] Sumy State University,
Rymskogo-Korsakova str., 2, Sumy, 40007, Ukraine.
e-mail: yanovskaanna@gmail.com

[2] Scientific-Research Institute of Mineral Fertilizers and Pigments of the
Sumy State University, 12, Kharkovskaya Str., Sumy, 40012, Ukraine

Reducing the agrogenic load on the environment requires, on the one hand, a reduction in the doses of applied fertilizers and plant protection products, and, on the other hand, to obtain sustainable and consistently high crop yields, the use of significant amounts of agrochemicals is required. One of the options for resolving this contradiction is the development of organo-mineral complexes of prolonged action, as components of which it is advisable to use natural minerals and compounds. This approach stimulates the efforts of researchers to use the composition of the coating with special properties, such as porosity, to retain moisture in the soil and the content of nutrients. The nutritional properties of the previously studied phosphate-glauconite concentrates are proposed to be enhanced by such a sorbent as diatomite, which is a sedimentary rock. A distinctive feature of this component is its porous structure and high content of silicon compounds, which have biogeochemical activity and improve nitrogen and phosphorus metabolism in plant tissues. Finely ground diatomite also finds independent use as a natural bioinsecticide. Microscopic studies of the presented samples of finely dispersed diatomite and encapsulated urea show that the diatomite powder is mainly particles no larger than 20 microns. At the same time, pores no larger than 600 nm are present on individual particles. Spectral analysis of the sample shows that the main element is silicon. The study of the surface of the phosphate-containing coating made it possible to determine that the inclusion of finely dispersed diatomite in the coating composition forms a denser porous structure. The presence of porous diatomite particles throughout the entire thickness of the encapsulated layer makes it possible to create a developed porous surface not only for the prolonging effect of the nitrogen core of the granule but also for the accumulation of soil moisture.

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Formation of reactive oxygen species as one of the triggers of antitumor action of nanocomplexes

Goltsev A.M., Bondarovych M.O., Babenko N.M., Gaevska Yu.O., Dubrava T.G., Ostankov M.V.

Cryopathophysiology and Immunology Department, Institute for Problems of Cryobiology & Cryomedicine of the National Academy of Sciences of Ukraine. Pereyaslavska Str, 23, Kharkiv-61016, Ukraine. E-mail:cryopato@gmail.com.

Experimental study of the antitumor effects of nanocomplexes (NCs), consisting of nanoparticles of $GdYVO_4$:Eu^{3+} and cholesterol, indicates the feasibility of their use in oncology practice. The mechanism of implementation of the antitumor effect of NCs may be associated with the formation of reactive oxygen species (ROS) with subsequent death of tumor cells, so the aim of the research was to study the pro-oxidant and antitumor properties of these NCs. The experiments were performed in Ehrlich ascites carcinoma (EAC) cells induced in BALB / c mice by intraperitoneal administration of $5x10^6$ cells / mouse in 0.3 ml of saline. On day 7 of culturing in the peritoneal cavity of mice, EAC cells were removed with a syringe and in vitro treated with NCs at the rate of 100 µl of NCs solution per 900 µl of EAC cells $1x10^7$ cells / ml at room temperature for 3 hours. The control was bone marrow (BM) cells, treated with NCs in a similar manner. ROS production was quantified by flow cytometry using the Fluorometric Intracellular ROS Kit (Sigma-Aldrich, USA), the level of metabolic activity of cells was found with the Cell growth determination kit MTT based (Sigma, USA), apoptotic and necrotic cells were numbered by FITC Annexin V Apoptosis Detection Kit I (BD, USA). The EAC cells before NCs treatment were found to have a basal level of ROS production at 12.16 ± 0.93%, which was twice higher than in BM cells. Treatment with NCs increased the number of ROS-positive cells in BM by 1.8 times and in EAC by more than 3 times compared to the corresponding basal levels of this index, which was a prerequisite for a deeper disorder of their functional state. Indeed, under the influence of NCs, the inhibition rate of metabolic activity of EAC cells by MTT test was almost 2 times greater than that of BM cells, that is a reflection of inhibition of NADP-H-dependent oxidoreductase enzymes of mitochondria. This led to a significant decrease (by 25%) in the number of living (An– / PI–) EAC cells, and their predominant death by necrosis. The results obtained can be taken into account when creating new strategies for cancer therapy.

Effect of Ag nanoparticles on cryopreserved mesenchymal stem cells from cartilage tissue

Volkova N.O.**, **Stepanyuk L.V., Goltsev A.M.

Institute for Problems of Cryobiology and Cryomedicine, NAS of Ukraine.
Pereyaslavska str.23, Kharkiv-61016, Ukraine.
E-mail: volkovana781@gmail.com

The nanoscale materials have a dose-dependent effect on biological objects. The finding of the presence/absence of Ag nanoparticles (AgNPs) cytotoxic action is an important direction of nanobiotechnological research. The effect of AgNPs on morphological characteristics, proliferative and antioxidant potentials of cryopreserved mesenchymal stem cells (CrMSCs) from cartilage tissue was investigated.

The AgNPs (Sigma-Aldrich, USA) with an average size of 15 nm were used in the study. CrMSCs from cartilage tissue were incubated with AgNPs at final concentrations of 4, 6, 10, 20 μg/mL for 1 hour. The control was cells without the influence of AgNPs (0 μg/mL). On the 1, 3, 7, and 10 days of cultivation the number of viable cells was determined by MTT test. Analysis of total antioxidant status (TAS) was performed using Randox test kit (UK). On the 10th day, the CrMSCs were fixed in a 4 % solution of paraformaldehyde followed by azure-II and eosin staining by Romanovsky-Giemsa. The results were processed with Student's t-test using Excel software.

The use of 4 and 6 μg/ml AgNPs did not influence on morphological characteristic, proliferative and TAS activity in CrMSCs from cartilage tissue. AgNPs at concentrations of 10 and 20 μg/mL decreased the TAS index (1.3 and 1.5-fold respectively) and proliferative potential (1.2 and 1.6-fold respectively) if compare with the control. The use of AgNPs at concentrations of 10 and 20 μg/mL led to changes in the morphological characteristics of CrMSCs from cartilage tissue in relation to control samples, namely signs of cytoskeletal dystrophy, cytoplasmatic granularity and vacuolization of nuclei. It was found that AgNPs in concentrations of 4 and 6 μg/mL are safe for CrMSCs from cartilage tissue, while increase up to 10 μg/mL has a toxic effect manifested by the change of proliferative, antioxidant activities and morphological characteristic.

Thus, the presented results are belonged to the field of applied nanobiotechnology, that spreads to field restorative medicine, mostly in creation of cartilage bioimplants.

The work was carried out within the framework of the target research program of the NAS of Ukraine "Genomic, molecular and cellular bases of development of innovative biotechnologies", agreement No. 2.2.6.132/21.

Biofunctionalization of semiconductor nanocrystals for the development of impediometric DNA sensors for early diagnosis of genetic diseases

Nesterenko E.O.[1]***, Grynko D.O.***[1,2]

[1] Institute of Molecular Biology and Genetics of the NAS of Ukraine
Zabolotnogo str. 150, Kyiv-03143, Ukraine

[2] V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine,
41, prospect Nauky, Kyiv-03680, Ukraine,
E-mail: dgrynko@gmail.com

The aim of the paper is the development of oligonucleotides biofunctionalization techniques for nanostructured electrodes with an array of CdS nanocrystals on its surface. Optimization of the biofunctionalization procedure is necessary for the formation of bioselective sensor elements based on semiconductor nanocrystals, thiolated oligonucleotides and low molecular weight thiols for the detection of specific nucleic acid sequences.

Based on the analysis of the scientific literature on the methods of immobilization of oligonucleotides on the surface of semiconductor CdS nanocrystals we can draw a conclusion that the most promising method is the direct binding of thiolated oligonucleotides to CdS. Experimental studies of CdS nanocrystals arrays with using experimental methods such as electric impedance spectrometry, and piezoelectric nano-weighing were performed to identify thiol immobilization processes.

The fact of functionalization is proved and the optimal conditions for CdS nanocrystals are clarified. Electrochemical studies of the processes of formation of molecular shells of the modPh oligonucleotide on the surface of electrodes with different morphology are carried out. The fact of functionalization is proved and the optimal conditions for CdS nanocrystals are determined.

The process of hybridization of oligonucleotide P1, which is complementary to modPh, on the surface of nanocrystals with the immobilized modPh layer is demonstrated. Range of experimentally tested P1 concentrations was from 0.001 nM to 100 nM in SSC buffer solution. Peculiarities of interaction are investigated for immobilized probe oligonucleotide modPh with complementary (P1), partially complementary (BCRex14) and non-complementary (npt02) nucleic acid sequences.

Piezo-mechanical impedance of electrode with nanosized CdS crystals immersed in bio-electrolyte

Nesterenko E.O.*[1]*, Bogoslovskaya A.B.*[2]*,
***Doroshenko T.P.*[2]*, Grynko D.O.*[1,2]**

[1] *Institute of Molecular Biology and Genetics of NAS of Ukraine ,*
150, Zabolotnogo Str., 03143 Kyiv, Ukraine.

[2] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine,*
41, prospect Nauky, 03680 Kyiv, Ukraine,
E-mail: dgrynko@gmail.com

The aim of the presented project is to develop of a new high informative technique for weighting of molecular shell on piezoelectric CdS nano-crystals [1] in the order of femto- grams and its application for DNA bio-sensors. The series of resonances in the range 1-10 MHz detected in the impedance spectra of conductive micro-wire electrode with nano-sized CdS crystals on its surface, which have been immersed into bio-electrolyte. The constructive and technological realization of a measuring flow cell is offered for experimental investigation. The cell is designed for single use, has a plastic body. The flow channel has a volume of up to 200 µl at a constant temperature in the range from 35 C to 85 C with a reproducibility of thermal stabilization of the electrolyte 0.1 C. The cell is equipped with two measuring electrodes, one of which is nanostructured and may be biofunctionalized with oligonucleotide. We demonstrated measuring procedure for surface density of molecular shell as well at the process of immobilization of modPh on surface of CdS nano-crystals, as hybridization of oligonucleotide P1, which is complementary to Ph. Range of oligonucleotides surface density was 0.15 - 10 nm^{-2} at experimentally tested P1 concentrations from 0.001 nM to 100 nM in SSC buffer solutions. This device responds to changes in the attached mass and viscous layer at the boundary crystal-electrolyte. The mass of nano-crystals is in the range of nano-grams, so the added mass of the order of pico-grams or less registered. The selectivity of the device is ensured at the biochemical level - when using, for example, hybridization of single-stranded DNA. If a monomolecular layer is covalently bound to the surface of nanocrystals, the added mass increased in the process of hybridization with complementary single-stranded DNA in the electrolyte and the resonance frequencies of the crystals were changed.

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C_{60} fullerene effect on the degree of tremor oscillations of muscle contraction in chronic alcoholic rats

Motuziuk O.[1], **Nozdrenko D.**[2], **Bogutska K.**[2], **Ritter U.**[3], **Prylutskyy Yu.**[2]

[1] *Lesya Ukrainka Volyn National University,*
ave. Voli, 13, 43025 Lutsk, Ukraine.
E-mail: cmoplutsk@gmail.com

[2] *Taras Shevchenko National University of Kyiv,*
Volodymyrska Str., 64, 01601 Kyiv, Ukraine.

[3] *Technical University of Ilmenau,*
Weimarer Str., 25, 98693 Ilmenau, Germany.

The effect of C_{60} fullerene aqueous solution (C_{60}FAS) on the degree of tremor oscillations of the muscle soleus in chronic alcoholic rats with duration of alcoholism 6 months was studied. Experimental animals once a day received 40% ethyl alcohol at a dose of 2 ml/100 g weight. C_{60}FAS at a dose of 1 mg/kg was mixed with an alcohol solution. Changes in the levels of tremor oscillations on stationary areas of muscle contraction were used as a marker to assess the level of miotic damage of the neuromuscular system, the severity of alcoholism in experimental animals and the therapeutic effect of C_{60}FAS.

The tremor of maximal power responses with peaks from 11% (on the first contractions) to 38% (on the tenth contraction) of the level of stationary retention of the achieved strength position was observed during the formation of smooth tetanus in chronic alcoholic rats. The usage of C_{60}FAS was shown to reduce the maximum amplitude of tremor oscillations by 18% on the first contractions and by 47% on the tenth contraction compared to the control. The positive dynamics of the therapeutic effect of C_{60}FAS on the quality of accurate positioning of the studied muscle under its long-term stimulation was revealed.

The established pronounced protective effect of C_{60}FAS on the dynamics of muscle contraction in the development of alcoholic myopathy in animals opens up prospects for its practical use as a fundamentally new nanostructured medicine in the treatment of miotic pathologies.

Self-sealing properties of phospholipid membranes after interactions with various nanostructures - MD study

***Raczynski P.*, Gorny K. and Dendzik Z.**

Faculty of Science and Technology, University of Silesia in Katowice,
41-500 Chorzow, Poland
Email: przemyslaw.raczynski@us.edu.pl

Biological membranes are very effective barriers created by nature to protect the interior of the cell from impact of the outside environment. Although the membranes are de-signed to prohibit entrance of molecules into the cell, many researchers try to deliver various substances to the cell via phospholipid bilayer [1]. They try to discover less-invasive, efficient techniques of the targeted delivery of cargo, such as medicines or markers, to living cells. Significant effort is being done to study the characteristics of the use of nano-based materials as systems which are able to facilitate this task [2]. Howev-er, during the process of the cargo delivery to the cell, the phospholipid bilayer can not be permanently damaged because this is equivalent to cell death. To get deeper insight into the self-sealing process of the bilayer we have indented it with carbon and silicon-carbide nanotubes, graphene bilayers and silicon nanocones using non-equilibrium steered molecular dynamics (SMD) simulations [3,4]. After the indentation process the indenter was removed and the mechanism of self-sealing of the phospholipid bilayer was examined.

Our results show high abilities of the self-sealing of the cell membrane. These results can be useful as it is the essential problem when it comes to the potential application of nanostructures as nanocontainers for targeted drug delivery. The damage done to membrane can be quantified by the number of extracted lipids or membrane bending. To evaluate the effectiveness of self sealing and overall impact of indentation process on membrane integrity we performed additional series of computer simulations to assess the time necessary for the membrane to seal itself (expel water from its interior). Some additional factors, like nanostructure orientation toward membrane were also taken into account when analyzing the effectiveness of membrane self sealing after nanoindetation process. Our results suggest that carbon based nanotubes could be considered as effectors in targeted drug delivery or biosesnsors.

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Sonosentetizing cytotoxic effects of C_{60} fullerene and Berberine towards cancer cells of different origin

Radivoievych A.[1,2]***, Prylutska S.***[3]***, Zolk O.***[2,4]***, Frohme M.***[1]***, Grebinyk A.***[1]

[1] *Division Molecular Biotechnology and Functional Genomics,*
Technical University of Applied Sciences Wildau,
Hochschulring 1, 15745 Wildau, Germany.
E-mail: mfrohme@th-wildau.de

[2] *Faculty of Health Sciences, joint Faculty of the Brandenburg University of Technology Cottbus – Senftenberg, the Brandenburg Medical School Theodor Fontane and the University of Potsdam, Germany.*

[3] *Department of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska 64, 01601 Kyiv, Ukraine.*

[4] *Institute of Clinical Pharmacology, Brandenburg Medical School, Immanuel Klinik Rüdersdorf, 15562 Rüdersdorf, Germany.*

Cancer sonodynamic therapy (SDT) is the therapeutic strategy that involves the use of sonosensitizers, which become cytotoxic upon exposure to high-frequency ultrasound (US). The spectrum of sonoluminescence that occurs during US propagation through the liquid overlaps with the absorbance spectrum of a carbon nanoparticle C_{60} fullerene (C_{60}) and an herbal alkaloid Berberine. That points on US as a matching option for activating its photosensitizing activity. In this study the effects of C_{60} and Berberine on viability of cancer cells of different origin was analyzed in the combination with 1 MHz US treatment.

A water colloidal C_{60} solution was obtained from the Ilmenau University of Technology [1]. The cells (human cervix carcinoma HeLa, human alveolar basal epithelial A549, human T lymphocyte Jurkat, mouse Lewis lung carcinoma LLC, and rat hepatoma H4llE) were treated with 20 µM C_{60} or Berberine for 24 h and irradiated with $\leq$ 200 W 1 MHz US during 90s. Then cell morphology and viability were estimated with a MTT assay and phase contrast microscopy respectively.

The obtained data pointed that US irradiation alone had no effect on cell viability, while cells irradiated with US in presence of C_{60} and Berberine had a decreased viability to 43% and 46% respectively. C_{60} was found to exhibit higher sonotoxicity towards LLC, HeLa and H4llE cells than Berberine. HeLa and LLC had more pronounced cell viability decrease under action of US irradiation and C_{60} among investigated cells of different origin. These results suggest that SDT with C_{60} and Berberine can become a promising approach for cancer treatment.

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Yttrium and lanthanum doped bioglass

Smolyak S.S., Karbivskyy V.L., Dubok V.A.

Department of Nanostructures Physics,
G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,
Kyiv-03142, Ukraine
E-mail: karb@imp.kiev.ua

The best material for bone regeneration is bioglass, in the manufacture of which the following composition can be used: 24,5% Na_2O, 24,5% CaO, 45% SiO_2, 6% P_2O_5. It is possible to change the material properties by varying the glass composition, taking into account the needs of a particular task [1, 2].

The following bioglass samples were synthesized for research: 60S (60% SiO_2, 36% CaO, 4% P_2O_5) and 45S5 (45% SiO_2, 24,5% Na_2O, 24,5% CaO, 6% P_2O_5). They show excellent characteristics in the restoration of bone tissue. Bioglass 60S, doped with La and Y, was synthesized by the sol-gel method to study the properties of such solutions.

Structural features and electronic structure of bioactive glass, including yttrium and lanthanum doped ones, were studied using the method of nuclear magnetic resonance on the ^{29}Si and ^{31}P nuclei. Solid state NMR spectra have been obtained for both static and rotated under magic angle (MAS) samples.

NMR allowed identifying the presence and ratio of phosphate and silicate groups in a network-forming polyhedron, with a different number of bridging oxygens.

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The main ways for metal nanoparticles degradation

Lopatko S.K., Chayka V.M.

National University of Life and Environmental Sciences of Ukraine Heroyiv Oborony st., 15, Kyiv - 03041, Ukraine
E-mail:lopatkos15@gmai.com

With the rapid development of nanotechnology, the production of metal nanoparticles, which subsequently enter agricultural lands in various ways, is also increasing. This article presents a review, mostly of foreign literature, to systematize knowledge about degradation pathways, mechanisms of nanoparticle penetration into the cell, their subsequent transport through tissues and interaction of metal nanoparticles with the environment in agrobiocenoses. Therefore, the main issue today is the possibility of destruction of nanotechnology products due to edaphic factors and products of metabolism of plants and microorganisms to avoid their accumulation in agrophytocenoses.

Physicochemical properties of metal nanoparticles (eg size, charge, shape, coating) and soil properties (eg pH, mineral composition, presence of organic acids, etc.) play an important role in elucidating the decay, transport, mobility and interaction of nanoparticles with soil components. . The main role in the formation of most morphological features of metal nanoparticles, which are the basis of nanoparticles, is played by the method of nanoparticle synthesis. In this way, potential risks of using metal nanomaterials can be anticipated and avoided.

Therefore, the main purpose of this review is to evaluate the possibilities of metal nanoparticles for degradation, describe the preconditions for biodegradation and note the main possibilities of using such properties in the agro-industrial complex.

Chemical modification of polystyrene surfaces for improving performaces of ELISA microtiter plates

***Shynkarenko O.V.*, Beketov G.V.**

*[1] Ye.V. Lashkaryov Institute of Semiconductor Physics (ISP),
NAS of Ukraine, Prospect Nauki, 41, Kyiv-03028, Ukraine
E-mail: o.v.shynkarenko@gmail.com*

Enzyme linked immunosorbent assay (ELISA), which is based on detection of marker biomolecules (antibodies, antigens, proteins and glycoproteins) in biological samples, is currently the most common laboratory diagnostic technique. Multilateral studies are aimed at further improving its performances. One of the core issues is the optimal immobilization of capture biomolecules at the surface of microplate wells, which rely on intermolecular interactions of biomolecule nanoparticles with the solid-phase substrate [1].

Chemical modification of ELISA microtiter plates is an efficient technique for improving reproducibility, sensitivity, and concentration range of biomolecule detection. We developed a modification method based on oxidative treatment of polystyrene surface, the predominant material for manufacture of microtiter plates, in aqueous solution of ammonium persulfate, $(NH_4)_2S_2O_8$ [2]. Our study is aimed at characterization of immobilization efficiency of target biomolecules in dependency of physical and chemical properties of modified surface [3]. The characterization techniques include the X-ray photoelectron spectroscopy, the surface plasmon resonance spectroscopy, and wettability measurements using axisymmetrical drop shape analysis (ADSA).

The obtained results show that the low-level hydrophilization of polystyrene surface essentially improves adsorption efficiency of biomolecules compared to the non-treated surface, while the higher level has an adverse effect. Possible explanations of these observations are discussed.

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Highly efficient biologically functionalized semiconductor electrodes based on nanostructured titanium oxide for DNA sensors

Shchurenko A.I.[1]***, Styopkin V. I.*** [1]***, Mamykin A.V.***[2]***, Kukla O.L.***[2]***,***
Nesterenko E.O.[3]***, Pyeshkova V.M.***[3]***, Grynko D.O.***[2,3]

[1] *Institute of Physics NAS of Ukraine.*
Prospect Nauki, 46, Kyiv-03028, Ukraine.

[2] *V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine.*
Prospect Nauki, 41, Kyiv-03680, Ukraine.

[3] *Institute of Molecular Biology and Genetics NAS of Ukraine.*
Zabolotnogo Str., 150, Kyiv-03143, Ukraine.
E-mail: dgrynko@gmail.com

A new low-cost technology for the production of porous nanostructured semiconductor electrodes is proposed [1], which may be the basis for the production of highly informative DNA sensors. Functionalization of such electrodes with a predetermined oligonucleotide provides selectivity of hybridization with the corresponding nucleotide sequence of DNA (target DNA). As a basis for such a sensor is used porous film of anodically oxidized titanium with different morphology (nano-tubs with a depth of 0.3 to 7 µm and a diameter of 200 to 400 nm). Technique of immobilization oligonucleotides on the porous titanium oxide films with thiolated oligonucleotides and low molecular weight thiols for the detection of specific nucleic acid sequences with impedance spectroscopy have been tested at presented report.

The process of hybridization of oligonucleotide P1, which is complementary to modPh, on the surface of nanostructured titanium oxide with the immobilized modPh layer is demonstrated. Range of experimentally tested P1 concentrations was 0.001 - 10 nM in SSC buffer solution. Peculiarities of interaction are investigated for immobilized probe oligonucleotide modPh with complementary (P1), partially complementary (BCRex14) and non-complementary (npt02) nucleic acid sequences.

The linear dynamic range of the developed DNA sensors is 0.001 - 10 nM. It is shown that the use of such electrodes provides the ability to reduce the limit of determination of specific nucleic acid sequences to 0.001-0.1 nM.

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Electrophoretic studies of proteins of erythrocytes membrane under influence of silver nanoparticles

Batyuk L.V.[1]***, Kizilova N.N.***[2]

[1] *Department of Medical and Biological Physics and Medical Information Science, Kharkiv National Medical University,*
4 Nauky Ave., Kharkiv, 61022, Ukraine.
E-mail: liliya-batyuk@ukr.net

[2] *V. N. Karazin Kharkiv National University, Kharkiv, Ukraine*

The application of silver nanoparticles (AgNPs) for treatments against different diseases is increasingly innovative and effective [1]. The venous blood erythrocytes of 20 patients with lung cancer and 20 healthy donors were used as the object of the study. The control group consisted of 20 practically healthy donors of the same age. The effect of AgNP preparations (diameter d~35 nm) on RBCs membranes in a physiological solution containing $65.25 \cdot 10^6$ cells per 1 ml of the reaction mixture was analyzed. Membranes of erythrocytes were obtained by the method of J. Dodge [2]. Isolation and separation of the membrane proteins of erythrocytes by one-dimensional disc-electrophoresis in a 10% polyacrylamide gel containing 1% sodium dodecyl sulfate was carried out according to the well-known Laemmli method [3].The resulting gels were scanned on a densitometer. Calculations of the percentage content of individual protein fractions (before and after its introduction of AgNP preparations in suspension in vitro) were performed based on the analysis of densitograms. Statistical processing was carried out using the t-criteria Students. Comparative analysis of the protein spectrum of erythrocyte membranes of blood of patients with cancer before and after AgNP preparations added revealed significant changes in the content of spectrin, ankyrin, and bands of proteins 2 and 3; in proteins of band of fractions 4.1, 4.2 and 4.9, protein of band 6 and protein of band 8.

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Two kinds of luminescence centers in low-temperature phosphorescence spectra of IPNV RNA

***Losytskyy M.Y.*[1], *Kravchenko V.M.*[1], *Rud Y.P.*[1,2],**
***Buchatskyi L.P.*[1,2], *Zaloilo O.V.*[1,2], *Yashchuk V.M.*[1]**

[1] *Taras Shevchenko National University of Kyiv,*
Volodymyrs'ka Str., 64/13, Kyiv, 01601, Ukraine.
E-mail: mlosytskyy@gmail.com

[2] *Institute of Fisheries of NAAS of Ukraine,*
Obukhivska Str., 135, Kyiv, 03164, Ukraine.

Viral infections are among the most important challenges for the modern world; thus the study of the properties of these nanosized biological objects is crucial for understanding the ways of fighting this challenge. Particularly, the electronic processes in viral nucleic acids and proteins determine the efficiency of the deactivation of viruses by electromagnetic irradiation. To understand these processes, spectral properties of viruses and their components (nucleic acids and proteins) should be studied. RNA viruses of fish are efficient models for the study of viral pathogenesis and its treatment. Important representative of this class of viruses is the infectious pancreatic necrosis virus (IPNV) which causes a highly contagious disease of salmonid fish. Earlier, spectral properties of IPNV virions, RNA and major capsid proteins were studied by us [1].

Here, we have studied the low-temperature luminescence properties of RNA molecules of IPNV in more details. The phosphorescence spectra of RNA reveal the presence of two kinds of luminescence centers, each of them manifested as structured phosphorescence spectrum with maxima near 402, 430 and 460 nm for "center I", and 415, 444 and 477 nm for "center II". The both centers have shifted excitation spectra, "center II" is also characterized by longer phosphorescence decay time compared to "center I". The nature of these centers and electronic processes in the RNA of IPNV were discussed.

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Photodynamic treatment of titanium dioxide nanoparticles is a convenient method of viral inactivation

Zahorodnia S.D.[1]***, Povnitsa O.Y.***[1]***, Artiukh L.O.***[1]***,***
Zahornyi M.M.[2]***, Ievtushenko A.I.***[2]

[1]*D. K. Zabolotny Institute of Microbiology and Virology of the NAS of Ukraine 154, Zabolotny str., 03143, Kyiv, Ukraine,*
E-mail: zagorodnya.sveta@gmail.com

[2] *I. M. Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, 3, Krhizhanovsky st., 03142, Kyiv, Ukraine,*
E-mail: earsen@ukr.net

The search for safe substances for humans and the environment and ways to inactivate pathogens is one of the priority areas of research. It is known that under the action of UV radiation, mesoporous titanium dioxide (TiO_2) produces active oxygen-containing radicals that can damage biological molecules of pathogens. Photodynamic inactivation is already used to inactivate enveloped viruses such as human herpes simplex virus, vesicular stomatitis virus, human immunodeficiency viruses, and hepatitis B and C viruses.

In this study, we evaluated the possibility of using photodynamic ultraviolet treatment of synthesized titanium dioxide nanoparticles to inactivate human adenovirus type 5 (HAdV5). Adenoviruses are known to be very resistant to ultraviolet radiation. The suspension of TiO_2 in aqueous-glycerol solution (concentration 10 mg/ml) was irradiated with UV light (BactoSfera OBB 15P OZONE FREE, Ukraine) at a distance of 20 cm, a wavelength at the peak 254 nm, power 15 W, peak - 4.5 W for 0, 5, 10, 20 and 30 minutes. Virus-containing material with a titer of 5.0 log10 $TCID_{50}$ / ml was added to the nanoparticles, a series of 10-fold dilutions was prepared, and Hep-2 cells were infected. After 3-4 days of cultivation using MTT analysis, virus titers were determined. Inactivation of adenovirus by UV-photoactivated nanoparticles led to a decrease in virus titer by 4.5 $\log_{10}$ after 5 min of irradiation.

Thus, we have shown that the virus without the enveloped – HadV5 can be effectively inactivated by photoactivated titanium dioxide.

Co-doped CdS quantum dots and their bionanocomplex with protein: interaction and bioimaging properties

Stolyarchuk I.D.[1]***, Wojnarowska-Nowak R.***[2]***, Nowak S.***[2]***,***
Romerowicz-Misielak M.[2]***, Kuzyk O.V.***[1]***,***
Dan'kiv O.O.[1]***, Stolyarchuk A.I.***[1]

[1] *Department of Physics Drohobych Ivan Franko State Padagogical University, 24 I. Franko Str., 82100 Drohobych, Ukraine.*
E-mail: i.stolyarchuk@dspu.edu.ua

[2] *Center for Microelectronics and Nanotechnology, University of Rzeszow, 16C Rejtana Str., 35-959 Rzeszow, Poland*

[3] *Department of Animal Physiology and Reproduction, Institute of Applied Biotechnology and Basic Sciences, University of Rzeszow, Werynia 502, 36100 Kolbuszowa, Poland*

Semiconductor nanoparticles or quantum dots (QDs) constitute significant materials for many areas of nano- and biotechnology. One of the main decisive parameters for the use of QDs in bionanotechnology is the functionalization of their surface with appropriate (bio)molecules to ensure the stability of colloidal solutions in combination with effective labeling of the corresponding biological objects. It is the combination of nanoparticles with selected biological or chemical ligands, such as proteins, antibodies or DNA sequences etc., that leads to the creation of highly functional bionanomaterials (bionanocomplexes), which opens up the broadest prospects for their use in bio- and nanomedicine [1].

In the present work, we report on spectroscopy studies of interactions between colloidal CdS:Co diluted magnetic semiconductor QDs and model proteins type of human serum albumin (HSA). To probe this interaction, in addition to conventional UV-Vis absorption and photoluminescence spectroscopic methods we have used micro-Raman spectroscopy and technique of magneto-optical Faraday rotation, which is important for case of nanoparticles with magnetic impurities. It was proved that, in all cases, the fluorescence quenching of HSA by the QDs depends on the size, temperature and electron-deformation interactions. The low toxicity as well as high stability of the QDs - HSA bioconjugates in the case of their using as bio-imaging probes for the 143b osteosarcoma cells has been demonstrated.

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Atheroma regression with intermittent pneumatic compression

Vasylyuk S.V*[1]*., Zaitsev D.V*[2]*.

[1] *Kiyv national Taras Shevchenko university, Physics faculty,*
Volodymyrska str., 60, Kyiv-09102, Ukraine.
E-mail: svetlanafvasylyuk@server.com

[2] *Kundiiev Institute of Occupational Health of the NAMS of Ukraine,*
75 Saksagansky str., Kyiv, 01033, Ukraine.

Intermittent pneumatic compression (IPC) is used in patients with peripheral arterial disease and critical ischemia for its ability to increase arterial blood flow and having benefit on plasma lipids. We predicted that, under compensated lipids ratio, IPC can promote the resorption of cholesterol deposits within 1.5-3 years [1].

A 54-year-old woman was admitted with complaints of frequent episodes of dizziness. The patient followed a diet, took omega-3 drugs and had a regular aerobic activity. An ultrasound examination revealed atheromas in the arteria carotis bifurcation, up to 10% on the right, and 30% on the left. IPC procedures lasting 72 minutes were carried out once a week for two years with no additional treatment. Each of 10 chambers was inflated for 1 s with the pressure 50 mm Hg. Two years later, an ultrasound scan was performed again by the same doctor and device. Atheromas decreased on the right up to 5% and on the left up to 25%.

The formation of stable laminar blood flow changes the expression of shear-dependent genes of endothelial cells to anti-inflammatory and anti-atherogenic [2]. Surface contacts augmentation leads to acceleration of cholesterol molecular transport, macrophage and endothelial progenitor cells migration [3].

The paper considers the approach of pulse waves modelling using soliton theory. The basic idea is that the real pulse wave nature is very similar to the properties of solitons. The central role is played by the elastic interaction properties between solitons and solitons with local perturbations.

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Development of targeted cosmetic products based on clay/ hydroxyapatite /vegetable raw composite materials

Paientko V.V.[1], ***Skwarek E.***[1], ***Matkovsky O. K.***[2],
Oranska O.I.[2], ***Gun'ko V.M.***[2], ***Babenko L.M.***[3]

[1] Department of Radiochemistry and Environmental Chemistry,
Institute of Chemical Sciences, Faculty of Chemistry,
Maria Curie-Skłodowska University,
3 Maria Curie-Skłodowska Sq., 20-031 Lublin,
E-mail: payentkovv@gmail.com

[2] Chuiko Institute of Surface Chemistry,
02000, Kiev, 17 General Naumov Street;

[3] M.G. Kholodny Institute of Botany,
2 Tereshchenkivska Street, 01004 Kyiv, Ukraine;

New forms of delivery of bioactive substances (BAS) are an important and urgent problem of modern pharmacology and cosmetology. The use of carriers for BAS allows one to obtain dosage forms with improved compatibility with biological fluids, controlled time of entry into the body, high storage stability, etc.

By creating composites that will provide the necessary content of BAS and their controlled release, we can reasonably hope to achieve positive results in this direction.

This paper proposes the creation of composites based on clay minerals and hydroxyapatite, which provide various forms of inclusion of the active substance by optimizing the composition and improving the methods of formation. Significant hydrophilicity of clays increases the moisture content in the materials and, as a consequence, increases the content of BAS. Acai (EUTERPE OLERACEAE (ACAI) BERRY) powder was chosen as a source of BAS.

It has been proposed composite materials clay / vegetable raw materials / hydroxyapatite. The safety indicators of components and composite materials are studied. The possibility of their use in cosmetics is substantiated. The hypoallergenicity of the studied systems is confirmed. Kinetic studies of BAS release can be used as a factor in regulating the direction of preventive action of cosmetics.

Acknowledgements: The research leading to these results are supported by project BPS/UKR/2022/1/00065/U/00001 (NAWA Солідарні з Україною).

Synthesis and properties of composite materials clay / hydroxyapatite / Mentha piperita powder

Paientko V. V.[1], Skwarek E.[1], Matkovsky O. K.[2], Oranska O.I.[2],
Gun'ko V.M.[2], Babenko L.M.[3], Bakaieva O.D.[4]

[1] Department of Radiochemistry and Environmental Chemistry,
Institute of Chemical Sciences, Faculty of Chemistry,
Maria Curie-Skłodowska University,
3 Maria Curie-Skłodowska Sq., 20-031 Lublin, payentkovv@gmail.com

2 Chuiko Institute of Surface Chemistry,
02000, Kiev, 17 General Naumov Street;

[3] M.G. Kholodny Institute of Botany,
2 Tereshchenkivska Street, 01004 Kyiv, Ukraine;

[4] Vinnitsia National Pirogov Memorial Medical University,
21018, Vinnitsa, St. Pirogova, 56; olya.bakaieva@gmail.com

A wide range of therapeutic and prophylactic properties of clay minerals creates the prospect of using them as components of shampoos in the development of new formulations

To increase the effectiveness of clays that are part of shampoos, it is advisable to use their compositions with vitamins and other biologically active substances (BAS). Mentha piperita powder was chosen as the source of BAR. This plant has excellent cosmetic properties. Mint leaves contain essential oil, as well as phenolic acids, calcium, phosphorus, iron, magnesium and vitamin A, which have a positive effect on the skin.

Samples of clay / hydroxyapatite / vegetable raw materials were obtained by the method of mechanochemical activation. The release of anthocyanins from plant raw materials and clay / hydroxyapatite / plant raw materials composite was studied by UV spectroscopy. To assess the level of safety of the obtained materials was used software product "Rana" - an information system designed to store and organize the composition data and calculate the development of cosmetics and other products or fillers, determine their level of safety in terms of component composition of the final mixture.

Composite materials based on clays and vegetable raw materials are offered. The hypoallergenicity of the studied systems is confirmed. Kinetic studies of BAS can be used as a factor in regulating the direction of preventive action of shampoos.

Acknowledgements: The research leading to these results are supported by project BPS/UKR/2022/1/00065/U/00001 (NAWA Солідарні з Україною)

Session 3

Nanochemistry and biotechnology

Influence of anneal temperature on morphology, structure and chemical composition of zinc oxide films printed by 3D printer

Yermakov M.S., Dobrozhan O.A., Opanasyuk A.S.

Department of Electronics and Computer Technology, Sumy State University.
Rimsky-Korsakov str., 2, Sumy, UA-40007, Ukraine.
E-mail: m.yermakov@ekt.sumdu.edu.ua

Zinc oxide (ZnO) is of considerable interest to researchers due to its feasibility. This material has high radiation, chemical and thermal resistance and in the future can be widely used in the creation of elements of transparent electronics, gas sensors, ultraviolet detectors and more. Zinc oxide is a straight-band n-type semiconductor belonging to the group of compounds A_2B_6, its band gap at 300 K is ~ 3.27 eV. ZnO films can be used as elements of high-efficiency electronic auto emitters. a variety of optoelectronic devices, liquid crystal displays, photodiodes, window and conductive layers of solar panels and other electronic devices due to the high conductivity and transparency in the visible spectrum.

ZnO films were obtained on the cover glass by printing ink based on a suspension of nanocrystals synthesized by the polyol method. Because the ink contained organic substances as solvents, it was annealed for one hour in air and vacuum to remove uncontrolled impurities after film application. The annealing temperature was varied in the range from 200 °C to 400 °C.

As a result of research, it was established that the films were nanostructured, contained zinc and oxygen atoms, and the distribution of these elements by area was uniform. In addition to the main components of the material, the method of EDAX in the layers also recorded the carbon that is part of the developed ink. In some cases, because the applied films were thin, a peak of the Na element belonging to the glass substrate was observed. It was found that the concentration of carbon in the films decreased with increasing annealing temperature. However, the results of the study show that we failed to burn all the carbon that got into the organic films, so the time of their annealing in future work should be increased. It should be noted that during annealing the adhesion of the films to the glass substrate deteriorated sharply. This is due to the occurrence of large thermal deformations in the system, as the coefficients of linear expansion of materials differ significantly (α_{sl} = 5.9 × 10-6 °C, αZnO = 29.0 × 10^{-6} °C).

Thus, the annealing conditions of printed ZnO films are established, which allow to burn out impurities without disturbing the nanostructured state of the layers.

Polyfunctionality of the influence of a complex nanocomposite bacterial preparation azogran on plant productivity

Kurdish I.K., Skorochod I.O., Roy A.O., Chuiko N.V., Chobotar'ov A.Yu., Parkhomenko N.J., Chobotar'ova V.V.

Zabolotny Institute of microbiology and virology of NAS of Ukraine.
154, Acad. Zabolotny St., Kyiv, 03143, Ukraine.
E-mail: ivan.kurdish2016@gmail.com

The complex nanocomposite bacterial preparation Azogran was created on the basis of the interaction of highly active nitrogen-fixing bacteria *Azotobacter vinelandii* IMV B-7076 and phosphate-mobilizing bacteria *Bacillus subtilis* IMV B-7023 with nanoparticles of the clay mineral bentonite. In the process of such interaction, bacterial cells are covered with bentonite particles, in doing so increases their viability during storage and adhesion to the surface of plant seeds during their bacterization before sowing into the soil. Such treatment of seeds increases their germination and the formation of seedlings.

The interaction of these bacterial strains with the bentonite nanocomposite significantly affects their physiological and biochemical activity. Thus, during cultivation of these bacteria in nutrient medium that contained 0.05–0.5 g/L of bentonite nanoparticles, the growth and ATPase activity of these strains increased significantly. At treatment of plants by this preparation the content of phenolic compounds increased in their organism. These biological active substances can reduce the levels of reactive oxygen species in plant tissues, which accumulate at negative environmental factors. Furthermore, inoculation of seeds by Azogran significantly increased the antioxidant enzymes (peroxidase, superoxide dismutase and catalase) activities, content of chlorophylls and carotenoids pigments in different plant species (barley, marigold, beans).

We are being shown that the use of the Azogran increases the resistance of plants to phytopathogenic microorganisms and viruses, as well as to phytophages. The use of this preparation significantly reduces the infection of potato by phytoviruses. The Azogran significantly reduces the spread of the Colorado potato beetle in the potato phytocenosis and leads to the death of more than 65% of the larvae of this phytophage. The use of the complex bacterial preparation Azogran in crop production has a significant effect on the growth and development of plants, improving their nitrogen and phosphorus nutrition, stimulating their growth with biologically active metabolites, including phytohormones. The use of the nanocomposite complex bacterial preparation Azogran in crop production significantly increases plant productivity.

Hydrogen bonds and molecular recognition

Blyzniuk I.M., Zhytnikova M.Yu., Miroshnychenko K.V.,
Semenov M.A., Shestopalova A.V.

1Biophysical Department, O. Ya. Usikov Institute for Radiophysics and
Electronics, Natl. Acad. of Sci. of Ukraine, Acad.
Proskury Street, 12, Kharkiv, 61085, Ukraine.
E-mail: avshestopalova1@gmail.com

The emergence and development of life on Earth are based on incredible physical and chemical stability and, at the same time, the unique conformational mobility of the molecular building blocks of life, namely, proteins and nucleic acids. These properties of biopolymers are the basis for the implementation of a variety of intermolecular interactions, the results of which are the high efficiency and selectivity of molecular biological processes, as well as fast and accurate mechanisms of reproduction of living organisms.

The mechanisms of accurate molecular recognition are directly connected with the formation of intra- and intermolecular hydrogen bonds in biomolecular systems. It is hydrogen (H-) bonds that underlie the interactions of biopolymers with the molecular environment and the formation of both nonspecific and specific intermolecular complexes. The specificity is usually due to the simultaneous formation of several H-bonds between the spatially complementary donor and acceptor groups, which form a unique pattern depending on the sequence of monomers of the biopolymer chain (for example, patterns of donor-acceptor groups in the major groove of DNA double helix). The formation of the nonspecific H-bonds in molecular biological systems is also necessary because they are the basis for the formation of the secondary structure of proteins, the formation of the "spine" of hydration in the minor groove of the DNA double helix, or for the implementation of the indirect mechanism of protein-nucleic acid recognition. The intra- and intermolecular H-bonds formation are the key factors influencing both the stability of the DNA-ligand and DNA-protein complexes. They determine the specificity and binding affinity of such complexes as well as define the successful molecular recognition. H-bonds are observed in different nanosystems, for example, in associates of organic molecules. In particular, the description of the molecular mechanisms of the stability of such associates is a necessary step for the prediction of the changes in the biological activity of some drugs upon interaction with target molecules. This information is also necessary for the implementation of targeted drug delivery using nanocomposites.

In conclusion, it should be emphasized that the implementation of the processes described above is substantially determined by the possibility of the formation and disruption of H-bonds typical of the nanosystems in which the processes occur. Apparently, H-bonds are one of the essential fundamental conditions for the successful self-organization of some nanosystems «from bottom to up».

Development and characterization of new biocomposite based on PTFE, TiO_2 and *Luffa cylindrica* fibers

Mounir Sahli1*, Steve Rudz[2], Khaled Chetehouna[3], Rabah Bensaha[1]

**corresponding author: sahlimounir@umc.edu.dz*

[1] *Constantine Ceramics Laboratory, Université des Frères Mentouri Constantine 1, Constantine, Algeria.*

[2] *GREMI, UMR 7344, Université d'Orléans/CNRS, F-18020, Bourges Cedex, France*

[3] *INSA Centre Val de Loire, Laboratoire PRISME, EA 4229, 18020 Bourges, France*

Abstract

The current research focuses on the use of *Luffa Cylindrica* fibers as a reinforcing agent in a fluoroplastic polymer matrix (PTFE) and TiO_2 nanoparticles as a photocatalytic agent in various mass fractions (percentage) for the development and physical characterization of new biocomposite materials. The three sample configurations are PTFE, TiO_2, *LC* = (65 : 5 : 30), (70 : 5: 25), and (60: 5: 35) % (in terms of mass fraction). Dynamic light scattering and laser Doppler velocimetry are used to determine the granulometry and zeta potential. Then, the structural and vibrational properties of the PTFE/TiO_2/*LC fiber* composites are both characterized by micro-Raman spectroscopy in an oblique backscattering configuration and FTIR spectroscopy. Finally, thermal properties are investigated using TGA and DSC. Among all the tested mass fractions, sample 2 (70% PTFE : 5% TiO_2 : 25% *LC*) offers the most interesting characteristics with a reasonable stability of colloidal dispersion and thermal degradation.

The next step in this work will be the characterization of this new biocomposite in terms of mechanical and tribological properties.

Keywords : luffa cylindrica, biocomposite, thermal degradation, PTFE, TiO_2.

Extraction of organosolv pulp and nanocellulose from post-harvest residues of corn

Barbash V.A.[1], Yashchenko O.V.[1], Yakymenko O.S.[1],
Horianoi V.A.[1], Myshak V.D.[2]

[1] *Department of Ecology and Technology of Plant Polymers,*
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prospect Peremogy, 37, Kyiv-03056, Ukraine.
E-mail: v.barbash@kpi.ua

[2] *Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine, Kyiv, Ukraine.*

Nanocellulose is a biodegradable material with high mechanical strength, transparency and chemical resistance, light weight and low coefficient of thermal expansion. Nanocellulose is widely used in industry to increase the mechanical strength and improve the barrier properties of paper and cardboard, polymer and cement composites, electric batteries and sorbents [1]. The study described the extraction of nanocellulose from corn pulp (OCP), obtained by environmentally friendly organosolv method of delignification of post-harvest corn residues by extraction with NaOH solution and cooking using a mixture of acetic acid and hydrogen peroxide [2]. A stable transparent nanocellulose gel was extracted from OCP by acid hydrolysis followed by ultrasonic treatment. It was found that an increase in the consumption of sulfuric acid, temperature and duration of the OCP hydrolysis process improves the quality indicators of corn nanocellulose. This dependence of nanocellulose quality indicators on the technological parameters of the hydrolysis process is typical for nanocellulose from other representatives of renewable plant materials (wheat straw, reeds, flax, hemp, kenaf, miscanthus) [3].

Morphological (SEM), structural (FTIR and XRD) and thermal characterization (TGA) of non-wood plant raw materials, OP and nanocellulose were carried out. Nanosizes of nanocellulose were confirmed by AFM and TEM methods. The values of particle sizes of nanocellulose and their mechanical properties (density, tensile strength) and transparency were established.

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NIR pentamethine cyanine dyes as fluorescent probes for live-cell imaging

Aristova D.[1], **Kot Y.**[2], **Chernii S.**[1], **Kot K.**[2],
Kompaniiets A.[2], **Yarmoluk S.**[1]

[1] *Institute of Molecular Biology and Genetics NASU,*
150 Zabolotnogo St., 03143 Kyiv, Ukraine.
E-mail: dar.arist@gmail.com

[2] *V.N. Karazin Kharkiv National University,*
4 Svobody Sq., 61022 Kharkiv, Ukraine.

Near-infrared (NIR; 650–900 nm) fluorescence imaging is an active and promising area for live-cell imaging. The NIR-emitted fluorescent dyes offer low energy of the excitation light, helping to avoid the phototoxicity effect and unwanted autofluorescent background. Therefore, it was decided as a promising study to evaluate NIR-emitted (675 – 710 nm) pentamethine cyanine dyes as fluorescent probes for live-cell visualization by fluorescence microscopy.

Spectral-luminescent properties of the dyes in a free state and the presence of nucleic acids and serum albumins were characterized. Dyes possess low to moderate fluorescence intensity in a free state, but it increases while binding to serum albumins up to 160 times with a quantum yield value equal to 42%. We have studied the ability of the dyes to stain live mesenchymal stem cells from rat bone marrow (MSC) at a concentration 1μM. The dyes can penetrate the cell but have different selectivity to cell compartments. Dyes 1753Sl and 1759Sl accumulate in intracellular vesicles. Furthermore, we have confirmed that the dye 1753Sl visualizes autophagosomes and can be a marker of cell aging. At the same time, cyanine dyes 1756Sl and 1872Sl accumulate in cell mitochondria. The selectivity of 1872Sl towards mitochondria does not depend on the depolarization degree of the mitochondrial membrane, while 1756Sl stains only mitochondria with depolarized membrane.

Besides this, we performed a cytotoxicity study that included measuring the level of reactive oxygen species (ROS), determining the degree of damage to the plasma membrane of cells, and detecting apoptosis. The presence of cyanine dyes 1753SI, 1756SI, 1872SI, and 1759SI at a working concentration of 1μM does not damage the plasma membrane, does not increase ROS content, and does not induce apoptosis of bone marrow mesenchymal stromal cells.

Thus, due to low cytotoxicity and selectivity to cell compartments, we can suggest the studied NIR-emitted pentamethine cyanine dyes as potential fluorescent probes to visualize live cells by fluorescence microscopy.

Promising nanobiotechnology to increase the shelf life of chicken eggs based on nanosilver preparation in hybrid carriers

Zheltonozhskaya T.[1]**, *Shevchenko L.***[2]**, *Permyakova N.***[1]**,**
Dovbnia Y.[2]**, *Klepko V.***[1]**, *Klymchuk D.***[3]

[1] *Department of Polymer Physics, Institute of Macromolecular Science of the NAS of Ukraine, 48 Kharkivske Shosse, 02160 Kyiv, Ukraine.*
E-mail: zheltonozhskaya@ukr.net

[2] *Department of Veterinary Hygiene, National University of Life and Environmental Sciences of Ukraine,*
15 Heroyiv Oborony St., 03041 Kyiv, Ukraine.

[3] *Laboratory of Electron Microscopy, M.G. Kholodniy Institute of Botany of the NAS of Ukraine, 2 Tereshchenkivska St., 01601 Kyiv, Ukraine.*

A simple and effective nanobiotechnology is proposed, aimed at reducing the endogenous and exogenous contamination of chicken eggs by opportunistic and pathogenic microflora in the processes of their formation and subsequent storage. The key element of this nanobiotechnology is a special preparation of nanosilver (d_{av}=2.4±1.0 nm), stabilized in biocompatible and biodegradable hybrid carriers (Figure), which is orally administrated to laying hens with drinking water.

In this paper, various aspects of obtaining a nanosilver preparation in hybrid solutions and possible changes in its state under the influence of factors such as the pH of the solution, the concentration of nanoparticles, the presence of NaCl as in a "physiological solution", as well as visible light are considered. The high stability of this preparation in hybrid

Then the results of systematic studies of the biological impact of the developed nanosilver preparation on the clinical condition of laying hens, morphological and biochemical parameters of their blood, as well as morphological, microbiological and chemical parameters of chicken eggs are represented. A striking effect of the selective accumulation of nanosilver in the eggshell was found without deterioration in the condition, blood parameters and productivity of laying hens.

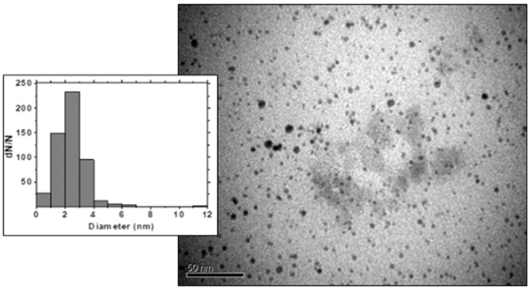

Fig. *TEM image of a nanosilver preparation in hydrophilic hybrid carriers*

The effect of cerium dioxide nanocrystals on the oxidative stress parameters in irradiated human skin mesenchymal stem cells-embedded scaffolds

Kot Yu.[1], Kot K.[1], Klochkov V.[2], Kavok N.[2], Yefimova S.[2], Trufanova N.[1,3], Petrenko O.[1,3], Tkachenko A.[4], Prokopiuk V.[3,4], Onishchenko A.[4], Kulyk M.[1]

[1] V. N. Karazin Kharkiv National University, biochemistry department,
4 Svobody Sq., Kharkiv, 61022, Ukraine.
E-mail: kot.juriy@gmail.com

[2] Institute for Scintillation Materials of NAS of Ukraine, Nanostructured
Materials Department named by Yu.V. Malyukin,
Nauky ave. 60, Kharkiv, 61072, Ukraine.

[3] Institute for Problems of Cryobiology and Cryomedicine of NAS of Ukraine,
Pereyaslavska 23, Kharkiv, 61015, Ukraine.

[4] Kharkiv National Medical University,
Nauky ave 4, Kharkiv, 61022, Ukraine.

Cerium dioxide nanocrystals (CeO_2) are today one of the most promising classes of antioxidant materials.

The aim of the study was to substantiate experimentally *in vitro* the possibility of using CeO_2 nanocrystals as an antioxidant for cell therapy of radiation burns.

Spherical CeO_2 nanoparticles (D=1-2 nm) were synthesized in the Nanostructured Materials Department named by Yu.V. Malyukin of Institute for Scintillation Materials of NAS of Ukraine.

The work was carried out on human skin mesenchymal stem cells-embedded scaffolds (hsMSCs-scaffolds). Cells subcultured until passage 3 (Eppendorf Galaxy 14S, 37°C, 5%CO_2, 99% RH) with viability of 86% (Invitrogen Countess Counter) were then seeded on a highly porous 3D cell culture polystyrene scaffold (Alvetex Scaffold, 96 well, REPROCELL) and cultured for 10 days until the culture density of 84%. 1 hour prior to irradiation, a suspension of nanoparticles was added to the culture medium (αMEM + 10% FBS, Gibco) to a final concentration of 10, 20 and 40 nM), and incubated for 1 hour (Eppendorf Galaxy 14S, 37°C, 5% CO_2, 99% RH).

After replacing the medium with nanoparticles free one, the cells were irradiated on the gamma complex Rokus AM (Co^{60}). The dose of irradiation was 0.75 Gy (104kV, 9mA, 0.2 Gy/min, duration of irradiation – 225 sec).

Two and six hours after irradiation, the fluorescence imaging (Olympus FV10iLIV confocal microscope, cellSense software), fluorimetric determination (Biotek FL600 reader, KC4 software) of the concentration of reactive oxygen species (ROS) (DCFDA, Ex/Em=495/529 nm), lipid hydroperoxides (MitoPeDPP, Ex/Em=452/470 nm), determination of the degree of DNA fragmentation by comet analysis (Mupid-exU System, Alpha Innotech Red™ Imaging System, CASPlab software), spectrophotometric determination (Biotek FL600 reader, KC4 software) of the enzymatic activity of superoxide dismutase and catalase (Abcam kits) were carried out in the hsMSCs - scaffolds.

It was shown that in the absence of irradiation, nanoparticles at concentrations of 10 and 20 nM do not cause changes in the studied parameters. The concentration of the nanoparticles 40 nM caused a decrease in cell viability by 7% after 6 hours of cultivation on a background of absence of changes in other parameters. This concentration also proved to be ineffective for maintaining the vitality of cells after irradiation - the number of living cells decreased both in the presence and absence of nanoparticles after 6 hours of cultivation by 28%. Pre-incubation with nanoparticles at a concentration of 10 and 20 nM resulted in an increase in the number of living cells in culture 6 hours after irradiation by 11% and 17%, respectively, compared with irradiated cells non- preincubated with nanoparticles.

In 2 and 6 hours after irradiation, the concentration of ROS and lipid hydroperoxides increased by 6.2 and 8.5 times, respectively, in the culture. The degree of fragmentation of nuclear DNA increased by 6.5 times. In this case, the activity of SOD and catalase decreased by 6 hours of observation for 3.6 and 5.8 times, respectively.

Pre-incubation with CeO_2 nanoparticles at all used concentrations resulted in a significant decrease in prooxidant indices in irradiated culture. Herewith, the most prominent protective effect was provided by the concentration of 20 nM – for 6th hour of cultivation after irradiation, the concentration of ROS and lipid hydroperoxides was respectively 46% and 29% less, and the activity of SOD and catalase was 71% and 108% higher than in irradiated culture without nanoparticles. At the same time, regardless of the concentration of nanoparticles, the degree of DNA fragmentation remained at the level of irradiated cells without nanoparticles, which apparently is either a consequence of long-term effects of ROS overproduction or the inability to fix defects by cell repair systems over the past observation time.

Thus, spherical nanoparticles CeO_2 (D=1-2 nm) at a concentration of 20 nM can be used in cell therapy of skin lesions to normalize the prooxidant-antioxidant balance.

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Study of Z-E isomerization of 6-methacryloxy-x'-metoxiaaurons

Martynes-Harsiia A., Iukhymenko N., Kolendo A.

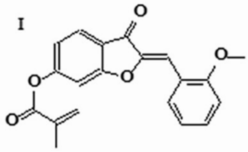
Taras Shevchenko National University of Kyiv, Faculty of Chemistry.
street Volodymyrska, 64, Kyiv, 01033 Ukraine.
E-mail: yukhimenko.n@gmail.com

The development of modern technologies raises the problem of creating new polymeric materials with a given set of properties that do not have known polymers. One of the current problems of modern polymer chemistry is the creation of "smart" polymers.

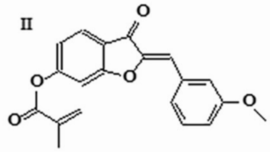
To create such polymers, we have synthesized new methacrylic monomers based on aurons.

The original phenylaurons were synthesized by the condensation reaction of 3-coumaranone with 4-hydroxybenzaldehyde in a mixture of DMF-ethanol solvents in alkaline medium [1]. Acylation of phenylaurons with methacrylic acid chloride in the presence of triethanolamine under cooling gave new methacrylic derivatives (I-III) [2].

I



II



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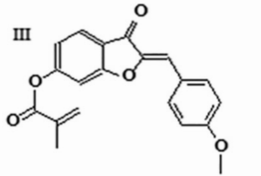


Studies of Z-E photoisomerization of new methacrylic monomers I-III under the action of UV radiation were performed in dioxane

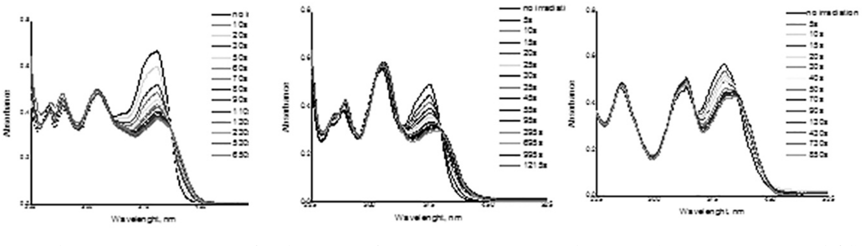


Fig. *Absorption spectra of solutions of monomers I-III in dioxane (C = 1 × 10^{-5} mol / l) at different irradiation times: a) (0 (curve 1) - 650 s (curve 14)), b) (0) (curve 1)) - 1215 s (curve 15)), s) (0 (curve 1) - 650 s (curve 14)) UV light (λmax - 500 nm)*

Based on the data obtained from the absorption spectra, the values of the reaction rate constants Z-E of photoisomerization of new methacrylic monomers of I-III monomers and half-lives were calculated. It is concluded that the substitution in the benzene ring affects the rate of the Z-E photoisomerization process.

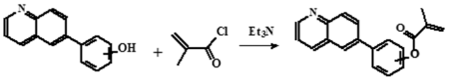
Synthesis of new metacrylic monomers based on quinoline-phenyl methacrylates for thermostabilization of polystyrene

Tymoshyk A., Martynes-Harsiia A., Iukhymenko N., Kolendo A.

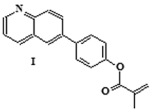
Taras Shevchenko National University of Kyiv, Faculty of Chemistry.
street Volodymyrska, 64 Kyiv 01033 Ukraine.
E-mail: yukhimenko.n@gmail.com

Polymeric materials are widely used in various fields of human activity, meeting the needs of industry, agriculture, medicine, culture and everyday life. To date, much attention is paid to the development of new polymeric materials with a given set of properties that do not have known polymers. One of the current problems of modern polymer chemistry is the creation of "smart" polymers.

To create such polymers, we have synthesized new methacrylic monomers based on quinoline-phenyl-methacrylates.



Acylation of quinoline-phenols with substituents in the 2nd and 3rd positions was performed with methacrylic acid chloride in the presence of triethanolamine and new methacrylic derivatives were obtained under cooling. (I-IV).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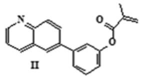
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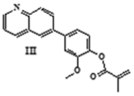
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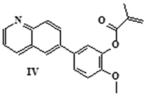
IV

Purification of new methacrylates was performed from a water-alcohol mixture, the yield was 60-80%. The structure of the compounds was proved by spectral methods.

Mechanism of methanol interaction with defects on graphene-like materials: quantum chemical study

Karpenko O.S.[1], **Bychko I.B.**[2], **Strizhak P.E.**[2]

[1] *Chuiko Institute of Surface Chemistry of the NAS of Ukraine,*
General Naumov Str., 17, Kyiv-03164, Ukraine.
E-mail: karpenkooksana@ukr.net

[2] *L.V. Pisarzhevsky Institute of Physical Chemistry of the NAS of Ukraine,*
Prospect Nauki, 31, Kyiv-03028, Ukraine.

Methanol conversion to dimethyl ether or formaldehyde are large-scale industrial processes. According to this, huge attention focused on finding ways to reduce the cost of relevant processes. Developing of the carbon catalysts for presented processes is one of the main route to reduce the cost of the methanol conversion. There are presented experimental works where carbon materials, particularly, carbon nanotubes [1], activated carbon, graphene materials are used as catalysts. However, reaction mechanisms of methanol conversion interaction in carbon materials is still under discussion.

This report presents the results of quantum chemical calculations by the method of density functional theory (DFT, B3LYP/6-31G+(d,p) with the involvement of Grimme dispersion correction) of the main elementary stages of methanol dehydration to dimethyl ether and dehydrogenation to formaldehyde on graphene-like materials (GLM). As models of GLM was used the polyaromatic molecule $C_{96}H_{24}$ (hydrogenated graphene) and its derivatives. Where considered two cases of methanol interaction: with point defects on $C_{96}H_{24}$ (single vacancy) and with $C_{96}H_{24}$ functionalized by oxygen functional groups like hydroxyl (–OH) and carboxyl (–COOH). The systems were tested under different conditions of multiplicity. Computed reaction profiles of the reactions were investigated. The role of the water molecule in the reaction of methanol dehydration to dimethyl ether was studied. Obtained results shows that active sites in dehydration reaction are hydroxyl and carboxyl group and in dehydrogenation reaction – single vacancy.

This work was supported by the National Research Foundation of Ukraine (grant 2020.02/0050).

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In silico and *in vitro* studies of combined actionof C_{60} fullerene with cis-Palladium(II)3-(2-pyridyl)-5-methyl-1,2,4-triazole

Grynyuk I.I.[1]***, Grebinyk A.G.***[2]***, Prylutska S.V.***[3]***, Hurmach V.V.***[4]***,***
Matyshevska O.P.[5]***, Prylutskyy Yu.I.***[4]***, Frohme M.***[2]

[1] *Igor Sikorsky Kyiv Polytechnic Institute,*
Peremohy av., 37, Kyiv 03056, Ukraine
E-mail: igrynyuk@yahoo.com

[2] *Technical University of Applied Sciences of Wildau,*
1 Hochschulring Str., Wildau, 15745, Germany

[3] *National University of Life and Environmental Science of Ukraine,*
Heroyiv Oborony Street, 15, Kiev 03041, Ukraine

[4] *Taras Shevchenko National University of Kyiv,*
64 Volodymyrska Str., Kyiv, 01601, Ukraine

[5] *Palladin Institute of Biochemistry of NAS of Ukraine,*
Leontovicha Street, 9, Kiev 01030, Ukraine

The creation of less toxic structural analogues of known effective drugs and their modulation by nanostructures in order to enhance the cytotoxic effect is relevant nowadays. Promising compound in this regard are *cis*-Palladium(II)3-(2-pyridyl)-5-methyl-1,2,4-triazole (*cis*-Pd(HL)C_{12}). C_{60} fullerene nanostructure can be a modulator of biological action of *cis*-Pd complex.

The aim of the work was to study interaction of DNA with cis-Pd(HL)Cl_2 separately and in combination with C_{60} fullerene and to estimate their influence on normal and leukemic cells.

Cis-Pd(HL)Cl_2 (the purity of compound was ≥98%) was synthesized at Taras Shevchenko National University of Kyiv (Ukraine). A highly stable water colloid solution of C_{60} fullerene (10^{-4} M, purity >99.5%) was synthesized at Technical University of Ilmenau (Germany).

By using computer modeling it was shown that cis-Pd(HL)Cl_2 form stable complexes with DNA separately and in combination with C_{60} fullerene.

Compound cis-Pd(HL)Cl_2 in range concentration 0,5 – 5 μM did not cause hemolytic effects. Erythrocytes hemolysis was observed in the presence 10 μM *cis*-Pd (HL)Cl_2, C_{60} fullerene prevented cis-Pd(HL)Cl_2-induce hemolytic effect.

Cis-Pd complex showed cytotoxic effect on leukemic CCRF-CEM cells at concentrations 1.5 μM after 72 h. 0.5 μM *cis*-Pd complex did not affect on the viability of CCRF-CEM cells, however, at the combined action with C_{60} fullerene this parameter decreased by 50% after 48 h incubation and kept at the same level within 72 h. Both significant decrease of CCRF-CEM cells number and their morphological changes were detected at combined action of *cis*-Pd complex and C_{60} fullerene.

Thus, *cis*-Pd complex showed a pronounced cytotoxic effect on leukemic cells, which was intensified at combined treatment with C_{60} fullerene.

Saponite based composite materials for removal of inorganic toxicants

Bondarieva A.**, **Yu J.**, **Tobilko V.

Department of Chemical Technology of Ceramics and Glass,
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute".
Ave. Peremohy 37, Kyiv-03056, Ukraine
E-mail: a.i.bondarieva@gmail.com

One of the most dangerous pollutants in groundwater and wastewater are inorganic toxicants in anionic forms. Nowadays, adsorption technologies are the most effective for treating water systems from contaminants of this type. For this reason, the important task is to modernise this technology constantly, including path obtaining new, highly efficient, low-cost and technologically simple sorbents.

Sorbents fulfil these requirements based on clay minerals. Among them is saponite (Sap), use of it is possible due to properties such as high surface area and cation exchange capacity. Nevertheless, the natural saponite is characterised by relatively low adsorption capacity. Therefore, the further modification of Sap is necessary to make it more competitive in its practical application. For this purpose, the use of iron (III) oxides-hydroxides is promising, which are characterised by high values of the specific surface area and increased reactivity due to a large number of hydroxyl centres.

This work aimed to obtain composite material based on natural saponite (Tashkiv deposit, Ukraine) to remove anionic forms toxicants from water systems. Modifications of saponite were performed with Co-doped iron-based layered double hydroxides subject to different molar ratios of clay:modifier.

The structure of materials is studied using physicochemical methods (X-ray powder diffraction and the low-temperature N_2 adsorption-desorption method).

The adsorption experiments were performed in the range of initial concentrations, under static conditions, at room temperature (20 ± 2 °C), and the ratio of solid and liquid phases S:L = 1:500. The equilibrium As(V) and Cr(VI) concentrations were determined by the inductively coupled plasma atomic emission spectroscopy (Thermo Scientific iCAP 7400 ICP-OES, USA).

The results showed that the synthesised materials have significantly higher sorption properties than the original saponite or ferrihydrite. It indicates the prospects for using such materials to purify contaminated water from heavy metal anions.

Analysis of the effect of $AlCl_3$ and $FeCl_3$ concentration in BSA solutions on the parameters of film textures upon reaching the isoelectric point

Glibitskiy D.[1]*, Gorobchenko O.*[2]*, Nikolov O.*[2]*, Cheipesh T.*[3]*,*
Dzhimieva T.[3,4]*, Zaitseva I.*[4,5]*, Zibarov A.*[6]*, Roshal A.*[6]*,*
Semenov M.[1]*, Khrebtova A.*[1]*, Glibitskiy G.*[1]

[1] *Department of biological physics, O.Ya. Usikov Institute for Radiophysics and Electronics, National Academy of Sciences of Ukraine,*
Kharkiv, 61085, Ukraine.
E-mail: dima.glib@gmail.com

[2] *Department of molecular and medical biophysics, School of radiophysics, biomedical electronics and computer systems, V.N. Karazin Kharkiv National University, Kharkiv, 61022, Ukraine.*

[3] *Chemical faculty, V.N. Karazin Kharkiv National University,*
Kharkiv, 61022, Ukraine.

[4] *V.N. Karazin Kharkiv National University, Kharkiv, 61022, Ukraine.*

[5] *O.M. Beketov National University of Urban Economy,*
Kharkiv, 61002, Ukraine.

[6] *Institute for Chemistry, V.N. Karazin Kharkiv National University,*
Kharkiv, 61022, Ukraine.

A method for assessing the effect of physicochemical factors on biopolymers by analyzing textures on films resulting from their dried solutions was previously presented. The main parameters for describing textures in this method are the specific length Lspec and the number of segments of zigzag patterns N_{segm}.

In the present work, analysis of the influence of different concentrations of $AlCl_3$ and $FeCl_3$ (from 0.1 to 0.4 mmol/l) on the change in texture parameters has been performed. It was found that with pH values going from 3.58 to 3.38, the decrease in N_{segm} and L_{spec} for $AlCl_3$ ranges from 5000 to 1800 and from 4.2 to 2.6, respectively. In $FeCl_3$ solutions, the decrease of pH from 2.8 to 2.46 results in decreasing N_{segm} and L_{spec} from 6400 to 0 and from 6 to 0, respectively.

The decrease in N_{segm} and L_{spec} correlates with the onset of BSA precipitation in solutions at pH < 3.7 ($AlCl_3$) and pH < 3 ($FeCl_3$), which may be due to the reentrant condensation in solutions due to a significant decrease in the absolute value of the protein surface potential.

Thus, it can be concluded that the dominant factor in the change in N_{segm} and L_{spec} is the change in the concentration of Al^{+3} and Fe^{+3} ions.

Nanostructural and biocolloid transformations of bottom sea sediments and physicochemical methods of their separation

***Panko A.V.*[1], *Kovzun I.G.*[1], *Prokopenko V.A.*[1],**
***Nikipelova O.M.*[2], *Tsyganovich O.A.*.[1]**

1 F.D. Ovcharenko Institute of Biocolloidal Chemistry of NAS of Ukraine,
42, Ak.Vernadskogo Blvd., Kyiv, Ukraine,03142. E-mail: gr.k.ibcc@ukr.net

2 Engineering and Technology Institute "Biotechnika" of NAAS of Ukraine,
26, Maiakska St, Khlibodarske, Odes'ka oblast, 67667

According to the experimental, and theoretical data obtained for the composing generalized physical, biocolloid-chemical, and microbiological models of transformation of marine sediment iron-aluminosilicates under the action of natural synergically correlating factors, the possibility of separating their components in different methods has been established, and that is generally confirmed by literature data [1, 2]. Improving such methods was done using previously developed [1] and partially generalized ideas about biocolloidal mechanisms of various silicates and metal oxides release from sediments. Thus, according to the obtained data, the separation of various oxides, such as iron and manganese, from iron-aluminosilicate precipitates is possible due to bacterial processes, which are further accompanied by chemical and physicochemical nanostructural transformations. Confirmation of such transformations is demonstrated by the example of synergically correlating parameters of viscosity, iron and manganese ion concentration, and microorganism count (CFU) for different iron-aluminosilicate model systems, as well as by changes in the microorganism count in biocenoses of natural dispersed iron-aluminosilicate compositions. Features of physicochemical methods of separation of biocolloidally treated sea and lake sediments are considered, which will allow obtaining of iron and iron-polymetallic concentrates based on Fe-Mn compositions without harmful impurities Si, S, P, and As.

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Bifunctional dextran conjugate with porphyrin- and cyanine-based telomerase inhibitors

Dubey L.V., Kuziv Ia.B., Kryvorotenko D.V., Negrutska V.V., Dubey I.Ya.

Institute of Molecular Biology and Genetics, NAS of Ukraine, 150
Zabolotnogo str., 03143 Kyiv, Ukraine
E-mail: dubey@imbg.org.ua

The majority of cancer cells express high levels of telomerase, the enzyme that synthesizes the telomeric DNA. Telomerase inhibitors have antitumor properties, so this enzyme is a promising target for antitumor therapy. Anticancer agents often suffer from toxicity, low specificity and poor water solubility. To overcome these issues, the drugs can be attached to some biocompatible hydrophilic polymers, such as polyethylene glycol or dextran.

We prepared a nanoconjugate of dextran polysaccharide (MW 40 kDa) bearing the simultaneously attached telomerase inhibitors of two classes, namely tricationic porphyrin TMP3 and cyanine LO13 [1]. Both drugs were functionalized with carboxyl groups. Dextran was modified with aminoalkyl linkers containing the disulfide bonds. It was treated with carbonyl diimidazole in DMSO-pyridine, and then the activated polymer reacted with cystamine. The COOH groups of TMP3 and LO13 derivatives were activated by the phosphonium reagent BOP in the presence of 1-hydroxybenzotriazole in dry DMF, and the active esters were sequentially coupled with amine-modified dextran in aqueous-organic medium (DMF/carbonate buffer, pH 8). The resulting conjugate structure is:

$$\textbf{Dex}\text{–OCONH(CH}_2\text{)}_2\text{SS(CH}_2\text{)}_2\text{NHCO(CH}_2\text{)}_n\text{–}\textbf{Inh}$$

(**Dex** – dextran, **Inh** – inhibitors, $n = 2$ for LO13 and 4 for TMP3)

The UV-Vis spectrum of dual conjugate contains the porphyrin and cyanine adsorption bands at 425 and 492 nm, respectively. TMP3 and LO13 content in various samples of the product was 10-15 μmol/g. This material is well soluble in water and sufficiently stable. Linker groups between dextran and the inhibitors contain the biolabile S-S bonds that can be cleaved in the cell by reducing agents like glutathione to release the drugs. The overnight treatment of the conjugate with 50 mM dithiothreitol (pH 7.5) resulted in the cleavage of both inhibitors from the polymer carrier. The study of biological activity of the conjugate is in progress.

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Antimicrobial properties of nanocomposite biomaterial for the treatment of purulent wounds and infected ulcers

Sukhodub L.F.,Kumeda M.O., Derevianko V.G., Sukhodub L.B.

Sumy State University

One of the important problems of modern surgery is the treatment of trophic ulcers of venous origin, which affect up to 3% of the population of industrialized countries. No less important is the issue of the ever-increasing resistance of microbial cells that contribute to the development of purulent-inflammatory processes to antibacterial drugs. All this encourages the search for new methods and materials for the treatment of purulent-inflammatory diseases without the use of antibiotics or with restrictions on their use, which determines the relevance of this problem. The proposed antiseptic biocomposite scaffolds can potentially be used for the treatment of patients suffering from purulent wounds and infected ulcers of the lower extremities of venous or arterial origin, including microcirculation disorders in diabetes. The apatite-polymer scaffold is a macroporous three-dimensional network formed by the polyelectrolyte interaction between macromolecules of polymers of natural origin - sodium alginate (Alg) and chitosan (CS), in the pores of which immobilized particles of calcium deficiency hydroxyapatite. The surface chitosan layer of the scaffold is additionally doped with divalent metal ions Ca^{2+}, Zn^{2+}, Mg^{2+}, Cu^{2+}, and Fe^{2+}, which form chelate complexes with CS and have enhanced antimicrobial action [1]. The figure shows the antimicrobial action of scaffolds containing metal ions in the form of growth inhibition zones of Gram-positive S. Aureus ATCC 25923 and Gram-negative E.

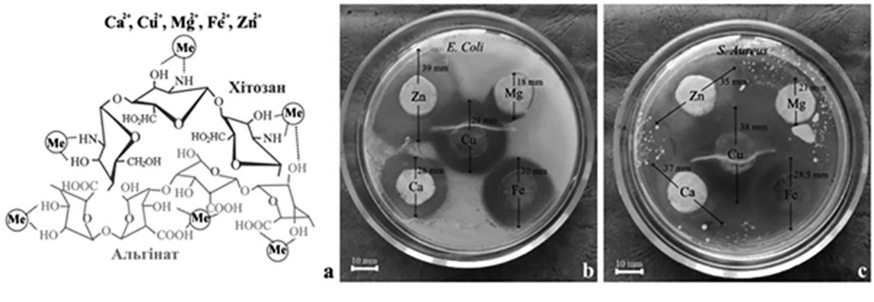

***Fig.**- a) scheme of interaction of polymer macromolecules with metals; b, c) the results of the study of antimicrobial activity of experimental samples.*

coli ATCC 25922 microorganisms. To assess the antiseptic ability of experimental samples against the studied test strains of microorganisms, the calculation of the integrated indicator (A) of their antimicrobial activity was performed [2]. The applied vector theory allowed to present A as a vector in n-dimensional space with coordinates in the form of a zone of growth inhibition for each test microorganism. The results showed that the value of A for samples containing ions Ca^{2+}, Zn^{2+}, Mg^{2+}, Cu^{2+}, Fe^{2+} is 1.85, 2.08, 1.1, 1.9, 1.65, respectively. Thus, according to the guidelines with an efficiency range of more than 1.5, all samples, except Mg^{2+} - containing, are those that show average antimicrobial activity, and Zn^{2+} - close to Chlorhexidine (2.07).

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The synthesis of irregularly shaped gold nanoparticles using natural polyphenols

Mariychuk R.[1], _Smolkova R._[1], _Eliašová A._[1],
Grishchenko L.M.[2], _Diyuk V. E._[2], _Lisnyak V.V._[2]

[1] *Department of Ecology, Faculty of Humanities and Natural Sciences,*
University of Prešov in Prešov, 17th November
Str. 1, 08001, Prešov, Slovakia.
E-mail: ruslan.mariychuk@unipo.sk

[2] *Taras Shevchenko National University of Kyiv, Volodymyrska Str. 62a,*
01601 Kyiv, Ukraine.

The synthesis of gold nanoparticles (AuNPs) using plant extracts has recently gained new importance due to its simplicity against the background of cost-effectiveness and environmental friendliness. Moreover, the biocompatibility of phytosynthesized AuNPs opens up opportunities for their biomedical applications. Biomolecules in the plant extract can reduce Au^{3+} cations to metallic gold (Au^0). But they also have an influence on the morphology of the forming AuNPs, determining size and shape. Control over the morphology of nanogold makes it possible to control the optical properties. Currently, the researchers focus their interest on the bio-synthesis of irregularly shaped AuNPs. They can find applications in biomedicine due to their response in the near-infrared region.

Despite the simplicity, the complexity of the composition of plant extracts requires an understanding of what role different biomolecules play in the formation, growth, and stabilization of AuNPs. The known protocol for the synthesis of irregularly shaped AuNPs (nanorods, nanostars, nanohexagons, etc.) requires the use of toxic surfactants. Therefore, the presented study was aimed at finding alternative shape-forming biomolecules from plant extracts, such as polyphenols.

Several polyphenols are the major components of Melissa extracts. Typically, they are peppery acid, rosmarinic acid, caffeic acid, gallic acid, and several others. These components were used to synthesize irregular AuNPs. The obtained nanocolloidal solutions were examined by UV-Vis-NIR spectroscopy and transmission electron microscopy. Molecular and structural transformations of organic compounds were studied by NMR analysis. The results showed that the form of AuNPs depends on various factors, such as the concentration and ratio of reagents, temperature, and pH level. The interplay between factors was analyzed, and the respective dependences were proposed.

Increased synthesis of biologically active components of medicinal mushrooms

Poyedinok N.L.[1], Galkin O.Yu.[1], Negriyko A.M.[2], Dubova H.Ye.[1]

[1] *National Technical University of Ukraine "I. Sikorsky Kyiv Polytechnic Institute"*
Peremohy Ave, 37, Kyiv-03056, Ukraine.
E-mail: hdubova16@gmail.com

[2] *Institute of Physics of National Academy of Sciences of Ukraine, 03028, Kyiv, Ukraine.*

The increased synthesis of biologically active substances (BAS) of medicinal mushrooms during cultivation is an urgent issue. Two ways of influencing the growth, metabolism and development of the mushroom *Inonotus obliquus* have been tested: laser irradiation (low intensity blue light) of mycelium and the addition of a colloidal solution of NPs (Ag, Fe, Mg) to the nutrient medium [1,2]. The peculiarity of the research involves a special method of preparing a colloidal solution of NPs by the method of electrospark dispersion. The effect of metal NPs on activators of biosynthetic activity has been studied in relation to many plants. However, the method of preparation by electrospark dispersion is more suitable for the use in the nutrient medium of mushrooms. MgNPs of the colloidal solution has led to the increase not only in melanin, but also in endopolysaccharides and flavonoids, which are precursors of other components, including aromatic ones. Some aromatic substances have a cytotoxic effect [3]. Laser irradiation has led to the increase activity of enzymes that are included in the synthesis of BAS. Each of these ways affects the fatty acid composition of the mushroom by changing the ratio of ω-3 to ω-6 fatty acids. The comparison of the effectiveness of methods of influencing mushrooms during growth has showed the importance of choosing metals for the preparation of colloidal solutions of NPs for cultivation of the *Hericium erinaceus, Lentinula edodes, Ganoderma lucidum.*

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The Spectral Properties Peculiarities of DNA-Ag ions system

Gryn D.V.*, *Yashchuk V.M.

Taras Shevchenko National University of Kyiv, Physics faculty,
Volodymyrs'ka str. 64/13, Kyiv, 01601, Ukraine.
E-mail: dm_gryn@ukr.net

DNA is vitally important macromolecule and often used in various fields of biochemistry, biology and medicine.

In many experiments the DNA fluo- and phosphorescence emission is observed and investigated.

It is well known the property of Ag^+ ions to accumulating on the DNA, from sepatate ions in solution to some small nano-clusters near DNA, and then to clusters and nanoparticles. This is often used in controlled nanoparticles grows on DNA used as a template.

In this work we analyze the influence of presence of Ag^+ ions on the DNA spectral properties.

Water solutions of DNA, and DNA-Ag samples of different DNA:Ag ratios were investigated at room and nitrogen (77K) temperatures.

The UV-vis spectra as well as fluorescence and phosphorescence spectra of DNA in presence of different quantity of Ag were compared to pure DNA spectra.

It is shown that Ag ions do not affect essentially on the DNA absorption. Presence of $AgNO_3$ in DNA water solution leads to sharp phosphorescence intensity increasing (more that 500x times at 77 K), compared to fluorescence, and also additional structure in phosphorescence spectra appears. This structure has been identified as adenine base phosphorescence.

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The use of metal nanoparticles of the platinum group to improve the analytical characteristics of enzyme biosensors for application in biotechnological industries

Shkotova L.V.[1]***, Dzyadevych S.V.***[1,2]

[1] Department of Biomolecular Electronics, Institute of Molecular Biology and Genetics, NAS of Ukraine, 150, Zabolotnogo Str., Kyiv-03143, Ukraine. E-mail: luda_shkotova@yahoo.com

[2] Institute of High Technologies, Taras Shevchenko Kyiv National University, 2 Hlushkova Ave., Kyiv-03022, Ukraine.

Nanomaterials have attracted much attention due to their electronic properties. In electrochemical biosensors, where the enzymes are integrated with electrodes, the direct electron transfer is difficult since the enzyme active sites are deeply buried in the protein matrix [1]. Nanomaterials are suitable for acting as "electronic wires" to shorten the electron transfer distance, enhance the electron transfer between the redox centers of enzyme and electrode surface and simultaneously retaining the biological activity of the redox enzymes, which allows the development of stable sensors [2].

The work is aimed at the development of a sensitive element of the biosensor, based on enzymes and amperometric electrodes modified with nanoparticles of the platinum group. The voltamperometric characteristics of the modified sensors were studied, the working characteristics of the biosensors were thoroughly analyzed, their stability and selectivity were investigated.

Application of bionanocomposites with promising properties opens new possibilities for the enzyme immobilization and the development of new electrochemical biosensors.

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Green biosynthesis of nanoparticles using *Lactobacillus*

Voloshyna I.M.[1]***, Shkotova L.V.***[2]***, Netiaha Y.***[1]***, Lastovetska L.***[1]

[1] *Department biotechnology, leather and furs, National University of Technologies and Design, 2 Nemyrovycha-Danchenka Str., Kyiv-01011, Ukraine, E-mail: i_woloschina@yahoo.com.*

[2] *Department of Biomolecular Electronics, Institute of Molecular Biology and Genetics, NAS of Ukraine, 150, Zabolotnogo Str., Kyiv-03143, Ukraine.*

Among modern various fields, nanoparticles are widely used in the medical and cosmetic industries. There are various ways to synthesize nanoparticles from Lactobacillus. Selected strains of microorganisms are effective and environmentally friendly substitutes for the synthesis of nanoparticles. One of the most important examples of the synthesis of nanoparticles is gold, which can be obtained by a simple redox reaction carried out in aqueous solution [1].

Another equally well-known metallic element for the nanoparticle synthesis is titanium oxide (TiO_2). The biosynthesis of TiO_2 is caused by ecological representatives of the human microflora, such as Lactobacillus sp. You can also use an alternative mechanism of TiO_2 nanoparticle biosynthesis, in which pH and the partial pressure of hydrogen gas (rH2) or the redox potential of the culturing solution are one of the important components in the process [2].

One of the vital metals for humanity is silver thanks to its antibacterial properties. Swift and environmentally friendly biosynthesis of silver nanoparticles using lactic acid bacteria is an economical way of finding solution, and any research in this area is promising [3, 4].

Zinc nanoparticles are particularly important for biological applications, as ZnO is listed as a generally accepted safe (GRAS) material [5].

Nanoparticle production is a unique biotechnological practice. This is a complex and multi-stage process. It is important for the development of medicine in the country. Current methods of biosynthesis are truly cost-effective and capable of producing nanoparticles. Optimization of modern methods of nanoparticle production is an urgent task in the field of biotechnology.

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Session 4

Physico-Chemical nanomaterials science

Decrystallization and stabilization of liquid bee honey during storage

Kurta S.A.*, *Khatsevich O.M.*, *Fedorchenko S.V.*, *Tagir M.

Chemistry Department of the Faculty of Natural Sciences,
Vasyl Stefanyk Precarpathian National University
Halytska Str., 201/320, Ivano-Frankivsk, Ukraine. E-mail: kca2014@ukr.net

The materials described in the article relate to the scientific field of food processing in the food industry and other fields related to the dilution, decrystallization of various solid and pasty products, in particular the dissolution of solid crystalline bee honey to a liquid consistency that can be used in dentistry for prevention and treatment of gum disease in gingivitis, periodontitis and periodontitis .. Natural bee honey, especially May, linden and acacia, contains a lot of fructose and can remain liquid in honeycombs sealed for 1-3 years. But honey extracted from honeycombs has a shelf life of only a few months, depending on the type and variety of honey. This is because honey contains up to 80% or more of fructose and glucose in a ratio of about 1: 1. The consumer characteristics of honey are almost unchanged, but its appearance becomes less attractive to consumers who want to see and consume it liquid and transparent. Therefore, the use of new methods and special conditions for cracking crystallized honey and preventing its natural crystallization, as well as conditions and means of storing honey in a liquid state for at least 1 year is an urgent problem in the food industry. Scientific activity and discussion of the achievements of ONAFT and the Department of Chemistry of Vasyl Stefanyk Precarpathian National University (Ivano-Frankivsk), contributed to the implementation of joint research and the introduction of a new type of food product - chewing gum "Honeycomb-Honeycomb". based on dissolved, liquid caramelized honey, which has a therapeutic and prophylactic effect and has pronounced therapeutic, anti-inflammatory, astringent, anti-infective, antimicrobial and antibacterial properties. The research provides for the possibility of creating and introducing new types of chewing gum based on liquid, dissolved honey, for the treatment, protection and prevention of dental diseases, primarily gingivitis, periodontitis and periodontitis.

Chemical, physicochemical and structural characteristics of liquid and crystallized (solid) honey depending on its thermochemical processing and duration of storage are investigated. There are 3 main factors that affect the rate of crystallization of honey: water content, pollen content and the ratio of glucose and fructose in honey. It was shown that by low-temperature isothermal accelerated treatment in a microwave reactor type MWR-SPR at 40°C, for 60s, it is possible to dissolve crystalline honey to a liquid state, which reduces the time for its dissolution in the classical method by heat transfer through the reactor wall from hot water. or electric heating from 4-12 hours. at the same temperature 50°C to 1 min, ie 240-600 times faster.

The properties, structure and qualitative and quantitative composition of the obtained liquid honey are investigated and compared with the properties of the original crystalline and liquid honey without processing. It is proved that the proposed accelerated treatment in a microwave reactor type MWR-SPR at 50°C, for 60s, retains a high diastase Gotha number -10-11. The content of hydroxymethylfurfural did not exceed 3-6 mg / kg of honey, which meets the requirements of DSTU for honey. And consumer organoleptic indicators of honey in a liquid aggregate state remain, within 1 year. At the same time, with the traditional method of crystallization (dissolution) of honey, these indicators are much worse, the diastase number decreases to 0-6, and the content of toxic hydrosimethylfurfural increases to 12-18 mg / kg, which significantly exceeds the permissible norms (DSTU 4497: 2005 Honey natural).

Analysis of the qualitative and quantitative composition of honey after low-temperature isothermal accelerated processing in a microwave reactor type MWR-SPR at 50°C, for 60s., Conducted by IR spectroscopy, showed the absence of significant qualitative changes compared to untreated honey. Microscopic studies confirmed a 10-fold reduction in the number and size of pollen particles. The size of the crystals of glucose and sucrose after such treatment is also reduced by 5 times. At the same time, the analysis of the mass distribution of sugar macromolecules by the method of angular distribution of the laser beam (NANODS CILAS) showed a decrease in the average particle size in the treated honey in 2 times compared with the crystallized samples. All this has a positive effect on the stabilization of liquid honey after dissolution (crystallization), when stored for 1 year.

Analysis of HSC and BSC (honey bioactivity) confirmed that in samples of liquid honey after crystallization by the proposed method, these values are reduced by half, which is much less than during the traditional method of heating by heat transfer. Analysis of the chemical and element-oxide composition of honey, performed by X-ray fluorescence spectroscopy, confirmed that the qualitative composition of honey treated by the proposed method is almost unchanged.

On the basis of samples of decrystallized liquid honey obtained by the new technology, a preventive chewing gum was created for the treatment of periodontal disease (gingivitis, periodontitis and periodontitis). Clinical studies of chewing gum samples based on a composition of liquid, caramelized honey, which were conducted at the Research and Training Center for Molecular Microbiology and Immunology of Mucous membranes of Uzhgorod National University in 2018-2019 to prevent and treat gingivitis, periodontitis and periodontitis in dentistry positive result in 72.5% of patients.

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Adsorption of cationic dye onto biocarbons: Kinetics and thermodynamic study

Bazan-Wozniak A.

Faculty of Chemistry, Adam Mickiewicz University in Poznań,
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland.
E-mail: aleksandra.bazan@amu.edu.pl

The rapid growth of the worldwide dye business has resulted in significant environmental issues, particularly water contamination. This industry released untreated waste containing synthetic organic dyes with high concentrations into the water sources. Organic dyes change the appearance and color of water. Moreover, some of them are recognized to be carcinogenic and mutagenic for humans and marine creatures. Organic dyes, due to their the vast diversity of their chemo-physical and structural properties, is a big challenge and no stand-alone method is able to decolorize dye wastewater completely. Nonetheless, adsorption is the most frequent method for dye removal because of its low cost, high efficiency, simplicity and absence of by-products [1,2].

The main objective was to develop low cost and effective adsorbent from residue after supercritical extraction raspberry seed to eliminate rhodamine B from water solution. Different experimental parameters like contact time, pH, and solution concentration were investigated to identify their effects on adsorption process. Additionally, different isothermal models such as Freundlich and Langmuir models were analyzed with adsorption data to understand the adsorption process. Adsorption kinetics was studied by fitting data of interparticle pseudo–first–order, and second–order kinetic models. Finally, thermodynamics of the sorption process was carried out to understand the practical applicability of the adsorbent for wastewater treatment from liquid pollutants.

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Phase stability of nanostructured materials under irradiation

Shirinyan A.S.**, **Bilogorodskyy Y.S., Krit O.M.

"Laboratory of composite materials of nuclear-hydrogen energy"
of Institute of Applied Physics of National Academy of Sciences of Ukraine.
Room 606, building 3, Prospect Nauki, 46,
Institute of Physics, Kyiv-03028, Ukraine.
E-mail: aramshirinyan@ukr.net, urabelogorodsky@ukr.net,
krit_o_m@ukr.net

Radiation stability of highly dispersed composite materials (NDCM) has been examined intensely in last years but it still remains not complete. A substantial increase of radiation tolerance can be expected in nanocrystalline materials compared to bulk solids with conventional grain sizes, assumed that interfaces NDCM can serve as sinks for vacancies and defects.

We aim to study the effect of vacancy swelling on phase stability of spherical Fe nanoparticle in an inert medium of NDCM. The thermodynamic approach based on the calculation of the Gibbs free energy of Fe nanoparticle for different phase states with vacancy-type defects is offered. Hereby size dependence for the radiation-induced concentrations of point defects is assumed [1]. We investigate radiation tolerance and phase transition bcc-Fe ↔ fcc-Fe depending on the particle size and other parameters [2].

A size dependence of phase transition of Fe nanoparticles on vacancy swelling is found showing the possibility of radiation-induced polymorphic transition, as well as the zone of radiation stability (tolerance) of Fe nanoparticles with respect to the phase transition. Competition between the energy of accumulated vacancies in the particle, the bulk energy of phase transformation and the surface energy of the particle is shown to be responsible for the specific behaviour of irradiated nanocrystalline Fe.

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Proflavin binding to LSMO nanoparticles at temperatures above and below the Curie point

Dukhopelnikov E.V., Blyzniuk I.N., Bereznyak E.G., Gladkovskaya N.A.

Institute for Radiophysics and Electronics NAS of Ukraine;
12 Akad.Proskury Str., Kharkiv, 61085, Ukraine.
E-mail: dukhopelnikov@gmail.com

Targeted drug delivery by a magnetic field is one of the promising trends in the use of magnetic nanoparticles. Lanthanum strontium manganese oxide nanoparticles (LSMO NPs) have recently been explored for similar use in anti-cancer therapy. The advantage of these nanoparticles is low Curie temperature (20-60°C). Therefore, LSMO NPs application makes it possible to combine two types of cancer treatment: drug delivery for chemotherapy and self-controlled hyperthermia.

Changes in the magnetic properties of LSMO NPs above the Curie point can also vary their loading with the drug. In this work, we studied the binding of a positively charged drug proflavine (Pf) with LSMO NPs at temperatures below and above the Curie point by spectrophotometric titration method [1].

The addition of Pf to non-modified LSMO NPs does not change the spectrum of the drug. The lack of binding is explained by the DLS data showing zero zeta potential of the nanoparticles' surface. To charge the surface and increase the colloidal stability of the suspension, we modified the surface of LSMO NPs with sodium citrate. We found that its optimal concentration in solution, which ensures the binding of the maximum amount of Pf, is equal to 2×10^{-3} M. The coating with sodium citrate creates a surface charge of the NPs equal to -40 (DLS data). By titration of modified LSMO NPs with Pf, the dependencies of the free Pf concentration on the total LSMO NPs concentration were obtained and fitted by the Langmuir equation [1] to determine the Pf-LSMO NPs binding parameters. The binding constant of Pf to LSMO NPs is $K_{bind}=2\times10^{4}$ M^{-1}. The complex formation at a temperature above the Curie point increases the degree of drug loading on the nanoparticle's surface from 110 drugs per one NP at 25°C to 150 ones at 60°C. It is caused by partial destruction of nanoparticle aggregates in suspension upon LSMO NPs losing their superparamagnetic properties.

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Galvanic waste processing by energy-saving ferritization with AC-magnetic field activation

Derecha D.O.[1,4], **Skirta Yu.B.**[1,2], **Samchenko D.M.**[3], **Kochetov G.M.**[3]

[1] *Institute of Magnetism, Natl. Acad. Sci. Ukraine and Min. Edu. Sci. Ukraine, Akad. Vernadsky Blvd. 36-b, Kyiv 03142, Ukraine*
E-mail: dderecha@gmail.com

[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Peremohy Ave. 37, Kyiv 03056, Ukraine*

[3] *Kyiv National University of Construction and Architecture, Povitroflotsky Ave. 31, Kyiv 03037, Ukraine*

[4] *Physico-technological Institute of Metals and Alloys, 34/1 Academician Vernadsky Blvd., Kyiv 03680, Ukraine*

The efficiency of the ac-magnetic field usage for resource-saving activation of the reaction mixture in the ferritization process with the extraction of heavy metals ions from galvanic waste has been confirmed. The one of the key parameters of the ferritization process - the ratio of the concentration of iron ions to the total concentration of other metal ions on the quality of galvanic waste processing has been investigated. It is determined that under the optimal processing conditions (ratio of concentrations of iron ions to other heavy metal ions 3.5 ÷ 4/1) the residual concentrations of heavy metal ions decrease to the values: $Fe^{2+;3+}$ - 0,1; Ni^{2+} - 0.26; Cu^{2+} - 0.2; Zn^{2+} - 0.19 mg / dm^3.

It is established that the AC-magnetic field activation provides the metal ions extraction degree of 99.96%, and also has undeniable energy advantages in comparison with thermal technique: the energy consumption is reduced by more than 60%. This indicates the suitability of purified water for reuse in galvanic production due to the requirements for the heavy metal ions content. Also, the structural studies of ferritic sediments shown that samples obtained at the ratio of heavy metal ions concentrations 4/1 phases characterized by the maximum content of crystalline ferromagnetic ferrite ($Ni_{0.53}Cu_{0.3}Zn_{0.17}Fe_2O_4$) ≥ 76% were detected.

The consumption of electricity for AC-magnetic field activation in comparison with thermal one is reduced by 60%. That makes possible to reduce the cost of this technique, and thus make it attractive for industrial applications.

Vortex motion of electrolyte at the electrolytic deposition of nickel in an external magnetic field

Derecha D.O.[1,5]***, Skirta Yu.B.***[1,2]***, Gerasimchuk I.V.***[1,2]***,***
Hruzevyich A.V.[1,3]***, Samchenko D.M.***[4]***, Kochetov G.M.***[4]

[1] *Institute of Magnetism, Natl. Acad. Sci. Ukraine and Min. Edu. Sci. Ukraine, Akad. Vernadsky Blvd. 36-b, Kyiv 03142, Ukraine*
E-mail: dderecha@gmail.com

[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Peremohy Ave. 37, Kyiv 03056, Ukraine*

[3] *Trypilska TPP, Promyslova Str. 1, Ukrainka 08720, Kyiv Rgn., Ukraine*

[4] *Kyiv National University of Construction and Architecture, Povitroflotsky Ave. 31, Kyiv 03037, Ukraine*

[5] *Physico-technological Institute of Metals and Alloys. 34/1 Academician Vernadsky Blvd., Kyiv 03680, Ukraine.*

The influence of the magnetic field on electrolysis, corrosion and other aspects of the interaction of metal surfaces with electrolytes attracts much attention nowadays. Earlier the effects of a significant acceleration of corrosion of metals in electrolytes in a constant magnetic field and the emergence of multi-vortex structures in electrolytes under the influence of a constant magnetic field were observed. Electrodeposition of metals has been successfully used to create surfaces with desired properties.

We observed and analyzed the vortex motion of the electrolyte during the electrolytic deposition of nickel on a ferromagnetic mesh electrode in an external magnetic field. The characteristic frequencies of rotation of the electrolyte were found by optical methods developed by us earlier. This rotation is in many aspects similar to the processes occurring during the dissolution of a steel ball in nitric acid in a magnetic field. The calculated spectrum shows maxima corresponding to the characteristic frequencies of the electrolyte motion. The most intense maxima correspond to the frequencies of 0.161 Hz, 0.337 Hz and 1.113 Hz. The presence of clearly pronounced maxima shows that the motion of the electrolyte is ordered, cyclical, and not chaotic.

The proposed method, with some modifications, can be used to study the frequency characteristics of the motion of liquids, gases and small objects without directly affecting the medium under investigation.

Synthesis and photophysical properties of indolenine styrylcyanine dye and its carboxyl-labeled derivative

<u>Chernii S.</u>^{1,2}***, Selin R.***^{1}***, Tretyakova I.***^{1}***, Dovbiy Y.***^{1}***,***
Chernii V.^{1}***, Pekhnyo V.***^{1}***, Kovalska V.***^{1,2}

[1] V.I. Vernadsky Institute of General and Inorganic Chemistry NASU,
32/34 Palladin Ave, 03-142 Kyiv, Ukraine

[2] Institute of Molecular Biology and Genetics NASU,
150 Zabolotnogo Street, 03143 Kyiv, Ukraine

**corresponding author chernii.sv@gmail.com*

Organic fluorescent dyes are widely used as a working medium in dye lasers, in analytical chemistry to determine the various trace elements, in photodynamic therapy, in tissue optics, in the analysis of cells, etc. Depending on the sphere of application of fluorophores their various properties: quantum yield and photostability, pH dependence, and fluorescence lifetime are essential [1].

Herein, two indolenine-based styrylcyanine dyes functionalized by the carboxyl group at the indolenine ring were synthesized and characterized. UV-VIS absorption and fluorescence spectra of these dyes in organic solvents (DMSO, ACN, MeOH) were studied.

The absorption maxima of the studied dyes in organic solvents are located in the range of 544-563 nm, and the molar extinction values were moderate in the range (5.3-7.7)×10^4 $M^{-1}cm^{-1}$ depending on solvent and dye structure. Dyes' fluorescence intensity in DMSO was 4-5 times higher than in MeOH and ACN. The emission maximum was shifted to the short-wavelength region for both dyes in MeOH (compared to DMSO and ACN). Depending on the solvent, the excitation was located in the range of 547-564 nm, with the emission in the range of 593-609 nm. The introduction of a carboxyl group in the indolenine ring leads to a bathochromic shift of the absorption maximum. These dyes can be further characterized as potential probes for biological application.

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Polymers and metal ions adsorption on the surface of biochars obtained from the nettle and sage herbs

Gęca M.[1]***, Wiśniewska M.***[1]*****, Nowicki P.***[2]

*[1] Department of Radiochemistry and Environmental Chemistry, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Sklodowska University in Lublin, M. Curie-Sklodowska Sq. 3, 20-031 Lublin, Poland, E-mail: *malgorzata.wisniewska@mail.umcs.pl;*

[2] Department of Applied Chemistry, Faculty of Chemistry, Adam Mickiewicz University in Poznań, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland.

Biochars are solids formed by biomass pyrolysis. They could be used as environmental friendly and low-costs adsorbents [1, 2]. Polymers and metals are wide used in modern industry. However these molecules are often toxic and dangerous for health. For that reason polymers and metals ions should be removed from water solutions. Adsorption of metal ions on the surface of activated carbons is commonly studied [3, 4]. However, polymers adsorption on these adsorbents is not widely described, so the presented research is innovative.

Poly(acrylic acid) and polyethyleneimine adsorption in the presence of metal ions on the surface of biochars obtained from the nettle and sage herbs was investigated. Studies were carried out in single and multi-component solutions. The influence of polymers on the metal ions adsorption was also checked. All these research allowed to assess the usefulness of biochars in real wastewater treatment processes.

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Indium deposited nanosystems formation on 2D layered chalcogenide crystals' surfaces

Galiy P.V.[1], Nenchuk T.M.[1], Ciszewski A.[2], Mazur P.[2], Dzyuba V.I.[1], Makar T.R.[1], Tsvetkova O.V.[1]

[1] Electronics and Computer Technology Department,
Ivan Franko Lviv National University,
50 Dragomanov Street, Lviv, 79005, Ukraine.
E-mail: galiy@electronics.lnu.edu.ua

[2] Institute of Experimental Physics, University of Wrocław,
pl. Maxa Borna 9, 50-204 Wrocław, Poland.

2D layered chalcogenide semiconductors, such as, InSe, In_4Se_3, InTe, Sb_2Te_3 are among newly emerging materials suitable for functional nanoscale devices applications [1]. It looks like that surface of 2D layered crystals are one among most perspective templates for self-assembling of metal nanostructures due to the solid state dewetting [2,3]. Because of intrinsic nature of van der Waals interlayer bonding, layered chalcogenide crystals' surfaces possess relatively good ambient stability, might be just easily obtained by cleavage even in UHV, and, thus, applied as template for fabrication of metal-semiconductor hetero nanosystems.

The studies of In deposition with further nanosystems formation were conducted using STM/STS data from Omicron NanoTechnology STM/AFM System. The studies included statistical analysis of STM data from large areas by standard roughness analysis tools from the WSxM software taking into account the distribution of pixels' height of the image depending on the degree of In deposition, as well as detailed analysis of high-resolution STM images. In consequence of our studies it was found that obtained indium nanostructures have got 0D or 1D dimensionality consistent with the nano relief of the initial crystals' patterns.

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Application of Nano-functional silicas in extraction of vegetable raw materials

***Raks V.*[1]*, Vasylchenko O.*[2]*, Myroniuk O.V.*[3]*, Sivolapov P.V.* [3]**

[1]*Taras Shevchenko National University of Kyiv, Ukraine*
[2]*National Aviation University, Kyiv, Ukraine*
[3] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" , Kyiv, Ukraine*
E-mail: pavlo.sivolapov@gmail.com

Novel silica-based solid phase extraction (SPE) cartridges with surface-immobilized of polyoxyethylated isooctylphenolic, polyethylene glycol octadecyl ether and polyethylene glycol hexadecyl ether groups were tested for extraction of components from vegetable raw materials. According to differential thermal analysis data, the grafted layer of silica-based SPE - cartridges is stable in O_2 flow up to 200 ºC. Its decomposition begins on exposure to O_2 at 210–300 ºC. Silica-based SPE - cartridges with satisfactory densities (20-30 $\mu mol \cdot g^{-1}$) are thermally stable and can contribute to the materials, desirable for analytical application. The purpose of the work was to analyze the methods used to find, isolate and identify polyol compounds from vegetable raw materials in recent years and compare with new approach using Nano-functional silicas.

Polyol compounds have a broad spectrum of action. They are used in the production of vitamin preparations, are involved in the regulation of intracellular calcium content, the transmission of hormonal signals, the catabolism of fats and the reduction of blood cholesterol, modulation of the activity of neurotransmitters. The most important biologically active polyol compounds are inositols. The main source from which inositols are derived is vegetable raw materials, namely alfalfa, as well as wheat sprouts, grapefruit, hazelnut and others. The paper deals with the extraction of polyols with organic and inorganic solvents, including in a Soxhlet apparatus, liquid pressure extraction, microwave extraction, and supercritical fluid extraction. The procedure of preliminary sample preparation and derivatization of polyols for their further separation and quantification is described. Modern chromatographic methods, that are used in the work with polyols, are analyzed. The possibility of using 1H nuclear magnetic resonance (NMR), ^{13}C and ^{31}P-NMR spectroscopy to identify the structure of polyol compounds, especially inositols, was demonstrated.

Study of biocarbons derived from residue after supercritical extraction of carrot seeds from adsorption of gaseous NO_2

Bazan-Wozniak A., Pietrzak R.

Faculty of Chemistry, Adam Mickiewicz University in Poznań,
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland.
E-mail: pietrob@amu.edu.pl

Human health is closely related to his environment. Air polluted is considered one of the major factors leading to many diseases such as cardiovascular and respiratory disease and lung cancer for the people. Besides, air pollution adversely affects the animals and deteriorates the plant environment. The sources of pollution vary from small unit of cigarettes and natural sources such as volcanic activities to large volume of emission from motor engines of automobiles and industrial activities [1]. That is why the search for new and more effective technologies for the environment purification is a continuous challenge. Recently, increasingly often carbon materials are used as effective adsorbents of pollutants from gas phases [2]. Porous materials have shown an enormous potential in a wide variety of applications due to their high specific surface area and porosity. Activated carbons are efficient adsorbents for gases and vapors [3].

The main aim of the study reported was to obtain cheap and effective biocarbons from the residue after supercritical extraction of carrot seeds and their comprehensive characterization by determination of textural parameters, content of surface oxygen functional groups and pH of their water extracts. The biocarbons were tested as potential adsorbents for the removal of gas pollutants represented by nitrogen dioxide. The effects of the methods of activation and variant of heating (microwave and conventional) on the physicochemical and sorption properties of the biocarbons were also examined.

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Electrical properties of p-CuCoO$_2$/n-Si heterojunction

Koziarskyi D.P., Koziarskyi I.P., Maistruk E.V.

Yuriy Fedkovych Chernivtsi National University,
2 Kotsubynsky st., 58002 Chernivtsi, Ukraine.
E-mail: d.koziarskyi@chnu.edu.ua

Delafossite (CuCoO$_2$) oxides have been widely testified to be used in the fields of translucent conductive oxides (TCO), solar cell devices, photocatalysis, and other optoelectronic devices as *p*-type semi-conductive materials [1]. The development of *p*-type TCO will give us possibilities that cannot be used with *n*-type materials alone, such as transparent *p-n* heterojunction, diodes, transistors [2].

Thin CuCoO$_2$ films (~ 200 nm thick) were obtained by RF magnetron sputtering on glass substrates and on plane-parallel *n*-Si plates. A stoichiometric mixture of CuO and CoO$_2$ was used to make the target. Substrate temperature $t_{\circ}$S = 380 °C, spraying was carried out in two stages t_1 = 15 min, P_1 = 180 W, t_2 = 15 min, P_2 = 200 W (t - spraying time, P - magnetron power). Its resistivity was ρ = 20 Ω·cm. The optical width of the band gap is E_g = 3.5 eV and absorption of light photons takes place by means of direct optical transitions.

Studies of *I-V*–characteristics of anisotype p-CuCoO$_2$/*n*-Si heterostructures at forward and reverse biases in the temperature range T = 299 – 343 K indicate the rectifying properties of the structures. The rectification ratio at $|V|$ = 0.7 V and T = 294 K was ~ 10^3. The diode characteristics of the heterostructure are due to the energy barrier $q\varphi k$ ~ 0.5 eV from the *n*-Si side. At forward biases of 0.05 $V < V <$ 0.4 V in the structure of p-CuCoO$_2$/*n*-Si the generation-recombination mechanism of current transfer prevails. At $V >$ 0.4 V the tunnel mechanisms of current transfer with participation of surface states prevail. The reverse current at biases – 2 $V < V <$ – 3kT/q V is determined by tunneling processes involving surface states. The p-CuCoO$_2$/*n*-Si heterostructure is photosensitive at reverse displacement under AM1.5 radiation conditions.

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Polarons and bipolarons in one-dimensional systems (arbitrary coupling)

Kashirina N.I.[1], Kashyrina Ya.O.[2], Korol O.A.[3], Roik O.S.[2]

[1] V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine.
Prospect Nauky, 41, Kyiv-03680, Ukraine.
E-mail: kashirina1506@gmail.com

[2] Taras Shevchenko National University of Kyiv,
Lev Tolstoy str., 12. Kyiv-01033, Ukraine.

[3] State University of Telecommunications.
Solomyanska str., 7. Kyiv-03680, Ukraine.

The energies of one-dimensional polarons and bipolarons (bound state of two polarons) are calculated in the region of intermediate and strong coupling of electrons with optical phonons.

The effective potential of the pair interaction of two polarons is calculated for various parameters of the electron-phonon coupling. Both singlet and triplet states of a two-electron system in the phonon field of a one-dimensional crystal are considered. It is shown that the exchange interaction of polarons has an antiferromagnetic character. As was shown in [1], both single-center and two-center configurations of 1D- strong coupling optical and acoustical bipolarons are stable in 1D- systems. This property distinguishes 1D- systems from 2D- and 3D- crystals, in which only one-center bipolarons are stable. 3D- graphs of electron density are constructed for both models of 1D- bipolarons. It is shown that the electron density distribution, as for the one-center and two-center configurations, is a curve with two well-defined maxima located along the line connecting the centers of the polarization wells of two 1D- polarons. This circumstance indicates that there is no fundamental difference between the two-center and one-center models of bipolarons in 1D- systems.

Variational calculations were performed using a multi-parameter basis of Gaussian functions with simply correlated multipliers. The variation was carried out by the random search method in combination with the Euler method.

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Restoration of the electron-phonon interaction function in an alloy molybdenum – rhenium

D'yachenko A.I.[1], Kalenyuk O.A.[1], Dmitrenko V.Yu.[2], Tarenkov V.Yu.[2]

[1] *G. V. Kurdyumov Institute for Metal Physics, NAS of Ukraine,*
36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine.

[2] *Donetsk Institute for Physics and Engineering Named after O. O. Galkin,*
NAS of Ukraine, 46 Nauky Ave., UA-03028 Kyiv, Ukraine.
E-mail: dmitrenko_v@ukr.net

The superconducting transition temperature of the Mo-Re alloy reaches to $T_C = 12–14$ K, which significantly exceeds the TC value for Mo ($T_C = 1$K) and Re ($T_C = 1.5$K) crystals [1]. The reason for such a strong increase of T_C is still not well understood. One of the most reliable and accurate methods for studying the mechanisms of electron-phonon interaction (EPI), including the tunneling density of states $N(\omega)=\mathrm{Re}\{\omega/[\omega 2-\Delta 2(\omega)]1/2\}$ ($\Delta(\omega)$ – complex parameter of the energy gap of a superconductor) and the function of the electron-phonon interaction $\alpha 2(\omega)F(\omega)$, is tunneling spectroscopy. A key limitation of this method is the preparation of the tunnel junctions. In this work, the EPI mechanism for the сплава $Mo_{0.73}Re_{0.27}$ alloy is studied for the first time by processing the characteristics of Ag-I-MoRe tunnel contacts, in which a dielectric layer I is formed on the natural MoRe oxide. The parabolic type of conductivity *dI/dV*, as well as a well-defined feature associated with the energy gap of the $Mo_{0.73}Re_{0.27}$ superconducting state and the features of the phonon spectrum, made it possible to reconstruct the EPI function of the $Mo_{0.73}Re_{0.27}$ alloy using the program [2]. The reliable values of the parameters of the energy gap, Δ, and the EPI constant, λ, in $Mo_{0.73}Re^{0.27}$ were obtained, which makes it possible to refine the parameter $\lambda(T_C)$ of the $Mo1–xRe_x$ alloys.

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Characteristics of charge carriers in 3,4-ethylenedioxythiophene oligomers (n=1–16)

Terebinska M.I., Filonenko O.V.,
Tkachuk O.I., Datsyuk A.M., Lobanov V.V.

Chuiko Institute of Surface Chemistry of the National Academy of Sciences of Ukraine, 17 Generala Naumova Street, Kyiv, 03164, Ukraine,
email: terebinska@ukr.net

A number of oligomers of 3,4-ethylenedioxythiophene (n=1–16) in charge states +1, +2, +3, and +4 were studied by the density functional theory method (B3LYP/6-31+G(d,p). Optimization of the spatial structure and calculation of the electronic structure of the cations of 3,4-ethylenedioxythiophene (EDT) oligomers were carried out using methods with and without spin limitation. It has been found that the ground electronic state of short oligomeric cations (n-EDT)$^{2+}$ and (n-EDT)$^{4+}$ ($n < 7$) corresponds to a spin-limited singlet state. The charge carrier in these oligomeric cations has the characteristics of a bipolaron. In contrast to small oligomers, in (n-EDT)$^{2+}$ with 7 n 14, the ground electronic state is also singlet, but unlimited in spin, and the charge carriers in them have the properties of a polaron pair. For the longest studied oligomers (n=15, 16) (n-EDT)$^{2+}$ and (n-EDT)$^{4+}$, as a result of singlet-triplet degeneracy, the ground electronic state is triplet, and the polaron pair becomes predominantly the charge carrier. For all considered cations with an odd charge (n-EDT)$^{1+}$ and (n-EDT)$^{3+}$, the ground electronic state turned out to be a doublet.

For n-EDT oligomers, the calculated C–C bond lengths between neighboring monomeric units are 1.433 Å, which is typical of the benzenoid phase. However, for (n-EDT)$^{1+}$ cations, the lengths of these bonds decrease monotonically from the ends of the chain to its center, reaching a value of 1.417 Å on the central bond, which is characteristic of the quinoid phase. In (n-EDT)$^{2+}$ dications, a similar dependence of bond lengths between monomer units is observed. For higher oxidation states (+3 and +4), the contribution of the quinoid phase increases and two separated polarons are formed at the ends of the oligomer chain.

Thus, the results obtained allow us to conclude that in oxidized EDT oligomers, at a high degree of doping, the conductivity is provided by the formation of two polarons at the ends of the chain.

Formation process of the nanoporous structure in porous ammonium nitrate granules: indicators of influence

Artyukhov A.E.[1]***, Volk I.I.***[1]***, Krmela J.***[2]***, Ospanov D.***[3]

[1]Sumy State University,
Rymskogo-Korsakova str., 2, Sumy, 40007, Ukraine.
E-mail: a.artyukhov@pohnp.sumdu.edu.ua

[2] Alexander Dubcek University of Trencin,
491/30, I. Krasku, 02001, Puchov, Slovak Republic

[3] Saken Seifullin Kazakh Agrotechnical University,
Zhengis Ave 62, 010000, Nur-Sultan, Kazakhstan

Obtaining granules of porous ammonium nitrate (PAN) as a component of industrial explosives is associated with the lack of reliable methods for controlling the process of nanopore formation.

In this work, the studies of the formation process of a nanoporous structure, begun in [1–3], are continued. The assessment of the quality of the nanoporous structure under various conditions for its preparation was carried out according to the data of microscopic analysis and the determination of the specific properties of PAN as a component of an industrial explosive.

The research results made it possible to determine the degree of influence of various technological indicators of the granulation and dehydration process on the nanoporous structure of PAN granules.

This work was carried out under the project "Technological bases of multistage convective drying in small-sized devices with utilization and heat recovery units," project No. 0120U100476.

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Optimization of the drying devices functioning in the process of forming the ammonium nitrate's nanoporous structure

Artyukhova N.O.[1]***, Krmela J.***[2]***,***
Artyukhov A.E.[1]***, Volk I.I.***[1]***, Ospanov D.***[3]

[1] *Sumy State University,*
Rymskogo-Korsakova str., 2, Sumy, 40007, Ukraine.
E-mail: n.artyukhova@pohnp.sumdu.edu.ua

[2] *Alexander Dubcek University of Trencin,*
491/30, I. Krasku, 02001, Puchov, Slovak Republic

[3] *Saken Seifullin Kazakh Agrotechnical University,*
Zhengis Ave 62, 010000, Nur-Sultan, Kazakhstan

The formation of nanopores in the volume of a granule of porous ammonium nitrate is a multistage process and is subject to the influence of many factors. At each stage (including the stage of dehydration at the stage of granulation, and final drying), the technological parameters of the implementation of the nanopore formation process and the design of the main technological equipment are subject to a detailed study.

In this paper, ways to optimize the operation of multistage shelf dryers with vertical sectioning of the working space due to the rational design of the shelves and the number of stages of contact with the drying agent are proposed.

Based on the research results, an algorithm for determining the optimal drying time, which would provide the necessary quantitative characteristics of the nanoporous structure and specific parameters of the PAS characteristic of the components of bulk industrial explosives was proposed.

This work was carried out under the project "Technological bases of multistage convective drying in small-sized devices with utilization and heat recovery units," project No. 0120U100476.

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Study of the role of alloying elements Cr, Ni, Fe, and Al in the improvement of high-temperature (700–800 °C) fracture toughness of Ti-based composites

Vasyliv B.D.[1]*, Kulyk V.V.*[2]*, Duriagina Z.A.*[2,3]*, Lyutyy P.Ya.*[2]*,*
Kovbasiuk T.M.[2]*, Vavrukh V.I.*[2]*, Trostyanchyn A.M.*[2]*, Vira V.V.*[4]

[1] *Department of Hydrogen Technologies and Alternative Energy Materials, Karpenko Physico-Mechanical Institute of the NAS of Ukraine, 5 Naukova str., Lviv 79060, Ukraine.*
E-mail: mechengin1111@gmail.com

[2] *Department of Materials Science and Engineering,*
Lviv Polytechnic National University,
12 S.Bandera str., Lviv 79000, Ukraine.

[3] *Department of Materials Engineering, The John Paul II Catholic University of Lublin, 14 Racławickie Al., Lublin 20-950, Poland.*

[4] *Department of Strength of Materials and Structural Mechanics, Lviv Polytechnic National University, 12 S.Bandera str., Lviv 79000, Ukraine.*

Advanced Ti-based composites are being used for manufacturing components of state-of-the-art power equipment as well as aircraft and rocket engines owing to their high strength-to-weight ratio and comparatively high fracture toughness in a temperature range of 20 °C to 650 °C. These materials have an advantage over conventional titanium alloys, an operating temperature of which is limited by 350–550 °C. This work is aimed at studying the role of alloying elements Cr, Ni, Fe, and Al in the improvement of high-temperature (700–800 °C) fracture toughness of Ti-based composites.

Ti–Al–X composites (X=Cr and/or Ni and/or Fe) were manufactured with electron arc smelting. The contents of alloying elements marked with X varied in a range of 0.2–41 wt%. Single-edge notch beam fracture toughness tests of specimen series were carried out in a temperature range of 20 °C to 800 °C. The microstructure and phase composition in relation to fracture toughness data and failure micromechanisms of the composites were analysed. The role of alloying elements Cr, Ni, Fe, and Al in the improvement of high-temperature fracture toughness of Ti-based composites was substantiated. It was found that both Ti–Al–Cr and Ti–Al–Ni composites of the optimal phase composition are promising in terms of fracture toughness for high-temperature (700–800 °C) applications.

Microstructure, high-temperature strength and fracture toughness of Ti–Si–X composites containing refractory phases

Vasyliv B.D.[1]***, Kulyk V.V.***[2]***, Duriagina Z.A.***[2,3]***, Lyutyy P.Ya.***[2]***,***
Kovbasiuk T.M.[2]***, Trostyanchyn A.M.***[2]***, Vira V.V.***[4]***, Vavrukh V.I.***[2]

[1] Department of Hydrogen Technologies and Alternative Energy Materials,
Karpenko Physico-Mechanical Institute of the NAS of Ukraine,
5 Naukova str., Lviv 79060, Ukraine.
E-mail: mechengin1111@gmail.com

[2] Department of Materials Science and Engineering, Lviv Polytechnic National University, 12 S.Bandera str., Lviv 79000, Ukraine.

[3] Department of Materials Engineering, The John Paul II Catholic University of Lublin, 14 Racławickie Al., Lublin 20-950, Poland.

[4] Department of Strength of Materials and Structural Mechanics, Lviv Polytechnic National University, 12 S.Bandera str., Lviv 79000, Ukraine.

State-of-the-art Ti–Si–X composites are being developed for applications in modern aircraft and rocket engines as well as power equipment owing to their comparatively low specific weight and high strength and fracture toughness in a temperature range of 20–650 °C. This work is aimed at improving mechanical characteristics of the composites, namely, strength and fracture toughness, and increasing their operating temperature range up to 700−800 °C.

Ti–Si–X composites (X=Al and/or Zr) were manufactured with electron arc smelting. The content of alloying elements varied in a wide range (0.8–2.5 wt% Al, 5–8 wt% Zr). Strength tests of specimen series were carried out under three-point bending in a temperature range of 20 °C to 1000 °C. Fracture toughness tests of single-edge notch beam specimens were performed in a temperature range of 20 °C to 900 °C. The chemical and phase compositions of the composites were determined, as well as their microstructure and failure micromechanisms in relation to mechanical behavior were analysed.

Based on the dependences of strength and fracture toughness on testing temperature for the specimen series as well as the microstructure and failure micromechanism analyses, it was found that the Ti_5Si_3 and complex $(Ti, Zr)_5Si_3$ refractory phases play a crucial role in enhancing fracture toughness of all the specimen series in the high-temperature (700–800 °C) range.

The role of dislocations in radiation-stimulated changes in the electrophysical and optical characteristics of silicon structures

***Lys R.M.*, Pavlyk B.V., Shykorjak J.A.**

Department of Sensor and Semiconductor Electronics, Ivan Franko National University of Lviv. Str. Tarnavskoho, 107, Lviv-79017, Ukraine.
E-mail: lys_r@ukr.net

The development of modern nanoelectronics in terms of significant reduction of elements makes increased demands on the state of the near-surface layer of silicon structures. After all, unstable processes that occur at the boundaries of the separation under the influence of external factors determine the operational parameters of these elements. The presence of point and linear defects can significantly affect the activity of the surface. This can affect the efficiency and durability of solar cells under the action of weak electromagnetic fields.

The aim was to form a surface-barrier and light-emitting structures (LES) based on *p*-Si crystals with different concentrations of dislocations on the surface of the semiconductor substrate and to investigate the change in their electrophysical and optical characteristics under the influence of X-rays. Changes in the surface resistance of silicon single crystals, volt-farad characteristics, the density of surface states, and electroluminescence of LES were analysed.

As the concentration of dislocations increases, the surface resistance of silicon increases. The reason is the process of generating the main charge carriers by linear defects. As the X-ray dose increases, the p-Si resistance increases further. The resistance of unirradiated and irradiated samples of solar silicon under elastic compression decreases. With increasing dislocation concentrations greater than 10^4 cm^2, there is a certain nonmonotonicity of charge accumulation at the Si-SiO$_2$ interface, which is associated with the additional influence of the mechanical field of dislocations and the electric field of the Cottrell cloud on X-stimulated changes in these structures.

It is shown that high concentrations of dislocations on the surface (111) of silicon are generated by the methods of plastic deformation and high-temperature annealing in an oxygen atmosphere. This allows creation of highly efficient radiating Al-Si(*p*) structures.

Effect of the bromination method of PAN carbon fibers on their interaction with ultrahigh-frequency electromagnetic radiation

Dovgan O.M.[1]***, Moiseienko V.A.***[1]***, Trachevskyi V.V.***[2]***,***
Mischanchuk O.V.[3]***, Diyuk V.E.***[1]***, Lisnyak V.V.***[1]***, Grishchenko L.M.***[1]

[1] *Taras Shevchenko National University of Kyiv,*
64/13, Volodymyrska St., Kyiv-01601, Ukraine.
liudmyla.grishchenko@gmail.com

[2] *Institute of Macromolecular Chemistry of NAS of Ukraine,*
Kharkivs'ke avenue, 48, Kyiv-02160, Ukraine.

[3] *O.O. Chuiko Institute of Surface Chemistry, NAS of Ukraine, Henerala*
Naumova St., 17, Kyiv-03164, Ukraine.

Carbon materials are widely used to obtain composite materials for personal protective equipment [1]. This work aimed to compare the effect of two bromination methods on the radio absorption properties of the resulting PAN-carbon fibers. We studied how the bromine modifier concentration impacts the magnitude of the attenuation of the power of electromagnetic radiation S_{21} and the voltage standing wave ratio (VSWR) in a wide frequency range for the samples of the brominated PAN-carbon fibers with a thickness of a single layer. We suggested that for the brominated PAN-carbon fibers obtained by the plasma chemical and the liquid phase methods, there is an "optimal" value of bromine concentration. Clearly, after reaching a certain amount of bromine in the composition of the brominated PAN-carbon fibers, all subsequent bromine addition has no prominent effect on the absorbing properties. They even harm the sample leading to wasteful use of the bromine modifier. In addition, the law of saturation of PAN-carbon fibers with bromine is the same for both modification methods. There is a general similarity in the behavior of modified PAN-carbon fibers with an increase in the frequency of electromagnetic radiation: the magnitude of the power attenuation S21 increases while VSWR decreases.

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Hydrophobization of the surface of carbon nanomaterials using the Diels–Alder reaction

Soloviov V.[1]***, Diyuk V.E.***[1]***, Vakaliuk A.V.***[1]***, Yatsymyrskyi A.V.***[1]***,***
Mischanchuk O.V.[2]***, Mariychuk R.***[3]***, Lisnyak V.V.***[1]

[1] *Taras Shevchenko National University of Kyiv,*
62a, Volodymyrska Str., Kyiv 01601, Ukraine, E-mail: vadiga@ukr.net

[2] *O.O. Chuiko Institute of Surface Chemistry, the National Academy*
f Science of Ukraine, Gen.
Naumova St., 17, General Naumov Str., 03164 Kyiv, Ukraine

[3] *Prešov Universirty in Prešov, Ul. 17 Novembra, 1, 080 01, Prešov, Slovakia*

Carbon nanomaterials (CNM) have high specific surface area and electrical conductivity. These CNM include nanoporous carbon sorbents those have unique mechanical properties and are non-toxic. So, one can use the CNM to solve the problems in chemical technology, ecology, and medicine. The chemical properties of CNM allow modifying the surface layer to improve material characteristics and obtain a variety of functional materials. The Diels-Alder (DA) reaction is very selective and runs between a diene and an unsaturated compound, which is a dienophile. The CNMs can contain both isolated carbon-carbon double bonds and conjugated carbon–carbon bonds, i.e., they can react with DA as both diene and dienophile. This work aims to study the ways of hydrophobization of the surface of various carbon nanomaterials: multilayer carbon nanotubes, carbon soot, activated carbon, and carbon fibers. The reactivity of active CNM centers in the reaction with 1,3-Cyclohexadiene (CHD) was investigated to address this issue. Barothermal treatment was used for effective modification, and the sample of CNM was autoclaved with CHD at 90–250 °C. Samples were investigated by miscellaneous methods, including SEM, adsorption of N2, TG/DTG, TPD MS, FTIR, and the Boehm titration. We show that the barothermal modification of CNM leads to the introduction into the surface layer of up to 2 mmol per gram of CNM of specific functional groups. The TG/DTG method has shown that at the least two forms of chemisorbing CHD can be formed when CNM is modified. The first chemisorbed form decomposes in the temperature range of 150–400 °C and refers to CHD grafted to the surface in line with the passaging of the DA reaction. The second form, with a decomposition temperature of more than 350–400 °C, corresponds to the thermal decomposition and destruction of chemisorbed products of partial pyrolysis of the modifying agent. The highest concentration of grafted CHD (up to 1.3 mmol per gram of CNM) was found for CNM modified at 200–250 °C. The process of pyrolysis of the surface layer of the modified CNMs was studied by the TPD MS method. As a result of modification of chemisorbed forms of CHD, the products of the partial destruction of CHD and the products of its dimerization are formed. The obtained materials have a hydrophobic surface and can be used for selective removal of non-polar molecules at adsorption purification.

The catalytic activity of phosphotungstic acid-carbon nanocomposites in the dehydration reaction of bioethanol

Soloviov V.[1]***, Diyuk V.E.***[1]***, Vakaliuk A.V.***[1]***, Tsapyuk G.G.***[1]***,***
Mischanchuk O.V.[2]***, Mariychuk R.***[3]***, Lisnyak V.V.***[1]

[1] *Taras Shevchenko National University of Kyiv,*
62a, Volodymyrska Str., Kyiv 01601, Ukraine, E-mail: vadiga@ukr.net

[2] *O.O. Chuiko Institute of Surface Chemistry, the National Academy*
of Science of Ukraine, Gen.
Naumova St., 17, General Naumov Str., 03164 Kyiv, Ukraine

[3] *Prešov Universirty in Prešov, Ul. 17 Novembra, 1, 080 01, Prešov, Slovakia*

Significant production volumes, ease of production, and low cost of bioethanol make it a valuable fuel additive and raw material for preparing important organic substances: diethyl ether, ethylene, ethylene oxide, propylene, butadiene, acetaldehyde, vinyl acetate, etc. Heteropolyacids are the most active catalysts for ethanol dehydration. They differ from other catalysts by significant acidity and high stability. Due to the low specific surface area, in the production of acid-based catalysts, heteropolyacids are usually loaded onto various carriers to increase their catalytic activity by increasing dispersion.

In this work, we investigated the activity and selectivity of nanocomposite catalysts. They were prepared using phosphotungstic acid (PTA) $H_3PW_{12}O_{40}$•nH_2O and various carbon materials, including activated carbon, carbon fibers, and carbon nanotubes. These catalysts were examined in the gas-phase reaction of ethanol dehydration and characterized by different methods: SEM, adsorption of N_2, TG/DTG, TPD MS, XRD, and FTIR.

We showed that the obtained nanocomposites are active catalysts in bioethanol dehydration. In the temperature range of 120-170 °C, the main product of dehydration is diethyl ether, and its maximum yield is 66%. In the temperature range of 190–230 °C, bioethanol can be dehydrated over catalysts to ethylene with 100% selectivity. Increasing the PTA content from 0.005 to 0.01 mmol per gram of support increases the yield of diethyl ether and decreases the temperatures of the formation of dehydration products. The temperature window of the diethyl ether formation expands by 10-30 °C when carbon fibers are used as a carrier. We prove that the use of oxidized carbon solids leads to a significant increase in the catalytic activity of the obtained composites, regardless of the content of the applied PTA. In the study of adsorption-desorption of ethanol, we found that oxygen-containing functional groups are surface centers of PTA immobilization and ethanol adsorption. Oxidation of the carrier surface is a method that improves the absorption of alcohol in the temperature range of 110-150 °C, increases the rate of dehydration, and increases the productivity of catalysts.

Effect of chlorination on the interaction of carbon fibers with electromagnetic radiation in the ultrahigh-frequency range

***Zhytnyk D.O.*[1], *Moiseienko V.A.*[1], *Mischanchuk O.V.*[2], *Matushko I.P.*[1], *Diyuk V.E.*[1], *Grishchenko L.M.*[1], *Boldyrieva O.Yu.*[1]**

[1] *Taras Shevchenko National University of Kyiv,*
64/13, Volodymyrska St., Kyiv-01601, Ukraine.
liudmyla.grishchenko@gmail.com

[2] *O.O. Chuiko Institute of Surface Chemistry, NAS of Ukraine,*
Gen. Naumova St., 17, Kyiv-03164, Ukraine.

Carbon materials are widely used as fillers to prepare composite materials for personal protective equipment and arm protection or can be integrated into stealth technologies [1]. But, there is almost no data on the effect of chemical modification on the nature of the interaction of carbon materials with electromagnetic radiation in the modern literature.

We used commercial carbon fibers (CFs) as starting material in this study. They were prepared by high-temperature carbonization of polyacrylonitrile (PAN) fibers. This work aims to study the effect of chlorination of PAN CFs on the radio wave absorbing properties of the resulting chlorinated PAN CFs. The chlorination process was performed with carbon tetrachloride vapor in an argon flow at 300 °C, 450 °C, and 600 °C. We investigated the temperature effect on the chlorination process and, therefore, on the chlorine concentration in the chlorinated PAN CFs on the microwave attenuation. We found that added chlorine has a crucial impact on the attenuation of the power of electromagnetic radiation S_{21} and the reflection coefficient of electromagnetic radiation S_{11}. This statement is true in a wide frequency range for a single layer of the chlorinated PAN CFs, considering that our studies were performed in the ultrahigh-frequency X and Ka bands. We proved that the attenuation magnitude and the reflection coefficient are increased with the chlorine concentration. Besides, their values are constants in a wide range of frequencies. This observation enables the construction of the latest generation of microwave attenuators; their attenuation can be programmed once by the chlorine concentration in the PAN CFs.

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Effect of boron doping on temperature dependence of Raman spectra of boron doped HPHT-diamond

Danylenko I.M.[1], ***Mozdalevskyi I.V.***[1,2], ***Nikolenko A.S.***[1], ***Strelchuk V.V.***[1], ***Starik S.P.***[3], ***Gontar O.G.***[3], ***Kovalenko T.V.***[3], ***Ivakhnenko S.O.***[3]

[1] V.E. Lashkaryov Institute of Semiconductor Physics NASU,
pr. Nauky 41, 03028 Kyiv, Ukraine
E-mail: igor.tesV@gmail.com

[2] Taras Shevchenko National University of Kyiv, Faculty of Physics,
Volodymyrska Street 64/13, 01601 Kyiv, Ukraine

[3] V. Bakul Institute for Superhard Materials NASU,
Avtozavodska str. 2, 04074 Kyiv, Ukraine

High hardness and stability of diamond, its excellent electrical and optical properties are of great importance for the development of the next generation of high-frequency and high power electronic devices. In particular, boron doped diamond (BDD) is of interest as *p*-type semiconductor. The dynamical behavior of optical phonons is important in terms of heat transfer, since electronic devices must efficiently dissipate heat to maintain operating temperatures. Temperature-dependent Raman spectroscopy is an effective non-contact method for measuring the temperature dependence of phonon lifetime. In this study, the effects of anharmonic decay (damping) of optical phonons in BDD are studied as a function of boron doping using micro-Raman spectroscopy through the modeling of temperature dependence of experimental phonon linewidth and frequency position. The type IIb BDD crystals with different level of boron doping were grown by the temperature gradient method under high pressure and high temperature (HPHT) in the Fe-Al-B-C system and multisectoral BDD plates of different orientation were prepared by laser cutting and mechanical polishing from. Undoped type IIa HPHT-diamond was studied for comparison. Micro-FTIR transmission spectroscopy was used to estimate the spatial distribution of uncompensated boron impurity $[N_a\text{-}N_d]$ in BDD plates through the analysis of boron-related absorption peaks. Theoretical modeling of temperature dependence of experimental phonon linewidth and frequency was performed in the temperature range of 78-373 K. Contributions of different mechanisms of anharmonic decay of optical phonons are considered. The predominant decay mechanisms and anharmonicity parameters of optical phonons are determined, which is of fundamental importance for the thermal conductivity of semiconductor materials.

Mechanochemical transformation of Pb_2MoO_5 single crystal into nano-dispersed state

Sydorchuk V.[1], **Khalameida S.**[1], **Khyzhun O.**[2]

[1] Institute for sorption and problems of endoecology of the NAS of Ukraine,
13 Gen. Naumova street, Kyiv-03164, Ukraine.
E-mail: svkhal@ukr.net

[2] I.M. Frantrevich Institute for Problems of Materials Science of the NAS of Ukraine, 3 Krzhyzhanovsky street, Kyiv-03142, Ukraine

Lead molybdate Pb_2MoO_5 belonging to the family of monoclinic compounds with a framework-type structure possesses excellent optical quality, high transparency throughout the visible spectral range, absence of optical damage and very promising intrinsic photoluminescence. Pb_2MoO_5 single crystals are considered as a very attractive material for application in acousto-optical devices, such as modulators, detectors and filters operating over the visible and middle infrared spectral regions. On the other hand, as a semiconductor, it is promising for application in photocatalysis in a nano-dispersed state. Therefore, transformation of its single crystal into nanosized state is an important scientific and applied task. Such transformation is possible by means of mechanochemical treatment. Particularly, high energy milling belongs to the effective method for preparation of oxide materials in nano-sized state.

Pb_2MoO_5 single crystal was subjected to mechanochemical treatment (MChT) in air and water at 500 rpm for 30 min using planetary ball mill. This contributes to the process of dispersion and surface activation, as indicated by studies carried out with XRD, nitrogen adsorption-desorption, XPS, FTIR and UV-Vis spectroscopy. As a result, nanopowders with crystallite size of 16-18 nm and specific surface area 1.9-3.5 m^2/g were derived.

Since Pb_2MoO_5 absorbs visible light and has band gap of about 2.5-2.6 eV, it was tested as photocatalyst in process of dyes degradation under visible irradiation. All milled samples exhibited photocatalytic activity under these conditions. Milled Pb_2MoO_5 nanopowder doped with 5% of bismuth oxide shown maximum activity: the rate constant degradation is $7 \cdot 10^{-5}$ s^{-1}. Employing XPS method, we have studied in detail changes in surface states when subjecting the Pb_2MoO_5 single crystal to MChT in air and water as well as when doping with bismuth oxide and found the correlation between binding energy values of the constituting atoms and photocatalytic activity of the Pb_2MoO_5 nanopowders.

Effect of $^{16}O^{6+}$ ion-irradiation on structural, magnetic properties, antistructural modeling of zinc nanoferrite

Parmar C.[1], Verma R.[1], Modak, S. S.[2], Mazaleyrat F.[3], Tatarchuk T.[4], Kane S.N.[1]

[1] *School of Physics, D. A. University, Khandwa road, Indore-452001, India*

[2] *Physics Department, Jaypee University of Eng. and Tech.,*
Guna 473226, India

[3] *SATIE, ENS Paris-Saclay, 4 Av. des Sciences,*
91190 Gif–sur–Yvette, France

[4] *Chemistry Department, Vasyl Stefanyk Precarpathian National University,*
Ivano-Frankivsk 76018, Ukraine
e-mail: tatarchuk.tetyana@gmail.com

Ferrimagnetic spinel ferrites with general formula $M^{2+}Fe^{3+}{}_2O_4$, display face centred cubic fcc structure, Fd_3m space group, and have two inter-penetrating sub-lattices tetrahedral *(A)*, octahedral *(B)*. Ferrites are important ceramic materials used in various applications including those in high frequency devices, microwave devices, gas sensing, multilayer chip inductors, in bio-medical applications etc. Tailoring their magnetic properties *(to design, develop suitable materials)* can be done by: i) a specific synthesis technique, ii) compositional variation, iii) thermal treatment/no-thermal treatment, ion irradiation etc. Ion irradiation is one of the novel techniques, known to affect material properties. So, we report effect of 80 MeV $^{16}O^{6+}$ ion irradiation *(Dose: $1\times10^{11} - 1\times10^{13}$ ions/cm²)* on structural, magnetic properties, antistructural-modeling of sol gel auto-combustion synthesized *"dry gel"* $ZnFe_2O_4$, monitored by x-ray diffraction (XRD), magnetic measurements.

Data analysis reveal that $^{16}O^{6+}$ ion irradiation leads to modification of: a) lattice parameter *(0.8400 – 0.8423 nm)*, b) grain diameter *(15.7 – 17.6 nm)*, c) Oxygen positional parameter *(0.3836 – 0.3846)*, inversion parameter *(0.1 – 0.3)*, d) re-distribution of Fe^{3+}, Zn^{2+} ions on A, B-site. Ion irradiation leads to reduction of: saturation magnetization *(0.40 – 7.88 Am²/kg)*, minor changes in coercivity, squareness ratio *(0.053 – 0.087)*. Results are interpreted in terms of ion-irradiation induced structural changes, resulting in alteration of magnetic properties. Antistructural modeling for the studied samples *(pristine, irradiated)* is used for describing the surface-active centers.

The effect of rare-earth metal oxide additives on crack growth resistance of fine-grained partially stabilized zirconia

Kulyk V.V.[1], Duriagina Z.A.[1,2], Vasyliv B.D.[3], Vavrukh V.I.[1], Kovbasiuk T.M.[1], Lyutyy P.Ya.[1], Vira V.V.[4]

[1] *Department of Materials Science and Engineering, Lviv Polytechnic National University, 12 S.Bandera str., Lviv 79000, Ukraine.*
E-mail: kulykvolodymyrvolodymyrovych@gmail.com

[2] *Department of Materials Engineering, The John Paul II Catholic University of Lublin, 14 Racławickie Al., Lublin 20-950, Poland.*

[3] *Department of Hydrogen Technologies and Alternative Energy Materials, Karpenko Physico-Mechanical Institute of the NAS of Ukraine, 5 Naukova str., Lviv 79060, Ukraine.*

[4] *Department of Strength of Materials and Structural Mechanics, Lviv Polytechnic National University, 12 S.Bandera str., Lviv 79000, Ukraine.*

Recently, the additives of rare-earth metal oxides are being used for obtaining partially stabilized zirconia ceramics aimed at applications in various high-temperature structural components. Corresponding sintering modes providing fine-grained microstructure formation are being developed. Due to the obtained correlations between the morphology parameters and resulting mechanical characteristics of ceramics it is possible to reach a unique combination of their functional properties.

In this work, zirconia ceramics stabilized with small percentages of rare-earth metal oxides have been studied in terms of sintering ability, elimination of the phase changes in zirconia, as well as employment of the transformation toughening mechanism during crack propagation. The metal oxides including rare-earth metal oxides (Y_2O_3, CoO, CeO_2, Fe_2O_3) were used as additives to reach a stabilizing effect on zirconia and manufacture ceramics with fine-grained microstructure. Series of ceramic specimens were prepared using conventional sintering in a temperature range of 1500 °C to 1850 °C with and without annealing. Fracture toughness test by indentation method and single-edge notch beam test under three-point bending were performed. Based on X-ray diffraction analysis and SEM studies of fracture surfaces of specimens it was concluded that the maximum transformation toughening effect revealed for ZrO_2–Y_2O_3–CoO–CeO_2–Fe_2O_3 ceramics was related to a distinct change in the fracture surface pattern.

Study of the effects of MgO additive and sintering temperature on mechanical behavior of fine-grained ZrO_2–MgO ceramics

Kulyk V.V.[1], *Duriagina Z.A.*[1,2], *Vasyliv B.D.*[3], *Vavrukh V.I.*[1], *Lyutyy P.Ya.*[1], *Kovbasiuk T.M.*[1], *Vira V.V.*[4]

[1] *Department of Materials Science and Engineering, Lviv Polytechnic National University, 12 S.Bandera str., Lviv 79000, Ukraine.*
E-mail: kulykvolodymyrvolodymyrovych@gmail.com

[2] *Department of Materials Engineering, The John Paul II Catholic University of Lublin, 14 Racławickie Al., Lublin 20-950, Poland.*

[3] *Department of Hydrogen Technologies and Alternative Energy Materials, Karpenko Physico-Mechanical Institute of the NAS of Ukraine, 5 Naukova str., Lviv 79060, Ukraine.*

[4] *Department of Strength of Materials and Structural Mechanics, Lviv Polytechnic National University, 12 S.Bandera str., Lviv 79000, Ukraine.*

Zirconia ceramics partially stabilized with various amounts of MgO have been studied. The aim of this work was to investigate changes in mechanical behavior of the ceramics depending on the sintering temperature and percentage of MgO additive. Conventional sintering of series of ceramic specimens in a temperature range of 1510 °C to 1850 °C with and without annealing was performed. A set of mechanical tests were carried out: (i) strength test of beam specimens under three-point bending; (ii) Vickers microhardness test; (iii) fracture toughness test by Vickers indentation (VI method); (iv) single-edge notch beam test under three-point bending (SENB method).

Among the materials studied, ZrO_2–2.5 mol% MgO ceramics sintered at 1850 °C showed the best crack growth resistance behavior for both VI and SENB methods. In contrast to other ceramic variants containing about 12–15 wt% c-ZrO_2 and 85–88 wt% m-ZrO_2, this material contained 58 wt% c-ZrO_2 and 42 wt% m-ZrO_2. Such a comparatively high percentage of c-ZrO_2 in this material variant caused a distinct difference in its mechanical behavior. Based on the obtained results of mechanical tests and the analysis of fracture surface morphology it was concluded that the fracture toughness of optimally fabricated ZrO_2–MgO ceramics is attributed to particle-crack interactions, which result in a transformation zone around the crack tip. An increase in crack growth resistance of this material variant was accompanied by a slight increase in its strength and microhardness.

Surface functionalization of nanoporous carbons with sulfur- and halogen-containing groups

Pryhunova O.[1]***, Grishchenko L.M.***[1]***, Zaderko A.N.***[1]***, Diyuk V.E.***[1]***,***
Mariychuk R.[2]***, Boldyrieva O.Yu.***[1]***, Lisnyak V.V.***[1,2]

[1] Taras Shevchenko National University of Kyiv,
62a, Volodymyrska Str., Kyiv 01601, Ukraine,
E-mail: lisnyak@univ.kiev.ua

[2] Prešov University in Prešov, Ul.
17 Novembra, 1, 080 01, Prešov, Slovakia

The introduction of two types of heteroatoms in the structure of carbon materials allows to change of the properties of the surface layer in a wide range and to obtain materials much better adapted to the specific application. Dual-doped carbons where one of the heteroatoms is fluorine are used mainly as electrode materials. Dual-doped carbons with S, N, Cl, and P heteroatoms are widely used in electrocatalytic processes, sensory, and catalysis. They are also integrated into the production of lithium-ion and sodium-ion batteries, and in supercapacitors.

In this work, the surface of nanoporous carbon (NC) was modified with $C_2F_4Br_2$ or CF_2Cl_2 freons in the gas phase process, which provides the introduction into the surface layer of 0.7–1.9 mmol of fluorine, 1.3–2.1 mmol of bromine, and 2.4–2.9 mmol of chlorine per gram of NC, as evidenced by elemental analysis and confirmed by NMR spectroscopy. The TGA method showed that the halogenated NCs have high thermal stability, and the thermal decomposition of surface groups is observed at temperatures above 500 °C. Modification with $C_2F_4Br_2$, compared with that of CF_2Cl_2, leads to the formation of a more active surface layer.

Acid-base catalysts obtained by sulfonation of halogen-containing NC have two temperature intervals of the thermal decomposition of the surface layer: 140–310 °C and 320–510 °C. It is shown that the determining effects of weight loss in these temperature ranges correlate with the catalytic activity of the obtained sulfonated NCs. The sulfonated NCs have been shown to have high catalytic activity in the isopropanol dehydration reaction. The temperature of 100% conversion of isopropanol to propylene for the most active sulfonated samples is 170–180 °C.

Features of the electrical properties of ZnO:Al/ZnS/*n*-CdTe heterojunctions

Maistruk E.V., Orletskyi I.G., Ilashchuk M.I., Koziarskyi I.P., Koziarskyi D.P.

Yuriy Fedkovych Chernivtsi National University,
2 Kotsubynsky st., 58002 Chernivtsi, Ukraine.
E-mail: i.koziarskyi@chnu.edu.ua

ZnS thin films are promising semiconductor materials for use in solar cells as a transparent front window or buffer layer. A high transmittance ($T = 85\%$) in the visible and near infrared ranges of the optical spectrum, a wide band gap ($E_g \approx 3.4$ eV), and better crystal lattice matching compared to CdS [1] with A^2B^6 substrates contribute to their use in buffer layer heterostructures based on CdTe.

ZnO:Al/ZnS/*n*-CdTe heterostructures were fabricated using freshly split crystalline CdTe substrates doped with Cl impurity (Cl concentration in the melt was $N^0Cl \approx 5{\cdot}1018$ cm^{-3}). The structures were fabricated by sequential deposition of thin films of ZnS (~ 0.2 μm) and ZnO:Al (~ 0.1–0.15 μm) by high-frequency magnetron sputtering of zinc sulfide and aluminum-doped zinc oxide targets.

Analysis of the I-V-characteristics of the studied heterojunctions at forward and reverse voltages in the temperature range $T = 296$–338 K showed the presence of the current rectification effect due to the potential barrier qφk = 0.72 eV. The mechanism of charge carriers passing through the barrier at forward biases is well explained on the basis of the theory of space-charge-limited currents, which arises due to the presence of shallow monoenergetic ($N_t \approx 10^{14}$ cm^{-3}) and deep (with exponential energy distribution) traps in the CdTe near-surface layer. The reverse currents are generated with the participation of the deep energy level $\Delta E = 0.76$ eV in the region of the base material depleted on the main charge carriers. A feature of the *C-V*-characteristics of ZnO:Al/ZnS/*n*-CdTe heterojunctions in the reverse bias region (at frequencies $f = 10$–1000 kHz) is the independence of the measured capacitance from voltage and its change with a change in the frequency of the excitation signal. The electrical properties of ZnO:Al/ZnS/*n*-CdTe heterojunctions are explained by the presence of a high-resistance CdS_xTe_{1-x} layer in the near-surface region of cadmium telluride, which is formed due to the diffusion of sulfur atoms during the fabrication of the structure.

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Two-band nature of superconductivity in molybdenum-rhenium alloys

***Shapovalov A.P.*[1], *Boliasova O.O.*[2], *Dmitrenko V.Yu.*[2], *Tarenkov V.Yu.*[2]**

[1] G. V. Kurdyumov Institute for Metal Physics, NAS of Ukraine,
36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine.

[2] Donetsk Institute for Physics and Engineering Named after O. O. Galkin,
NAS of Ukraine, 46 Nauky Ave., UA-03028 Kyiv, Ukraine.
E-mail: dmitrenko_v@ukr.net

The class of multiband superconductors (SCs) includes not only the ‘classical’ two-band MgB_2, but also such as high-temperature SCs. The discovery of another two-band SC, $Mo_{1-x}Re_x$, with a conventional electron-phonon pairing mechanism allows a more detailed study of the nature of multi-band superconductivity, the unique dynamic characteristics of which can manifest themselves in various functional devices.

Characteristics of $Mo_{1-x}Re_x$ alloys [1] indicating two-band nature of superconductivity were obtained from the measurements the electronic heat capacity and the magnetic field penetration depth. The Andreev spectroscopy gives an unambiguous result in terms of a microscopic nature of the investigated superconducting state. In this report, a series of experiments were carried out to study the conductivity of $Mo_{0.52}Re_{0.48}$-Ag (S-N) contacts. Point contacts of the Andreev type are prepared by the sliding electrode method of a silver needle on a MoRe film, or a MoRe needle in contact with a silver electrode. From the obtained Andreev spectra for both film and bulk samples of the MoRe alloy, the two energy gaps have been restored: a large Δ_{MoRe} =2.45 mV and a small $\Delta L \approx$ 0.34 mV. A similar conclusion was obtained from the experiments on temperature dependence of the heat capacity of this SC [1]. The ratio $2\Delta_0/kTc = 4.2 \pm 0,1$ indicates a strongly coupled nature of superconductivity in the bulk and film of $Mo_{0.52}Re_{0.48}$.

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Nanoelastics of Ge1-xSnx films driven by composition and structural relaxation

Malyuta S.V.[1,2]***, Lytvyn P.M.***[1]***, Kuchuk A.V.***[1]***,***
Kondratenko S.V.[3]***, Mazur Yu.I.***[4]

[1] *V.E. Lashkaryov Institute of Semiconductor Physics NASU,*
41 Nauky pr., 03028 Kyiv, Ukraine
E-mail: serhiy.malyuta@gmail.com

[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37 Peremohy, av. 03056 Kyiv, Ukraine*

[3] *Taras Shevchenko National University of Kyiv,*
64 Volodymyrs'ka St., 01601, Kyiv, Ukraine

[4] *Institute of Nano Science and Engineering, University of Arkansas,*
Fayetteville, AR, 72701, USA

Recently, there has been increased interest in $Ge_{1-x}Sn_x$ compounds as the material for mid-range infrared optoelectronics. There is a fundamental possibility to control the bandgap ranging from semiconductor to semimetal. The transition from the indirect to direct-band gap configuration is relatively easy to implement, increasing the tin content over 6.5 at. % in these alloys. Within the last few years, significant progress has been made in the development of GeSn-based lasers, photodetectors, emitting diodes, and transistors. Nevertheless, the $Ge_{1-x}Sn_x$ structural stability is a case to solve. A large number of dislocations of various types, surface segregation of tin atoms, and phase separation of metastable GeSn layers decrease a conductivity channel and increase the density of non-radiative recombination centers.

Nanomechanical properties, in particular elastic characteristics, of GeSn thin films are extremely important in the problem of deformation engineering of their band structure. Nonmonotonic dependences of Young's modulus value for the $Ge_{1-x}Sn_x$/Ge/Si nanostructures with variations in their composition and thickness are revealed by the "atomic force" indentation. It is shown that for $Ge_{1-x}Sn_x$ films of subcritical thicknesses and small x (1÷5%) the changes in Young's modulus are caused by the change in the composition. With the onset of plastic relaxation for the mean values of x (5÷8%), the increase of Young's modulus correlates with the amount of dislocation hardening effect. The phase separation processes and the segregation of tin on the surface at the supercritical thicknesses and high Sn content (~ 12%) lead to Young's modulus decreasing with increasing $Ge_{1-x}Sn_x$ film thickness.

Flooding of massive samples and thin films of the Gd-Fe system

Prysyazhnyuk V.I.

Department of Metal Physics of Ivan Franko National University of Lviv.
Kyrylo & Mephodiy Street, 8, Lviv-79005, Ukraine
E-mail: viktor.prysyazhnyuk@lnu.edu.ua

In materials science, a new tend of chemical and thermal treatment of metals is intensively developing, which consists in the use of hydrogen as a technological environment in the process of processing functional materials. Such hydrogen technologies are based on the laws of the influence of hydrogen on phase transformations in metals, including polymorphism, atomic ordering and the formation and decay of intermetallic phases and hydrides. A known process that affects the formation of the phase-structural state of the material is HDDR (hydrogenation, disproportionation, desorption, recombination). If you complete the HDDR process at different stages, you can get very different results.

The Gd-Fe_2 compounds and films and two flood schemes were used for the study – 1) The crushed Gd-Fe_2 samples were under a pressure of $2x10^6$ Pa for 168 hours at room temperature. 2) The crushed samples of Gd-Fe_2 were under a pressure of 10^6 Pa for 30 minutes at temperatures of about 700K. In the first case, hydrogen penetrated the lattice, deforming it. The amount of absorbed hydrogen depends on how finely ground our powder, in the case of thin films, the amount of absorbed hydrogen increases sharply compared to the mass of the "absorber". Electrographic studies of films before and after flooding indicate that such films have become finer. When heating the flooded samples, the reverse process of hydrogen evolution was observed, as evidenced by chemical analysis of the air in the heating chamber. It is possible to use such multi-layered structures to create hydrogen batteries. In the second case, hydrogen reacts with Gd-Fe_2 to form GdH_2 and GdH_3 plus free Fe. As evidenced by the destruction of the sample (turned into powder) and diffraction studies. Unfortunately, the second method is not very productive for films. But such hydrogen treatment can be used to influence the magnetic properties of the obtained powders, because it forms an anisotropic structure of magnetic materials.

Photocatalytic performance of mixed lithium niobates-tantalates prepared by mechanochemical methods

Sydorchuk V.*[1]*, Sugak D.*[2]*, Hurskyi S.*[3]*, Samsonenko M.*[1]*,
***Khalameida S.*[1]*, Vasylechko L.*[2]**

[1] *Institute for Sorption and Problems of Endoecology, NAS of Ukraine, 14 Naumov St, Kyiv-03164, Ukraine.*
E-mail: mashuna.08@gmail.com

[2] *Lviv Polytechnic National University,*
12 Bandera St., 79013 Lviv, Ukraine

[3] *Institute for Energy Research and Physical Technologies,*
Clausthal University of Technology, 19B Am Stollen, Goslar, Germany

Lithium niobate LN and tantalate LT are among the most frequently used materials of functional electronics. Recently $LiNb_{1-x}Ta_xO_3$ (LN-LT) solid solutions have been studied, since they offer the prospects for combining the advantages of both pure materials. The nanoparticles of LN-LT can be more attractive for some practical applications. As the wide-gap semiconductors, LN and LT powders are also prospective photocatalysts under UV irradiation. High energy milling belongs to effective method for preparation of oxide materials in nano-sized state. It promotes activation of reagents and their interaction with perovskite phase formation.

Thus, dry milling of Li_2CO_3-Nb_2O_5-Ta_2O_5 mixtures with different ratio of oxides at 600 rpm for 15 h results in formation of intermediates consisting predominantly of X-ray amorphous and low-crystalline niobates-tantalates [1]. After next calcinations at 700ºC, intermediates are converted into perovskites with a solid solution structure and a particle size of 20-80 nm.

Since both obtained intermediate and pure perovskite powders absorb visible light and have band gap within 3.00-3.25 eV, they were tested as photocatalysts under visible irradiation in process of dyes degradation in aqueous media. Calcined high-crystalline niobates-tantalates show moderate photocatalytic activity. At the same time, as-milled intermediates and especially those after hydrothermal treatment exhibited high performance, apparently due to the higher specific surface area. Praseodymium-doped sample has the highest activity which is obviously associated with smallest value of the band gap.

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Surface relief gratings in methacrylic polymers containing quinoline-based azo-dyes

Chomicki D.[1]***, Czaplicki R.***[1]***, Kharchenko O.***[2]***, Smokal V.***[2]***,***
Krupka O.[2]***, Derkowska-Zielińska B.***[1]

[1] *Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5/7, 87-100 Toruń, Poland.E-mail: chomicki@doktorant.umk.pl*

[2] *Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska 60, 01033 Kyiv, Ukraine*

Azobenzenes are constituted of two phenyl rings linked by an azo (–N=N–) bridge. One of their most important features is reversible trans-cis photoisomerization reaction, which leads to very interesting phenomena [1].

When azobenzene molecules are attached to the polymer chain and the material is excited with a polarized laser beam, the occurring intensity gradient causes of mass transport of the polymer chains. This phenomenon can be used for surface patterning of the azobenzene-containing polymers. Especially, when the sample is illuminated with the interference pattern, it leads to surface relief grating (SRG) formation on the surface of the material [2]. SRG formation can be used in many applications such as holographic data storage devices, fiber couplers, as well as fabrication of nanostructures from other materials [3,4]. For this reasons, development of new materials with improved grating formation efficiency and stability continuously interests scientists.

We will show surface relief grating formation in methacrylic polymers containing quinoline-based azo-dyes. SRGs were recorded using two-beam interferometric setup that allows to measure the time evolution of diffraction efficiency. The inscribed patterns were examined with atomic force microscopy. We observed that we can modify the surface relief formation dynamics, final diffraction efficiency as well as surface modulation depth by changing the substituents present in the azo-dye moiety.

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Molecular Dynamics Simulation of the Formation of Extended Defect Structure in 3C-SiC Thin Films on Si(001) Substrates

Sarikov A.[1]***, Marzegalli A.***[2]***, Barbisan L.***[3]***,***
Scalise E.[3]***, Montalenti F.***[3]***, Miglio L.***[3]

[1] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine.*
41 Nauki avenue, 03028 Kyiv, Ukraine.
E-mail: sarikov@isp.kiev.ua

[2] *L-NESS and Department of Physics, Politecnico di Milano,*
via Anzani 42, 22100 Como, Italy.

[3] *L-NESS and Department of Materials Science, University*
of Milano-Bicocca, via R. Cozzi 55, 20125 Milan, Italy.

Thin films of cubic silicon carbide (3C-SiC) epitaxially grown on Si(001) substrates are promising for power device applications. However, the electronic quality of such films is strongly affected by large amount of extended defects, such as stacking faults (SFs) and partial dislocations (PDs), formed during film growth.

This work presents the results of a detailed study of the formation of extended defect configurations during growth of 3C-SiC films on Si(001) substrates using molecular dynamics (MD) simulations. First, a synergetic approach based on the application of the Vashishta and the analytical bond order potentials for simulation of large-scale PD and SF transformations, and the local atomic configurations of dislocation cores, respectively, is proposed and validated. Using this approach, the evolution and interaction of partial dislocations and stacking faults are simulated as directly related to the 3C-SiC growth technology. The processes under study are described in terms of the orientations of the Burgers vectors and mutual arrangements of partial dislocations terminating stacking faults. A number of experimentally observed phenomena are explained including: (i) stabilization of multiple stacking faults by PD complexes, leading to the formation of hexagonal SiC inclusions (4H and 6H) in 3C-SiC, (ii) formation of preferential shapes of multiple SFs; and (iii) annihilation of stacking faults with formation of characteristic SF intersection patterns. Obtained results provide a comprehensive understanding of how the technological conditions of growing epitaxial 3C-SiC films on Si(001) substrates result in the experimentally observed extended defect configurations in them. These results are important for further development of 3C-SiC growth technology to improve the electronic quality of obtained films.

Effect of Intensifying Additives on the Properties of Celsian Ceramics

Lisachuk G.V., Kryvobok R.V., Voloshchuk V.V.

National Technical University "Kharkiv Polytechnic Institute".
Kyrpychova str., 2, Kharkiv-61002, Ukraine.
E-mail: valenty93vol@gmail.com

The creation of radio-transparent ceramic materials with a set of high performance characteristics is currently an urgent need for modern aviation and rocket and space industries. Modern technologies make it possible to obtain materials with different properties by modifying them with different additives.

In this work, the effect of intensifying additives on the properties of Celsian ceramics is studied. The oxides SnO_2, Li_2O and Cr_2O_3 and the eutectic additive $SnO_2 – Li_2O$ were used as intensifiers. Additives were added to the mixture in the amount of 0.5 - 2 wt.% over 100 wt.%. Firing was carried out at temperatures of 1,200°C, 1,250°C and 1,300°C with holding at the maximum temperature for 1 hour. The assessment of the effect of additives on the sintering of the Celsian phase was studied by comparing the physical and dielectric properties of the test samples. Structural-phase features of the samples were studied by X-ray phase analysis and scanning electron microscopy.

The results of studying the microstructure of test samples obtained at a temperature of 1,200°C, containing the eutectic additive $Li_2O – SnO_2$ (1 wt.%), indicate the presence of monoclinic Celsian crystals evenly distributed in the glass phase and single closed pores up to 40 μm in size, the presence of which is explained by the accelerated mode firing with a short interval of isothermal exposure. A positive effect of the addition of $SnO_2 – Li_2O$ on the low-temperature activation of the process of synthesizing the Celsian phase and obtaining a densely sintered ceramic material has been established.

It has been established that, in terms of its dielectric properties, the obtained ceramic material belongs to radio-transparent materials. Celsian ceramics synthesized at a low temperature of 1,200° C with an exposure of 1 hour and with the addition of 1 wt. % $SnO_2 – Li_2O$, is characterized by the following properties: water absorption – 7.1%, apparent density – 2.6 g/cm^3, dielectric permittivity – 8.7, dielectric loss tangent – 0.09.

Laser-stimulated reversible structural modification of surface As-enriched As-S nanolayers

Kondrat O.B.[1], **Holomb R.M.**[1,2], **Mitsa V.M.**[1], **Tsud N.**[3], **Vondráček M.**[4], **Mitsa O.V.**[1], **Matolin V.**[3], **Veres M.**[2]

[1] *Information Control Systems and Technologies Department, Uzhhorod National University. 88000 Uzhhorod, Ukraine. E-mail: oleksandr.kondrat@uzhnu.edu.ua*

[2] *Wigner Research Centre for Physics, Hungarian Academy of Sciences, 1121 Budapest, Hungary.*

[3] *Charles University, Faculty of Mathematics and Physics, Department of Surface and Plasma Science, V Holešovičkách 2, 18000 Prague, Czech Republic.*

[4] *Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 21 Prague, Czech Republic.*

The $As_{45}S_{55}$ nanolayers were prepared *in-situ* in preparation chamber of Materials Science Beamline (MSB, Elettra–Sincrotrone Trieste) by thermal evaporation of bulk glass powder and deposition onto a silicon substrate. The atomic composition, local structure, and their characteristics, as well as reversible structural changes during thermal annealing and laser illumination by monochromatic coherent light with over band-gap photon energy of *in-situ* fabricated $As_{45}S_{55}$ nanolayers were examined by synchrotron radiation photoelectron spectroscopy [1]. It was established that the structure of as-deposited sample is slightly enriched by As. *In situ* thermal annealing rearranges the structure of As-S film and leads to the formation $As\text{-}S_3$ and $As\text{-}Se_2As$ s.u. following by dissociation of s.u. with As-As bonds. From the other hands, *in situ* over band-gap laser illumination increases the contribution of $As\text{-}S_2As$ s.u. in the structure of As-Se nanolayers even more then in the as-deposited film. The "thermal annealing" - "laser illumination" of As-S nanolayers performed in cycle mode reveals the reversibility of the structural changes.

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Metal-based nanocrystalline materials condensed from the vapor phase

Kozyrev A., Grechanyuk V., Grechanyuk I.,
Matsenko A., Kovalchul Yu.

Department of Chemistry, Kyiv National University of Construction
and Architecture. Povitroflotsky Ave., 31, Kyiv-03037, Ukraine.
E-mail: artem.v.kozyrev@gmail.com

Experimental study of methods for obtaining nanocrystalline molybdenum- and copper-based materials on from two independent crucibles on a stationary and rotating substrate [1] has been done. The interaction of the separating layer with condensed Cu-Mo materials was investigated. The influence of substrate material, surface roughness, temperature of the substrate, evaporation rate of starting materials on the mechanical properties of Cu-Mo condensed materials, partially described in [2, 3], was analyzed. It is determined certain content of molybdenum, exceeding which the strength dramatically decreases due to the formation of pores, and it was shown that an increase in the substrate temperature from 700°C to 900°C makes it possible to prevent this effect.

Due to the determination of mechanical characteristics of condensed composite materials obtained on rotating substrates with different surface roughnesses, it was found that a decrease of the roughness of the substrates leads to an increase in the ultimate tensile strength and elongation. It was found that structural defects in the form of rods formed on micro-droplets ejected from the evaporator are the cause of reduced strength and ductility of condensed composite materials. It was establish that the regularities of formation of the technological layer of Cu-Mo condensate depend on the thickness of the separating layer of calcium fluoride.

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The use of ferrocene as a source of iron nanoparticles – an effective catalyst for the production of carbon nanotubes

Sviatenko A.*[1]*, Filonenko D.*[1]*, Nebesnyi A.*[1]*, Khovavko A.*[1]*,
***Strativnov E.*[1]*, NieGuochao*[2]*, Minitskyi A.*[3]*, Barabash M.*[4]**

[1] Department of thermo-chemical processes and nanotechnologies
Gas Institute of National Academy of Sciences
39 Degtyarivska str., 03113 Kyiv, Ukraine
E-mail: ingaskiev@gmail.com

[2] School of Physics and Telecommunication Engineering,
Yulin Normal University, Yulin 537000, China

[3] National Technical University of Ukraine 'Igor Sikorsky Kyiv
Polytechnic Institute' 37, Prospect Pobedy, UA-03056 Kyiv, Ukraine

[4] Technical Centre of National Academy of Science of Ukraine,
13, Pokrovs'ka Str., UA-04070 Kyiv, Ukraine

This paper presents the results of studying the process of carbon nanotubes (CNTs) synthesis in a converted gas (CG) atmosphere in a flow-type quartz reactor by the method of chemical vapor deposition CVD using ferrocene decomposition products as a catalyst. The products of air conversion of natural gas served for CNTs synthesis. Target carbon was obtained by disproportionation of carbon monoxide. The temperature regime for CNTs growth was about 650 °C and was chosen as optimal for the iron catalyst.

A schematic of a laboratory unit for CNTs synthesis is shown in Fig. 1.

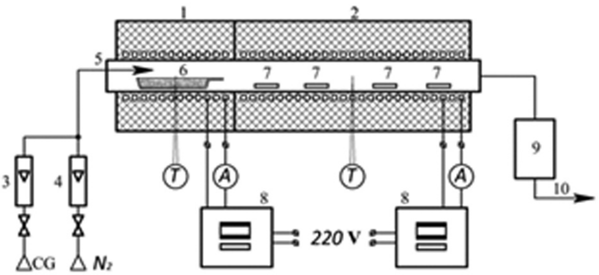

Fig.1. *Scheme of an experimental unit for studying CNTs deposition on dispersed iron particles in a converted gas atmosphere. 1- electric furnace for evaporation of ferrocene; 2- electric furnace for zone heating of CNTs growing; 3,4 - flowmeters and valves for converted gas and nitrogen supplying; 5- quartz reactor; 6- boat with ferrocene; 7- ceramic rods – deposition centers; 8- control system; 9- filter; 10- outcoming gas.*

Only precise control of the composition of the gas mixture and the ratio of the carbon source – carbon monoxide to hydrogen, as well as the temperature regime allows CNTs obtaining practically without external carbon impurities in the form of amorphous carbon.

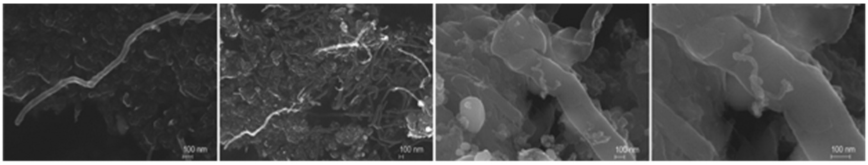

Fig. 2. *SEM photo of obtained CNTs*

Experiments have shown that dispersed iron particles obtained from ferrocene have a high reactivity, in many respects not inferior to freshly reduced iron, which, due to its low reduction temperature, has a developed surface and, as a consequence, is one of the most effective catalysts for carbon deposition. But the process of preparing such a catalyst is a rather laborious and energy-consuming process, which consists in multiple repetitions of oxidation-reduction cycles in order to obtain the most developed substrate surface for CNT deposition.

As a percentage of one unit of iron, approximately 14 weight units of carbon were obtained in the form of CNTs. The results on the yield of the target carbon product confirmed the possibility of using ferrocene as an effective catalyst for the growth of CNTs, as well as the possibility of using this technology on an industrial scale.

The effect of electrolytic aggregation of Au nanoparticles on optical characteristics of $AgInS_2/ZnS$ QDs modified with oligonucleotides

Nesterenko Y.O.[1], *Rachkov O.E.*[1], *Kozoriz K.O.*[2], *Borkovska L.V.*[2],

[1] *Institute of Molecular Biology and Genetics of NASU,*
150 Zabolotnogo Str., 03680 Kyiv, Ukraine
E-mail: anen.cheshir@gmail.com

[2] *V. Lashkaryov Institute of Semiconductor Physics of the NAS of Ukraine,*
45 Prospect Nauky, 03028 Kyiv, Ukraine.

The interaction of exciton in semiconductor nanocrystal, the so-called quantum dot (QD), with plasmon of metal nanoparticle (NP) is widely used in optical sensors for detection of biological and chemical substances in the solutions. Here, we present the results of investigations of the influence of electrolytic aggregation of gold nanoparticles (Au-NPs) on optical characteristics of the $AgInS_2/ZnS$ QDs modified with oligonucleotides. The QDs were stabilized with mercaptoacetic acid and glutathione, and the Au-NPs were processed with lipoic acid and mercaptohexanol. The QDs and Au-NPs were modified, respectively with 19-bases (MP-SH) and 26-bases (SH-DP) thiolated oligonucleotides. The nanoobjects were placed in buffer solutions SSC of different multiplicity (0.1×, 0.25×, 0.5×SSC).

The photoluminescence (PL) spectra of QD modified with oligonucleotides (MP-QDs) show a wide band in the yellow-red spectral region caused by radiative recombination of carriers via the levels of defects in the QDs. The adding of Au-NPs modified with oligonucleotides (Au-DP) resulted in the decrease of PL intensity. This was accompanied by the changes in optical absorption. Specifically, the increase in absorption recorded at 620 nm and 690 nm took place. The effect enhanced as the multiplicity of buffer solution increased and was ascribed to formation of aggregates of Au-NPs and QDs. In fact, formation of aggregates of Au-NPs caused the change of frequency of surface plasmon resonance (SPR) which manifested in the appearance of absorption “shoulder” at about 620 nm.

The process of aggregate formation depended on type of QD’s stabilizing ligand. In particular, for the solutions of Au-DP and glutathione stabilized MP-QDs stored for 24 hours a precipitation on the bottom of the tube was observed and accompanied with complete quenching of the PL intensity.

The effect should be taken into account when the sensor system for detection of specific sequences of nucleic acids in solutions is developed.

Synthesis and lower critical solution temperature behavior of chitosan and N-isopropylacrylamide graft copolymers

***<u>Babelyte M.</u>*[1], *Liudvinaviciute D.*[1], *Navikaite-Snipaitiene V.*[1], *Rosliuk D.*[1], *Rutkaite R.*[1], *Samaryk V.*[2]**

[1] *Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu Rd. 19, Kaunas 50254, Lithuania.*
E-mail: migle.babelyte@ktu.edu

[2] *Department of Organic Chemistry, Lviv Polytechnic National University, Stepana Bandery St. 14, Lviv, Ukraine.*

Chitosan (CS) is nontoxic, biocompatible and biodegradable, pH-sensitive polymer with antimicrobial activity. Because of these properties, it is an interesting biopolymer which can be further modified *via* grafting reactions. One of the most attractive compounds which can be used for grafting of chitosan is N-isopropylacrylamide (NIPAAm). Poly(N-isopropylacrylamide) (PNIPAAm) is highly thermo-sensitive polymer and shows sharp solubility changes in water around a specific temperature which is known as lower critical solution temperature (LCST). Beyond 32 ºC PNIPAAm turns into precipitate which can be composed of nanosized particles. Therefore, the graft copolymers with CS in the backbone and NIPAAm in the side chains could have dual stimuli responsive behavior and may be interesting in terms of drug delivery system.

In this study, chitosan-graft-N-isopropylacrylamide (CS-g-NIPAAm) copolymers were synthesized by free-radical polymerization in aqueous solution using potassium persulfate (PPS) as an initiator. By changing the molar ratio of CS:NIPAAm from 1:0.25 to 1:10 the copolymers with different grafting ratio were prepared. The obtained CS-g-NIPAAm copolymers were characterized by FTIR, H-NMR spectroscopy and other techniques. Moreover, the LCST behavior of synthesized copolymers was assessed by cloud point, particle size and fluorescence spectroscopy analysis.

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Investigation and mathematical modeling of time-dependent and kinetic parameters of the electrode relaxation processes

***Vyshnevska Yu.P.*[1], *Brazhnyk I.V.*[2]**

[1] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute".

37K20, Peremohy Ave., Kyiv, 03056, Ukraine.
E-mail: vishnevsk@ukr.net

[2] Gimasi SA.
4, Piazzale Roncàa, Mendrisio, 6850, Switzerland.

Investigation of complex electrochemical systems that involve intermediate products or multistage redox reactions constitute a challenging topic. Available electroanalytical methods inextricably rely on the corresponding theoretical models for the correct interpretation of the experimental data. Moreover, the model limitations are found to be increasingly pronounced while shifting from well-studied systems with bulk materials toward novel heterogeneous and nanostructured materials. Experimental methods based on the analysis of the relaxation processes have a number of advantages when compared to traditional chronopotentiometry. For instance the potential *vs*. time charts does not suffer from the influence of the ohmic component. In addition, it is usually sufficient to apply relatively low polarization that does not shift the electrochemical system from the stationary condition to such an extent as in case of chronopotentiometry where much higher current densities should be applied to reliably identify the transition time.

Still, available theoretical models that describe relaxation processes are found to be mainly focused on the charge distribution within double layer for the determination of its capacitance, lacking adequate representation for the diffusion portion of the relaxation. In present study, a set of relations has been obtained analytically for the analysis of the potential *vs*. time relaxation curves - for the case of thin electrolyte layer and for semi-infinite diffusion. Proposed approach includes a solution of the diffusion problem using Fick’s second law as a theoretical basis implying assumption that after current cut off the charge does not pass through the electrode-electrolyte interface, and the reactants concentrations obeys the Sand equation (for the galvanostatic regime of polarization). The Nernst equation has been used for obtaining the potential *vs*. time relation on the basis of the surface concentration vs. time dependence. Obtained relations may be used for investigation of the kinetics of electrode processes in various cases like ion intercalation, electrochemical alloy formation, anodic metal dissolution and beyond.

Microbiological resistance of ceramics in different mycobacterial surrounds

***Kuzminchuk A.V.*, Dontsova T.A.**

National Technical University of Ukraine"Igor Sikorsky Kyiv Polytechnic Institute", Peremohy Ave, 37, Kyiv-03056, Ukraine.
E-mail: email.of. kuzminchuk.a@gmail.com

The usage of ceramic filtering elements for water treatment in home point-of-entry or field filters nowadays isn't widespread, but looking forward on amount of advantages, we can suppose it in nearest time. List of advantages includes long operating term, possibility of regeneration, less harmful waste. Nowadays it looks encouraging according to sustainable development trends.

The main factors affecting properties are variety and content of additives, sintering time and properties. During research ceramic filtering element with good filtering properties were obtained and investigated.

Base materials are kaolin and diatomaceous earth, as natural components with minimal processing, additives as borax, soda ash, barium sulfate, starch and etc. were used.

We studied influence of these factors by x-ray analysis to gain optimal surface parameters of material and suspension filtering capacity to analyze these main factors.

Proceeding from results of study we can suppose that material is suitable for point-of-entry home water and field water filters which can be effective for purifying even difficult water.

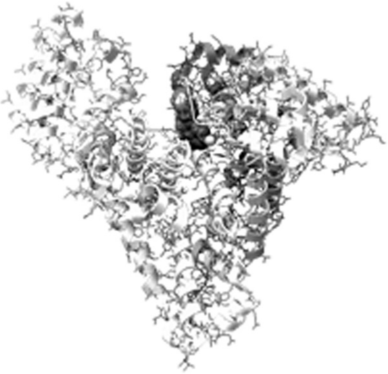
Mechanisms of the Interaction of Bovine Serum Albumin with Quercetin

Goncharova O.O.[1]***, Dmytrenko O.P.***[1]***, Lesiuk A.I.***[1]***,***
Kulish M.P.[1]***, Pavlenko O.L.***[1]***, Kanyuk M.I.***[2]

[1] *Physics Faculty, National Taras Shevchenko University of Kyiv, Glushkova prosp., 4, Kyiv-03039, Ukraine.*
E-mail: lesyuk.andrey@gmail.com

[2] *Palladin Institute of Biochemistry of the National Academy of Sciences of Ukraine, Leontovycha str, 9, Kyiv-01601, Ukraine.*

The peculiarities of the complexation of the macromolecule of bovine serum albumin (BSA) and quercetin (Quer) were investigated. The obtained experimental data of the fluorescence spectra of aqueous BSA-Quer solutions indicated a static mechanism of the fluorescence quenching with the formation of molecular complexes. The established values of the binding constant K_A and the number n of binding sites allowed to determine the thermodynamic parameters ΔH and ΔS of the interaction of molecules. Their values indicated the hydrophobic nature of the binding in the complex, which was confirmed by the results of modeling by molecular dynamics. The binding energy ΔG=-30.37 kJ/mol was calculated by the molecular docking method, which agrees well with the results obtained from the fluorescence spectra. The distance from Quer to the fluorescent tryptophan amino acid residues of the BSA molecule determined from the spectra by Forster theory corresponds to the simulation results. By the molecular dynamics of the BSA-Quer complex the temporal stability of the binding mode was shown and the conformational changes of the immediate amino acid environment of Quer as a result of the interaction were analyzed.



Space-charge polarization phenomena in single crystal and ceramics of bismuth sodium titanate

Sidak V.M.[1], Trubitsyn M.P.[2]

[1] *Biomedical Physics and Informatics Department, Dnipro State Medical University, Vernadsky str. 9, Dnipro-49044, Ukraine*
E-mail: vasylsidak@gmail.com

[2] *Department of Experimental Physics, Oles Honchar Dnipro National University, Gagarina ave. 72, Dnipro-49010, Ukraine*

Bismuth sodium titanate $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) is a lead-free relaxor ferroelectric which electrical properties in broad temperature and frequency ranges are determined by polar nanometer sized clusters [1]. NBT is considered as promising material for use in functional electronics due to high dielectric permittivity, piezoelectric and pyroelectric coefficients. Previously, slow dielectric relaxation with a specific frequency dispersion was observed in NBT crystals around 670 K [2]. Dielectric anomaly disappeared after the heat treatment in air (870 K) and could be restored by the subsequent treatment in vacuum (1070 K). To explain the unusual $\varepsilon(T, \omega)$ dependences, the thermal decay of the dipole centers was taken into account. The data obtained showed that the relaxation of ε was determined by the defects based on oxygen vacancies (V_O). The observed non-equilibrium polarization processes earlier were related to dipole centers formed by Ti ions that captured electrons and located near V_O. However, the typical values of permittivity in maximum ($\sim 10^4$) are too high for dipole defects contribution and more likely evidence for space-charge polarization phenomena. Similar giant permittivity is actively studied and discussed for another compounds of perovskite family [3]. To obtain the information on the mechanisms of the assumed space-charge polarization, we study and compare the data on slow dielectric relaxation in NBT single crystal and ceramics.

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The effect of heterovalent dopants on ionic conduction in amorphous and nanocrystalline lithium heptagermanate

Trubitsyn M.P.**, **Bochkova T.M.,
Koptiev M.M., Volnianskii M.D.

Institute for Energy Efficient Technologies and Materials Sciences,
Oles Honchar Dnipro National University,
Gagarina ave. 72, Dnipro-49010, Ukraine.
E-mail: trubitsyn_m@ua.fm

Electrical conductivity of lithium heptagermanate $Li_2Ge_7O_{15}$ crystal is mainly determined by Li ions interstitials moving along the channels within Ge-O lattice framework [1]. Heterovalent doping with 3d-group ions (Mn, Cr) noticeably changes ionic conduction in $Li_2Ge_7O_{15}$ crystal due to appearing charge compensating Li ions vacancies or interstitials [2]. Preparing amorphous and nanocrystalline $Li_2Ge_7O_{15}$ compounds in [3] allowed to increase ionic conduction drastically as compared with crystal. At first combined influence of doping and nanometer structuring on ionic transport was studied in [4]. It was demonstrated that introducing small amounts of heterovalent dopants (Cr, Mn, Cu, Al, Gd) had only minor effect on ionic conduction in amorphous and nanocrystalline samples [4]. It was argued that in the disordered structures of glassy and nanocrystalline compounds there were much more weakly bound Li ions as compared with doped crystals. In this work we study ionic conduction in amorphous and nanocrystalline $Li_2Ge_7O_{15}$ doped with heterovalent impurities which can be introduced in much higher concentrations than considered in [4]. Such dopants cause presence of non-stoichiometric excess Li ions which weakly bound to Ge-O structural framework and notably increase conductivity.

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Synthesis of TiO_2/MOFs Nanostructures

Zhou Z., Dontsova T.A., Potaskalov V.A.

National Technical University of Ukraine"Igor Sikorsky Kyiv Polytechnic Institute", Peremohy Avenue, 37, Kyiv, 03056, Ukraine.
E-mail: t.dontsova@kpi.ua

Metal-organic frameworks (MOFs) are a class of porous materials with periodic network structures constructed by self-assembly of organic ligands and metal units via coordination bond bridges [1]. Like zeolites and inorganic porous molecular sieves, MOFs are also porous materials with a large specific surface area. However, the metal and organic ligands that make up MOFs come in different types and structures, and at the same time, the ways in which the metal nodes and organic ligands are coordinated are different. Therefore, MOFs with different pore sizes and specific physicochemical properties can be obtained by artificial regulation [2].

MOFs have become a hot research point in gas adsorption, gas storage, gas separation and long-term drug release [3]. In addition, MOFs exhibit photochemical properties similar to typical semiconductors such as TiO_2 and ZnO due to their unique structural properties. Therefore, MOF materials are also widely used in the field of photocatalysis.

The metallic elements of MOFs are usually transition metals. The main reason is that transition metals contain a large number of unfilled d- and f-electron orbitals, and coordination numbers range from 2 to 7, allowing for various secondary building blocks such as tetrahedron, octahedron and dodecahedron. As research has deepened, the metal blocks have been expanded from traditional transition metals to alkali and alkaline earth metals, further expanding the types of MOFs.

We synthesized titanium (IV) oxide nanoparticles by hydrothermal method from titanium propoxide. Organometallic compounds of copper, nickel, zinc, and zirconium were chosen as MOFs for modification. The obtained nanostructures were examined radiographically and for porosity.

Translated with www.DeepL.com/Translator (free version)

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Temperature transformation of the ferroelectric P(VDF-TrFE) copolymer phase structure

***Yampolskiy A.L.*, Makarenko O.V., Lendiel V.V.**

Taras Shevchenko National University of Kyiv
(64/13, Volodymyrs'ka Str., Kyiv 01601, Ukraine)
E-mail: uv365nm@ukr.net

Charge-sensitive atomic force microscopy is employed to study the structure of P(VDF-TrFE) copolymer deposited onto a thin noble metal layer on glass substrate. This material is known for its ferroelectric properties and is attractive for variety of modern applications.

P(VDF-TrFE) can exist in four conformations, and the ferroelectric properties are most pronounced in the β-phase, which is of interest [1]. The effect of thermal annealing on the structure of such polymers is studied.

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Electrochemical hydrogenation properties of Ni/Co-C composites

Vlad Kh.I.[1]***, Verbovytskyy Yu.V.***[1]***, Bogatyrov V.M.***[2]***, Zavaliy I.Yu.***[1]

[1] Karpenko Physico-Mechanical Institute of the NAS of Ukraine.
Naukova Str., 5, Lviv-79060, Ukraine.
E-mail: kristinavlad1998@gmail.com

[2] Chuiko Institute of Surface Chemistry, NASU,
17 General Naumov Str., Kyiv 03164, Ukraine.

Metallic nanoparticles of Ni and Co are of great interest due to features of their magnetic and catalytic properties arising from a small size and high specific surface area [1]. They are used also as binders for the negative MH-electrode preparation of Ni-MH batteries. Metallic powders reduce the internal resistance of the electrodes, provide electrical contact and thus help increase the discharge capacity and improve the reversibility of charge-discharge processes. It should be note that some of Ni/Co-based nanomaterials possess its own high electrochemical capacity and can be effectively used for preparation of MH-electrodes.

Nickel and/or cobalt carbon nanoparticles were synthesized from polystyrene and metal salts using pyrolysis method [2]. The morphology, structural features and electrochemical hydrogenation properties of the obtained nanomaterials were investigated by scanning electron microscopy, X-ray powder diffraction, galvanostatic charging-discharging, volt- and chrono-amperometry. The crystallinity of the synthesized Ni/Co-C nanoparticles was confirmed by the X-ray diffraction. Ni/Co-C composites were obtained by mixing with carbonyl nickel, pressed into pellets. Electrochemical parameters (discharge capacity and cyclic stability) were studied and their substantial dependence from the Ni/Co ratio was shown. The obtained results will be analyzed and compared with those for Ni-Co nanoparticles synthesized by other methods.

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Effect of alkali metals ions on sol-gel transformation in solution of hydroxypropylcellulose

**Sobchuk A.O.[1], Lazarenko M.M.[1], Kovalchuk V.I.[1], Nedilko S.G.[1],
Gryn S.V.[2], Scherbatskyi V.P.[1], Tkachev S.Yu.[1], Andrusenko D.A.[1],
Lazarenko M.V.[3], Yablochkova K.S.[1], Alekseev O.M.[1]**

[1] *Taras Shevchenko National University of Kyiv, Physical Faculty,
Volodymyrska St. 64/13, Kyiv 01601, Ukraine.
E-mail: litrboychik@gmail.com*

[2] *Taras Shevchenko National University of Kyiv, Institute of High
Technologies, Volodymyrs'ka St. 64/13, Kyiv 01601, Ukraine.*

[3] *National University of Food Technologies,
Volodymyrs'ka St. 68, Kyiv-01601, Ukraine*

The sol-gel transformations in the water solutions of hydroxypropylcellulose (HPC) are widely known, but they still are in field of intensive researches. The peculiarity of these solutions is their ability to change considerably their optical, rheological and other physical properties under influence of different external factors. Considerable scientific interest is caused by demand of modern technologies of the new type of materials, so-called "smart materials". Physical and chemical properties of "smart materials" can be tuned by changes of certain parameters, such as temperature, pH level, electrical and magnetic fields, etc.

The HPC-water systems could be used as example of the systems of this sort due to formation of aggregates of hydroxypropylcellulose with different size and shape, highly sensitive to temperature, pH and presence of electrolytes. So, addition of electrolytes in HPC-water solutions leads to significant changes in their electrical properties and causes influence on sol-gel transformations.

The aim of the present work is to study the influence of alkali metals ions (IA group) on the physical properties of the solution and sol-gel transformations in the HPC-water solution. The measurements of conductivity, viscosimetry, dynamic light scattering (DLS) method, turbidimetry, absorption and luminescence spectroscopy were used to characterize systems under study.

It was shown that the range of structure transformations shifts to lower temperatures (in the overall range 40..50 °C) in presence of the alkali metals ions (Li^+, Na^+, K^+, Rb^+, Cs^+). Besides, an formation of bigger particles of polymer was observed.

Vapor-condensed composite materials Ni-Al_2O_3, $NiCr$-Al_2O_3 with oxide nanophase

Grechanyuk V., Grechanyuk M., Chornovol V., Kozyrev A., Kovalchuk Yu.

Department of Chemistry, Kyiv National University of Construction and Architecture. Povitroflotsky Ave., 31, Kyiv-03037, Ukraine.
E-mail: missvik@ukr.net

High-speed electron-beam evaporation of metals and non-metals in vacuum (the deposition rate of atomic or molecular flows on a substrate can reach 150 μm/min) is a relatively new direction in materials science. These processes are currently widely used mainly for the application of protective coatings to gas turbine parts. New materials obtained by condensing vapor flows on a substrate heated to a certain temperature include dispersion-strengthened, layered, and porous materials [1-3].

The structure and physico-mechanical properties of bulk composite materials condensed from the vapor phase with a dispersed oxide nanophase: $Ni – Al_2O_3$, $NiCr$-Al_2O_3 in a wide (up to 40% wt.) range of Al_2O_3 concentrations are studied in this work. The dependences of the physico-mechanical properties of composites on the temperature of the substrate on which vapor flows are deposited are established. It is shown that in the above range of oxide nanophase concentrations, there is a smooth transition from dispersion-strengthened to microporous materials. The influence of the deposition temperature and vacuum annealing time on the morphology, micropore volume, and mechanical properties of the composites has been studied.

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Influence of the In-Ga substitution on the physical properties of layered $CuInP_2S_6$ crystals

Ban H., Gal D., Haysak A., Molnar A.

Department of the Physics of Semiconductors, Uzhhorod National University,
Voloshina Str. 54, Uzhhorod, 88000, Ukraine
E-mail: alexander.molnar@uzhnu.edu.ua

Layered crystals of the $Me1Me_2P_2S_6$ family are promising 2D functional materials for nanoelectronics. One of the most interesting of them is $CuInP_2S_6$ and solid solutions based on it.

We investigated the temperature dependence of the dielectric constant of 80%$CuInP_2S_6$- 20%$CuGaP_2S_6$ solid solution in the temperature range 80-450 K and the frequency range $10 \div 10^5$ Hz. To determine the potassium content, we used the method of extraction-photometric determination [1]. As can be seen in Figure 1, the phase transition temperature for this composition is 318K, which is 3 degrees higher than that of a pure crystal $CuInP_2S_6$. At temperatures below 200K (more precisely, at 120-140K at 10 kHz), a "step" is observed on the temperature dependence of the real part of the dielectric constant, and a maximum on the temperature dependence of the imaginary part of the dielectric constant. Such dielectric dispersion is typical for dipolar glasses.

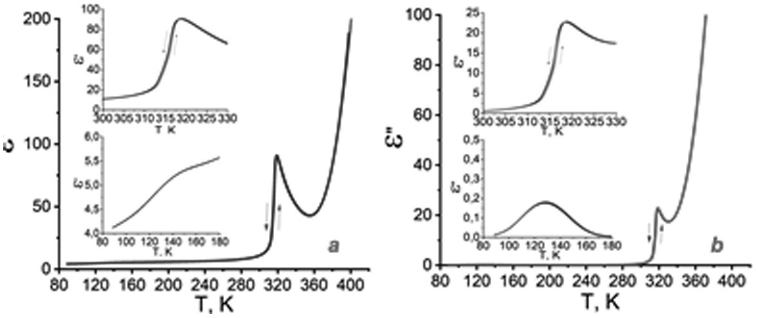

Fig. 1. *Temperature dependency of real a and imaginary b parts of complex dielectric permittivity* $\varepsilon^* = \varepsilon' - i \cdot \varepsilon''$ *of 80%*$CuInP_2S_6$*- 20%*$CuGaP_2S_6$ *solid solution.*

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Selected physicochemical properties of hydroxyapatite and white - blue clay composite

Skwarek E.[1], Broda E.[1], Payentko V. V.[2], Liedienov N.A.[2], Pashchenko A.V.[2], Levchenko G.G.[2], Kowalska K.[1]

[1] *Faculty of Chemistry, Maria Curie-Sklodowska University,*
M. Curie-Sklodowska Sq. 3, 20-031 Lublin, Poland,

[2] *Chuiko Institute of Surface Chemistry of NAS Ukraine,*
17 General Naumov Str, Kyiv, Ukraine.
e-mail:ewunias@hektor.umcs.lublin.pl

Hydroxyapatite (HAP) composites are very important biomaterials, which can be applied in various life areas. HAP composite with white clay was prepared and studied using X-ray diffraction, nitrogen adsorption, Fourier transform infrared spectroscopy (FTIR), potentiometric titration, and quasi-elastic light scattering and zeta potential measurements. The values of pH_{pzc} (point of zero charge) and pHIEP (isoelectric point) characteristic of the electrical double layer depend strongly on the white clay addition to HAP. Comparative studies of hydroxyapatite, white clay and composite by nitrogen adsorption and FTIR methods showed that in most cases composite has the properties nearly intermediate between hydroxyapatite and white clay taken for the synthesis; however, certain non-additivity is observed for the characteristics due to precipitation of HAP onto clay particles that changes the HAP formation conditions in comparison to HAP formation alone. Thus, changes in the condition of the composite preparation allow one to control the characteristics of the final materials [1,2].

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Features of hysteresis of wetting of a solid substrate by a nanodroplet

***Burian S.A.*[1,2], *Zubariev O.M.*[1], *Kovalchuk V.I.*[2],**
***Yaroshchuk A.E.*[3], *Isaiev M.V.*[4]**

[1] *Faculty of Physics, Taras Shevchenko National University of Kyiv,*
Volodymyrska str. 64/13, Kyiv-01601, Ukraine
E-mail: burian_sergii@knu.ua

[2] *F.D. Ovcharenko Institute of Biocolloidal Chemistry of the National*
Academy of Sciences of Ukraine,
Vernadskoho Ave. 42, Kyiv-03142, Ukraine

[3] *Institució Catalana de Recerca i Estudis Avançats, pg. L.Companys 23,*
Barcelona-08010, Spain

[4] *Université de Lorraine, CNRS, LEMTA, 54000 Nancy, France*

Understanding the dynamics of three-phase contact-line movement is crucial for the description of processes important for numerous technological issues related to nuclearization, evaporation, percolation etc [1,2]. In this context, from a microscopic point of view, phenomena of hysteresis of wetting angle on smooth surfaces are still not fully understood.

In our talk, we will consider the shape of a nanoscopic droplet located on a solid substrate in an external force field applied parallel to the surface. The cylindrical cap shape of the droplet was chosen to minimise the impact of three-phase line curvature. Molecular dynamics simulations were chosen as the main tool for the evaluation of droplet shape.

As a main result of our simulations, a contact-angle hysteresis on atomistic smoothed surfaces was observed. Dependences of droplet velocity, receding and advancing contact angle on the magnitude of external field were also investigated. An analytical model postulating adsorption of water molecules on the solid substrate was developed to explain the characteristic features of the droplet shape.

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Morphology and Growth Mechanisms of CdTe Thin Film

Nykyruy L.I.[1], Yavorskyi R.S.[1], Wisz G.[2], Sawicka-Chudy P.[2],
Vakaliuk I.V.[1], Naidych B.P.[1], Yavorskyi Ya.S.[1]

[1] Vasyl Stefanyk Precarpation National University,
T. Shevchenko Str. 57, Ivano-Frankivsk-76018, Ukraine.
E-mail: ivanna.maliarska@pnu.edu.ua

[2] Institute of Physics, College of Natural Science, University of Rzeszów,
1 Pigonia Street, 35-317 Rzeszów, Poland.

The photovoltaics is a popular and actively developing industry. The most common are materials based on silicon in the amorphous, nanocrystalline, polycrystalline phases and polycrystalline chalcogenide (sixth group) semiconductor compounds. The third class of new compounds is based on organometallic dyes and polymers [1]. The main characteristic that determines the parameters of the photovoltaic cell is the electrical efficiency. This parameter depends on the length and intensity of the incident sunlight, the type of photovoltaic cells, composition materials, and the components used in the solar module. Among chalcogenide materials, CdTe has higher temperature and radiation stability. This makes the material suitable for use at higher temperatures and resistant to ionizing radiation.

Thin films were grown on glass and (100) silicon substrates by physical vapor deposition technique at constant evaporation and substrate temperatures. The thickness was determined by the time (τ = (30–570) sec) of condensate deposition. Morphological and structural properties of CdTe thin films were studied using Atomic Force Microscope (CSM Instruments) and Scanning Electron Microscope (Vega 3 Tescan).

The morphology of the surface of cadmium telluride thin films was investigated by atomic force microscopy in periodic contact mode. The surfaces of the films have a "scaly" shape with normal dimensions of about 25 - 45 nm, which are more clearly distinguished on glass substrates. Analysis of the surface morphology of CdTe films indicates Stransky-Krastanov growth mechanism. After the growth of several layers of material, the formation of individual islands becomes predominant and then their growth continues.

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Monte Carlo simulation of bond-random spin-crossover compounds

Gudyma Iu.V., Yarema V.S.

Physical, Technical and Computer Sciences Institute,
Yuriy Fedcovich Chernivtsi National University,
Chernivtsi 58012, Ukraine.
E-mail:yugudyma@gmail.com

Spin-crossover (SCO) complexes are the transition metal coordination compounds with the electronic configuration ranging between 3d4 and 3d7 (manganese, iron, chromium, and cobalt) in (pseudo)octahedral surroundings. The variation of some external stimuli causes the reversible phase transition from low spin (LS) diamagnetic state to high spin (HS) paramagnetic state in SCO materials. The SCO is one of the best examples of molecular electronic bistability [1].

Intermolecular interactions are mediated by small molecular distortions that lead to some randomness of bonds. This leads to a treating intermolecular interaction as random bond [2]. Our model is a random-bond version of the well-known pseudo-spin model of spin-crossover solids, and is similar to the Edwards-Anderson model with the external field.

The Ising-like model of spin-crossover solid compounds with random bonds has been studied by intensive numerical Monte Carlo simulation. A numerical solution to the problem is found and analyzed. The six typical cases of the temperature behavior of spin-crossover compounds for random intermolecular bonds have been studied.

Random distribution of intermolecular coupling results in the peculiarity of cooperative behavior, such as narrowing hysteresis loops or their vanishing or a more complex quasi-spin glass state. Our investigations could be helpful in the understanding of various patterns in real SCO systems.

The successful implementation of the described approach for providing a facile way to include random intermolecular interactions paves the way for future research about the role of such interactions within SCO compounds.

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Decrystallization and stabilization of liquid bee honey during storage

Kurta S.A.**, **Khatsevich O.M., Fedorchenko S.V., Tagir M.

Chemistry Department of the Faculty of Natural Sciences ,
Vasyl Stefanyk Precarpathian National University
Halytska Str., 201/320, Ivano-Frankivsk, Ukraine. E-mail: kca2014@ukr.net

The materials described in the article relate to the scientific field of food processing in the food industry and other fields related to the dilution, decrystallization of various solid and pasty products, in particular the dissolution of solid crystalline bee honey to a liquid consistency that can be used in dentistry for prevention and treatment of gum disease in gingivitis, periodontitis and periodontitis .. Natural bee honey, especially May, linden and acacia, contains a lot of fructose and can remain liquid in honeycombs sealed for 1-3 years. But honey extracted from honeycombs has a shelf life of only a few months, depending on the type and variety of honey. This is because honey contains up to 80% or more of fructose and glucose in a ratio of about 1: 1. The consumer characteristics of honey are almost unchanged, but its appearance becomes less attractive to consumers who want to see and consume it liquid and transparent. Therefore, the use of new methods and special conditions for cracking crystallized honey and preventing its natural crystallization, as well as conditions and means of storing honey in a liquid state for at least 1 year is an urgent problem in the food industry. Scientific activity and discussion of the achievements of ONAFT and the Department of Chemistry of Vasyl Stefanyk Precarpathian National University (Ivano-Frankivsk), contributed to the implementation of joint research and the introduction of a new type of food product - chewing gum "Honeycomb-Honeycomb". based on dissolved, liquid caramelized honey, which has a therapeutic and prophylactic effect and has pronounced therapeutic, anti-inflammatory, astringent, anti-infective, antimicrobial and antibacterial properties. The research provides for the possibility of creating and introducing new types of chewing gum based on liquid, dissolved honey, for the treatment, protection and prevention of dental diseases, primarily gingivitis, periodontitis and periodontitis.

Chemical, physicochemical and structural characteristics of liquid and crystallized (solid) honey depending on its thermochemical processing and duration of storage are investigated. There are 3 main factors that affect the rate of crystallization of honey: water content, pollen content and the ratio of glucose and fructose in honey. It was shown that by low-temperature isothermal accelerated treatment in a microwave reactor type MWR-SPR at 40°C, for 60s, it is possible to dissolve crystalline honey to a liquid state, which reduces the time for its dissolution in the classical method by heat transfer through the reactor wall from hot water. or electric heating from 4-12 hours. at the same temperature 50°C to 1 min, ie 240-600 times faster.

The properties, structure and qualitative and quantitative composition of the obtained liquid honey are investigated and compared with the properties of the original crystalline and liquid honey without processing. It is proved that the proposed accelerated treatment in a microwave reactor type MWR-SPR at 50°C, for 60s, retains a high diastase Gotha number -10-11. The content of hydroxymethylfurfural did not exceed 3-6 mg / kg of honey, which meets the requirements of DSTU for honey. And consumer organoleptic indicators of honey in a liquid aggregate state remain, within 1 year. At the same time, with the traditional method of crystallization (dissolution) of honey, these indicators are much worse, the diastase number decreases to 0-6, and the content of toxic hydrosimethylfurfural increases to 12-18 mg / kg, which significantly exceeds the permissible norms (DSTU 4497: 2005 Honey natural).

Analysis of the qualitative and quantitative composition of honey after low-temperature isothermal accelerated processing in a microwave reactor type MWR-SPR at 50°C, for 60s., Conducted by IR spectroscopy, showed the absence of significant qualitative changes compared to untreated honey. Microscopic studies confirmed a 10-fold reduction in the number and size of pollen particles. The size of the crystals of glucose and sucrose after such treatment is also reduced by 5 times. At the same time, the analysis of the mass distribution of sugar macromolecules by the method of angular distribution of the laser beam (NANODS CILAS) showed a decrease in the average particle size in the treated honey in 2 times compared with the crystallized samples. All this has a positive effect on the stabilization of liquid honey after dissolution (crystallization), when stored for 1 year.

Analysis of HSC and BSC (honey bioactivity) confirmed that in samples of liquid honey after crystallization by the proposed method, these values are reduced by half, which is much less than during the traditional method of heating by heat transfer. Analysis of the chemical and element-oxide composition of honey, performed by X-ray fluorescence spectroscopy, confirmed that the qualitative composition of honey treated by the proposed method is almost unchanged.

On the basis of samples of decrystallized liquid honey obtained by the new technology, a preventive chewing gum was created for the treatment of periodontal disease (gingivitis, periodontitis and periodontitis). Clinical studies of chewing gum samples based on a composition of liquid, caramelized honey, which were conducted at the Research and Training Center for Molecular Microbiology and Immunology of Mucous membranes of Uzhgorod National University in 2018-2019 to prevent and treat gingivitis, periodontitis and periodontitis in dentistry positive result in 72.5% of patients.

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Low-temperature modification of amorphous metallic alloys Fe-(Me)-Si-B

Hula T.H.[1]***, Hertsyk O.M.***[1]***, Kovbuz M.O.***[1]***, Yezerska O.A.***[2]***,***
Pandyak N.L.[3]***, Tashak M.S.***[4]

[1] *Faculty of Chemistry, Ivan Franko National University of Lviv,*
Kyryla and Mefodiya Str., 6, Lviv-79005, Ukraine.
E-mail: djunjer1@gmail.com

[2] *Fraunhofer Institute for Manufacturing Technology and Advanced*
Materials, Wiener Strasse 12, 28359 Bremen, Germany.

[3] *Ukrainian National Forestry University,*
Gen. Chuprynka Str., 103, Lviv-79057, Ukraine.

[4] *Lviv Polytechnic National University,*
S. Bandery Str., 12, Lviv-79013, Ukraine.

Rapid cooling, which is used in the technology of production amorphous metallic alloys (AMA), inhibits the diffusion processes in the solid phase [1]. As a result, amorphous metallic alloys do not have such defects as secondary phases, segregations, which are usually formed due to diffusion during slow cooling. Therefore, AMAs are considered to be ideal chemically homogeneous alloys, highly corrosion resistant, able to withstand extreme conditions and those could be nanostructured under temperature treatment. Applying of such alloys in conditions of extreme temperatures, for example, in the space industry, requires an investigation of the dependence of structural and electrochemical parameters of amorphous alloys $Fe_{80,0}Si_{6,0}B_{14,0}$ (AMA-1); $Fe_{78.5}Ni_{1.0}Mo_{0.5}Si_{6.0}B_{14.0}$ (AMA-2); $Fe_{73,1}Cu_{1,0}Nb_{3,0}Si_{15,5}B_{7,4}$ (AMA-3) and $Fe_{59}Ni_{26}Cr_{6,6}Mo_{0,9}V_{1,6}W_{0,3}Si_{3}B_{2,9}$ (AMA-4) from low temperature treatment at 77 K.

X-ray investigation of AMA samples Fe-(Me)-Si-B cooled at T = 77 K showed that after such low-temperature treatment there are no significant changes in the structure [2]. Evaluation of the microhardness of samples exposed to low temperatures showed that cooling AMA-2 and AMA-3 to T = 77 K increases the microhardness of such alloys, for multicomponent AMA-4 change is nonlinear. AMA-2 was the least sensitive to cooling. One-hour exposure at T = 77 K strengthened the surface of AMA-3 most significantly, while for multicomponent AMA-4 one- and three-hour exposure reduced the strength of the alloy surface. Fluctuations in the hardening coefficients for the investigated amorphous alloys in the vicinity of the unit demonstrate the high mechanical stability of the AMA surface.

Stabilization of electrochemical parameters in 0,5 M aqueous solution of NaCl amorphous metallic alloys after cooling them at T = 77 K promotes their further investigation in other aggressive environments.

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Supported Ir nanoparticles as catalyst for water electrolyzers: from synthesis to real application.

***Blanco Redondo L.**, Lobko Y., Matolínová I., Matolín V.*

Charles University, Faculty of Mathematics and Physics,
Department of Surface and Plasma Science.
V Holesovickach 2, 180 00, Prague 8, Czech Republic
E-mail: lublare93@gmail.com

In water electrolyzer systems, the positive electrode is one of the most important components, where the oxygen evolution reaction (OER) occurs. In this process, the water molecules are split into oxygen ions, protons, and electrons, and the oxygen gas is produced on the anode surface [1]. The state-of-the-art materials that catalyze OER are nanostructured ruthenium, iridium, and their oxides, but their cost and scarcity require reduction and enhancement of their utilization [2]. One morphological approach consists of the dispersion of the active material in a support in order to increase their mass activity. However, due to the high potential reached during operating conditions for water splitting, support materials have to possess a high corrosion resistance. Titanium oxides are good candidates because of their high thermal and chemical stability, low cost, and commercial availability [3]. But their poor electrical conductivity ($\sim 10^{-6}$ S cm^{-1}) makes the design of an active and stable catalyst a non-trivial task.

In this work, Ir nanoparticles have been reduced on the surface of TiO_2 nanoparticles, and a complete analysis of their morphological, chemical, and electrochemical properties has been carried out, including testing in-situ in a single cell water electrolyzer. The results show a successful performance of the supported Ir nanoparticles comparable to the pure Ir black nanoparticles but with an active metal loading five times lower. In addition, insights about the metal-support interaction have been studied to have a better knowledge about the catalyst properties.

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Study of the effects of the microstructure, contact stress and temperature on the area specific resistance of fuel cell materials

Podhurska V.Ya.[1]***, Vasyliv B.D.***[1]***, Milewski Ja.***[2]***, Skibiński Ja.***[3]***,***
Dybiński O.[2]***, Martsinchyk A.***[2]***, Rebis Ja.***[3]

[1] *Department of Hydrogen Technologies and Alternative Energy Materials,*
Karpenko Physico-Mechanical Institute of the NAS of Ukraine,
5 Naukova str., Lviv 79060, Ukraine.
E-mail: podhurskavika@gmail.com

[2] *Institute of Heat Engineering, Warsaw University of Technology,*
21/25 Nowowiejska str., Warsaw, 00-665, Poland

[3] *Faculty of Materials Science and Engineering, Warsaw University*
of Technology, 141 Wołoska str., Warsaw, 02-507, Poland

A fuel cell is a promising source of energy based on direct transformation of chemical energy into electricity. Traditionally, this device comprises a set of single fuel cells united in a stack. A single fuel cell consists of a dense electrolyte and porous electrodes applied to its opposite sides. Along with single fuel cells, an important component of the stack is the current collector, as it serves to supply gas mixtures and conduct electricity. The contact resistance between the current collector and the electrodes serves as a crucial characteristic of the fuel cell system determining its efficiency. Contact electrical resistance depends on the materials of the components and the clamping force. This work is aimed at studying the effect of microstructural parameters of the current collector and electrode materials and the applied load on the contact electrical resistance between them.

The change in the contact electrical resistance between the current collector and anode materials during heating and cooling under different contact stresses (0.09 MPa and 0.45 MPa) was studied.

As a result of experimental measurements, the kinetic dependences of the area specific resistance (ASR) of the nickel anode on the temperature in the operating temperature range of a fuel cell of 20–600 °C were obtained for heating and cooling cycles in air under loads of 49.05 N and 245.25 N, which correspond to the levels of contact stresses in bulk material 0.09 MPa and 0.45 MPa. It was found that at a temperature of 600 °C, the ASR of the nickel anode under contact stress of 0.45 MPa is 2.3–3 times lower than that under contact stress of 0.09 MPa.

Water evaporation from cellulose based materials with different pore sizes

***Brytan A.V.*, Alekseev O.M. Andrusenko D.A.,**
Lazarenko M. M., Vasylyuk S.V. Zabashta Yu. F.

Department of Molecular Physics, Physics Facult,
Taras Shevchenko National Kyiv University,
64/13 Volodymyrska str., Kyiv, 01601, Ukraine,
E-mail: a_britan@ukr.net

The water evaporation from the porous materials surface is the process that significantly depends on the material spatial structure and the pores geometric parameters distribution. This fact is caused by the mass and heat transfer processes within the volume depend on such type parameters and can differ meaningly for materials with different pores types [1,2].

The work represents data of experimental investigation of water evaporation from different materials surfaces in the air for atmospheric pressure and different values of ambient temperature (50, 60, 70 and 80 C). For pore size influence investigation cellulose-based materials with various pore sizes were chosen: filter paper, fabric, and bandage.

In the experiments sample mass dependences on time were measured at the time during water was evaporating from its surface. By using obtained experimental data water concentration in material (moisture content) time dependences were calculated. A simplified model of the water diffusion process inside the samples was proposed. The activation energies of water molecules diffusion in these materials were determined.

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Sensitivity of the alkylsulfid-terminated difunctionalized iron(II) clathrochelate to a conformation of transport protein albumin

Chornenka N.V.[1]***, Losytskyy M.***[2]***,***
Kovalska V.B.[2]***, Gumienna-Kontecka E.***[3]

[1] V.I. Vernadsky Institute of General and Inorganic Chemistry NASU, Kyiv, Ukraine.
e-mail: nina.v.chornenka@gmail.com

[2] Institute of Molecular Biology and Genetics, NASU, Kyiv, Ukraine.

[3] Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland.

Iron(II) clathrochelates, which are the three-dimensional cage complexes containing an encapsulated Fe^{2+} ion, were shown to acquire an intensive circular dichroism signal – induced CD (ICD) spectra – upon binding to some proteins, particularly albumins. Changes in the shapes and in the intensities of these spectra reflect both the conformation transitions of proteins macromolecules and their structural alterations. Here, ICD response of alkylsulfid-terminated diribbed-difunctionalized iron(II) clathrochelate (Fig. 1a) on the presence of serum bovine albumin (BSA) at pH 7.9 (1, 2 at Fig. 1b) and pH 4.3 (3, 4 at Fig. 1b), and clathrochelate-to-BSA concentration ratios 1:2 (1, 3 at Fig. 1b) and 2:1 (2, 4 at Fig. 1b) was studied. While for pH 7.9 clathroshelate ICD spectra were similar for both protein concentrations and contained two positive (near 350 and 530 nm) and one negative (near 450 nm) maxima, in the case of pH 4.3 lower protein concentration leads to drastic changes in ICD spectrum, namely the mirror reflection of the bands. We believe that partial conformation transition of BSA macromolecule leads to appearing of additional sites on BSA macromolecule for clathrochelates binding at higher clathrochelate-to-BSA concentrations ratio.

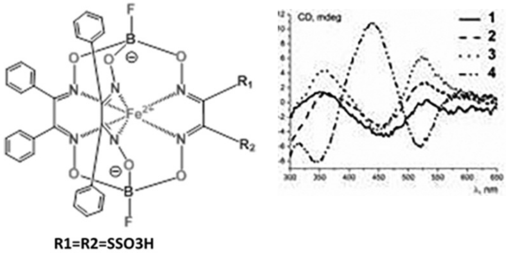

Fig.1. *Structure of clathrochelate (a) and ICD spectra of the BSA – clathrochelate assemblies (b).*

The project leading to these results has received Funding from the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska-Qurie grant agreement No 778245.

Features of hysteresis of wetting of a solid substrate by a nanodroplet

Burian S.A.[1,2]***, Zubariev O.M.***[1]***, Kovalchuk V.I.***[2]***,***
Yaroshchuk A.E.[3]***, Isaiev M.V.***[4]

[1] *Faculty of Physics, Taras Shevchenko National University of Kyiv,*
Volodymyrska str. 64/13, Kyiv-01601, Ukraine
E-mail: burian_sergii@knu.ua

[2] *F.D. Ovcharenko Institute of Biocolloidal Chemistry of the National*
Academy of Sciences of Ukraine,
Vernadskoho Ave. 42, Kyiv-03142, Ukraine

[3] *Institució Catalana de Recerca i Estudis Avançats, pg. L.Companys 23,*
Barcelona-08010, Spain

[4] *Université de Lorraine, CNRS, LEMTA, 54000 Nancy, France*

Understanding the dynamics of three-phase contact-line movement is crucial for the description of processes important for numerous technological issues related to nuclearization, evaporation, percolation etc [1,2]. In this context, from a microscopic point of view, phenomena of hysteresis of wetting angle on smooth surfaces are still not fully understood.

In our talk, we will consider the shape of a nanoscopic droplet located on a solid substrate in an external force field applied parallel to the surface. The cylindrical cap shape of the droplet was chosen to minimise the impact of three-phase line curvature. Molecular dynamics simulations were chosen as the main tool for the evaluation of droplet shape.

As a main result of our simulations, a contact-angle hysteresis on atomistic smoothed surfaces was observed. Dependences of droplet velocity, receding and advancing contact angle on the magnitude of external field were also investigated. An analytical model postulating adsorption of water molecules on the solid substrate was developed to explain the characteristic features of the droplet shape.

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First-principles study of two-dimensional haeckelite BeO monolayer

Piatnytskyi D.M.[1]***, Afanasieva T.V.***[1,2]

[1] Taras Shevchenko University of Kyiv,
Glushkova Avenue 4G, Kyiv-03187,
Ukraine.
E-mail: taifumerang03@gmail.com

[2] Physical Electronics Department, Institute of Physics of the NAS of
Ukraine. Prospect Nauki, 46, Kyiv-03039, Ukraine.
E-mail: tetiana.v.afanasieva@gmail.com

The two-dimensional (2D) materials have drawn great attention in material science due to their exotic electronic properties. II-VI semiconductors are interesting candidate materials for the tailoring of two-dimensional hexagonal structures. Recently, a two-dimensional BeO hexagonal monolayer on Mo(112) support was obtained [1]. The alternative two-dimensional materials like several graphene allotropes, GaN, and NbS_2 haeckelites have been predicted to be stable using theoretical investigation. Haeckelite-like structures and line defects also have been observed in different freestanding materials and on support. These new 2D materials have attracted interest in opening the possibility to find semiconductor materials with unexplored properties.

First-principles density functional theory calculations were performed to investigate the stability, electronic properties, and catalytic activity of two-dimensional haeckelite BeO monolayer (containing 8-4 membered rings). The calculations were carried out using the ABINIT package. The optimized geometry, band structure, local density of states (LDOS), binding energies, and charge density were calculated. The interatomic distances between Be and O atoms are 1.48 and 1.56 Å. The lattice parameter is found to be 5.20 Å. The conduction band minimum is at Gamma point. The indirect band gap for the freestanding haeckelite BeO monolayer is found to be 5.48 eV by GGA-PBE calculation. The direct band gap at G point was estimated to be 5.71 eV. The catalytic activity of the BeO monolayers was investigated. So, the interaction of the haeckelite BeO structures with hydrogen and carbon monoxide molecules were simulated. The binding energies for H_2 and CO molecules on the haeckelite BeO monolayer were obtained.

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Study of point-defect complexes reconstruction in silicon near-surface layers under the ion implantation process

Slobodzyan D.[1]***, Kushlyk M.***[1]***, Luchechko A.***[1]***, Lys R.***[1]***,***
Shpotyuk Ya.[1,2]***, Mahlovanyi B.***[2]***, Żyłka M.***[3]***, Żyłka W.***[4]

[1] *Department of Sensor and Semiconductor Electronics,*
Ivan Franko National University of Lviv,
107, Tarnavskoho Str., 79017 Lviv, Ukraine;

[2] *Institute of Physics, University of Rzeszow,*
1, Pigonia Str., 35-310 Rzeszów, Poland

[3] *Department of Aerospace Engineering, Rzeszow University of Technology,*
8, Powstańców Warszawy al., 35-959 Rzeszów, Poland;

[4] *Institute of Materials Engineering, University of Rzeszow,*
1, Pigonia Str., 35-310 Rzeszów, Poland;
E-mail: dmytro.slobodzyan@lnu.edu.ua

Today, silicon is an important material for the manufacture of electronic devices for various purposes. Therefore, a significant number of scientific publications devoted to the study of its properties have accumulated over the past few decades. However, the regular miniaturization of the elements stimulates an increase in the level of requirement for the perfection of the internal structure of silicon, as well as for the reliability of devices based on it. This, in turn, sets a high priority for the study of silicon nanoscale complexes especially Si clusters to improve the properties of nanostructured materials.

P-type Cz-Si was used for the studies. Samples have been cut from a single crystal silicon disk with flat surfaces orientation (111).

The aim of the work was to form a surface-barrier (SBS) and light-emitting structures (LES) and to investigate the change in their electro physical and optical characteristics under the influence of irradiation.

Defect formation processes on the surface and subsurface layers of silicon crystals were analysed by IR spectroscopy.

Structural studies of silicon morphology were performed with an LUMAM I-3 optical microscope and a Solver P47-PRO atomic-force microscope.

Electrophysical properties of SBS were studied by measuring and analysing current-voltage characteristic (IVC) and high-frequency capacitance-voltage characteristic (CVC) curves. Optical properties of LES were studied by measuring and analysing electroluminescence spectra.

A model for the reconstruction of nanoscale defective complexes of the near-surface silicon layer was proposed.

Sol-gel derived $ZnAl_2O_4$ nanopowders co-doped with Cr^{3+}, Er^{3+} and Yb^{3+} ions

Hreb V.[1], **Lutsyuk I.**[1], **Zelinskiy A.**[2], **Luchechko A.**[2],
Shpotyul M.[1], **Vasylechko L.**[1]

[1] *Lviv Polytechnic National University,*
Bandera 12, 79013, Lviv, 79013, Ukraine

[2] *Ivan Franko National University of Lviv,*
Universytetska 1, Lviv, 79000, Ukraine
E-mail: vasyl.m.hreb@lpnu.lviv.ua

Low-temperature citrate sol-gel method was used for the synthesis of nanocrystalline $ZnAl_2O_4$ spinel-based phosphors co-doped with Cr^{3+}, Er^{3+} and Yb^{3+} ions. A series of triple-doped materials of nominal composition $ZnAl_{1.994}xO_4$:$Cr_{0.003}Er_{0.003}$Ybx ($x = 0.009$, 0.015 and 0.021) were obtained from stoichiometric amounts of $Al(NO_3)3{\cdot}9H_2O$, ZnO, $Cr(NO_3)_3{\cdot}9H_2O$, Er_2O_3 and Yb_2O_3 as initial precursors. In contrast to the traditional high-temperature solid-state synthesis, the applied method allowed to obtain phase-pure nanopowders of all three series of materials with Cr^{3+}:Er^{3+}:Yb^{3+} ratios of 1:1:3, 1:1:5 and 1:1:7 at a minimal heat treatment temperature of 700 °C. The average grain size derived from X-ray diffraction data increases from ~33 nm after initial crystallization of materials at 700 °C up to 73-75 nm in the materials heat-treated at 1200 °C. Spot-check investigation of sample morphology by scanning electron microscopy revealed a platelet-like structure with plates formed by dense packed near spherical grains of 50-150 nm diameter. The unit cell dimensions of triply doped $ZnAl_2O_4$:Cr,Er,Yb materials are systematically higher than those for RE-free $ZnAl_2O_4$:Cr samples, thus proving effective incorporation of the large Er^{3+} and Yb^{3+} ions into $ZnAl_2O_4$ lattice. Analysis of obtained structural results shows that the heat treatment temperature affects the lattice parameter of the spinel structure, which decreases gradually for all three series of the triple doped $ZnAl_2O_4$:Cr:Er:Yb powders, becoming practically equal after final annealing at 1200 °C. This observation can be explained (i) by limited solubility of RE ions in $ZnAl_2O_4$ crystal matrices and/or (ii) by partial redistribution (inversion) of Al and Zn cations in the tetrahedral and octahedral positions of spinel structure.

The excitation spectra of the $ZnAl_2O_4$:Cr:Er:Yb phosphors consist of three wide bands, which correspond to the $^4A_2 \rightarrow {}^4T_1$ and $^4A_2 \rightarrow {}^4T_2$ transitions in Cr^{3+} ions in octahedral sites. The evolution of the luminescent characteristics of three series of triple-doped spinel-type materials on the Cr/Er/Yb ratio as well as on the heat treatment temperature of the powders is discussed.

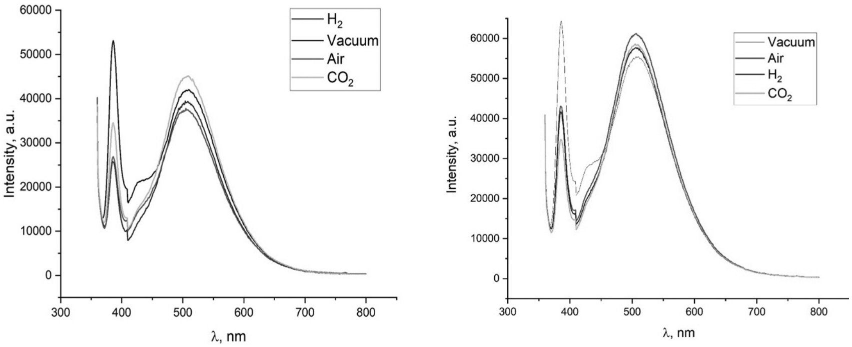
Acknowledgment: The work was partially supported by the National Research Foundation of Ukraine (grant no. 2020.02/0373) and supported by the Ukrainian Ministry of Education and Science under Project no. 0121U107736 (DB/MODUS)

Photoluminescent properties in different gas ambient of ZnO nanopowders doped by Mo and V

Venhryn Yu.I., Serednytski A.S., Popovych D.I.

Pidstryhach Institute for Applied Problems of Mechanics and Mathematics
NAS of Ukraine. Naukova str., 3b, Lviv-79060, Ukraine.
E-mail: popovych@iapmm.lviv.ua

The researches structural, morphological and photoluminescent properties of *ZnO* nanopowders doped by *Co* and *V* obtained using pulsed laser reactive technology is carried out. Electron microscopy and X-ray diffractometry were conducted to determine the structure, shape, and size of the nanoparticles. Investigation the peculiarities of photoluminescence (PL) in different ambient of *Mo* and *V* doped *ZnO* nanopowders was carried out. Changing the gas environment leads to a significant change in the intensity of the PL spectra and its deformation, that can be used in the gas sensors. The PL spectra of all sample consist strong emission bands located in the UV-range and broad non-elemental emission band in the visible region from 410 to 600 nm (Fig. 1). The decomposition of PL spectra into elementary bands shows the presence elementary peaks of 430, 520 nm. The influence of the impurity and the gas medium on the redistribution of elementary luminescence bands intensities was investigated.



a) *b)*

Fig.1. *Photoluminescent spectra in different ambient of ZnO nanopowders doped by a) Mo b) V.*

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Raman mapping few-layer MoS_2 to develop flexible electronics

Qiu Y.[1]***, Chen W.***[1]***, Babichuk I.S.***[1,2]***, Babichuk I.V.***[3]***, Yang J.***[1]

[1] *Faculty of Intelligent Manufacturing, Wuyi University,*
529020, Jiangmen, P.R. China.
E-mail: 48489797@qq.com (Qiu), ivan@szu.edu.cn

[2] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine,*
03680, Kyiv, Ukraine.

[3] *National Center "Minor academy of sciences of Ukraine",*
04119, Kyiv, Ukraine.

Molybdenum disulfide (MoS_2) as the most typical member of the transition metal dichalcogenides family has attracted increasing attention recently due to its extraordinarily different material properties compared with conventional bulk materials. The MoS_2 possesses a high Young's modulus, high strength, and outstanding carrier mobility. By exploiting the unique mechanical and mechanoelectrical transduction properties, MoS_2 can be used in wide-ranging applications, including flexible electronics and strain sensors.

One of the main tasks at the beginning of the investigation was to optimize the parameters of the synthesis of MoS_2 monolayer without defects over a large area. The synthesis of high-quality defect-free monolayer depends on many factors, such as the type of substrate, the quality of the starting material, pressure, temperature, gas flow, and so on. The chemical vapor deposition (CVD) method was used for the synthesis. Another direction was the development of a protocol for the transfer of these layers on the prepared flexible substrate. One of the transfer methods was the use of a layer of poly-(methyl methacrylate) (PMMA) coated by spin coating method on MoS_2 and growth substrate (SiO_2/Si) to lift off the PMMA/MoS_2 stack.

The used of Raman spectroscopy demonstrated the mono and few-layer MoS_2. Raman mapping showed the high-quality MoS_2 monolayers (Fig. 1), but not a large areas and only flakes.

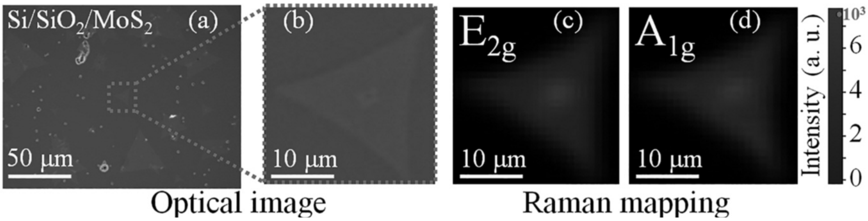

Fig. 1. *(a) The optical photo of surface MoS_2 flakes grown on SiO_2/Si substrate by CVD method. (b) The mapping area of MoS_2 flake. (c-d) The Raman mapping of E_{2g} and A_{1g} bands corresponds to the area in the optical photo.*

Reduction of combustibility of the polyurethane matrix of microwave-absorbing composite materials

Guzii S.G.[1]***, Khodakovskyy O.V.***[2]***, Kurska T.M.***[3]

[1] *V. Bakul Institute for Superhard materials of NAS of Ukraine,*
Avtozavodskaya Str., 2, Kyiv-04074, Ukraine.
E-mail: sguziy2@gmail.com

[2] *National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute», Peremohy Ave., 37, Kyiv-03056, Ukraine.*

[3] *Odessa Polytechnic State University,*
Shevchenko Ave., 1, Odessa-65044, Ukraine.

One of the promising areas of modern materials science is the creation of new polymer nanocomposite materials in the form of electromagnetic screens [1] and coatings designed to absorb and scatter electromagnetic waves with a frequency of 10 - 70 GHz from household and industrial appliances and equipment. Given that in such material, as a binder is a polymer, there is a natural question to reduce its combustibility in critical operating conditions, for example, at the time of fire. Therefore, based on the scientific achievements of the authors [2] and the experience of world practice of fire protection, as an object of study was adopted intumescent system (IC) of traditional composition [3]. Based on statistical data processing, regression equations were obtain and isoparametric diagrams of changes in the physical properties of the polymeric binder from changes in variable factors were constructed. The method of superimposition of replicas of isoparametric diagrams established the optimal range of concentrations of IC additives that meet the requirements of normalized parameters, namely: PFA from 15 to 17%, PE from 9 to 11.5% and MA from 11 to 14%. The introduction of IC components in the specified percentage allows reducing the combustibility of polyurethane varnish by 12.5 times compared to the original.

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Session 5
Nanostructured surfaces

Properties of multilayer aluminum-doped indium saving ITO thin films deposited by sputtering method

Petrovska S.S.[1], Sergiienko R.A.[2], Ilkiv B.I.[1],
Nakamura T.[3], Ohtsuka M.[3]

[1] Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine, Krzhyzhanovski Str., 3, Kyiv-03142, Ukraine.

[2] Physico-Technological Institute of Metals and Alloys, Vernadsky Ave., 34/1, Kyiv-03142, Ukraine.

[3] Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan.
E-mail: makoto.ohtsuka.d7@tohoku.ac.jp

Multilayer (ML) aluminum-doped indium tin oxide (ITO) thin films with reduced to 50 mass% indium oxide content were prepared by co-sputtering of the ITO50 and Al_2O_3 targets in mixed argon-oxygen atmosphere onto very thin layer of conventional ITO (ITO90) deposited on glass substrates preheated at 523 K (ITO50:Al_2O_3/ITO90). Present work demonstrates the influence of the oxygen flow rate and heat treatment on optical, electrical, and structural properties of ML ITO50:Al_2O_3 thin films. It was found that as-deposited ML ITO50:Al_2O_3/ITO90 thin films sputtered in pure argon showed the decrease of the volume resistivity (445 μΩcm) in 1.6 times in comparison with single layer (SL) ITO50:Al_2O_3 thin films deposited at optimal conditions and in 6.3 times as compared with SL ITO50:Al_2O_3 thin films sputtered in pure argon atmosphere. Minimal volume resistivity in ML ITO50:Al_2O_3/ITO90 thin films can be achieved when depositing in pure argon atmosphere in contrast to undoped ML ITO50/ITO90, iron-doped ML ITO50:Fe_2O_3/ITO90 and ITO50:Fe_3O_4/ITO90 thin films, which need mixed argon-oxygen atmosphere to reach minimal values of volume resistivity. ML ITO50:Al_2O_3/ITO90 thin films deposited in pure argon atmosphere showed average transmittance larger than 85 % in the visible range. On the other hand, these films deposited in mixed argon-oxygen atmosphere showed average transmittance larger than 90 %. ML ITO50:Al_2O_3/ITO90 thin films showed polycrystalline $In_4Sn_3O_{12}$ structure in as-deposited state and after heat treatment at 523 K. Peaks corresponding to aluminum oxide were not revealed on XRD patterns of ML ITO50:Al_2O_3/ITO90 thin films.

Iron-doped indium-saving indium tin oxide thin films deposited by DC sputtering method using Fe_3O_4 target

Petrovska S.S.[1], Sergiienko R.A.[2], Ilkiv B.I.[1], Nakamura T.[3], Ohtsuka M.[3]

[1] *Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine, Krzhyzhanovski Str., 3, Kyiv-03142, Ukraine.*

[2] *Physico-Technological Institute of Metals and Alloys, Vernadsky Ave., 34/1, Kyiv-03142, Ukraine.*

[3] *Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan.*
E-mail: makoto.ohtsuka.d7@tohoku.ac.jp

Iron-doped indium-saving ITO50:Fe_3O_4 thin films were deposited onto glass substrates unheated and preheated at 523 K by co-sputtering of ITO50 and Fe_3O_4 targets at different oxygen flow rates (0-0.3 sccm) and subsequently heat treated.

It was found that minimal value of volume resistivity was obtained for ITO50:Fe_3O_4 thin films deposited on preheated substrates (PHS) at oxygen flow rate of 0.2 sccm that is 14 times lower than that of ITO50:Fe_3O_4 thin films deposited on unheated substrates (UHS) at the same oxygen flow rate.

The transmittance of both ITO50:Fe_3O_4 (PHS) and ITO50:Fe_3O_4 (UHS) thin films was improved with increasing oxygen flow rate. Doping of indium saving ITO thin films with Fe_3O_4 allows increasing transmittance. Average transmittance was above 85 % in visible range for both ITO50:Fe_3O_4 (PHS) and ITO50:Fe_3O_4 (UHS) thin films.

ITO50:Fe_3O_4 (PHS) thin films crystallizes at lower heat-treated temperature than ITO50:Fe_3O_4 (UHS) thin films, however undoped ITO50 (PHS) thin films deposited at the same oxygen flow was crystallizes in as-deposited state. Doping with Fe_3O_4 does not change the structure of undoped ITO50 (PHS) thin films.

Arithmetical mean height (S_a) and root mean square height (S_q) of as-deposited ITO50:Fe_3O_4 (PHS) thin films were 0.52 nm and 0.67 nm, respectively.

Formation of submicron relief structures on the surface of sapphire substrates

***Kryuchyn A.A.*, Rubish V.M., Shihovets O.V., Pankratova A.V.**

Institute for Information Recording of the NAS of Ukraine.
M. Shpak str 2, Kyiv-03113, Ukraine.
E-mail: kryuchyn@gmail.com

Microrelief structures on the surface of sapphire substrates are widely used in the manufacture of LEDs, diffractive optical elements and long-term storage media. Most epitaxial structures for LEDs are grown on profiled sapphire substrates, which allows to achieve high efficiency in 1.5-2 times of light output from LEDs [1]. Microrelief diffraction optical elements (DOE) are formed on sapphire substrates, designed to operate at high radiation powers and temperatures [2]. Microrelief sapphire substrates are also proposed to be used to create long-term data storage media. The formation of relief on the surface of the sapphire substrate is difficult due to its high chemical resistance. The proposed methods of creating a relief on the surface of the sapphire substrate can be divided into two groups - the formation of microrelief in the material of the substrate and obtaining a microrelief image in the material applied to the surface of the sapphire substrate. To create a microrelief on the surface of sapphire substrates can use the method of nanospheres lithography [3].The main problems in creating a microrelief on the surface of sapphire substrates are the removal of static electric charge in the process of ionic-chemical etching of substrates and obtaining a protective mask with windows of specified sizes, through which etching of sapphire substrate. To create submicron relief structures on the surface of sapphire substrates, we used two-layer masks consisting of chromium and photoresist films. Elements of submicron sizes were formed on the photoresist layer by direct laser writing. The chromium film was chemically etched through windows in the photoresist. Plasma-chemical etching through a two-layer mask produced relief elements on the surface of a sapphire substrate with dimensions (0.3–0.7) µm and depth (0.1–0.2) µm.

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Investigation mobility of current carriers from temperature for CdTe and PbTe thin films

***Mazur M-Y.M.*[1], *Mazur T.M.*[2], *Mazur M.P.*[2]**

[1] *National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute», Prosp. Peremohy, 37, Kyiv, Ukraine*

[2] *Department of General and Applied Physics, Institute of Architecture, Construction and Energy, Ivano-Frankivsk National Technical University of Oil and Gas, Karpatska, 15, Ivano-Frankivsk-76019, Ukraine.*
E-mail: tetiana.mazur@nung.edu.ua

Promising materials for their creation of active elements of micro- and optoelectronics, such as sources of infrared radiation of the optical spectrum, detectors of X- and γ- radiation, thermoelectric energy converters, are films of cadmium and lead telluride [1]. In the study of transport phenomena in semiconductor films, the dependence of thickness properties is well known, due to the fact that, along with bulk mechanisms of current carrier scattering, processes on the surface play an important role. In addition, in a number of thin films, the scattering of current carriers on grain boundaries dominates, since the total surface of crystallites can exceed the film surface by several orders of magnitude.

Films were obtained by hot wall deposition on glass substrates according to [2]. The thickness of the films was determined by the spraying time. The structure of the films was studied by X-ray and electron microscopic methods. The electrical conductivity of the films was measured at direct current in the temperature range 77–300 K. All films, regardless of temperature and grain size, had hole conductivity. The main parameters that determine the grain size in thin films are the film thickness and the substrate temperature. By reducing the film thickness to 0.05 μm and reducing the substrate temperature to the temperature of liquid nitrogen, it is possible to obtain films with a grain size $\approx 2\ 10^{-7}$ cm.

The structure of the films was studied by electron microscopy and diffraction, as well as optical metallography. The electrical parameters of the films were measured by the compensation method in constant electric and magnetic fields. The measurement was carried out on separate films of different thicknesses. The current through the samples was $\cong 0.1$ mA. The magnetic field was directed perpendicular to the film surface at an induction of 0.8 Tesla. The measured sample had four Hall and two current contacts.

Based on the results obtained, it can be argued that certain activation energies are associated with potential barriers at grain boundaries, which lead to a decrease in hole mobility with decreasing temperature. It should be noted that the experimental results are in good agreement with the theoretical calculations of the

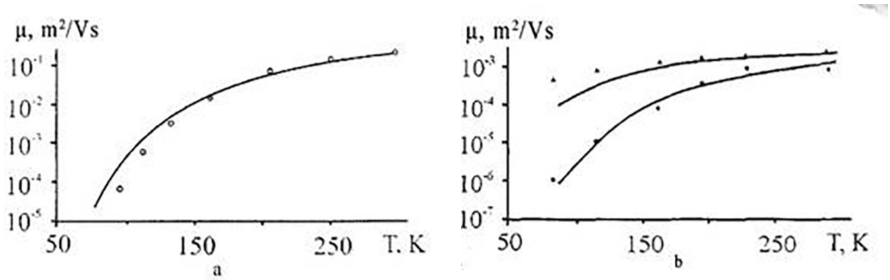

Fig. 1. *Dependence of current carrier concentration on temperature for p-CdTe (a) ($L=10^{-4}$ cm) and p-PbTe (b) thin films (1 – $L=10^{-6}$ cm, 2 – $L=10^{-7}$ cm) (points – experiment, solid line – calculation by formula)*

effective value of mobility, which indicates the validity of the choice of a physical model for a nanostructured material. The decrease in carrier mobility due to scattering at barriers is the reason for the decrease in conductivity with decreasing temperature, Fig. 1.

Thus, in p-CdTe and p-PbTe films, the dominant role in transport phenomena is played by processes at grain boundaries associated with the formation of potential barriers and thermionic emission of current carriers.

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Unusual magnetoresistane changes of thin deuterium-covered W(100) plate under high-temperature annealing

***Bordeniuk I.V.*, Sologub S.V.**

Department of Adsorption Phenomena, Institute of Physics of the NAS of Ukraine. Prospect Nauki, 46, Kyiv-03028, Ukraine.
E-mail: ibordeniuk@gmail.com

Changes of the magnetoresistance (MR) of thin (~100 μm) W(100) plates covered with saturated deuterium coverage at T = 4.2 K during isochronous (~1 s) annealing were examined by static skin-effect and transversal magnetoresistance techniques. MR changes due to modification of specularity of surface scattering of conduction electrons by submonolayer deuterium desorption/ordering (Fig. 1, T = 5 – 800 K) [1] and *unusual, partially reversible, MR changes of the plate with atomically clean surfaces at annealing temperatures T = 1250 – 2650 K (Fig. 1) were found.*

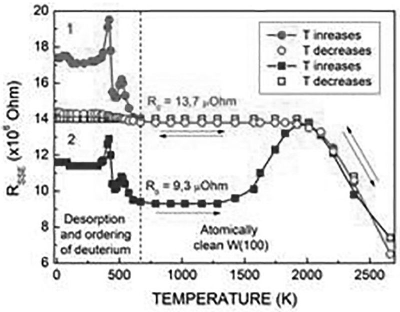

Fig. 1. *Change of the MR of the W(100) plate covered by deuterium at T ≈ 5 K due to isochronous annealing.*

Reasons of the unexpected high-temperature effect, in particular, the deuterium-induced change of surface and bulk structure of tungsten plates caused by high-temperature “flashes” and penetration of deuterium into the subsurface area of tungsten, are discussed.

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Study of the nanostructure of the mixed adsorption layer of heavy metal and diclofenac on the surfaces of synthetic zeolites and their carbon composites

Medykowska M.[1], Wiśniewska M.[1*], Szewczuk-Karpisz K.[2], Panek R.[3]

[1] Department of Radiochemistry and Environmental Chemistry, Faculty of Chemistry, Maria Curie- Sklodowska University,
Maria Curie-Sklodowska Sq. 3, 20-031 Lublin, Poland,
*E-mail: *malgorzata.wisniewska@mail.umcs.pl;*

[2] Institute of Agrophysics, Polish Academy of Sciences,
Doświadczalna 4, 20-290 Lublin, Poland;

[3] Department of Building Materials Engineering and Geoengineering,
Faculty of Civil Engineering and Architecture, Lublin University of Technology, Nadbystrzycka Street 40, 20-618 Lublin, Poland.

Diclofenac is one of the most popular over-the-counter nonsteroidal anti-inflammatory drugs (NSAIDs). Compared to other NSAID analgesics, it is well tolerated, does not accumulate in tissues, and rarely causes serious side effects. It has been estimated that its annual global consumption is about 940 tons. For this reason, it is one of the more common pharmaceuticals in raw sewages [1]. Other common contaminants in wastewater are heavy metals, which enter there due to many ways e.g. from agriculture and textile industry. For this reason, it was decided to investigate the adsorption capacity of zeolites and their composites with carbon towards diclofenac as well as heavy metals (Pb(II) and Zn(II)) in mixed systems of adsorbates, which better reflect the nature of wastewater samples.

Therefore, adsorption, desorption and kinetics measurements were performed. Furthermore, the interaction mechanisms of heavy metal ions and drug molecules with solid surfaces were determined based on the results of electrokinetic studies. The conducted studies showed that the investigated materials are characterized by high application potential and great possibilities of future usage.

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Influence of laser treatment on the characteristics of martensitic transformation in Fe-Ni-Ti-Al alloy

Bondar V., Danilchenko V., Dzevin Ie.

G.V. Kurdyumov Institute for Metal Physics NASU,
Kyiv, 03142, Vernadsky blvd.,36, Ukraine
Tel.: +38 044 424 3577
E-mail: danila@imp.kiev.ua

The influence of pulsed laser treatment (LT) on the structural-phase state and completeness of martensitic γ-α (f.c.c.-b.c.c.) transformation in the metastable Fe-Ni-Ti-Al alloy has been studied. It is established that LT in the melting mode activated martensitic transformation (MT) in the near-surface alloy layer. The influence of the size effect and nanosized austenitic grains and the structural state of austenite on the ability of LT to activate MT in the near-surface layer of melted alloy is analyzed.

Laser melting austenitized the near-surface layer of the quenched biphasic alloy and consequently weakened the layer relative to the volume. After subsequent cooling in liquid nitrogen, the near-surface layer due to the formation of additional martensite received a more significant strengthening compared to the volume.

Catalytic activity of acetazolamide on electroreduction of In(III) in chlorates(VII); use of a nanostructured cyclic renewable film of liquid silver amalgam electrode (R-AgLAFE)

<u>Nosal-Wiercińska A.</u>**, Martyna M., Pawlak A.

Department of Analytical Chemistry, Institute of Chemical Sciences,
Faculty of Chemistry, Maria Curie-Skłodowska University,
Maria Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland
*E-mail: *agnieszka.nosal-wiercinska@mail.umcs.pl*

The use of an innovative electrode with a cyclic renewable film of liquid silver amalgam R-AgLAFE is an excellent alternative to HDME, as it guarantees similar quality and performance parameters to HMDE [1] and fits into the current trend of green chemistry.

Acetazolamide is one of the most important drugs used in the treatment of secondary glaucoma [2]. Therefore, there is a need to study the mechanisms of action of this drug or search for new systems of controlled release.

The influence of acetazolamide (ACT) on multi-step In(III) ion electroreduction was investigated using both voltammetry and impedance methods.

It was observed that acetazolamide catalyzes the electroreduction of In(III) ions.

Since the „cap – pair" effect provides a significant increase in the sensitivity of the quantification of both the depolarizer (In(III) and the ligand (ACT) hence the proposed procedure may be of paramount importance for evaluating the progress of treatment and building a mechanistic model of the effects of this drug on the human body.

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Ab initio studies of the gas adsorption on the surface CdSe1-xSx ultra-thin films

Kashuba A.I.[1], **Semkiv I.V.**[1], **Andriyevsky B.**[2],
Ilchuk H.A.[1], **Kashuba N.Yu.**[1], **Petrus R.Yu.**[1]

[1] *Lviv Polytechnic National University,*
12, S. Bandera Str., Lviv-79013, Ukraine
E-mail: andrii.i.kashuba@lpnu.ua

[2] *Koszalin University of Technology,*
2, Sniadeckich Str., Koszalin 75-453, Poland

Substitutional solid-state solutions with a general formula $CdSe_{1-x}S_x$ attract a considerable interest of researchers from both fundamental and applied viewpoints. Recently, extensive studies have been conducted which are aimed at manufacturing highly efficient CdS/CdTe solar cells, in which CdS thin films serve as a 'wideband optical window'. Ternary $CdSe_{1-x}S_x$ films are promising in this respect at least because they enable changing and combining basic physical characteristics of the initial binary compounds CdSe and CdS in a controlled and predictable manner.

Semiconducting compounds of AIIBVI group represent also promising materials for different sensors. In particular, they can be utilized as working elements of gas sensors. Potentials of the binary compounds CdS and CdTe as gas sensors have been analyzed, e.g., in the work [1]. This has been done for the particular cases of nanorods deposited on Ti substrates and thin films. In spite of these achievements, the main properties of the $CdSe_{1-x}S_x$ system associated with its possible sensor applications have not yet been elucidated.

All of our calculations, including geometry optimization and calculations of total energy, energy spectra, density of states and adsorption configuration of gases, were performed with a functional density functional theory (DFT). Thin films of $CdSe_{1-x}S_x$ were modeled on the basis of a 'parent' CdSe compound with wurtzite crystal structure. The electronic band structure and the main optical properties obtained theoretically in this work are compared with the experimental data known from the literature, which reveals a fair agreement with the experiment.

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Model calculations of nanolayer heating of a substance under the action of irradiation

Shmeleva L.V., Suprun A.D.

Department of Theoretical Physics, Faculty of Physics,
Taras Shevchenko National University of Kyiv.
Volodymyrska Street, 64/13, Kyiv-01601, Ukraine.
E-mail: lshmel@univ.kiev.ua

The paper considers the process of laser heating of a local area of an arbitrary metal surface. In previous researches, we studied the processes accompanying such an effect. The previously developed model takes into account both the elastic response of the medium and the temperature response to a powerful external impact.

The modeled temperature dependences were analyzed for several technological applications using asymptotic approximations. In fact, the general analytical solutions depend on the coefficients of reflection and scattering of radiation by the surface, and these coefficients themselves also have a significant temperature dependence. As a result, the obtained equations for describing the surface heating process transform to transcendental. This leads to the need to use numerical methods to refine the temperature dynamics of the surface under intense laser irradiation.

Theoretical and numerical prediction of the results of laser exposure, both destructive and non-destructive, on various surfaces of materials today is extremely important. Laser technologies are used in many areas. Currently, one of the important areas is research related to the use of optical sensors. Here the laser ray falls on a metal layer of nanoscale thickness. Since the accuracy of such sensors is important, the effect of temperature on measurement results must be investigated. Considering that the thicknesses of the films used in surface plasmon resonance sensors are nanosized, the problem is further complicated. This is due to taking into account the dependence of the temperature of the nanosized metal layer on the absorption coefficient. These studies have been carried out and analyzed in the work.

The temperature dependences of the heating of a smooth (mirror) nanolayer and a nanolayer with irregularities or foreign inclusions was calculating in this proceedings. The obtained results are compared with previous results, where the temperature dependence of the optical coefficients was not considered.

Ion nanostructuring of crystal surfaces and processes of self-organization

Zayachuk D.M.

Lviv Polytechnic National University,
S. Bandera Str., 12, Lviv-79013, Ukraine
E-mail: zayachuk@polynet.lviv.ua

Ion beam treatment is widely used for structuring the surface of solids, which is of great practical importance for various technical and technological applications. The main approach suggested to describe the process of individual surface structure formation under impact of ion beam bombardment is top-down, based on etching of solid surface by energetic ions, the sputter yield of which depends on the local surface curvature. In this report the issue of interaction of ion beams with a crystalline surface is considered from the point of view of impact on nanostructuring of the sputtering surfaces of the processes of self-organization of the planes of high reticular density and easy cleaving basing on the results of our recent studies of SnTe and PbTe crystals [1,2].

SnTe and PbTe crystals are characterized by the same planes of high reticular density. SnTe crystals do not cleave, and for PbTe crystals the planes of high reticular density are also planes of easy cleavage. As a result the prolonged treatment of surfaces of these compounds with ion beams leads to the dominance of different ion-induced structures on their sputtering surfaces. In the case of SnTe, sharpened cones dominate on the structured surface. In the case of PbTe, sharpened conical structures are transformed into pyramidal structures. Their shape and lateral surface condition are determined by the crystallographic orientation of the sputtering surface and the self-organization of the planes of high reticular density in the process of formation of the pyramidal structure facets. The mechanisms of self-organization and the interplay between the reticular density of the sputtered surfaces and the surfaces of the lateral facets of ion-induced pyramidal nano- and microstructures are analyzed.

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Ni nanostructures on semiconductor surfaces

Smolyak S.S., Karbivskyy V.L., Karbivska L.I., Shvachko N.K.

Department of Nanostructures Physics,
G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,
Kyiv-03142, Ukraine
E-mail: karb@imp.kiev.ua

The formation mechanism of nickel nanorelief on the silicon surface (plane-111) during thermal evaporation in vacuum was investigated (all images on JSPM-4500 tunneling microscope were acquired in constant current mode). After the first deposition cycle (1 sec.), nickel forms islands with a height of about 0.11 nm (fig. 1). After increasing the application time to three seconds, a percolation effect is observed, in this case, nickel nanoparticles completely cover the silicon substrate, which corresponds to 4 - 5 metal monolayers.

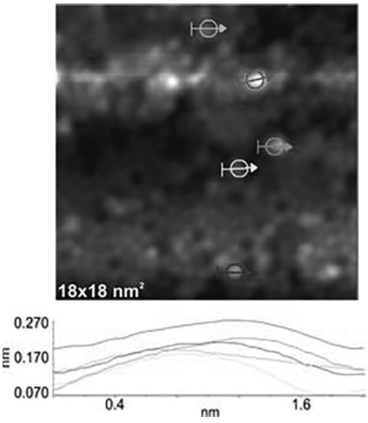

Fig. 1. *Ni nanostructures deposited for 1 sec. on the Si (111) surface.*

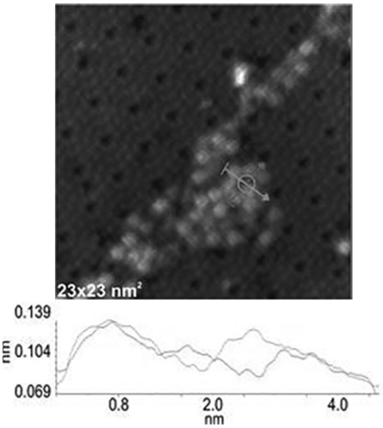

Fig. 2. *Nanoformations of nickel on Si (111) at T=1150 ºC.*

It was found that nanoformations have a nearly spherical shape and form clusters consisting of approximately 5 - 10 nickel nanoparticles. This shape is typical for liquid metal droplets, which flatten on impact with the substrate. With an increase in the deposition time to *5 sec.*, an almost twofold increase in the height of nanoparticles is observed, while the longitudinal and transverse dimensions remain almost unchanged. A significant interaction of Ni nanostructures with the substrate was found. After significant heating of the surface, partial desorption of Ni is observed (fig. 2). The nanostructures obtained after thermal loading form an intermediate $NiSi_2$ phase.

In general, the formation of transition metal silicides on single-crystal surfaces is an important problem for microelectronics. Among the many interesting technological properties, one can note their importance in connection with the formation of a silicon-silicide phase boundary in a Schottky contact [1].

One of the important characteristics in the analysis of surface-applied nanostructures is sub-roughness, which refers to the coating nano-geometry and determines its important performance properties, in particular wear resistance, strength, chemical resistance and other properties. Sub-roughness is determined using precision techniques and research tools such as atomic resolution scanning probe microscopy. The nature of sub-roughness is determined by the internal structure of the solid, its defects and the processes of interaction of the surface with the environment. As a result of an increase in the deposition time, the parameters of the initial sub-roughness can change as a result of relaxation processes in the structure, which is accompanied by the processes of growth and transformation of clusters. In this case, the elements are segregated to the surface, changing the electronic structure and properties of the surface.

Conclusions

The parameters of sub-roughness (R_a, R_q, R_{zjis}, R_z, S_{ratio}) for coated surfaces and their dependence on the technological parameters of application have been established. It is shown that there is an increase in the size of clusters with the general preservation of the tendency for an increase in the maximum difference between the peaks and valleys at ten points.

Nickel on the surface of silicon forms stable chemical complexes $NiSi_2$ of spherical shape, which are characterized by a monomodal distribution in size with an average diameter of 1.0 nm.

The linear ordering of spherical clusters is determined by the presence of twinning boundaries.

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Natural zeolites modified with silver nanoparticles as promising sorbents with antibacterial properties

Patrylak L.K.[1,2]***, Yakovenko A.V.***[1]***, Nizhnik B.O.***[1,2]***,***
Pertko O.P.[1]***, Povazhnyi V.A.***[1]

[1] Department of Catalytic Synthesis, V.P Kukhar Institute of Bioorganic Chemistry and Petrochemistry of NAS of Ukraine.
Murmanska Str., 1, Kyiv-02094, Ukraine E-mail: lkpg@ukr.net

[2] Depatment of Technology of Inorganic Substances, Water Treatment and General Chemical Technology, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute".
Peremohy ave., 37, Kyiv-03056, Ukraine

Today, more than eighty types of natural zeolites are known [1, 2]. The latter, in contrast to synthetic zeolites, usually contain a number of impurities from other rocks. Clinoptilolite, as a zeolite of the gaylandite group, finds considerable application [3] in various fields. It is one of the most stable and common natural zeolites in the world, deposits of which are available in Transcarpathia. The shortcomings of the porous structure of the clinoptilolite, on the other hand, limit the widespread usage of Ukrainian natural zeolites.

The aim of this study was to use a complex modification of natural zeolites to obtain promising silver-containing antibacterial sorbents with improved porosity.

The original rock was clinoptilolite-type zeolite from the Sokyrnytsia deposit (Transcarpathian region). The first stage of its modification was the expansion of the pores by four times dealumination/decationation by ethylenediamine tetraacetic acid. This gentle treatment increased the SiO_2/Al_2O_3 ratio from 7.3 to 8.7, increased the specific surface area to 90 m^2/g, and the micropore volume to 0.036 cm^3/g. Additionally, the sample was doped with silver in the amount of 1 wt% using silver nitrate. The obtained zeolite sample is a promising sorbent with antibacterial properties.

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UV degradation of water repellency on nanostructured aluminum and steel surfaces

Myronyuk O.*[1]*, Rodin A.*[2]*,
***Vanagas E.*[3]*, Baklan D.*[1]*, Raks V.*[4]**

[1] *National Technical University of Ukraine "Igor Sikorsky*
Kyiv Polytechnic Institute".
Prosp. Peremohy, 37, Kyiv-03056, Ukraine.
E-mail: d.baklan@kpi.ua

[2] *State research institute Center for Physical Sciences and Technology,*
Savanorių ave. 231, Vilnius-02300, Lithuania.

[3] *Evana Technologies, UAB,*
Mokslininkų st. 2A, Vilnius-08412, Lithuania.

[4] *Taras Shevchenko National University of Kyiv,*
Volodymyrska St 64/13, Kyiv- 01601, Ukraine.

The use of nanotextured metal surfaces treated with low-energy organic substances is potentially effective in many applications, including outdoor surfaces exposed to solar UV radiation. Undoubtedly, the assessment of the sustainability of superhydrophobic properties when exposed to UV light is one of the key stages in the further development of this technology. The reporting phase of the research was aimed at creating a model of scalable surfaces. The surfaces of steel and aluminum were textured with a femtosecond laser to impart hybrid micro-nano roughness using the procedures described in [1] and [2]. Immediately after laser processing, steel surfaces contain anisotropic LIPSS textures with elements of 80-200 nm, and aluminum surfaces - 50-200 nm. These surfaces were treated with alkoxy silanes. Water repellency was evaluated by measuring the critical surface energy (25 mJ/m^2), water contact angles (greater than 155°) and sliding angles. The project has received funding from the Research Council of Lithuania, agreement S-LU-22-3, and the Ministry of Education and Science of Ukraine in the scope of the bilateral Lithuania-Ukraine program of cooperation.

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Chemical etching of InSb crystals using I_2 + methanol or DMF compositions

Malanych G.P.

Semiconductor Chemistry Department,
V.Ye. Lashkaryov Institute of Semiconductor Physics of the NAS of Ukraine.
Prospect Nauki, 41, Kyiv-03028, Ukraine.
E-mail: galya.malanich@gmail.com

The quality and condition of the surface play an important role in the technology of manufacturing semiconductor devices. The chemical etching is a usual method of the cleaning and the texturing of the substrate surfaces.

InSb (112) crystals were used for the investigations. The single-crystalline ingots were cut into 25 mm^2 size substrates using the string cutting with diamond coating. In order to achieve the nanosized relief, the samples were treated in the following sequence: mechanical grinding, chemical-mechanical polishing (CMP) and in-process washing (after each stage of the treatment) and chemical-dynamic polishing (CDP). The cutting-induced surface deformation layer was partially removed by mechanical grinding with aqueous slurries of M10 to M5 and ASM 1/0 abrasive powders. The disturbed during cutting and grinding layer with the thickness of 100-150 μm was removed by CMP using non-abrasive etchant. CMP was carried out on a glass polisher covered with lawn cloth at a continuous supply of etchant (2-3 ml·min^{-1}) for 3 min and a pressure on the plates in 2-3 kPa. CDP was the finish stage of the substrate modification. It was carried out in the reproducible hydrodynamic conditions using the disk rotation method. The dissolution rate of crystals was defined using the electronic indicator TESA DIGICO 400. In-process washing of the crystals was carried out after every treatment stages in $Na_2S_2O_3$ and NaOH solutions and distilled water.

The interaction between the semiconductors and the I_2 + methanol or DMF etchants was studied using the CDP. It was found that in the studied concentration range (6-18 mass.% I_2 in DMF) with increasing I_2 content, the dissolution rate of InSb increases from 0.4 to 7.7 μm.min^{-1}, forming a polished surface with a mirror luster. The dependence of PbTe dissolution rates in the range of concentrations of 3-15 mass.% I2 in methanol was studied. It was determined that with increasing iodine content from 3 to 12 mass.%, the dissolution rate increases from 1.8 to 9.6 μm.min^{-1} A further increase in the content of I_2 to 15 mass.% in the etching composition leads to a decrease in the etching rate of the samples to 1.4 μm.min^{-1}. As a result of the CDP, the polished surface is formed with Ra < 5 nm.

Effect of Zn-BEA zeolites dealumination on their catalytic perfomance in propane dehydrogenation to propylene with CO_2

Orlyk S.M.[1], Chedryk V.I.[1], Kyriienko P.I.[1],
Kapran A.Yu.[1], Balakin D.Yu.[2], Dzwigaj S.[3]

[1] L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine,
31 Prosp. Nauky, 03028 Kyiv, Ukraine.
E-mail: ayukapran@ukr.net

[2] Institute of Physics, NAS of Ukraine, 46 Prosp. Nauky, 03028 Kyiv, Ukraine.

[3] Laboratoire de Réactivité de Surface, Sorbonne Université-CNRS, UMR 7197, 4 place Jussieu, Paris, F-75005, France.

Oxidative dehydrogenation processes of alkanes, in particular propane to propylene with CO_2 (DHP-CO_2), is considered a promising alternative to the oil-based cracking processes of propylene production [1, 2].

The influence of preliminary dealumination of BEA zeolite on the acid-base characteristics of Zn-BEA compositions and their catalytic properties in the DHP-CO_2 process is studied.

Full pre-dealumination of starting BEA specimen followed by incorporation of zinc cations in the T-positions of the zeolite framework is shown to cause a halving in the total acidity and basicity of the ZnSiBEA sample compared to ZnAlBEA.

The ZnSiBEA catalyst, characterized by a more developed mesoporous nanostructure and specific surface area, the predominance of acidic (Zn^{2+} cations) and basic (O_2- anions and oxygen vacancies) sites of medium strength as well as an absence of protonic acid centers in contrast to ZnAlBEA and partially dealuminated ZnAlSiBEA specimen, is superior to them concerning the achieved selectivity of 74% and yield of 22% with respect to propylene produced.

Regeneration of the ZnSiBEA zeolite by calcining *in situ* is shown to provide an increase in the selectivity to 94% and yield to 30% with reference to propylene in the DHP-CO_2.

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Investigation of frontal functional nanolayers of solar silicon using electrochemical technologies of porous silicon

***Skrypnyk I.I.**, Yerokhov V.Yu., Druzhinin A.A., Nichkalo S.I.*

Department of Semiconductor Electronics,
Lviv Polytechnic National University,
S. Bandera Str., 12, Lviv-79013, Ukraine
E-mail: v.yerokhov@gmail.com

The study of all stages of formation of the porous structure based on the chosen technology and identification of patterns that affect the characteristics of the obtained nano-, meso- and macropores are very important, as most parameters of porous layers are laid at the initial stage. When using porous silicon as a textural and anti-reflective coating, the porous layer is formed directly on the surface of silicon and together with the antireflective coating. It must also provide passivation of the surface of the solar cell (SC).

Silicon surface texturing, both chemical and electrochemical etching, is an integral part of modern high-performance silicon SC technology. The texture on the front surface of the SC not only reduces reflection losses, but also helps to capture long-wavelength light in the structure of the SC, thereby expanding its operating spectral range and increasing the short-circuit current.

Electrochemical hydrogenation in hydrogen-enriched electrolytes may be a more effective method of improving the passivating properties of PSi [1]. With this treatment, efficient hydrogenation of broken bonds at the interface between PSi/monocrystalline, polycrystalline or multicrystalline silicon can be achieved, which will help reduce the rate of surface recombination. Compared with other methods of hydrogen saturation, electrochemical hydrogenation has a number of advantages. First, it can be combined with the anodizing process and does not complicate the technology of SC manufacturing. Second, electrochemical hydrogenation is a controlled process that allows hydrogen atoms to penetrate the semiconductor volume to a given depth and passivated broken bonds without damaging its crystal lattice. In order to improve the passivating properties of PSi layers used in SC, a study of the process of electrochemical hydrogenation of PSi was performed both on p-type silicon substrates with a resistivity of 0.1–10 Ω×cm and on substrates with formed emitter transition n^+-p conductivity.

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Structural transformations in oxide ceramic coatings formed on aluminum alloys in silicate electrolyte

Posuvailo V.M.[1]***, Koval'chuck I.V.***[1]***, Ivasenko I.B.***[1]***,***
Kanyuk Yu.I.[1]***, Iurkevych R.M.***[2]

[1] *Physico-Mechanical Institute of NAS of Ukraine.*
Naukova Str. 5, 79601 Lviv, Ukraine.
E-mail: vposuvailo@gmail.com

[2] *Hetman Petro Sahaidachyi National Army Academy.*
79012 Lviv, Ukraine

X-ray phase analysis of oxide ceramic coatings formed on the alloys D16T and AK9M2 in the process of plasma electrolyte oxidation in the electrolyte (KOH (3 g/l), Na_2SiO_3 (2 g/l) is fulfilled. It is established that at the beginning of the coating synthesis (after 5 min) there is a transformation of the crystal lattice of aluminum with the formation of the compound $Al_{3.21}Si_{0.47}$ in the surface layers of both alloys. After 1h of synthesis, the corresponding oxide ceramic coatings on alloys D16T and AK9M2 contain the following phases: α-Al_2O_3 (corundum), γ-Al_2O_3 and $Al_2O_3 \cdot SiO_2$.(sillimanite). When increasing the synthesis time to 2 h there is a partial conversion of sillimanite ($Al_2O_3{\cdot}SiO_2$) to mullite ($3Al_2O_3{\cdot}2SiO_2$) in the coatings on the alloy AK9M2. The study of the surface microstructure showed a uniform growth of oxide ceramic coatings and an increase of Si areas due to the formation of SiO_2 and the formation of a low-temperature substitution compound $Al_{3.21}Si_{0.47.\,T}$he image segmentation method was used to analyze the pore sizes and the probable distribution and size of bit channels. It is established that the minimum pore size is approximately 0.9 μm.

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Ab initio study of the effect of metal doping on electronic properties of $(ZnO)_n$ (n= 96, 120) nanoclusters

Bovhyra R.V.[1]***, Popovych D.I.***[1]***, Bovgyra O.V.***[2]

[1] *Pidstryhach Institute for Applied Problems of Mechanics and Mathematics*
NAS Ukraine, Naukova 3-B, Lviv, Ukraine
E-mail: bovhyra@gmail.com

[2] *Ivan Franko National University of Lviv, Faculty of Physics,*
Kyrylo and Mefodiy 8, 79005-Lviv, Ukraine

The results of ab initio density functional theory studies of energy spectrum and ground state parameters of zinc oxide nanoclusters $(ZnO)_n$ ($n = 96, 120$), doped with different metals (Co, Cu, Ni) are presented. Calculations were performed using ultrasoft pseudopotentials in the basis of plane waves. To describe the exchange-correlation energy of the electrons, we used a generalized gradient approximation with Hubbard corrections (GGA+U) in Perdew, Burke and Ernzerhof parameterization. Optimization of the nanocluster structure was performed using conjugate gradient method. No symmetry restrictions were used during structure optimization.

The first task in this research, was figuring out the best placement position for the doping atoms. The two main configurations of the placement of Co, Cu and Ni atoms on the surface of the optimized $(ZnO)_{96}$ and $(ZnO)_{120}$ nanoclusters were considered: zinc atoms were substituted by the doping atoms; oxygen atoms were substituted by Co, Cu and Ni atoms. After relaxation procedure, the changes in the structural geometry of all studied nanosystems were observed. For the $(ZnO)_n$+M(Zn) systems (n=96, 120; M=Co, Cu, Al) as well as $(ZnO)_n$+M(O) (n=96, 120; M=Co, Cu, Al) systems, we observed significant drop in the energy gap value (E_g) compared to the pristine nanoclusters. Formation energy (E_f) was calculated for both placement positions researched in this study. The obtained results were then compared with the values obtained in our previous studies for $(ZnO)_n$ (n=34, 60) nanoclusters [1].

The negative values for the formation for $(ZnO)_n$+M(Zn) indicate the exothermic character of the doping process while the positive formation energy value is corresponds to the endothermic process. Because of that, for our study the most favorable placement position for our doping atoms is configuration when a metal atom M (M=Co, Cu, Al) replaces the Zn atom.

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Obtaining of CO_2 conversion catalytic activity electrodes Cu/AuNPs by galvanic replacement

***Zozulya G.I.*, Kuntyi O.I., Shepida M.V., Mazur A.S.**

Department of Chemistry and Technology of Inorganic Substances,
Lviv Polytechnic National University.
Bandera Str., 12, Lviv-79013, Ukraine.
E-mail: gzozula@ukr.net

Electrochemical reduction of CO_2 is one of the directions of its utilization and efficient synthesis of CO, CH_4, HCOOH, CH_3OH, etc. The cathodic conversion in aqueous solutions is the most studied. This doesn't ensure proper selectivity of the target products and their formation rate. In the last decade, much attention has been paid to non-aqueous solutions in which the synthesis of specified substances with high yields can be realized [1].

Reduction of CO_2 is carried out on catalytically active electrodes, including copper cathodes (Cu/MNPs) modified with high-efficiency metal nanoparticles (Ag, Au, Pt, Pd). One of the methods of their controlled preparation is a galvanic replacement in non-aqueous solutions [2].

The results of AuNPs deposition studies on a copper surface by galvanic replacement in organic aprotic solvents (DMSO, DMF, AN) is present in this work. The dependence of the deposited nanoparticles geometry and their distribution on the copper surface on the nature of the solution, the concentration of Au precursor ($HAuCl_4$), the duration of the process, as well as the action of the ultrasonic field was studied. It is shown that the main factors of the controlled formation of gold nanostructures are the concentration of $HAuCl_4$ and the duration of galvanic replacement. Ultrasonic is mainly a factor in speeding up the process.

The dependence of the catalytic activity of the obtained Cu/AuNPs cathodes for CO_2 reduction in acetonitrile solutions on the size of AuNPs and the density of their filling of the copper surface is shown. Based on them, conditions are established that ensure high speed and efficiency of electrochemical reduction of CO_2.

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The influence of PEO-modes on morphology and composition of doped nanocomposites

**Karakurkchi A.V.[1], Sakhnenko M.D.[2], Korogodskaya A.M.[2],
Yermolenko I. Yu.[2], Yar-Mukhamedova G.Sh.[3]**

*[1] National Defense University of Ukraine named after Ivan Cherniakhovskyi,
Povitroflotskyi Ave. 28, Kyiv-03049, Ukraine.
E-mail: anyutikukr@gmail.com*

*[2] National Technical University "Kharkiv Polytechnic Institute",
Kyrpychova Str. 2, Kharkiv-61002, Ukraine.*

*[3] Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh
National University, 050040, Al-Farabi av., 71, Almaty, Kazakhstan.*

Plasma-electrolytic oxidation (PEO) of valve metals in alkaline complex electrolytes allows the formation of multifunctional materials (nanocomposites). These materials synergistically combine the characteristic properties of the oxide matrix and auxiliary components [1].

PEO was carried out on the alloy VT1-0 in diphosphate electrolytes with the addition of salts of transition and refractory elements. It is shown that the starting density of oxidation current is the main factor influencing the operating voltage of PEO, which is the main technological parameter of the formation of composite systems. It is established that increasing the operating current density and the use of the "decreasing power" mode allows to accelerate the process of incorporation of the dopant metal into the TiO_2 matrix during PEO. It is proved that increasing the oxidation time to 30 minutes contributes to the enrichment of the surface layers of the target component. So, it is possible to flexibly control the process of plasma-electrolyte synthesis of coatings due to the variation of the component composition of the electrolyte and technological parameters *(j, U, t)*. The morphology of the surface layer is transformed from torus-like (characteristic of TiO_2) to unevenly rough or globular with increasing content of the additive component. The presence of oxide phases of the base metal (titanium) and oxides of dopant metals in the synthesized coating was established for the studied systems. This, in combination with the results of AFM analysis, allows to position the formed coatings as nanocomposites.

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Theoretical prediction of adsorption characteristics of cellulose molecules on the surface of carbon nanostructures

Borysyuk V.[1]***, Isokov T.***[1]***, Hizhnyi Yu.***[1]***,***
Nedilko S.G.[1]***, Shegeda M.***[1]***, Zhydachevskyy Ya.***[2]

[1] *Taras Shevchenko National University of Kyiv,*
Volodymyrska Street 64/13, 01601, Kyiv, Ukraine
E-mail: borysyukviktor@gmail.com

[2] *Institute of Physics Polish Academy of Sciences,*
al. Lotników 32/46 Warsaw, Poland

Currently, the optical characteristics of nanocomposite materials based on cellulose and carbon nanostructures (CNSs) are being actively studied [1]. Despite intensive studies, several key problems regarding the peculiarities of the interaction of the components of nanocomposites "cellulose-CNSs" still remain unsolved. These are, in particular, the questions regarding the types of bonds formed in the material between components, the mutual influence of the components on their physical (electronic, optical, and other) properties, and the role of individual components' in formation of the properties of material.

Our studies were carried out in the form of the electronic structure calculations performed by the quantum chemical method in the DFT approximation [2]. The calculations revealed the mechanisms of the cellulose molecul adsorption on the surface of carbon nanotubes CNT(5,5) and single-layered graphene sheets, both bare and doped with boron or nitrogen. Binding energies and inter-nuclear distances between components were calculated and analyzed.

Calculation results were discussed in view of the possible influence of doping and surface functionalization of carbon nanostructures on cellulose optical (light absorption) characteristics. Perspectives for the efficient doping and surface functionalization of nanostructured carbon materials are revealed.

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Peculiarities of the formation of functional oligomer brushes onto a glass surface in dilute and semi-dilute regimes

Izhyk O.B.[1]***, Kostruba A.M.***[2]***, Balaban O.V.***[1]***,***
Volianiuk K.A.[1]***, Mitina N.Ye.***[1]***, Zaichenko O.S.***[1]

[1] *Lviv Polytechnic National University.*
St. Bandera str., 12, Lviv - 79013, Ukraine.
E-mail: oleh.b.izhyk@lpnu.ua

[2] *Lviv National Stepan Gzhytsky University of Veterinary Medicine and Biotechnology, Pekarska str., 50, Lviv – 79010, Ukraine.*

Thin-film technology where the polymer brushes are used as a structural unit to give new functional properties, enhance existing ones, or create a template for nanofillers, still faces the one fundamental problem: packing density. It relates to polymer solutions where the correlation length between random polymer coils depends on the concentration, temperature, solvent quality. Our particular interest focused on the formation of a sandwich-like structure where the first layer of surface-active oligomer possessing functional sites could be used as a precursor layer for subsequent molecular design of other layers via surface-initiated radical polymerization or non-radical reaction of addition or intermolecular interaction between first and second layers. This approach provides an ability to control the porosity of sandwich-like brushes, optical, conductive, or dielectric characteristics of polymer-inorganic composites. Such techniques as ellipsometry, surface tension measurements, scanning electron microscopy, viscosimetry, dynamic light scattering were used for the study of slide surface modification and polymer solutions. Poly(vinyl pyrrolidone) brushes possessing terminal epoxide and peroxide groups were used. It was revealed that the properties of tethered oligomer brushes correlate with supramolecular structures existing in polymer solution in dilute and semi-dilute regimes. The overlapping concentration was predicted theoretically and confirmed experimentally. The length of polymer brushes and refractive index of film rise with an increase in concentration and time of adsorption. Moreover, the increase in surface tension indicates enhancing of the packing density. In general, the thickness of polymer brushes is in the range of 13-24 nm, while the refractive index is from 1.450 to 1.480. This information is important for the formation of sandwich structures for possible antireflective coating, conductive or luminescent thin-film composites.

Effect of implantation of Ho and Nd ions on the physical properties of thin ZnO films

Oberemok O.**, **Melnik V., Dubikovskyi O., Gudymenko O., Kosulya O., Romanyuk B., Kolomys O.1, Sabov T., Maksimenko Z.

Department of Ion Beam Engineering, V. Lashkaryov Institute
of Semiconductor Physics of NAS of Ukraine,
41, prospect Nauky, 03028, Kyiv, Ukraine.
E-mail: ober@isp.kiev.ua

The large exciton binding energy of 60 meV and wide band gap energy of 3.37 eV at room temperature promote the use of ZnO thin films as a host photonic material in the creation of sensor and light-emitting devices [1]. Ho or Nd doping is a promising method for engineering of ZnO film optical properties due to the large number of energy levels of elements. The incorporation of these elements into the ZnO crystal lattice occurs in the form of the replacement of Zn^{2+} ions by Ho^{3+} and Nd^{3+} ions. The built-in ions have more large radii that leads to distortion of the ZnO structure during annealings. Ion-beam implantation of elements with subsequent thermal treatments is a promising method for controlling the distribution of dopants in the ZnO film. This work is devoted to elucidation of the optical, structural, and phase changes caused by Ho and Nd ion implantation in a ZnO host film.

Analyzed polycrystalline ZnO films are an array of vertical highly oriented nanorods on the Si (100) surface. It is ascertained that the Ho or Nd ion implantation leads to an improvement in the level of crystallinity of ZnO nanorod arrays. Threshold temperatures for displacement of Ho or Nd dopants outside the nanorods are 750°C and 600°C, respectively. It is shown that the implanted dopants are almost uniform distributed over the ZnO film thickness and accumulate at the SiO_x/Si interface at high-temperature annealing. The assumption that neodymium, unlike holmium, has time to oxidize during intergranular diffusion has explained the formation of thinner silicon oxide at the ZnO/Si interface. Thus, the use of Ho and Nd impurities as an activator and sensitizer in light-emitting ZnO nanostructures requires the use of thermal activation modes in which both dopants will remain in ZnO nanocrystals.

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Temperature dependence of coherence lengths for optimally-doped $YBa_2Cu_3O_{7-\delta}$ thin films

***Petrenko E.V.*[1], *Omelchenko L.V.*[1], *Solovjov A.L.*[1,2],**
***Terekhov A. V.*[1], *Kolesnichenko Yu. A.*[1], *Sergeyev D.M.*[3]**

[1] Department of Point-Contact Spectroscopy,
B. Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Nauky Ave., 47, Kharkiv-61103, Ukraine.
E-mail: petrenko@ilt.kharkov.ua

[2] Institute for Low Temperatures and Structural Research of PAS,
ul. Okolna 2, P.O. Box 1410, 50-950 Wroclaw, Poland.

[3] Department of Physics, K. Zhubanov Aktobe Regional State University,
A. Moldagulova Prospect, 34, Aktobe-030000, Kazakhstan.

A high value of superconducting transition temperature T_c in cuprate high-temperature superconductors (HTSCs) is likely due to a small size of Cooper pairs, which is determined by the short in-plane coherence length $\xi_{ab}(0)$ [1]. It is well established that, due to anisotropy, ξ_{ab} is approximately an order of magnitude larger than the coherence length along the c-axis ξ_c. Interestingly, in cuprates, the exact temperature dependence of both ξab and ξ_c above and, more surprisingly, below Tc has not yet been fully elucidated. To determine $\xi_{ab}(T)$ and $\xi_c(T)$, it is necessary to obtain the temperature dependences of the upper critical magnetic field $\mu_0H_{c2}(T)$, preferably in a wide temperature range and in a magnetic field applied parallel to either the *ab*- plane or the *c*-axis, since the coherence lengths and the upper critical field are mutually correlated.

For the first time, having calculated the upper critical fields $\mu_0Hc_2(0)$ of the optimally doped YBCO film both within the Ginzburg-Landau (GL) [2] and Wertamer-Helfand-Hochenberg (WHH) [3] theories, we report results concerning the temperature dependences of the coherence lengths in the ab-plane $\xi_{ab}(T)$ and along the *c*-axis $\xi_c(T)$. The effect of a small coherence length on the behavior of Cooper pairs will be discussed during the conference in detail.

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Surface morphology and optical properties of ZnMeO (Me: Co, Ni) thin films prepared by RF - sputtering

***Stolyarchuk I.D.**, **Dan'kiv O.O.**, **Hadzaman I.V.**,*
***Stolyarchuk A.I.**, **Krypak A.O.**, **Kuzyk O.V.**,*

Department of Physics, Drohobych Ivan Franko State
Pedagogical University, 24 I.Franko str.,
82100 Drohobych, Ukraine.
E-mail: i.stolyarchuk@dspu.edu.ua

Zinc oxide (ZnO) based materials demonstrate attractive properties for different modern technological applications. ZnO has a wide band gap and a high exciton binding energy (Eg = 3.37 eV; Eb = 60 meV). For this reason ZnO is good candidate for optoelectronic applications and, also, for detection of harmful and toxic gases. Many recent publications have been dedicated to transition metal (Mn, Co, Ni) doped ZnO from point of view searching of room temperature ferromagnetic ordering due to magnetic ion doping. There is also suggestion that doping ZnO with transition metals could be promise way to enhance the gas sensor sensitivity.

In this work, we report on the fabrication of undoped ZnO and ZnMeO (Me: Mn, Co, Ni) thin films by RF-plasma sputtering technique. Content of transition metals in the deposited films has varied in range of 0 – 10 %. X-ray diffraction (XRD), transmission electron microscopy (TEM) and atomic force microscopy (AFM) were main techniques for structural and morphological analysis of the fabricated samples. According to HR-TEM and AFM analysis the ZnCoO thin films are composed of closely packed nanocrystallites with nanorod shape, whereas the ZnNiO thin films show uniform columnar microstructure. The shift of the absorption edge due to decrease the energy band gap Eg with increasing cobalt content and complex dependence of the energy band gap on content of nickel was observed in optical absorption spectra of the studied films.

The revealed morphological features and related optical properties are very important for applications in gas sensors since surface roughness is directly proportional to the gas sensitivity due to the increased contact area with gaseous specious. As for example, the carbon monoxide and ethanol gas sensing properties (response and recovery times) of the ZnMeO (Me: Co, Ni) thin films were investigated and the obtained results and sensing mechanisms are discussed.

Corrosion-mechanical properties of structural steels with surface nanostructure

***Maksymiv O.V.*[1], *Kyryliv V.I.*[1], *Chaikovs'kyi B.P.*[2], *Gurey V.I.*[3], *Zvirko O.I.*[1]**

[1] Karpenko Physico-Mechanical Institute of the NAS of Ukraine,
5, Naukova St., Lviv 79060, Ukraine.
E-mail: okyryliv@yahoo.com

[2] Stepan Gzhytskyi National University of Veterinary Medicine and
Biotechnologies, 50, Pekarska St., Lviv 79010, Ukraine.

[3] Lviv Polytechnic National University,
12, Bandery St., Lviv 79013, Ukraine.

The most widely used method of formation of nanocrystalline structures (NCS) is severe plastic deformation (SPD) which allows obtaining bulk and surface NCS. Mechanical-pulse treatment (MPT) is among them. It generates SPD by high-speed friction. Strengthened surface layer with NCS formed by MPT owns modified structural-phase state and chemical composition due to its alloying from special technological media (TM) which are supplied in the friction contact zone during MPT. MPT of structural low-alloy steels provides rising of surface hardness, strength, wear resistance, resistance to fatigue, corrosion fatigue and contact fatigue failure. NCS also prevents hydrogen penetration into the substrate being hydrogen permeation barriers [1]. The influence of different types of TM (mineral oil, tap water and air) during MPT on fatigue and corrosion fatigue of 45 steel and contact durability of 20XH3A steel were studied in the paper.

The fatigue and corrosion fatigue in artificial sea water of 45 steel after MPT using air and mineral oil as TM were studied. It was indicated that MPT increased its fatigue strength in 1.3 times and corrosion-fatigue strength in 2.2 times compared with grinded specimens. It should be noted that type of TM during MPT didn't influence significantly on fatigue strength limit, whereas air as TM provided corrosion-fatigue limit σ_{-1} = 160 MPa compared with mineral oil σ_{-1} = 140 MPa. The same regularity was observed during contact durability investigations of 20XH3A steel in tap water and industrial oil. It was showed that contact durability of 20XH3A steel specimens (cementation + quenching + tempering at 150 °C, HRC 59…60) after MPT in air is higher than after MPT in mineral oil or tap water.

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The morphology investigation of the cadmium sulphide thin films for solar cell applications

Vakaliuk I.V., Nykyruy L.I., Ilnitsky R.V., Naidych B.P., Yavorskyi R.S., Matkivskyi O.M., Katanova L.O.

Vasyl Stefanyk Precarpathian National University,
T. Shevchenko, 57, 76-018, Ivano-Frankivsk, Ukraine
E-mail: ivanna.maliarska@pnu.edu.ua

The solar cells on the basis of cadmium telluride (CdTe) have recommended themselves as a perspective thin film technology of the future market of renewable energy. In spite of that the Silica solar cells are still dominant, CdTe occupies about 7% of the this market and is the first of technologies of the second generation which has effectively carried out a jump to the mass introduction.

In the solar cells based on cadmium telluride the n-type of conductivity CdS layer (2.4 eV bandgap) directly contacts with p-CdTe and form p-n heterojunction. The CdS layer is not a photoelectricity active layer but has a «window» function. The solar irradiation penetrates under CdS into the photoelecticly active CdTe layer (absorber). As a rule, the CdS layer must be as thin as possible in order to permit to the best part of photons with energy, higher than its bandgap, to reach the CdTe and, therefore, to provide the higher values of photoelectric current. But too thin CdS layer increases the possibility of a local by-passing.

The CdS thin films were deposited onto glass substrates by the method of the open evaporation in vacuum. The SEM analysis used for morphology investigation of the obtained polycrystal CdS thin films. It has been determined that scales type of the surface structure characteristic for smaller widths of films. The presence and the size of these plates are directly depended on the time of deposition. Specifically, it has been concluded that the increasing of the deposition time results in the decreasing of the lateral size of scales: from about 30 μm during the deposition time 60 sec to about 20 μm during the deposition time 90 sec. Due to the reduction of the surface plates in size, we can assume that with increasing of deposition time, the process of their fusion begins. A further increase of the deposition time leads to blurred outlines of such plates, and for the thickest films they are absent.

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Structure and properties of carbon-containing nanostructured coatings on metal surfaces obtained by electric discharge in gas and electric explosion of electrical conductors

Vinnychenko D.V.[1]***, Nazarova N.S.***[1]***, Boguslavskii L.Z.***[1]***,***
Chuschak S.V.[1]***, Adamchuk Y.O.***[1]***, Chuschak A.V.***[1]***, Vyshnevskyi O.A.***[2]

[1] Pulse Electrotechnical Systems Department, Institute of Pulse Processes and Technologies of NAS of Ukraine.
Bogoyavlensky av. 43a, Mykolaiv - 54018, Ukraine
E-mail: vdvvvs@gmail.com

[2] Department of diamond, M. P. Semenenko Institute of Geochemistry, Mineralogy and Ore Formation of NAS of Ukraine. Academician Palladin Ave., 34, Kyiv - 03142, Ukraine

The method of electric discharge treatment of carbon-containing gases [1] allows to obtain a nanostructured coating of almost the same size particles that form micrometer globules. Nanocarbon coating has no impurities. Particle sizes is no more 40 nm. This coating is X-ray amorphous and attenuates X-rays at wavelength $\lambda_{K\alpha}$= 0,154178 nm on average by 51%.

Electric discharge through a metal conductor in carbon-containing gas [2] allows to obtain a nanostructured composite coating, which consists of carbon, metal and carbide globules and is uniform in particle size. The particle sizes obtained from tungsten wires are 40 nm, and from titanium wires - 100 nm. The hardness of the substrate surface is significantly increased due to the applied coating.

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Morphological changes of structures with surface quantum dots under the gamma irradiation

Moskvin P.[1], Rashkovetskyi L.[2], Strilchuk O.[2], Svezhentsova K.[2], Kryzhanivskyy V.[1]

[1] *StateUniversity "Zhytomyrskapolitechnika",*
103 Chudnivska str.,10005, Zhytomyr, Ukraine
E-mail: moskvinpavel56@gmail.com

[2] *V.Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 41,*
Prospect Nauky, 03680, Kyiv, Ukraine
E-mail: ostrilchuk@gmail.com

The AFM image of the $In_{0.4}Ga_{0.6}As/GaAs$ structures surface with quantum dots (QD) before and after their interaction with γ-irradiation within 10^5 - 10^8 rad was analyzed. The influence of γ-radiation on the geometric parameters of nanorelief for QD structures was established. The MFA method [1] was used to quantify the variation of the geometric parameters of surface nanoforms depending on the dose of γ-irradiation. The dependences of the Renyi's numbers and fractal ordering parameters on the irradiation dose were found. It is shown that with increasing radiation dose there is a blurring (destruction) of interfaces of QD, which correlates quantitatively with a decrease in the values of Renyi's numbers for surface area and volume of surface nanoforms. The study of the width of multifractal spectra (fractal ordering parameter) showed the rearrangement of the fractal structure of the surface as different doses of radiation exposed to it.

The obtained results are in good agreement with the spectral dependences of initial and irradiated structures with surface $In_{0.4}Ga_{0.6}As/GaAs$ QDs [2]. At low irradiation doses (105 rad) there is an increase in the intensity of PL caused by an improvement in the crystal quality of the structure (the "low doses" effect). Increasing the radiation dose to 10^6 -10^7 rad leads to the accumulation of radiation defects and the appearance of radiation-induced defect levels near the QDs/wetting layer interfaces, which are an additional channel for transferring carriers from the wetting layer to QDs, and causing a significant magnification in PL intensity. Increasing the radiation dose to 10^8 rad enhances the role of diffusion processes increases the mobility of both growth defects and radiation-stimulated defects, which leads to the destruction of QD boundaries, resulting in a sharp decrease or disappearance of PL intensity.

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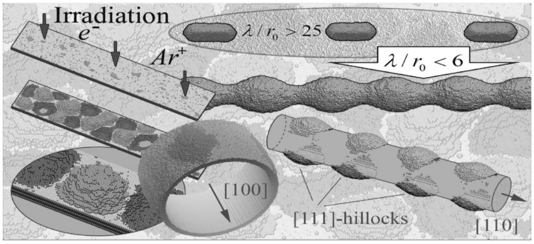
Controlled self-ordering in the dynamics of forming periodic quasi-one-dimensional

***Bereznykov O.V.*, Gorshkov V.N.**

National Technical University of Ukraine, Igor Sikorsky Kyiv Polytechnic Institute, 37 Prospect Peremogy, Kiev 03056, Ukraine.
E-mail: alexber36@gmail.com

The spontaneous formation of transversely modulated 1D- structures occurs either during the disintegration of nanowires into separate fragments or during the diffusion deposition of atoms onto their surface. In both versions, the main mechanism providing a fairly strict periodicity in the arrangement of the forming nanoclusters is surface diffusion of atoms. At a given temperature, T, the dynamics of the process corresponds to a decrease in the free energy, F, of the system: $dF=dU-TdS<0$. In our work, physical mechanisms are shown that can be controlled both in cases where the decrease in free energy is associated with a decrease in internal energy, U, and cases when this is achieved due to the dominant increase in entropy, S, despite the accompanying increase in U. The transition between these two regimes can be carried out by intensifying the surface diffusion of atoms by external irradiation of the nanowire (by electrons or ions but avoiding noticeable heating), which leads to the forced formation of periodic perturbations on the wire surface as a result of the well-known roughening transition (RT) effect.



The results obtained by us on the basis of the kinetic Monte Carlo model show that the indicated diversity in the dynamics of the system corresponds to the same diversity in their morphology at the final stage of evolution. We have demonstrated, for example, that for a given orientation of a nanowire relative to its internal crystal structure (variants of FCC, BCC and diamond-like crystal structures are considered), the period of its breakup can be significantly changed both upward and downward, up to the formation of super-short-wavelength "frozen in time" surface perturbations (unduloids), the occurrence of which corresponds to overcoming the threshold of the so-called energy instability of the surface. The variety of morphologies in the synthesis of one-dimensional systems and methods for controlling their parameters are demonstrated in the case of diffusion deposition of germanium or silicon atoms onto a silicon/germanium nanowire.

Incoherent structures in lithium submonolayer films on tungsten and molybdenum (112) faces

Zayika S.O.[1], **Loburets A.T.**[1], **Fedorus A.G.**[2]

[1] *Yuri Kondratyuk Poltava Polytechnic National University.*
Pershotravnevyj Ave, 24, Poltava-36004, Ukraine.
E-mail: zaikasvetlana@gmail.com

[2] *Institute of Physics of the NAS of Ukraine.*
Prospect Nauki, 46, Kyiv-03039, Ukraine.

In two-dimensional submonolayer metal-on-metal adsorbed films, different structures can form even at low coverages. This is possible because of values of electronegativities of adatoms and adsorbent will be significantly different [1]. Initially, a structure of the films is consistent with a periodic potential of the surface. As the coverage degree θ increases, such a consistency begins to be lost. Reasons are a lateral interaction of adatoms and their size. A vivid example of such films is lithium adsorbed on anisotropic grooved (112) faces of tungsten and molybdenum [2]. Maximum coverage, at which the structures remain consistent with the substrate, is half of the monolayer with a structure $p(1\times2)$. Applying a mathematical model of surface diffusion created by us in a homogeneous film, we found that a formation of a coherent structure $p(1 \times 2)$ leads to a very sharp decrease of a diffusion coefficient if there are no defects in such a film. The film becomes incoherent in the range of coverages $0.5 < \theta < 1$. Rectangular at $\theta = 0.5$ elementary cell becomes oblique-angled one due to a displacement of rows of adatoms. This is accompanied by loss of a distant order, i.e. a hexatic phase is formed. In real systems, a similar phenomenon was observed by authors [3] in a range of coverages $0.66 < \theta < 0.85$ by measuring the intensity of LEED profiles. In contrast to modern research, a transformation of the structure in the two-dimensional crystalline phase was studied.

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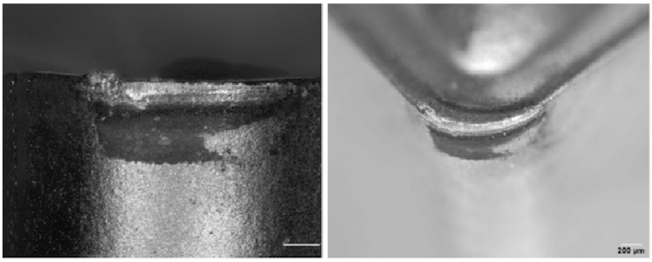
Experimental study of the characteristics of vacuum-arc multilayer coatings based on tungsten

Serdiuk I.V., Stolboviy V.O.

National Science Center "Kharkiv Institute of Physics and Technology"
of the NAS of Ukraine. Str. Akademicheskaya, 1, Kharkiv-61108, Ukraine.
E-mail: iraserduk@kipt.kharkov.ua

The development of high-level industry since the beginning of the 20th century has led to the research of more convenient materials. Superalloys solve many problems, but they create some new: the harder they are, the more difficult it is to machine them. Finding cutting tools that can resist the process of machining them enough time is a big issue. After a few seconds, the contact area between the workpiece and the cutting tool become very hot (700-1100°C) and the forces in action quickly wreck the surface of the tool. In general, very hard substrate of the cutting tool alone is not enough, and a protective layer – a coating – must be added. Chemical reactions, physical wears and the degradation process during machining is yet not fully understood and the aim of our work is to experimentally study them. Developed coatings are deposited by PVD (Physical Vapor Deposition) method and have a thickness of about 6 to 18 microns. Their properties depend strongly on technological parameters of deposition method that implies the spraying of elements from different cathodes at lower temperatures (around 350°C). We will study nitride-based multilayered multicomponent coatings like WN/NbN, WN/CrN and others. The good quality of each layers combined by doing double, triple or even multi-layers. The early-stage degradation of such protective surface can be explained in various ways including abrasive, adhesive, diffusional, chemical and oxidational processes. We have observed mechanical wears and cracks, droplets and a few case of diffusion (fig.1).



(a) flank face *face (b) 45°observation*

***Fig. 1**: Flank wear. Cutting tool with WN-CrN vacuum-arc coating*

Due to the extreme conditions encountered while turning, those processes develop almost immediately and are therefore very demanding for the tools.

Session 6
Nanooptics and photonics

Kinetic and Electrostatic Control of Electroluminescence in Molecular Junctions

Leonov V. O., Shevchenko Ye. V., Petrov E. G.

Bogolyubov Institute for Theoretical Physics of NAS of Ukraine,
14-b Metrolohichna str. Kyiv, 03143, Ukraine
e-mail: leogluck@gmail.com

Physically, electroluminescence (EL) can be observed during the resonant transmission of electrons from the r-th electrode to the r' -th electrode. In such a process, energy E_s of excited singlet level of a molecule has to fall in the intervals $E+(V_b, V_G) + \mu_r > E+(V_b. V_G) + \mu_r$ (1) or $E+\mu_r > E\_(V_b. V_G) > E_s + \mu_{r'}$ (2) (μ_r is the chemical potential of the $r=(1,2)$ -th electrode). The electrostatic control of EL is achieved by shifting the position of the energy levels $E+(V_b, V_G)$ and $E\_(V_b, V_G)$ associated with a positively or negatively charged molecule. Thus, by changing the magnitude and polarity of V_b and V_G, conditions are reached under which inequalities (1) and (2) are fully, partially, or not at all fulfilled. In addition, it is necessary to reduce the quenching of EL caused by the interaction of the fluorophore with the electrodes. This is achieved with the help of spacers that create tunnel barriers between the fluorophore and the surface of each of the electrodes. A charge hopping through tunneling barriers is the determining factor controlling the kinetics of charge transmission processes in the 1F2 system. The corresponding hopping rates are expressed in terms of parameters $\Gamma_L^{(r)}$ and $\Gamma_H^{(r)}$,which determine the broadening of the LUMO and HOMO levels respectively. In asymmetric 1F2 junctions where $\Gamma_L^{(r)}$ and $\Gamma_H^{(r)}$ can differ markedly in magnitude. Therefore, the kinetics of electron transfer significantly depends on the polarity V_b , so that the EL becomes bipolar. The population of the excited singlet level of the molecule, P_s , depends significantly on the voltage polarity. We have shown [1,2], that under conditions (1) and (2) control over EL can be achieved via the variation of P_s. Thus, in addition to the electrostatic control of EL (via bias and gate voltages), a kinetic mechanism for regulating EL in photoactive nanoscale molecular junctions is proposed.

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Optical Properties of Chromophore-Containing Methacrylate Based Polymers

Krupka O.[1,2], **Kharchenko O.**[1], **Smokal V.**[1], **Karout H. EL.**[2],
Andrushchak A.[3], **Sahraoui B.**[2]

[1]Department of Chemistry, Taras Shevchenko National University of Kyiv,
60 Volodymyrska, 01033 Kyiv, Ukraine
E-mail: oksana_krupka@yahoo.com

[2] Laboratory MOLTECH-Anjou, CNRS UMR 6200, University of Angers,
2 Bd Lavoisier, 49045 Angers CEDEX, France

[3] Institute of Applied physics and Nanomaterials science, Lviv Polytechnic
National University,12 Bandery Street, 79013, Lviv, Ukraine

The development of innovative technologies and nanoegineering applications requires the involvement of new low-cost, efficient materials and to establish new technical methods. Synthesis of polymers with desired and expected properties on the one hand and technical processes based on the interaction of light with polymers with polymers, on the other hand, have become important for the various application. Polymeric materials are used in very broad areas as nonlinear optical materials, core materials for optical waveguides, photoresists materials, field effect transistors, photoswitches, materials for optical memories, solar cells and so on. Nonetheless, the photochromic polymers have a special place among wide range synthetic organic polymers. These polymers are transformed from one form to another and have a different absorption spectrum upon the absorption of light and vice versa either thermally or by the absorption of light. Nevertheless, photochromic changes can be based on various photochemical and photophysical processes and may induce conformational changes in linear polymers containing appropriate chromophoric groups. Hence, these transformations lead to changes in the physical properties of polymers such as dipole moment, geometrical structure at the molecular level, changes in the refractive index. For instance, polymeric materials containing azobenzene groups, diarylethenes, coumarines, fulgides attract the main interest because of their excellent performance. This study promotes the better understanding of the structure-property relationship with possible prediction of NLO properties of polymers. The results of the NLO investigation (second and third harmonic generation) of high-quality thin films of chromophore containing methacrylic polymers will be presented. Strong dependence of the NLO response upon the structure of the polymers has been found, which is related to a different charge transfer occurring within the side-chain fragments.

Extremely narrow resonances in defect containing photonic structures for metrology, sensoring, collimation, signal processing and spectroscopy

Glushko, E.Ya.

Semiconductor Photonic Structures Lab., Institute of Semiconductor Physics
of NAS of Ukraine Nauki Prsp., 45, Kyiv -03028,
scientist.com_eugene.glushko@mail.com

A planar photonic resonator containing unitary defect in the middle of the structure can exhibit a system of extraordinary narrow resonance peaks of transmission on the background of perfect reflection. Here, the properties of standing modes inside the polyethylene (polypropylene)/silicon plane resonators in the total intrinsic reflection region and unusual manifestations of THz transmission spectra in centimeter and millimeter wavelength range were studied. It is shown that the angle and frequency half-widths of the resonance peak can be less than 10^{-9} of the magnitude of angle and frequency in dependence on the number of periods. This allows one to form collimated beams with the divergence measured in a fraction of a microdegree. It is shown that a plane resonator containing a central defect transforms the frequency divided peaks into the outgoing-transmitted beams of various directions like a prism transforms light. This opens the way for precision measurements of angle and frequency distribution of THz radiation. It is proposed to use the existing extremely sharp peaks of transmission in planar resonators containing a central defect for aims of spectroscopy and metrology. A new spectroscopy technique is proposed based on the existing sharp transmission resonances using the conception of accumulating reservoir of electromagnetic field.

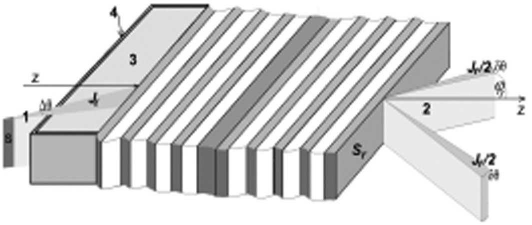

Fig. 1. *Under investigation is a planar layered* $(Si/PE)_n/D(Si/PE)_n/Si$ *photonic crystal resonator containing a central defect. 1, monochromatic diverged incident beam* $\boldsymbol{J}_l$*; 2, collimated outgoing beams* $\boldsymbol{J}_r/2$*, 3, electromagnetic field reservoir; 4, mirror walls of the reservoir; φr, output angle; Δθ and δθ are the input and output divergence of beam, correspondingly.*

An extra-high extent of collimation resulting from the usage of defected photonic resonators gives an opportunity to form long and stable channels of communication and energy transportation in the THz frequency range.

Photonic structures have a wide spectrum of applications in science and technology such as night-vision applications, safety and defense, sensing, communication applications, signal processing and many other areas. A great attention attracts the resonator properties of photonic structures. Some extraordinary forms of reflection and transmission occur inside the area of perfect reflective reflection windows occur in photonic crystal (PhCr) resonators accompanied by extremely sharp local resonances of transmission. The system under consideration is shown in Fig. 1. A monochromatic diverged incident beam $\boldsymbol{J}_1$ passes from the source S into the resonator $(Si/PE)_n/D(Si/PE)_n/Si$ through an electromagnetic field reservoir (EFR). The latter allows one in a lossless process to concentrate inside the radiation of different directions with the angular white noise distribution. The source frequency should be matched with the calculated resonant curve which occupies interval *(590.76, 692.75) GHz* at the chosen geometrical sizes of resonator. Depending on the quality of the source, the initial beam divergence $\Delta\theta$ may be large enough. The task is to collimate a diverging monochromatic beam. After interaction with resonator, any wave with a wavevector out of the transmission peak zone reflects back into the EFR space whereas waves inside the peak angular interval pass through the collimator with a significantly lowered divergence $\delta\theta$. We suppose that a stochastic angular distribution of field is created inside the EFR and distribution of power along the axis OX is homogeneous. Owing to the perfect mirror walls of the reservoir the density of field inside the EFR increases up to state of saturation when the energy flux of the output beam $\boldsymbol{J}_r$ plus flux of losses become equal to energy flux of the input beam $\boldsymbol{J}_l$. A very close problem was considered in [1] for a resonator contacting with metal: a *90 GHz* beam being initially diverging in a wide angle interval has decreased its divergence up to *0.4*° in the vicinity of the direction *22.5*° after passing the metalized silicon-propylene resonator. An advantage of a metalized resonator is its ability to form narrow transmission resonance lines against the background of perfect reflection. The reason is the uniform mirror metallic reflection in the entire frequency interval. The disadvantage is the inevitable loss of power, which leads to a reduction in the output power of the THz searchlight. The considered above semiconductor-dielectric structures are characterized by the practically absent heat losses or scattering in the transparency region of materials. Therefore only the geometrical losses caused by escaping of radiation through the resonator faces are retained and as well as that inside the source of THz radiation. We are taking into account two possible channels of energy leakage: through the lateral sides of the PhCr and one more arising due to the reverse flow immediately through the source window. We suppose here that the intensities of radiation J_l and J_r reflected or transmitted through the resonator are proportional to the average density of energy inside the EMW reservoir. The characteristic time τ of the energy accumulation process depends on the input and output sections, the angle dependence of transmission for the chosen frequencies in the vicinity of *600 GHz*, and volume of the EMW reservoir. For the adopted parameters: $I_l = 0.1\ W/cm^2$, source section $12.5\ cm^2$, output section $12.5\ cm^2$, EMW reservoir volume $1257 cm^3$ τ equals approximately *3.78 ms*. The ratio of energy loss on the reservoir walls and the reverse flow through the source section was taken as 28%. As a result, we have a strongly collimated beam with the angular HWHM $\delta\theta$ close to *0.123 μDeg* and output intensity $J_r = 0.07142\ W/cm^2$. Our evaluations show that electromagnetic energy of saturation inside the electromagnetic box depends on the leakage through the windows. In the considered case, the accumulated inside the EFR energy approximately equals to *4.723 mJ* and the saturation is practically reached during $\approx 35\ ms$ with the characteristic time $\tau \approx 3.778\ ms$. The resonant curve angular HWHM essentially depends on the structure optical contrastivity and the number of periods.

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Processing the analytical optical signals by the means of the system of the nickel nanostripes, deposited on the glass substrate and the chromium nanofilm

Sizhuk A.[1]***, Oberemok Y.***[1]***, Savenkov S.***[1]***, Xiaohong C.***[2]***,***
Zhenjie Z.[2]***, Zhuo S.***[2]***, Malyshev V.***[1]***, Prokopenko O.***[1]

[1]*Taras Shevchenko National University of Kyiv,*
Glushkova ave. 4g, Kyiv, Ukraine
E-mail: andrii.sizhuk@gmail.com

[2] *Shanghai East China Normal University, Shanghai, China*

In this work the reflection properties of the system of the nickel nanostripes, deposited on the glass substrate and the chromium nanofilm, are discussed. The method of processing the analytical (analog) and digital optical signals by the means of the system is proposed.

Thermal influence from the absorption of optical flux on the indications of the sensor "prism - gold nanolayer - water"

Suprun A.D., Shmeleva L.V.

Department of Theoretical Physics, Faculty of Physics,
Taras Shevchenko National University of Kyiv.
Volodymyrska Street, 64/13, Kyiv-01601, Ukraine.
E-mail: lshmel@univ.kiev.ua

In previous our studies, the thermal effect of laser radiation on the sensory effect of the three-layer structure "prism - gold - water" was analyzed. The presence of water in this structure is due to the fact that in many of these sensors, water is one of the components of the analyte. This is especially true for biosensors. In addition, for water, the dependence of the refractive index on temperature and wavelength in practically significant ranges (0÷100ºC and 300÷1000 nm, respectively) is well studied.

It is known that the influence of a laser radiation flux on a metal nano layer can lead to its heating and to the same heating of nearby water layers. In previous investigations, the approximation of an infinite absorption coefficient of the gold layer was considered. This approximation showed a significant influence on the thermal effect of radiation on the sensor indications. But the infinite absorption coefficient model significantly levels the specifics of gold. Such a model does not difference metals by their absorption coefficient.

In this research, the finiteness of the absorption coefficient for gold and the influence of this circumstance on the heating of the gold nanolayer were taken into account. It was found that as the absorption coefficient decreases in the sense of the inequality $k < \infty$, the amount of radiation flow, required to reach the same temperature as for $k = \infty$, increases. This means, in particular, that taking into account the finiteness of the absorption coefficient makes it possible to significantly expand the range of measuring the flux for the sensory effect.

The range of radiation flux at which the effect of temperature on the sensory effect can be neglected also increases. The magnitude of the sensory effect itself also increases both in terms of the wavelength and in terms of the resonant angle of incidence.

Express algorithm for calculating the sensory effect of a three-layer optical circuit in comparison with the transfer matrix method

Suprun A.D., Shmeleva L.V.

Department of Theoretical Physics, Faculty of Physics,
Taras Shevchenko National University of Kyiv.
Volodymyrska Street, 64/13, Kyiv-01601, Ukraine.
E-mail: lshmel@univ.kiev.ua

Usually, the matrix transfer (MT) method is used to calculate complex optical systems. This method, on the one hand, makes it possible to calculate quite complex (multilayer) systems, although it is several approximate. And, on the other hand, it is quite accurate and allows practically modulate a real experiment.

But a significant flaw of the MT method is that it requires significant computer power. Moreover, the more complex the system in terms of the number of layers, the more unwieldy its numerical realization. This always leaves open the question of finding less unwieldy, but at the same time sufficiently accurate express algorithms (EA) for finding the sensor values of the resonant wavelength and the resonant angle of incidence.

Three-layer scheme (Kretschman) "prism - gold nano layer - dielectric" was considered, as having the simplest structure and, at the same time, for it the EA are known to calculate the resonant wavelength and resonant angle of incidence. The results of direct calculation using MT and the results of calculation using EA are compared. The optimal mode in calculations by the TM method was chosen from the condition of the maximum relation of the depth of the minimum of the reflection coefficient to its half-width.

Comparison of the results of calculations by both methods showed the coincidence of the values of the resonant wavelength and the resonant angle of incidence for the three-layer scheme.

This allows us to talk about the search for similar algorithms for more complex systems, for example, for four-layer schemes often used in today’s investigates using a graphene layer.

Structures influence on the optical properties of gold films on Ge underlayers

***Bihun R.I.*, Lyahovych T.I.**

Ukraine, Lviv, Ivan Franko Lviv national university, 50 Dragomanov st.

The electron transport in thin conductive metal layers and interaction with electromagnetic radiation are the subject of interest of modern micro-, nanoelectronics and nanoplasmonic industries [1]. Size effect significantly affects physical properties of nanoscale films. Metal films of a few nanometers thickness are promising as ohmic conductors with high transparency, both in the visible and in infrared wavelengths. Therefore, they are very attractive for modern transparent electronics. Since thin metal layer can be both in continues and disperse phase (island) state, the question remains open about the conditions of transition from one state to another. The thickness of the metal film at which the transition from disperse to continues state is observed called critical percolation thickness d_c. It is known that in the region of critical transition the metal film exhibits abnormal optical and electrical properties that can be explained within the percolation model [2-3]. The possibility of influence dc thickness percolation threshold will provide ohm conductive metal connectors with extrimly high optical transparency in a range of thicknesses $d < 2$-3 nm.

The Au metal films and Ge underlayers of nanometer thickness were deposited with thermal evaporation method on the bare glass substrate under high vacuum condition ($P \sim 10^{-7}$torr) at the room temperature under "quench condense" regime [1]. Mass thicknesses of investigated films have been assessed by the shift of the resonance frequency of the quartz oscillator. Transmittance and reflectance spectra were measured by broadband spectrophotometer Shimadzu UV-3600.

The analysis of the size dependence of gold films transmittance (for wavelengths 1100 nm, 1500 nm, 1900 nm and 2500 nm) which were deposited on a clean glass substrate and on a glass substrate precoated with germanium underlayer with mass thickness of 0,5 nm have showed that the value of d_c for gold films deposited on a clean glass substrate is 6,4 nm, while for similar samples deposited on Ge underlayers with mass thickness of 0,5 nm, is $d_c = 4$ nm.

The analysis of infrared absorption of investigated gold samples showed the existence of maximum absorption for percolation transition thickness. In particular, it was found that for gold film deposited on a clean glass substrate the absorption maximum is $A = 0{,}21$, and for similar samples deposited on germanium underlayers the absorption maximum is $A = 0{,}3$. The observed behavior is caused by higher crystalline structure and more effective level of substrate occupation with gold film. Before percolation transition metal film is consisted with isolated islands, where the electronic subsystem is localized. The higher concentration of isolated islands, the more electrons is involved in plasmon resonance which leads to a high absorption ability of metal condensate.

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Immobilization-induced enhancement of S_2 fluorescence of near-infrared dyes due to interaction with carbon quantum dots

Dimitriev O.P.[1]***, Piryatinski Yu.P.***[2]***, Sharanov I.P.***[3]***, Slominskii Yu.L.***[3]

[1] V.Lashkaryov Institute of Semiconductor Physics NAS of Ukraine,
pr. Nauki 41, Kyiv, Ukraine.
E-mail: dimitr@isp.kiev.ua

[2] Institute of Physics NAS of Ukraine,
pr. Nauki 46, Kyiv, Ukraine.

[3] Institute of Organic Chemistry NAS of Ukraine,
5 Murmanska St., Kyiv, Ukraine.

Anti-Kasha emission, i.e., the emission from S_n (n>1) excited levels, of infrared chromophores which possess intensive absorption and S1 emission in the near-infrared (NIR) region, but which are spectrally silent in the visible, is a challenging task for relevant applications in actual fields, such as energy conversion, bio-imaging, sensitization of solar cells, optical sensors, etc. Here we demonstrate a dual emission of NIR tricarbocyanine dyes with a bright green S_2 fluorescence, which is relatively weak for the free dye molecule but whose quantum yield increases by 2-4 times, together with a strong enhancement of the spontaneous rate of S_2 fluorescence, whereas the quantum yield of S_1 emission decreases by 2-7 times, respectively, as a result of immobilization of the dye molecule via interaction with carbon quantum dots. The above spectral changes are shown to depend on the terminal and meso-groups of the dye and the solvent used. The dye immobilization due to interaction with carbon quantum dots is shown to cause freezing of rotational degrees of freedom of the molecule as indicated by suppression of the dye hot band absorption-assisted anti-Stokes S_1 emission. The observed enhancement of the S_2 fluorescence and its rate is discussed in terms of immobilization-induced emission and a Purcell effect, respectively.

Liquid crystal control of the electromagnetic wave propagation through metal-multilayer dielectric structure

Zadorozhnii V.I., Reshetnyak V.Yu.

Taras Shevchenko National University of Kyiv;
64/13, Volodymyrska Street, City of Kyiv, Ukraine, 01601.
E-mail: v.i.zador@gmail.com .

We consider metal- multilayer dielectric structure consisting of a glass layer, thin silver layer, liquid crystal and alternating high (TiO_2) and low (SiO_2) refraction index quarter-wave layers (Bragg reflector). There is a layer of SiO_2 between the silver layer and the liquid crystal (LC). The tilt angle of the liquid crystal is changed by applying an electrical voltage to the LC layer.

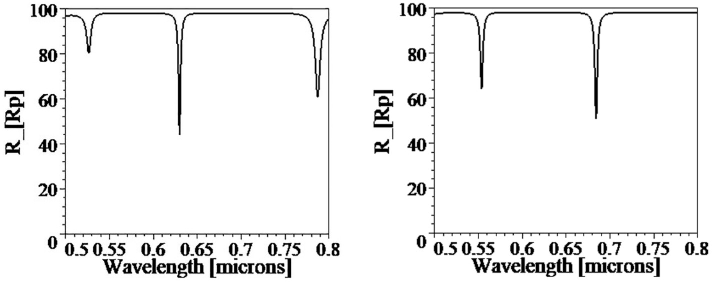

Fig.1 *(left)* $\theta_{LC}=0°$, *(right)* $\theta_{LC}=90°$.

Under certain conditions, a narrow, deep dip can be observed in the reflectivity spectrum of the system (Fig 1), the spectral position of which can be adjusted by changing the tilt angle of the liquid crystal director. The numerical modeling was carried out using the transfer matrix method. Structures like this may be attractive for various applications, e.g. sensors [1-3].

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Effect of J-aggregate formation in liquid crystal matrix on their optical properties

Sorokin A.V.**, **Grankina I.I., Kasian N.A., Lisetski L.N., Yefimova S.L.

Yu.V. Malyukin Nanostructured Materials Department,
Institute for Scintillation Materials of NAS of Ukraine,
Nauky Ave. 60, Kharkiv, 61072, Ukraine
E-mail: sorokin@isma/kharkov.ua

Ordered luminescent molecular aggregates of dyes (so-called J-aggregates), primarily cyanine, merocyanine and porphyrin, form a wide class of luminescent nanoclusters, which are characterized by ultrahigh extinction coefficients, efficient energy migration and electron excitation, extremely high coefficients of cubic susceptibility etc. The unique optical properties of J-aggregates are related to the exciton nature of their electronic excitations of the Frenkel type. This phenomenon is possible only due to the high degree of ordering of molecules in chains, in fact translational symmetry, which is achieved due to the flat structure of molecules from which J-aggregates are formed. In fact, J-aggregates can be attributed to low-dimensional molecular crystals. Unlike bulk crystals, the exciton properties of J-aggregates are highly dependent on the degree of molecules disorientation in the chains or static disorder. Thus, the structure, and hence the optical properties of J-aggregates are largely determined by their microenvironment, which can be used to create J-aggregates with specified optical properties. At the same time, a number of studies have shown that in nanostructured media the J-aggregates luminescence can be significantly quenched due to the growth of static disorder.

In this work, the J-aggregate formation of anionic cyanine dye TDBC in the liquid crystal (LC) matrix 5CB has been studied using optical spectroscopy. The absorption spectra of the TDBC dye formed in LCs shown that the J-band is more intense and narrower. Simultaneously, lifetime increasing has been found for that case. The spectral changes can be associated with static disorder decreasing caused by the spatial restriction in the matrix. Photostability of this matrix is of major importance for a variety of applications, such as material sensing and fluorescence imaging. Herein, we demonstrated that TDBC J-aggregates formed in LCs are much more photostable comparing with ones in solution.

Interaction between Molecular Aggregates Incorporated in Layered Polymer Films

***Pisklova P.V.*[1,2], *Ropakova I.Yu.*[1], *Viagin O.G.*[1], *Yefimova S.L.*[1], *Sorokin A.V.*[1]**

[1] *Yu.V. Malyukin Nanostructured Materials Department, Institute for Scintillation Materials of NAS of Ukraine,*
Nauky Ave. 60, Kharkiv, 61072, Ukraine

[2] *Institute of Physics, University of Rostock,*
Albert-Einstein-Str. 23, 18059 Rostock, Germany
E-mail: polinkapisklova@gmail.com

Molecular aggregates of cyanine and some other dyes are nanosized luminescent clusters formed by organic molecules. They were discovered in the late thirties of the last centuries by E. Jelley and called in his honor J-aggregates [1]. Due to the high ordering of monomers within J-aggregates and strong intermolecular coupling between monomers, the electronic excitations of J-aggregates are the Frenkel excitons delocalized over a certain number of monomers. Thus, the exciton coherence length is one of the most important characteristics of J-aggregates, taking effect on the exciton bandwidth and exction lifetime. As a result, the spectroscopic properties of J-aggregates are quite different from that of the constituting molecules. J-aggregates are characterized by a narrow absorption band (J-band) red-shifted to the monomer one, nearly resonant luminescence with a much shorter luminescence decay time than that of monomers, due to the exciton superradiation effect.

The unique features of J-aggregates provide their wide applications in various fields, such as photonics, sensorics, photovoltaics, etc. In particular, the strong photon absorption of J-aggregates and their high exciton mobility allow to realize an impressive energy transfer between J-aggregates and obtain a significant pumping of dyes gaining their bright luminescence.

Some advantages can be obtained for J-aggregates placed into thin polymer films like layered polyelectrolyte ones. The additional dye pumping can be achieved by electromagnetic field confinement in the nanoscale region near the J-aggregates due to the formation of the surface exciton polariton in such molecular aggregates [2]. However, the features of such pumping in the case of J-aggregates used as the energy trap is not clear.

Therefore, the present work is devoted to studying the interaction between two types of dyes, TDBC and TCC, with similar structures in aqueous solutions and thin polymer films. It has been experimentally confirmed that by placing the J-aggregates in different layers separated by polymer film spacer, efficient energy transfer can be achieved with TDBC J-aggregates as an energy donors and TCC J-aggregates as energy acceptors.

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Variations of the initial charge composition and physical properties of the single crystals of PbO – MoO_3 system

<u>Bochkova T.M.</u>[1], Bondar D.S.[1], Trubitsyn M.P.[1], Volnyanskii M.D.[1], Volnyanskaya I.P.[2]

[1] *Physics of Active Dielectric Crystals Laboratory, Oles Honchar Dnipro National University, prosp. Gagarina 72, Dnipro, 49010, Ukraine*
E-mail: tbochkova@meta.ua

[2] *Prydniprovs'ka State Academy of Civil Engineering and Architecture, str. Chernyshevsky 24A, Dnipro, 49600, Ukraine*

Lead molybdate ($PbMoO_4$) and double lead molybdate (Pb_2MoO_5) are perspective materials for acousto-optical devices. These applications require good optical quality and high radiation resistance. However, the crystals grown from the melt in air by the conventional Czochralskii technique, as a rule, have specific color and demonstrate photochromism after irradiation with UV light. Such undesirable phenomena can be associated with nanometer sized phase inclusions, coordination complexes based on intrinsic defects and/or impurities. Comprehensive study of the typical defects is of high importance to obtain PbO – MoO_3 single crystals more suitable for practical applications. It is known that $PbMoO_4$ exhibits vacancy disorder due to violation of stoichiometry and oxygen exchange with surrounding atmosphere. One can expect that an increase in the volatile component in the composition of the charge helps to prevent the formation of cation vacancies. Regarding Pb_2MoO_5, there is no any information on this issue.

Lead molybdate possess the scheelite-type crystal structure of the tetragonal system (space group $I\,4_1/a$). The lattice of Pb_2MoO_5 is monoclinic (space group *C 2/m)*. Both crystals contain the characteristic molecular anionic groups $(MoO_4)^{2-}$ with almost the same Mo – O distance. The similarity and differences in the structure of crystals determine the features in their optical and electrical properties.

In this work we report the data on study of $PbMoO_4$ and Pb_2MoO_5 single crystals grown by Czochralskii method using of the initial charge composition with deviations from the stoichiometric ratio of components. The influence of some excess of lead, as well as of molybdenum in the charge, on the optical absorption, photochromic and photodielectric effects in the crystals is discussed. The effect of growing conditions, doping, and high temperature annealing on the properties of crystals $PbMoO_4$ and Pb_2MoO_5 is also considered.

Polarization degree of freedom for guided waves

Yermakov O.[1]***, Polevoy S.***[2]

[1] Department of Computer Physics, V. N. Karazin
Kharkiv National University, 61022, 4 Svobody Square, Kharkiv, Ukraine.
E-mail: oe.yermakov@gmail.com

[2] Radiospectroscopy Department, O.Ya. Usikov Institute for Radiophysics
and Electronics NASU,
61085, 12 Acad. Proskury Str., Kharkiv, Ukraine.

The spectrum of electromagnetic plane waves in any isotropic homogeneous medium is twice degenerate with respect to polarization at any frequency and in any direction, because the dispersions of TE- and TM-polarized eigenmodes are absolutely the same. The operational principle of any bulk classical polarizer is based on the removal of the polarization degeneracy by using an anisotropic slab. Miniaturization and planar technologies lead to the high localization of the electromagnetic signal in the plane of propagation. However, at the same time, the degeneracy is removed. So, there is no polarization degree of freedom for planar photonic devices with in-plane electromagnetic wave propagation. It significantly limits the functionality of flat optical and planar photonic devices.

In this work, we aim merging the polarization degeneracy and high localization for guided waves propagating within an all-dielectric metasurface. Namely, we theoretically study the periodic subwavelength array of cylinders with high refractive index and demonstrate the broadband TE-TM polarization degeneracy of its guided modes. This concept can be transferred to the optical and infrared ranges using other material platforms and opens new opportunities for the polarization control of guided waves such as metasurface-based waveguide polarizer [1]. These results could potentially become a platform for new generation of planar photonic polarization devices.

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Optical characterization of Al_2O_3-YAG based eutectics: effect of plates thickness

Komarenko D.O.[1]***, Siryk Yu.V.***[2]***, Ilchenko S.G.***[1]***, Multian V.V.***[1]***,***
Vovk O.M.[2]***, Nizhankovskyi S.V.***[2]***, Gayvoronsky V.Ya.***[1]

[1] *Advanced Materials Nonlinear Optical Diagnostics Lab., Institute of Physics NAS of Ukraine,*
Prospect Nauky 46, 03028, Kyiv, Ukraine
E-mail: vlad@iop.kiev.ua

[2] *Institute for Single Crystals, National Academy of Sciences of Ukraine,*
Nauky Ave. 60, Kharkiv, Ukraine

Eutectics Al_2O_3-YAG and Al_2O_3-YAG:Ce are crystalline materials in which phases of the YAG garnet and Al_2O_3 sapphire penetrate each other, being formed during simultaneous growth. These eutectic crystals are characterized by a complex morphology, the so-called "china script" in which it is difficult to determine between phase intervals with different refractive indices. High dispersivity of the material increases path of the incident light beam and the efficiency of its capture by active cerium ions. The light emanating from a crystal after its irradiation consists of two components: the primary beam (usually 450 nm) and the beam obtained as a result of absorption and emission on active Ce^{3+} ions. Superposition of the scattered primary radiation with the emitted one is perceived by the human eye as white light. Both spectral components have different scattering mechanisms.

We have investigated efficiency of the elastic optical scattering and photoinduced extinction [1] of the pulsed laser radiation in Al_2O_3-YAG:Ce (0.25% wt. Ce) plates with optically quality polished interfaces against their thickness (0.5 – 2 mm) in visible and near IR ranges . It was obtained nonmonotonic dependence – 1 mm plate demonstrated the highest total transmittance decrease of the laser beam at 1064 nm among others. Magnitude of the reduction is crucially depends of the laser beam radius and its wavefront curvature.

Meanwhile angular resoluted elastic optical scattering analysis at 532 nm revealed a minimal spreading of the transmitted light (67 deg, FWHM) in 1 mm Al_2O_3-YAG:Ce plate in comparison with 86-94 degs for the rest ones.

Obtained results can be applied for the light convertors based on Al_2O_3-YAG:Ce eutectics optimization.

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Structural and photoluminescence properties of β-Ga_2O_3 nanocrystals obtained by mechanosynthesis

<u>Luchechko A.</u>[1*], Vasyltsiv V.[1], Kushlyk M.[1], Slobodzhan D.[1], Baláž M.[2], Cebulski J.[3], Szmuc K.[4], Szlęzak J.[3], Shpotyuk Y.[1,3]

[1] Department of Sensor and Semiconductor Electronics,
Ivan Franko National University of Lviv,
Tarnavskogo Str., 107, Lviv 79017, Ukraine.
[*]E-mail: andriy.luchechko@lnu.edu.ua

[2] Institute of Geotechnics of the Slovak Academy of Sciences
Watsonova str., 45, 04001, Košice, Slovakia

[3] Institute of Physics, University of Rzeszow, Rzeszow, 35-959, Poland

[4] Institute of Materials Engineering, University of Rzeszow,
Rzeszow, 35-959, Poland.

The gallium oxide (β-Ga_2O_3) is a promising material for application in power electronics, solar cells, UV photodetectors, transparent electrodes, flat panel displays, and UV phosphors. Nanosized Ga_2O_3 has great potential application in optoelectronic nanodevices and gas sensors.

In this work, a series of β-Ga_2O_3 nanocrystals have been successfully obtained by the high-energy ball milling method, changing the milling conditions of the initial powder of gallium oxide. The obtained nanocrystalline powders have been characterized by multi-experimental methods including X-ray diffraction, transmission electron microscopy, energy-dispersive X-ray spectroscopy, and luminescent spectroscopy.

XRD patterns show mainly a single β-Ga_2O_3 phase (a monoclinic crystalline structure with a space group of C2/m) formed in the milling process with a small amount of α-Ga_2O_3 phase. The grains of irregular shape were identified with the TEM technique. HRTEM images confirmed the formation of the β-Ga_2O_3 nanocrystals with a size distribution of 50-120 nm.

Luminescence bands with maxima at about 380, 425 and 490 nm were observed in photoluminescence spectra. The blue shift of the emission maxima at the excitation in the fundamental absorption edge under the different milling conditions was detected. The excitation spectra are observed in the wavelength range from 230 to 400 nm and also depend on obtaining conditions of nanopowders.

Microstructure and properties of β-Ga_2O_3 ceramics

Luchechko A.[1]***, Vasyltsiv V.***[1]***, Shpotyuk Ya.***[1,2]***, Kostyk L.***[1]***,***
Kushlyk M.[1]***, Slobodzhan D.***[1]***, Hreb V.***[3]***, Vasylechko L.***[3]***, Cebulski J.***[2]

[1] *Department of Sensor and Semiconductor Electronics,*
Ivan Franko National University of Lviv,
Tarnavskogo Str., 107, Lviv 79017, Ukraine
E-mail: andriy.luchechko@lnu.edu.ua

[2] *Institute of Materials Engineering, University of Rzeszow,*
Rzeszow, 35-959, Poland

[3] *Lviv Polytechnic National University,*
Lviv, S. Bandera St., 12, 79013, Ukraine

The growing need for energy-saving devices motivates researchers to explore new materials and optimize existing ones. Gallium oxide is a promising material with semiconductor properties for application as an efficient phosphor emitting in UV and visible spectral regions [1]. Modification of β-Ga_2O_3 by doping with different metal ions and/or annealing in the oxidizing and reducing atmospheres allows for controlling the structural, electrical, and spectral characteristics.

In this work, β-Ga_2O_3 ceramic samples have been synthesized via a solid-state reaction method at 1200°C. The samples were characterized using XRD analysis, electron microscopy, optical and luminescence spectroscopy as well as the measurement of electrical characteristics.

Rietveld's refinement of β-Ga_2O_3 ceramics confirms that samples are stabilized in monoclinic symmetry with C2/m space group. In this ceramic, the main peak of luminescence excitation is observed in the region of the absorption edge (260 nm) and the low-intensity peak is in the region of transparency with a maximum near 370 nm. The emission spectrum shows three host emission peaks located at 380, 420, and 480 nm with different relative intensities under these excitation wavelengths. Photoluminescence of ceramics at room temperature is mainly due to the recombination of electrons and holes through donor-acceptor pairs. Such ceramics has promising applications in devices of power electronics and UV-optoelectronics. The influence of annealing in a vacuum on structural, electrical, and luminescent properties, as well as on the morphology of the surface of β-Ga_2O_3 ceramics is discussed.

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The threshold of laser-induced damage of image sensors in open atmosphere

Matsnev I.V., Derzhypolska L.A., Derzhypolskyi A.G., Chumak O.O., Khodakovsky V.M., Negriyko A.M.

Laser Spectroscopy Department, Institute of Physics of the NAS of Ukraine.
Prospect Nauki, 46, Kyiv-03039, Ukraine.
E-mail: matsnev.igor@gmail.com

Studies on the action powerful laser radiation on image sensors are still of great interest regarding protection of sensors and opto-electronic devices, in spite of rather long history of these researches [1]. The new aspects of interactions of laser radiation and sensor matrices are related with permanent grows of electronic integration and nanoscale sizes of single elements on microchips. The early well studied processes of interaction of powerful laser radiation with the bulk materials are not enough for the description of the details of interaction nano- pico- and femtosecond laser pulses with micro- and nanosized structure of optical sensor matrix.

We are presented here the results of detailed studies of interaction of pulsed laser radiation with CCD and CMOS matrices in open atmosphere. The open atmosphere conditions is rather important for evaluation the practical energy threshold for damage of sensor at the field applications [2]. The experimental results of the action powerful laser light onto the image sensors at the open atmosphere are demonstrated. The estimations of atmosphere turbulence onto the threshold energy will be presented. The video camera operation damage without sensor surface structural damages was observed.

The results could be used in the developments of the optical sensors protection measures and improvement of sensor robustness.

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Session 7

Nanoobjects microscopy

Classification of the crystallization modes of amorphous films

Bagmut A.G., Bagmut I.A.

Department of Physics of the National Technical University
“Kharkiv Polytechnic Institute” of Ukraine. NTU “KhPI”
2, Kyrpychova str., 61002, Kharkiv, Ukraine.
E-mail: agbagmut@gmail.com

Based on “in situ” electron microscopic studies with the method of video recording of phase transformations, following polymorphous crystallization modes in amorphous films have been identified according to their structural and morphological characteristics (Table).

Layer polymorphous crystallization (LPC) mode describes the nucleation and growth of a single-crystal layer in the field of the electron-beam impact on amorphous film (Fig. 1). In this case $\delta_0 = D_0/a_0$, where a_0 is a cell parameter of the growing crystal. D0 is an average crystal size at a time $t = t_0$ (t_0 is characteristic unit of time), after which the volume of the amorphous phase decreases by the factor of e = 2.718. For LPC mode δ_0 is about several thousand (2000-5000) [1].

Island polymorphous crystallization (IPC) mode describes the nucleation and growth of a polycrystalline layer. In this case $\delta_0 = D_0/\Omega^{1/3}$, where Ω is the volume of the crystal unit cell. For IPC mode δ_0 is about several hundred (100-1100).

Intermediate mode between LPC and IPC. For this case δ0 ~ 1100-2000.

Dendrite polymorphous crystallization (DPC) mode describes the nucleation and growth of dendrite in amorphous layer. In this case also $\delta 0 = D_0/\Omega^{1/3}$, where Ω is the volume of the crystal unit cell. For DPC mode δ_0 ~ 3868.

Mode	Film	Deposition method	δ_0
LPC	Sb_2S_3	Thermal evaporation	4992
	Cr_2O_3	Laser evaporation	3107
	V_2O_3	Laser evaporation	4553
	Ta_2O_5	Laser evaporation	3659
IPC	ZrO_2	Ion-plasma evaporation	118
	ZrO_2	Laser evaporation	904
	Yb_2O_2S	Electron evaporation	1030
Intermediate	Ta_2O_5	Laser evaporation	1783
DPC	HfO_2	Laser evaporation	3868

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Magnetohydrodynamic treatment and optimization of alloying complex of Al-Si-Mg casting alloys

Monastyrska T.O.[1], Berezina A.L.[1],
Molebnyi O.A.[1], Fikssen V.M.[2]

[1] *G.V. Kurdyumov Institute for Metal Physics of the NAS of Ukraine,*
Vernadsky Blvd. 36, Kyiv-142, 03680, Ukraine
E-mail: monast@imp.kiev.ua

[2] *Physico-Technical Institute of Metals and Alloys of the NAS of Ukraine,*
Vernadsky Blvd. 34/1, Kyiv-142, 03680, Ukraine

The possibility of improving the structure and properties of aluminum cast alloy based on Al-Si-Mg due to the melt treatment in the magnetohydrodynamic installation [1, 2] has been studied in this work. Also, the optimization of the chemical composition and select the optimal modes of heat treatment of the alloys to improve the structure and complex of properties was carried out. It was shown that the most effective alloying element which improve the strength characteristics of Al-Si-Mg alloy is lithium. It was found that the introduction of lithium into the alloy in the amount of 0.2% leads to the modification of the Al-Si eutectic and provides the increase in the yield strength and tensile strength by 15%, while the ductility increases more than three times as much as compared to that of the base alloy.

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Peculiarities of nanoscale structural defects in multisectoral HPHT-diamond plates reviled by selective etching

Lytvyn P.M.[1]***, Strelchuk V.V.***[1]***, Nikolenko A.S.***[1]***, Malyuta S.V.***[1]***,***
Danylenko I.M.[1]***, Gontar O.G.***[2]***, Kovalenko T.V.***[2]***,***
Suprun O.M.[2]***, Ivakhnenko S.O.***[2]

[1] *V.E. Lashkaryov Institute of Semiconductor Physics NASU,*
pr. Nauky 41, 03028 Kyiv, Ukraine
E-mail: Igor.tesV@gmail.com

[2] *V. Bakul Institute for Superhard Materials NASU,*
Avtozavodska str. 2, 04074 Kyiv, Ukraine

Boron doped diamond (BDD) due to its unique physical properties is promising material for high-power and high-frequency electronics. However, the performance of diamond-based devices could be significantly affected by defects having non-uniform distribution within the BDD crystal. In this study, BDD crystals were obtained by temperature gradient method at high pressure and high temperature (HPHT) conditions in Fe-Al-B-C system. Multisectoral BDD plates oriented along the growth axis were produced by laser cutting and mechanical polishing. The growth faces of BDD crystals and multi-sector plates were studied at different stages of selective etching by Atomic-Force Microscopy (AFM), Kelvin-Probe Force Microscopy (KPFM) and Spreading Resistance Microscopy (SRM). Selective etching was carried out in a melt of KOH and KNO_3 at a temperature of 550°C, that allowed to investigate the defects in the early nanoscale (~1-2 nm in relief) stages of their appearance way before they can be detected by optical microscopy. Dependence of etching rate on boron concentration allowed for visualizing the intersectoral boundaries. Both dislocations etch pits in the form of hexagons and protrusions in the form of triangles associated with agglomerates of impurity defects were revealed. No variation in size, orientation, and density of defects was revealed at the intersectoral boundaries. The concentration of agglomerates remains constant, while the density of growth dislocations increases from seed to surface. The dislocation density near the surface was estimated at 105 - 106 cm^{-2}. Dislocation pits are often decorated with clusters of impurity defects. The defects are electrically neutral and are activated when bias potential is applied. Both pits and impurity agglomerates demonstrate lower SR in the probe-surface contact relative to the overall level of sector resistance. These changes in SR are less than 20 % of the difference in SR at intersectoral boundaries. A comparison is made of the defects on the growth faces of BDD crystals and corresponding plates.

Signal filtering with additive and multiplicative noise by orthogonal Legendre polynomials

***Fitio V.M.*, Petrovska H.A.**

Lviv Polytechnic National University.
S. Bandera str., 12, Lviv-79013, Ukraine
E-mail: volodymyr.m.fito@lpnu.ua, halyna.a.petrovska@lpnu.ua

Nowadays digital holographic interferometry is increasingly used to study macro-objects and micro-objects and phenomena. There is determination of surface roughness, study of micro-displacements, determination of part quality in MEMS, study of periodic microstructures, microscopy of living objects, and etc. In digital holographic interferometry, the first measuring stage is optical and the second is digital. The resolution of digital holographic microscopy can be limited by the parameters of the digital camera as well as the optical channel noise.

In this paper, the possibility of using orthogonal Legendre polynomials to filter noisy signals is investigated. It is possible to filter the signals in the interval [0, a] by scaling and shifting. Moreover, noise can be both the additive and the multiplicative. It is shown that Legendre polynomials can be successfully used for filtering interferograms and phase maps in digital holographic interferometry. Filtration is based on choosing the optimal number of polynomials at the signal approximation. Direct filtering of digital holograms (high spatial frequency of digital hologram signal) and phase maps (phase jump to π for certain coordinates) is impractical as several hundred polynomials must be used for filtering. It increases the time of numerical calculations. Therefore, in digital holographic interferometry it is necessary to directly filter the amplitudes of the fields calculated from the digital hologram. Further, interferograms and phase maps can be calculated from the filtered amplitudes of the object different states.

It should be noted that interferograms also can be directly filtered by Legendre polynomials. If the minimum distance between adjacent local minima (maxima) for the real or imaginary part of the signal is equal to Δl, then for a satisfactory approximation of such a signal by Legendre polynomials requires $6/\Delta l$ polynomials. Multiplicative noise filtering requires more time for computer calculations than additive one. Legendre polynomial filtering efficiency is improved if the noise signal has harmonic components with a frequency that is higher than the frequency of the useful signal.

Polymorphous crystallization of amorphous films of Ta_2O_5

***Bagmut A.G.*, Bagmut I.A.**

Department of Physics of the National Technical
University "Kharkiv Polytechnic Institute" of Ukraine. NTU "KhPI" 2,
Kyrpychova str., 61002, Kharkiv, Ukraine.
E-mail: agbagmut@gmail.com

The purpose of this work is the electron microscope study with "in situ" video recording of crystal growth in amorphous films of Ta_2O_5 and the systematization of crystallization reactions according to structural and morphological features. Amorphous films were obtained by pulsed laser sputtering of Ta targets in oxygen atmosphere. Phase transformations and structural analysis were performed by the methods of TEM, using microscopes EM-100L and PEM-100-01, operating at the accelerating voltage of 100 kV. The process of crystallization of the films was recorded from the screen of the electron microscope with Canon Power Shot G15 camera in the video recording mode with the frame rate of 30 s^{-1}.

Formation of the crystalline film took place polymorphically [1] at the constant crystal growth rate, but at different crystallization modes, that is due to local non-homogeneity of amorphous film. During layer polymorphous crystallization mode a single crystal was formed in the region of study. A quadratic time dependence of the fraction of crystalline phase was observed and the relative length was ~ 3659.

During island polymorphous crystallization mode a polycrystalline film was formed in the region of study. Time dependence of the crystallization centers density was described by the curve with saturation, time dependence of the fraction of the crystalline phase had the exponential character, described by the Johnson-Mail-Avrami-Kolmogorov equation. The relative length was ~ 416.

Interjacent character of crystallization is characterized by the nucleation and growth of several (3-4) disoriented crystals. Time dependence of the fraction of the crystalline phase was approximated by the polynomial of the third power. The relative length was ~ 1783.

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Session 8.

Nanoplasmonics and surface enhanced spectroscopy

Raman investigations of $Cu_2MgxZn_{1-x}SnS_4$ films with different chemical composition

Yermakov M.S.[1]*, Pshenychnyi R.M.*[1]*, Opanasyuk A.S.*[1]*,*
Klymov O.V.[2]*, Muñoz-Sanjosé V.*[2]

[1] *Department of Electronics and Computer Technology,*
Sumy State University. Rimsky-Korsakov str.,
2, Sumy, UA-40007, Ukraine.
E-mail: m.yermakov@ekt.sumdu.edu.ua

[2] *Department of Applied Physics and Electromagnetism,*
University of Valencia, C / Dr. Moliner 50, 46100 Burjassot, Spain.

Currently, Cu_2ZnSnS_4 is considered a promising material for the absorption layers of solar cells (SC) of the third generation. However, despite a large number of studies, the efficiency of photo converters based on it does not exceed 10%. The main reason for this is the low value of the no-load voltage compared to the width of the bandgap of the material, which is associated with the formation of anti-structural defects SnZn. One way to overcome this disorder is to replace Zn with Mg in the crystal lattice of the semiconductor, giving new options based on the $Cu_2MgxZn_{1-x}SnS_4$ compounds.

To create a precursor, saline solutions in stoichiometric amounts of $CuCl_2$: $Zn(CH_3COO)_2$: $MgCl_2$: $SnCl_2$: $(NH_2)_2CS$ = 2 : 1-x : x : 1 : 4 were slowly added to the thiourea solution. As a result of mixing the initial solutions, transparent molecular precursors with an x value in the range from 0 to 0.4 were obtained. The films were obtained by application using the technique of spray pyrolysis. Studies of the elemental composition of the films thus obtained showed the following values of the concentrations of CMg atoms in the samples: 0%, 3.91%, 5.77%, 3.94%, 6.70%, corresponding to the 0, 10, 20, 30 and 40% of nominal Mg content.

The Raman investigation of samples with Mg nominal content up to 20% shows that they have three main peaks at frequencies of 295 cm^{-1}, 337 cm^{-1}, and 372 cm^{-1}, which correspond to the reference data for pure kesterite compounds. With a further increase in Mg content, a new peak intensity appeared at a frequency of 350 cm^{-1}, which may indicate the presence of a secondary phase of Cu_2SnS_4. In addition a shift of the A1 peak from the frequency of 337 cm^{-1} to the frequency of 317 cm-1 was detected. This shift is explained by the replacement of smaller radii of Zn^{2+} ions with larger Mg^{2+} ions.

We have shown the availability of the spray pyrolysis technique for the synthesis of $Cu_2MgxZn_{1-x}SnS_4$ films, with a controlled ratio of Zn to Mg content.

Luminescence and Raman studies of nanostructures based on $(SiO_x–Sm)_n$ multilayers

Michailovska K.V., Dan’ko V.A., Indutnyi I.Z.,
Shepeliavyi P.E., Sopinskyy M.V.

V. Lashkaryov Institute of Semiconductor Physics Natl. Acad. of Sci. of Ukraine. 45 Prospect Nauky, 03028 Kyiv, Ukraine.
E-mail: danko-va@ukr.net

In recent years Sm-doped materials are widely studied for a variety of optoelectronic application such as optical waveguides, white LEDS, solar cells, X-ray imaging, etc. It is known that the introduction of Sm into oxide glasses contributes to the modification of their structure and properties. As shown by our previous studies, the doping of silicon oxide layers with samarium by co-evaporation of SiO and Sm in vacuum accelerates the formation of silicon nanoparticles (ncs-Si) during annealing of these films in air. In this work, we study the PL and Raman spectra of $(SiO_x–Sm)_n$ multilayer films obtained by alternate vacuum evaporation of SiO and Sm onto different substrates (c-Si, SiO_2 and Al_2O_3). The number of pairs of nanolayers *(n)* for the studied samples was 10, the total thickness of the structure was 400 nm. Annealing of the samples was carried out in air in the temperature range of 500–970 ºC for 30 min, resulting in diffusion of Sm into the SiO_x layers and thermally stimulated formation of ncs-Si, additionally stimulated by the samarium impurity. The content of Sm in the studied samples was 1.5 wt. %.

The photoluminescence (PL) spectra of $(SiO_x–Sm)_{10}$ films annealed at different temperatures were measured and compared with the spectra of SiO_x:Sm samples obtained by coevaporation of SiO and Sm, as well as with SiOx films of the same thickness, annealed under similar conditions. It is shown $(SiO_x–Sm)10$ films exhibit the brightest PL and are more stable with time of storage. In these films, the transition of ncs-Si from the amorphous state to the amorphous-crystalline state begins to manifest itself already at $T_{an} \geq 600$ ºC. Studies of the Raman spectra of annealed $(SiO_x–Sm)_{10}$ films confirmed the presence of crystalline ncs-Si in the samples and made it possible to estimate the average size of nanocrystals (~3.6 nm). Decomposition of the Raman spectrum into component bands made it possible to detect a band in the region of 495–510 cm^{-1} and associate it with local variations of the oxygen environment on the ncs-Si–SiO_x interface in the SiO_x matrix. The mechanisms of participation of Sm in the processes of SiO decomposition and passivation of the surface of formed ncs-Si are discussed.

Excitation of surface plasmon polaritons on aluminum-coated diffraction gratings formed on an inorganic chalcogenide photoresist: influence of surface relief profile

Indutnyi I.Z., Mynko V.I., Sopinskyy M.V., Danko V.A. and Lytvyn P.M.

V. Lashkaryov Institute of Semiconductor Physics Nat. Acad. of Sci. of Ukraine. 45 Prospect Nauky, 03028 Kyiv, Ukraine.
E-mail: indutnyy@isp.kiev.ua

Historically, the first and most studied plasmonic structures are metallic periodic structures (diffraction gratings), in which the excitation of surface plasmon polaritons (SPPs) was observed for the first time more than a century ago. The processes of SPP excitation in such structures have been intensively studied in recent decades. In a number of theoretical and experimental studies, it was found that the shape of SPP resonances in the angular dependence of the intensity of reflected light changes significantly when the grating groove profile deviates from a sinusoid. Therefore, in this work we experimentally studied the relationship between the groove profile of aluminum gratings and the shape of SPP resonances in the angular dependences of the intensities of specular reflection and diffracted radiation in the -1 order of diffraction. Gratings for studies with a period $a = 700$ nm were formed on films of $As_{40}S_{30}Se_{30}$ chalcogenide photoresist by means of interference lithography and vacuum thermal deposition of an opaque aluminum layer about 80 nm thick. The grating groove profile was varied during their fabrication by varying the time of exposure and selective etching.

It has been established that for the +1 order SPP resonance, an increase in the contribution of higher harmonics to the Fourier transform for the surface profiles of the gratings under study mainly affects the shape and amplitude of plasmon resonances in the angular dependence of diffracted radiation. At the same time, for -2 order SPP, a significant increase in the amplitude of SPP resonances is observed both in specular reflection and in diffracted radiation. This is due to the appearance in the Fourier transform of a component having a wave vector twice as large as the wave vector of the fundamental harmonic of the grating, and much higher efficiency of direct excitation of -2 order SPP through this component. It is shown that the integral efficiency of +1 order SPP excitation depends on the grating groove profile and decreases with increasing deviation of the grating relief profile from the sinusoid.

Plasmon phenomena in a metal nanotube of variable thickness

***Malysh R.O.*, Korotun A.V.**

National University "Zaporizhzhia Polytechnic",
Zhukovskogo st., 64, Zaporizhzhia, Ukraine.
E-mail: andko@zp.edu.ua

Nowadays metal nanotubes due to the occurrence of surface plasmon resonances (PPR) are widely used, in particular, as optical sensors [1]. Note that if plasmon resonances in cylindrical metal shells are well studied (see, for example, [2]), then the question of excitation of PPR in metal shells of variable thickness is insufficiently studied. Therefore, the analysis of the influence of the nonconcentricity of the shell boundaries on the PPR frequencies in the optical frequency range is an urgent task.

The approach to solving this problem consists of the following stages:

1) the electrostatic problem for determination of potentials in a cover, kernel and out of a cover is solved;

2) the polarizability of the studied nanostructure is determined;

3) PPR frequencies are determined from the condition of zero of the real part of the denominator of the expression for polarizability.

Note that knowing the polarizability, it is possible to determine such observed quantities as the absorption and scattering cross sections of a metal nanotube of variable thickness.

The study of the frequency dependences of the porosity showed the presence of additional resonances caused by the nonconcentricity of the shell boundaries. In addition, it was found that the absorption and scattering cross sections significantly depend on the amount of shear of the centers of the dielectric nucleus and the entire nanotube.

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Spectral quality factor of sensory sensing elements on SPR in the form of metal nanowire

***Lutsenko Yu.I.*, Karandas Ya.V., Korotun A.V.**

National University "Zaporizhzhia Polytechnic",
Zhukovskogo st., 64, Zaporizhzhia, Ukraine.
E-mail: andko@zp.edu.ua

The rapid development of nanotechnology has led to a shift in sensory research towards nanometer scales [1]. In particular, SPR sensors have become widely used, which make it possible to detect very small amounts of substances and adapt to the analysis of a wide range of different chemical and biological objects.

Modern technologies allow the use of metal nanoparticles as sensitive elements. For optimal selection of nanoparticles use such characteristics as figure of merit:

$$\mathrm{FOM} = \frac{S_\omega}{\gamma_{\mathrm{eff}}}$$

where γ_{eff} – effective relaxation rate,

$$S_\omega = 2\surd T_m \frac{\partial\omega_{sp}}{\partial T_m}$$

– spectral sensitivity.

In expression (2) ω_{sp} – SPR frequency, T_m – dielectric constant of the environment.

Note that due to the fact that 1D-structures are asymmetric, they excite longitudinal and transverse surface plasmons, and, accordingly, spectral sensitivity, effective relaxation rate and spectral quality factor are diagonal tensors of the second rank:

$$S_\omega^{\perp(\square)} = 2\surd T_m \frac{\partial\omega_{sp}^{\perp(\square)}}{\partial T_m}$$

$$\mathrm{FOM}^{\perp(\square)} = \frac{S_\omega^{\perp(\square)}}{\gamma_{\mathrm{eff}}^{\perp(\square)}}$$

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Dielectric function of a metal nanosphere covered with a layer of adsorbed molecules

Maniuk M.S., Smirnova N.A., Korotun A.V.

National University ”Zaporizhzhia Polytechnic“,
Zhukovskogo st., 64, Zaporizhzhia, Ukraine.
E-mail: andko@zp.edu.ua

Currently, metal nanoparticles of various shapes, including spherical, due to their unique optical properties are widely used in biology and medicine [1]. Thus, the problem of determining the expansion of the plasmon resonance line of a spherical metal nanoparticle, the surface of which is covered with a layer of adsorbed molecules, is of considerable interest. In this case, the interface decay channel of surface plasmons makes a significant contribution to the surface relaxation rate.

This effect is due to an increase in the local density of states induced by adsorbed molecules near the Fermi level of nanoparticles. Note that the correct description of these factors requires consideration of interband and intraband transitions of electrons, as well as the tensor nature of the surface relaxation rate. Therefore, taking into account these considerations, in the expression for the effective parameter describing the degree of loss of coherence during electron scattering on the surface, it is necessary to take into account the term associated with the presence of the adsorbed molecular layer:

$$\gamma^{\perp(\square)}=A_{\perp(\square)}\frac{\nu_F}{R}$$

where ν_F is the Fermi velocity of electrons; R is the corresponding lateral size of the nanoparticle, and

$$A_{\perp(\square)}=A^{\mathrm{size}}+A_{\perp(\square)}+A_{\perp(\square)}^{\mathrm{interface}}$$

In formula (2), the first term is due to the scattering of electrons by the nanoparticle on its surface, and the origin of the second term is due to the presence of an adsorbed layer on the surface of the nanoparticle.

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Plasmonic nanocavity metasurfaces based on femtosecond laser-nanostructured patterns perspective for the enhanced optical response of organic and biological molecules

Berezovska N.[1]***, Dmitruk I.***[1]***, Yeshchenko O.***[1]***, Kudrya V.***[1]***,***
Stanovyi O.1, Tomchuk A.[1]***, Hrabovskyi Ye.***[1]***,***
Golovynskyi S.[2]***, Xue B.***[2]***, Qu J.***[2]***, Dmytruk A.***[3]

[1] *Faculty of Physics, Taras Shevchenko National University of Kyiv.*
Volodymyrska Street, 64/13, Kyiv-01601, Ukraine.
E-mail: n_berezovska@univ.kiev.ua

[2] *College of Physics and Optoelectronic Engineering, Shenzhen University.*
518060 Shenzhen, P. R. China.

[3] *Department of Photon Processes, Institute of Physics of NAS of Ukraine.*
Prospect Nauky, 46, Kyiv-03028, Ukraine.

Plasmonic nanocavity metasurfaces based on femtosecond laser-induced periodic surface structures (LIPSSs) with noble metal nanoparticles (NPs) in near-field proximity can provide excitation of plasmon gap mode and respective electromagnetic (EM) field enhancement that causes an increase of the spectroscopic signal by up to several orders of magnitude in surface enhanced Raman scattering (SERS) or surface-enhanced fluorescence (SEF). That has been demonstrated on adsorbed species of biomolecules of low concentration [1].

Within the scope of present report, we study an efficiency of the application of LIPSSs either directly fabricated on metallic surfaces or obtained on semiconductor substrates subsequently coated with metallic gold or silver films for highly sensitive fluorescent label-free detection and imaging of biomolecules (nucleotides) or dyes (Rhodamine 6G) at room temperature. We discuss the most relevant parameters for the generation of different LIPSSs, as well as an impact of shape and size of metal NPs placed in the vicinity of metal or metal-semiconductor substrate on the efficiency of formation of plasmonic "hot spots", i.e. the spatial areas with highly intense EM field where the huge plasmon enhancement occurs.

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Surface plasmon oscillations control by nematic liquid crystal reorientation

Yakovkin I.I., Ledney M.F.

Taras Shevchenko National University of Kyiv, Faculty of Physics,
Department of Theoretical Physics. 03127, Kyiv, Hlushkova Avenue, 4
E-mail: yakovkinii@gmail.com

We present the study of the surface plasmon polariton propagation properties control by imposing a reorientation in the adjacently located nematic liquid crystal. A plane nematic liquid crystal cell, initially oriented homeothropically, is placed into a static electric field parallel to the substrates. Due to the influence of the electric field the liquid crystal starts to deviate from the initial orientation, posing a change in the dielectric function of the liquid crystal cell. One of the substrates of the liquid crystal cell contacts with a thin metal coating, on the interface with which the surface plasmon polariton can propagate. The properties of the surface plasmon polariton (most importantly the effective refraction index) are reflecting the change of the liquid crystal orientation.

The calculation of the surface plasmon polariton properties in such structure were performed both analytically, using an adapted perturbation technique presented in [1], as well as by direct numeric solution of the Maxwell's equations. The dielectric function of the investigated structure is determined by the principal values of the dielectric permittivities as well as by the director profile of the liquid crystal. The latter is calculated by minimizing the free energy of the liquid crystal cell, as described in [2].

The performed calculations show that the effective refraction index of the surface plasmon polariton as a function of the external electric field strength can possess a hysteresis-like behavior. That is, the effective refractive index is an ambiguous function of the electric field strength, and its value is highly influenced by the previous states of the system. The parameters and criteria for such hysteresis to occur are calculated. Such phenomenon is likely to prove useful in constructing plasmonic switches and basic memory units.

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SERS-application of Ag nanoparticles synthesized from bio-extracts

Mazur N.V.[1], Smirnov O.E.[2,3], Kovalenko M.S.[2], Dzhagan V.V.[1], Yefanov V.S.[1], Yeshchenko O.A[4], Dzhagan V.M.[1,4], Yukhymchuk V.O.[1]

[1] *V. Lashkaryov Institute of Semiconductors Physics,*
National Academy of Sciences of Ukraine, Kyiv, Ukraine.
E-mail: nazarmazur@isp.kiev.ua

[2] *ESC "Institute of Biology and Medicine",*
Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

[3] *Institute of Plant Physiology and Genetics, National Academy of Sciences of Ukraine, Kyiv, Ukraine*

[4] *Physics Department, Taras Shevchenko National University of Kyiv,*
Kyiv, Ukraine,

Long-standing intense research on synthesis and functionalization of Ag nanoparticles (NPs) is due to the unique combination of antibacterial, optical, electrical, and catalytic properties, stimulating various applications. Most progress is currently made in the area of anti-pathogen applications and applications based on localized surface plasmon resonance (LSPR), such as sensors and SERS-substrates (surface-enhanced Raman spectroscopy). Among numerous synthesis routes, there is an increasing number of reports on phytosynthesized silver NPs, based on an extract of different parts of plants.

Here we report application of mycosynthesized Ag NPs, obtained using Ganoderma lucidum fruit body extract as the bioreducing and stabilizing agent, as a substrate for Surface-Enhanced Raman Scattering (SERS). Stable Ag NPs colloids with distinct plasmonic resonance in UV-blue range (Fig. 1a,) were obtained for a broad pH range (5-11). At very acidic conditions, pH=2.5, synthesis efficiency drops but the formation of plasmonic NPs still takes place. All the NP samples were tested as a SERS-substrate, using standard dye analyte, rhodamine 6G. In addition to the dependence of the enhancement efficiency on the NP synthesis conditions, we observe spectral effects that can be related to the adsorption geometry of the molecule on the NP surface in different conditions, in particular, in solution and after drying the Ag NP/analyte composite on the substrate.

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Plasmonic response modelling of sensors composed of two noble metal layers separated by a dielectric

Yampolskiy A.L., Makarenko O.V.

Taras Shevchenko National University of Kyiv,
Faculty of Physics, Department of Optics
(64/13, Volodymyrs'ka Str., Kyiv 01601, Ukraine)
E-mail: uv365nm@ukr.net

Using a plasmon resonant dip in light internal reflection curves underlies one of the methods for measuring the refractive index of a medium. The method makes it possible to determine changes in the refractive index with sensitivity of about 100…170 deg/RIU [1, 2]. Further improvement of such sensors operational characteristics is very relevant.

Exploiting of multilayer structures makes it possible to significantly improve the accuracy of refractive index determining by utilizing the interference effects of coupled modes excitation in metal layers. Usual design circumstance of such sensors is invariable thickness of all the layers forming the structure.

The aim of the authors was to consider the simplest structure that allows changing the distance between the layers. Its optical characteristics are compared with a conventional sensor based on a single noble metal layer, and changes analysis caused by variation in the dielectric layer thickness, is carried out.

P(VDF-TrFE), known for its ferroelectric and piezoelectric properties, was chosen as a material that can change its thickness. Voltage application to the metal layers surrounding the polymer, allows one to vary the distance between the layers and optical characteristics of the sensor.

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Nitrogen-doped graphene oxide nanocomposite with silver nanoparticles as a SERS detector

***Menshova E.P.*, Dzhanabekova R.Kh.,**
Ibrayev N.Kh., Seliverstova E.V.

Institute of Molecular Nanophotonics, Karaganda Buketov University.
St. University, 28, 100024 Karaganda, Kazakhstan
E-mail: menshovayevgeniya@gmail.com

The creation of active substrates for Raman scattering is an urgent task for determining "trace" amounts of analytes. We prepared SERS-active substrates based on nitrogen-doped graphene oxide (NGO) with silver nanoparticles (NPs) and studied the Raman spectra of R6G on the composite surface.

The composite was synthesized by a 2-stage method based on an ammonia complex [1]. In the SEM images, the NGO sheets are covered with spherical Ag NPs, the size of which is 80 – 120 nm. It correlates with the data obtained on the absorption spectrum with a maximum at 490 nm.

Raman spectra (Confotec MR 520) showed that during the synthesis of the nanocomposite, a large number of topological defects are formed in graphene oxide. Also, the spectrum of the nanocomposite differs from the spectrum of NGO by the presence of additional peaks at 600 and 1800 cm^{-1}, which are characteristic of the residual products of ammonia [2] and ascorbic acid [3].

The studied SERS-active substrates are capable of amplifying the R6G signal (10^{-5} mol) by a factor of 35.92 relative to the dye signal on NGO without Ag NPs. Even at a low dye concentration of 10^{-9} mol, peaks at 611, 771 and 1125 cm^{-1} can be identified, associated with in-plane and out-of-plane vibrations of the aromatic ring and C-H vibrations in the plane, as well as bands 1189, 1310, 1360, 1508, and 1649 cm^{-1} related to the stretching vibrations of aromatic C–C bonds [1]. We believe that the high sensitivity of detection is associated not only with the SERS effect, but also with additional sorption of the analyte.

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Mechano-chemical modification of β-Ga_2O_3 and β-Ga_2O_3:Eu micropowders by plasmonic nanoparticles

Kushlyk M.[1], *Slobodzian D.*[1], *Luchechko A.*[1],
Shpotiuk Ya.[1,2], *Baláž M.*[3]

[1] *Ivan Franko National University of Lviv,*
79017, 107 Tarnavskoho Str., Ukraine

[2] *Institute of Physics, University of Rzeszów,*
1, Pigonia str., 35-959 Rzeszów, Poland

[3] *Institute of Geotechnics SAS, Watsonova 45, 04001 Košice, Slovakia*

In recent years, increasing interest has been given to the synthesis of metal-oxide-semiconductors, such as monoclinic gallium oxide (β-Ga_2O_3). Especially, β-Ga_2O_3 semiconductor nanomaterials are attractive candidates as active elements for advanced nanoscale devices due to their unique electronic and optical properties, low effective density, high specific surface area, and shell permeability that are important in many technological applications such as photonics, sensors, solar energy conversion, and electrochemical energy storage, etc. On the other hand, much attention has been paid to the plasmonic effect of metal nanoparticles (NPs) formed in close vicinity to the recombination centres. Combining a thin conversion layer with silver plasmonic nanostructures leads to increased donor absorption and emission efficiency.

The structural, morphological, chemical and optical properties of β-Ga_2O_3 and β-Ga_2O_3:Eu (pure and modified by Ag NPs) powder composites were investigated by X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy as well as photoluminescence spectroscopy (PL) and Raman spectroscopy. The results show that the properties of obtained β-Ga_2O_3 composites were strongly influenced by the chamber material and rotation speed. Thus, different crystalline sizes (from 5 um to 300 nm) were obtained, where the bigger particle size show's the greater bulk emission. In the case of β-Ga_2O_3 powder doped with Eu, an opposite result was obtained. Also, it needs to note, that higher luminescence intensity was obtained for the pure composite prepared in the ZrO_2 chamber. It is partially caused by the presence of tungstate and carbon atoms in Ga_2O_3 powders as well as low content of α-Ga_2O_3 phase.

It is determined that modification with Ag NPs requires increasing the mechanosynthesis time up to 4 h at a low rotation speed (~300 rpm). The absorption spectra show the existence of two modes of plasmon resonance for silver nanoparticles in the β-Ga_2O_3 matrix with relatively high intensity. One of them is a quadrupole mode (with λ_{max} near 360-370 nm) and another one is a dipole mode whose maximum is in the range from 450 to 480 nm. It leads to a redshift of the PL band for plasmonically modified Ga_2O_3 powders in the direction of the plasmon resonance maximum, with 20% of intensity enhancement.

Session 9.
Nanoscale physics

Domain wall with Bloch point in ferromagnetic cylindrical nanowire

***Shevchenko A.B.*[1], *Barabash M.Yu.*[2]**

[1] *G.V. Kurdymov Institute of Metal Physics of the NAS of Ukraine,*
Vernadskogo pr., 36, Kyiv-03142, Ukraine

[2] *Technical Centre of the NAS of Ukraine,*
Pokrovskya str., 13, Kyiv-04070, Ukraine
E-mail: mbarabash@nasu.kiev.ua

The study of ferromagnetic nanowires (FNs) is an important task of nanoscale physics due to their unique properties. Among the wide variety of FNs, here we consider cylindrical nanowires, in which the formation of domain walls (DWs) takes place. It is clear that thermodynamic and magnetocaloric properties of cylindrical FNs [1-3] depend on DW magnetic structure. In this condition we will study DWs whose structure is characterized by Bloch point (BP).

Using the indefinite Lagrange multiplier method the BP magnetic structure near its singularity center was determined [4]. It is shown that the behavior of the magnetization vector of Bloch point is affected by the symmetry of the system. It is found the critical radius of FN which ensnares the formation of a DW with BP. Given criteria is agree with the conclusion made in [5] regarding the critical radius of a permalloy cylindrical nanowire. Obtained results may be used in new methods for diagnosing both FNs and the magnetic structure of DWs in them.

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Structure of nanoclusters and density of solutions of rigid-chain polymers

Bulavin L.A., Zabashta Yu.F., Lazarenko M.M.,
Alekseev O.M., Vergun L.Yu.

Taras Shevchenko National University of Kyiv.
64/13, Volodymyrska Street, City of Kyiv, Ukraine, 01601
E-mail: LienaVergun@univ.net.ua

As is known, a feature of the polymer solution is the presence of nanoclusters. The nanoclasters are nanosized aggregates consisting of a polymer chain and related solvent molecules. The literature mainly refers to (see, for example, [1], etc.) nanoclusters formed by flexible chains. Instead, this report considers nanoclusters containing rigid chains.

A continuous model of polymer solution is proposed. According to this model the solution is considered as a set of three phases: solvent and two phases, which make up the nanocluster, namely, the core and the boundary layer.

The formulas that relate the density of the solution with the densities of these phases are derived. The temperature dependence of the density of the aqueous solution of hydroxypropylmethylcellulose (typical representative of the class of rigid chain polymers) is experimentally investigated. The experiment was performed on a Density meter: Anton Paar DMA 4500 M in the range of 293 K-353K.

Based on the obtained experimental data using the derived formulas, and data borrowed from [2], a structural model of a rigid-chain nanocluster was built. For such model the core has a cylindrical shape and is formed by a threefold chain, and the boundary layer is formed by water molecules. The orientation of water molecules changes with increasing temperature.

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Theoretical study of nonlinear spin waves in magnetic multilayers with metasurfaces

Gerasimchuk V.S.[1], ***Gerasimchuk I.V.***[1,2]

[1] *Faculty of Physics and Mathematics, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",*
Peremohy Ave. 37, Kyiv 03056, Ukraine

[2] *Department of Physics of Meso- and Nanocrystal Magnetic Structures, Institute of Magnetism, Natl. Acad. Sci. Ukraine and Min. Edu. Sci. Ukraine, Akad. Vernadsky Blvd. 36-b, Kyiv 03142, Ukraine*
E-mail: igor.gera@gmail.com

The multilayer magnetic structures are widely investigated regarding their potential technological applications. Recently, magnetic film micro- and nanostructures have been intensively studied as possible candidates for the creation of promising devices for spintronics and magnonics. Of particular interest are multilayer periodic structures with magnetic ordering which have pronounced anisotropic properties. In turn, the presence of metasurfaces (thin layers) in layered structures with different magnetic properties and different ratios of layer thicknesses is the requirement for the formation of spin-wave excitations localized at the metasurfaces between the contacting magnetic layers [1]. Earlier, the analysis of such excitations was limited to linear on the oscillation amplitude approximation, but now the study of nonlinear spin-wave excitations and their properties become actual. Due to the new technological possibilities of the creating of periodic nanostructures, the investigations of the propagation of nonlinear spin waves localized near thin layers of the magnetic material in a system of thin plane parallel magnetic layers (plane magnetic defects) are of great practical interest.

In the present work, we study analytically the localization of nonlinear waves propagating in a five-layer magnetic structure along the alternating wide and thin layers with different single-ion anisotropies in them. We find the exact solutions for spin wave localized states, the total number of elementary excitations localized in the system and its total energy as functions of the scaling variable characterizing the distance between the plane magnetic defects. We present all these dependences in the universal scaling forms valid for different values of the characteristic of magnetic defects.

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Electrostatics of a nanowire heterostructure radial p-i-n diode

Borblik V.L.

Department of electrical and galvanomagnetic properties of semiconductors,
V.Lashkaryov Institute of Semiconductor Physics of the NAS of Ukraine.
Prospect Nauki, 41, Kyiv-03680, Ukraine.
E-mail: borblik@isp.kiev.ua

Semiconductor nanowires are used mostly in the form of multilayer structures in which material and/or doping type change either in radial or axial direction. In particular, nanowires with *p-n* junctions have found broad application as radiation detectors, solar cells, light emitting device and lasers. It has been shown that the radial core-shell nanowires have certain adventures compared with axial ones [1].

In many cases, *p-i–n* structures prove to be more effective than simple p-n structures because they extend a region of the built-in electric field. Theoretical analysis [2] has shown that electric field in *i*-layer of the radial *p-i–n* diode is inhomogeneous and its maximum value can be both lower and higher in comparison with electric field in equivalent planar *p-i–n* diode.

However often not homo but hetero *p-i–n* diodes are used in the applications. Therefore it is of interest to consider electronic properties of the radial heterostructure *p-i–n* diode.

In *p-i–n* structure symmetrical on doped materials (i.e. when *p*- and *n*- layers are made of the same semiconductor), entering into p-n junction of the *i*-layer with larger dielectric constant than that of the doped layers lowers electric field in it, and entering of *i*-layer with smaller dielectric constant - raises the field. Besides, it is turn out that entering i-layer into p-n junction extends the electric field region not always. At middle doping levels, depletion widths of the p- and *n*- layers so decrease under entering *i*-layer that total thickness of the electric field region does not increase practically.

In *p-i-n* structure asymmetrical on doped materials, two different cases are possible: 1) the core material has narrower gap in comparison with material of the external shell and 2) reverse situation. The second-type structure provides significantly higher built-in electric field in the *i*-layer than the first-type structure does.

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Properties of electron states in open multi-cascade nanostructure: S-matrix, transmission coefficient and probability function methods

Seti Ju., Vereshko E., Voitsekhivska O., Tkach M.

Department of Theoretical Physics and Computer Simulation,
Yuriy Fedkovych Chernivtsi National University,
2, Kotsyubinsky Str., 58012, Chernivtsi, Ukraine
E-mail: vereshko.yevheniia@chnu.edu.ua

The problem of quasiparticles states in low-dimensional structures, for a long time, has been purely fundamental. It became practically important only after the creation of first devices based on nanostructures (quantum well infrared photodetectors, quantum cascade detectors, quantum cascade lasers, etc.). This has significantly intensified theoretical research in the field of nanostructure physics. In the majority of papers, due to the complexity of analytical and numerical calculations, structures with a small number of nano layers were studied, while complicated multi-cascade nanostructures were not observed. Therefore, the properties of the basic elements of nano devices containing dozens of cascades are still not completely studied.

The aim of the proposed paper is to study the spectral characteristics of an electron in a multi-cascade open nanostructure [1]. The models of effective mass and rectangular potentials based on the solutions of Schrödinger equation in three different approaches (transmission coefficient (D), scattering matrix (S) and probability distribution function (W)) are used for the calculation of the resonant energies and widths of electron quasi-stationary states. The analysis of the spectral characteristics as functions of the number of cascades show that in the simplest single-cascade nanostructure the resonant energies and widths of the electron states in all three approaches coincide with an accuracy not less than 0.1%. If the number of cascades increases, it leads to the formation of bands. The number of resonant energies in the band is equal to the number of cascades in the S-matrix approach, while in D- and W-approaches – it is smaller. Also, it is established that in the S-approach the sum of resonant widths of electron states in each band is independent of the number of cascades and coincides with the width of the corresponding quasi-stationary state in single-cascade structure, while in D- and W-approaches the sum of widths in the bands only decreases.

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Quantum theory of energetic parameters in two-well nanostructure, being a main operating element of broadband photodetector functioning in far IR range

Tkach M.V., Hutiv V.V., Seti Ju.O., Voitsekhivska O.M.

Department of Theoretical Physics and Computer Simulation,
Yuriy Fedkovych Chernivtsi National University,
2, Kotsyubinsky Str., Chernivtsi-58012, Ukraine,
E-mail: hutiv. vasyl@chnu. edu. ua.

For the stable operation of quantum nanostructures, being the main elements of broadband photodetectors functioning in a very far infrared range, they should demonstrate peculiar characteristics: provide high detective properties over the whole width of the absorption band in the desired range of electromagnetic field energies at minimum dark current. Due to the significant mismatch in the size of the unit cells of anisotropic materials of quantum wells and barriers, it is difficult to produce stable high-quality photodetectors. Therefore, intensive research is underway into such isotropic materials, whose quantum wells and barriers have well-matched unit cell sizes and, with the optimal geometric design, can meet these requirements for the successful operation of QWIPs.

In the proposed paper, a quantum mechanical calculation of the electron spectrum, wave functions and oscillator forces of quantum transitions under the action of an absorbed electromagnetic field in a nano heterostructure consisting of two wide quantum wells, but with an inverted internal structure of potential profile is performed. The results of numeric calculation show that by choosing the geometric parameters of the inner profile (widths and heights of the inner quantum wells and barriers) of the main element of photodetector, it is possible to ensure such ratio between the width and the maximum of absorption band range, which optimizes the operation of broadband detector in the demanded far IR range, as the "window" of atmospheric transparency.

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Why plasmon enhancement coefficient is different for light absorption, scattering and luminescence effects?

Dolgov L.[1], Kiisk V.[1], Sildos I.[1], Fesenko O.[2], Dramicanin M.[3], Wu M.[4]

[1] *Institute of Physics, University of Tartu, W. Ostwaldi Street 1, Tartu 50411, Estonia, email: leonid.dolgov@ut.ee*

[2] *Institute of Physics, NAS of the Ukraine, Prospect Nauki 46, Kyiv 03680, Ukraine*

[3] *Vinca Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, Belgrade 11001, Serbia*

[4] *MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry, Sun Yat-sen University, Guangzhou 510275, P. R. China*

Minute addition of metal nanoparticles or metal nanolayers to dielectric material can drastically change its optical properties. Light induced collective electron plasma oscillations localized near metal-dielectric interface can sufficiently enhance intensity of light absorption, scattering and luminescence in such materials at resonance frequencies. For example, pronounced several order plasmonic increase in intensity of Raman light scattering for material, contacting with noble metal nanoparticles [1], give hope on the same manner promising effects in light absorption (plasmonic solar cells [2]) and light emission (nano-lasers and SPASERs [3]). However, values of light intensity enhancement reported for these effects are different in different literature sources. This report both inspects selected publications related to plasmonic enhancement of light absorption, scattering and luminescence and discusses original results obtained by corresponding author in partnership with several scientific groups from Ukraine, Serbia, China and Estonia.

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Influence of the conductive polymer matrix on the structural and optical properties of metalloquinolates and their derivatives.

Sypniewska M.[1]***, Gondek E.***[2]***, Pokladko-Kowar M.***[2]***, Kaczmarek-Kedziera A.***[3]***, Apostoluk A.***[4]***, Smokal V.***[5]***, Szczesny R.***[3]***, Derkowska-Zielinska B.***[1]

[1] Institute of Physics, Faculty of Physics, Astronomy and Informatics,
Nicolaus Copernicus University in Torun,
Grudziadzka 5, Torun 87-100, Poland
E-mail:msyp@doktorant.umk.pl

[2] Department of Physics, Cracow University of Technology,
Podchorążych Str. 1, 30-084 Krakow, Poland;

[3] Faculty of Chemistry, Nicolaus Copernicus University in Torun,
Gagarina 7, Torun 87-100, Poland

[4] Univ Lyon, INSA Lyon, ECL, CNRS, UCBL, CPE Lyon, INL, UMR5270,
69621 Villeurbanne, France

[5] Department of Chemistry, Taras Shevchenko National University of Kyiv, 60
Volodymyrska, 01033, Kyiv, Ukraine

In this work, we investigated the optical and structural properties of metalloquinolates and their derivatives thin layer. The 8-hydroxyquinoline derivatives are a group of compounds with rich and varied activity. These compounds contain the 8-hydroxyquinoline moiety, which is consist of two rings system: carbocyclic and pyridine rings with hydroxyl group substituted at position-8 [1]. The 8-hydroxyquinolines are good chelating agents that form complexes with a wide variety of metal ions such as Zn^{2+}, Co^{2+} and Al^{3+} due to the proximity of the hydroxyl group to the heterocyclic nitrogen [2]. These properties make the 8-hydroxyquinoline derivatives (i.e. metalloquinolates with/without a styryl fragment) a privileged structure with various physical and chemical properties.

The goal of this work is to investigate the optical and morphological properties of polymer matrix thin layers containing methylquinoline (Meq) and styrylquinoline (STq) by using UV-Vis and IR spectroscopies, as well as SEM technique. Photoluminescence (PL) properties of fabricated films were also analyzed. Layers were deposited on silicon substrate using the spin-coating method. The obtained results will consist of the systematic view of the photo-physical properties for Meq and innovative photoactive materials with a styrilquinoline moiety.

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The exciton spectrum of the quantum dot - quantum ring semiconductor nanostructure in an electric field

***Hnidko I.S.*, Gutsul V.I., Koziarskyi I.P., Makhanets O.M.**

Yuriy Fedkovych Chernivtsi National University,
Kotsyubynsky St. 2, Chernivtsi-58002, Ukraine
E-mail: hnidko.ihor@chnu.edu.ua

The intensive development of nanotechnology has made it possible to create new nanostructures with clear geometric shapes. In particular, structures containing quantum dots and nanorings have already been created and are being intensively studied [1].

In this work, we investigate a nanostructure consisting of a cylindrical semiconductor quantum dot (quantum well, GaAs medium), which through a finite potential barrier ($Al_xGa_{1-x}As$ medium) is tunnel-connected to a coaxial cylindrical nanoring (quantum well, GaAs medium).

Assuming that the lattice constant and the dielectric constant of the nanosystem elements differ slightly from each other, a model of effective masses and rectangular potentials is used to calculate the electron and hole spectra. These values are considered known in all areas of the nanosystem. All theoretical calculations were performed in a cylindrical coordinate system that is appropriate for this case. The corresponding stationary Schrödinger equations for noninteracting electrons and holes in the absence of an electric field are solved analytically exactly. Radial wave functions are obtained as a linear combination of the Bessel, Neumann and modified Bessel functions. The stationary Schrödinger equations for quasiparticles in the presence of an electric field are not analytically solved. For their approximate solution, the unknown wave functions are sought in the form of a decomposition over a complete set of cylindrically symmetric wave functions, and the energy of the electron or hole is found from the solution of the corresponding secular equation. Since the interaction energy between an electron and a hole is much less than the sum of the size-quantized energies of the corresponding quasiparticles, the exciton binding energy is found using perturbation theory.

The dependences of the energies of the electron, hole, and exciton on the magnitude of the electric field strength are analyzed.

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Charge transport through superconducting nanodevices

Belogolovskii M.[1,2], **Zhitlukhina E.**[3], **Seidel P.**[2]

[1] *Kyiv Academic University, National Academy of Sciences of Ukraine,*
36 Vernadsky blvd., 03142 Kyiv, Ukraine
E-mail: belogolovskii@ukr.net

[2] *Institut für Festkörperphysik, Friedrich-Schiller-Universität,*
Helmholtzweg 3, 07743 Jena, Germany

[3] *O. O. Galkin Donetsk Institute for Physics and Engineering, National*
Academy of Sciences of Ukraine, 46 Nauki Avenue, 03028 Kyiv, Ukraine

Any practically used device includes a combination of different materials and/or potential barriers. This makes it important to study and understand new characteristics which appear in the interface region of the materials. When the devices are nanoscale, quantum effects become increasingly important and through the superconductor (S), non-locality and quantum coherence enter in a natural way. This work discuss a scattering matrix formalism to quantum electron transport in complex nanoscale multilayers formed by materials with different charge orderings. We argue that such approach is typically more transparent and efficient for coherent conductors than conventional kinetic equation and Green's function methods and demonstrate it on the example of five-layer planar $NI_1NS_1I_2S_2$ heterostructures where N is a non-superconducting nm-thick conducting film, which can be also magnetically ordered, and I is an insulating barrier.

The idea behind the scattering approach to quantum charge transfer in meso- and nanowires is to decompose the problem into elementary scattering events and calculate their total contribution by summing coupled convergent series. In our case, we have composite terms from interfaces between two contacting films, leakage through barriers, and specific backscattering effects from the superconductor known as Andreev retroreflections. The calculations are carried out sequentially with the inclusion of new elements and taking into account their influence according to the formulas for the probabilities of charge passage through a two-barrier system and reflection from it. If the transfer probability of the entire structure is calculated, then its conductivity can be found using the well-known Landauer formula.

We used numerical results for $NI_1NS_1I_2S_2$ nanodevises to explain unusual conductance features observed previously by various groups that aimed to induce superconductivity in proximized materials with a non-trivial electronic structure. Benchmark experiments to prove that the features discussed do indeed reflect theoretically expected signatures of exotic physical phenomena as Majorana zero modes or Andreev bound states in unconventional superconductors are proposed.

Structural features of aqueous solutions of alcohols

Atamas N.[1, 2], **Taranyik G.**[3]

[1] *Taras Shevchenko National University of Kyiv,*
Kyiv 01601, Ukraine
E-mail: atamasphys@mail.univ.kiev.ua

[2] *Institute of Physical Chemistry Polish Academy of Sciences,*
Kasprzaka 44/52, 01-224 Warsaw, Poland

[3] *International European University, Kyiv 03187, Ukraine*

At a recent time, there has been more and more attention to the study of the mechanisms that regulate hydrophobic and hydrophilic interactions in water, which determine the main causes of the behavior of aqueous solutions of biological macromolecules. Monohydric alcohols, which have both hydrophilic (hydroxyl OH groups), and hydrophobic groups (methyl and ethyl groups) allow to be considered as simple model systems to obtain information on the behavior of biomolecules in water. In addition to the above, in the course of studies of the concentration-structural features of aqueous solutions of monohydric alcohols with the use of Monte Carlo method, the following goals have been being achieved: to study the effect of the hydrophilic properties of alcohols on changes in the structural characteristics of aqueous solutions at various concentrations of alcohol; to build up the model representations for the structure of aqueous solutions of alcohols at various concentrations. On the basis of the studies carried out the following have been established: (1) in an aqueous solution of ethyl and propyl alcohols at $X_{al} \cong$ (< 0.05 ppm of the ethyl alcohol, and 0.04 ppm of propyl alcohol), the alcohol molecule does not change the percolation properties of the network of HB between water molecules;(2) the value of the dipole moment of an alcohol affects the structural characteristics of clusters of alcohol molecules in water at $X_{al} \cong$ (0.2-0.25) ppm.;(3)· at $X_{al} > 0.3$ ppm. it occurs the structure of clusters is rearranged from alcohol molecules into structures similar to reverse micelles. The number of alcohol molecules that form reverse micelles does not depend on the structure, and dipole moment of alcohol molecules, and is equal to 4 ;(4)· at $X_{al} \cong$ (0.6 - 0.8) ppm rupture of micelles formed by alcohol molecules occurs. At these concentrations there can also exist free alcohol molecules, and half-chains of four alcohol molecules as well.

Defect structure and kinetic properties of $CdSe_xTe_{1-x}(x=0.1)$ solid solution: ab initio calculation

Malyk O.P.[1], Syrotyuk S.V.[1]

[1] Semiconductor Electronics Department, Lviv Polytechnic National University. Bandera Street, 12, Lviv-79013, Ukraine.
E-mail: omalyk@ukr.net

$CdSe^xTe_{1-x}$ possesses unique physical properties necessary for photovoltaic converters of solar energy, namely, a required band gap width and needed absorption coefficient value. The optical and electrical properties of this material (in particular, the absorption coefficient and the transport phenomena) strongly depend on the structure of intrinsic and impurity point defects. Therefore, the study of the $CdSe_xTe_{1-x}$ defects structure is an actual applied problem. In literature there is a wide range of works where the ab initio approach is used to calculate the structure of defects. However, a common disadvantage of these works is the absence of connection between the structure of point defects and the kinetic characteristics, which determine the electronic properties of the material. In the proposed study the point defects in n-$CdSe_{0.1}Te_{0.9}$ are considered, namely: Cd_{Te}, Cd_{Se}, Te_{Cd}, Se_{Cd}, V_{Te}, V_{Se}, V_{Te}–Cd_{Te}, V_{Se}–Cd_{Se}. To calculate the energy spectrum of the ideal and defect structure the supercell method was used on the base of the ABINIT code. To establish the temperature dependence of the energy spectrum of an ideal and defect supercell an empirical formula for the temperature dependence of the band gap was used [1]. By choosing a mixture of the usual exchange-correlation GGA potential and the Hartree-Fock exchange potential a coincidence of experimental and theoretical values of the band gap was achieved at 0 and 300 K. The description of the transport phenomena in n-$CdSe_{0.1}Te_{0.9}$ was performed on the basis of short-range electron scattering models [2,3]. For crystals with defect concentration $1\times10^{14}\div 1\times10^{18}$ cm^{-3} the temperature dependences of electron mobility and Hall factor in the range 15 – 400 K are calculated.

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Magnetic field effect on the optical properties core-shell type II quantum dot

***Holovatsky V.A.**[1]*, ***Chubrei M.V.**[1]*, ***Duque C.A.**[2]*

[1] *Department of Theoretical Physics and Computer Modelling,*
Chernivtsi National University after Yuriy Fed'kovych.
Kotsiubynsky str, 2, Chernivtsi-58002, Ukraine

[2] *Grupo de Materia Condensada-UdeA, Facultad de Ciencias Exactas*
y Naturales, Instituto de Física, Universidad de Antioquia,
Medellín AA 1226, Colombia
E-mail: v.holovatsky@chnu.edu.ua

This study presents a simple model within the effective mass approximation to describe the magnetic field impact on the energy structure and interband optical quantum transitions in type-II ZnTe/CdSe spherical quantum dots. The dependencies energy spectra and wave functions of an electron and hole on the magnetic field are calculated by the diagonalization method for spherical quantum dots different sizes.

It is shown that the magnetic field violates the spherical symmetry of the system and takes off the degeneration of energy spectrum with respect to the magnetic quantum number. The energy of the electron in the states with $m \geq 0$ increases when magnetic field enhances; for the states with $m<0$ these dependences are non-monotonous (decreasing at first and then increasing). Moreover, the ground state of electron, which localized in the spherical shell CdSe, is formed alternately by the lowest states $m=0, -1, -2, \ldots$ with increasing the induction of magnetic field [1-2] (Aharonov Bohm effect). The hole is localized in the core and it ground state $m=0$ at all range magnetic field value.

The absorption coefficient and oscillator strength of the quantum transitions are calculated as function of the magnetic field induction [3].

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Optical absorption in core-shell quantum antidot with donor impurity under applied co-directed electric and magnetic fields

Chubrei M.V., Holovatsky V.A., Holovatska N.H.

Chernivtsi National University after Yuriy Fed’kovych.
Kotsyubynsky, 2, Chernivtsi - 58012, Ukraine.
E-mail: chubrei.maryna@chnu.edu.ua

The dependence of the energy spectrum on the size of nanoparticles, the effect of external fields, and impurity presence in nanoparticles give great potential for the practical application of quantum dots in optoelectronic systems such as light-emitting diodes and flat light-emitting panels, lasers, photodetectors, cells of solar panels and photoelectric converters.

Theoretical studies of the co-directed electric and magnetic fields influence on an electron energy spectrum and wave functions are fulfilled in the multilayer spherical quantum dot (MSQD) $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ with off-center donor impurity. The calculations were done within the effective mass approximation and the nanosystem rectangular potential profile by the matrix method using the exact electron wave functions in the nanosystem without the external fields and impurity effects [1]. In this paper it was investigated external fields combined effect and core size on the electron energy spectrum, binding energies of an off-center hydrogenic donor impurity and optical absorption coefficients.

For the electron energy spectrum, the ground state shifts to a lower energy region as the electric field strength increases. The magnetic field shifts all energy levels to a higher energy region. The magnetic field effect is stronger for larger nanostructures.

The linear $\alpha^{(1)}(\omega)$, third-order nonlinear $\alpha^{(3)}(I,\omega)$ and total optical absorption coefficients are defined by taking into account quantum transitions from ground to several excited states. The results show that external fields and impurity presence effects cause significant changes on the optical absorption coefficient. For nanosystems with a bigger core, the external fields effect is stronger. The absorption coefficients maximums shift to the region of higher energies with the increase of the magnetic field induction.

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Spin-reorientation phase transition and nonequilibrium thermodynamics of compensated ferrimagnet $ErFeO_3$

Zubov E.E.[1,2]

[1] *Kyiv Academic University, National Academy of Sciences of Ukraine,*
36 Vernadsky blvd., 03142 Kyiv, Ukraine
E-mail: eezubov@ukr.net

[2] *Vasyl' Stus Donetsk National University,*
21 600-Richchya Str., 21021 Vinnytsia, Ukraine

Orthoferrites with a general formula RMO_3, where R and M are rare-earth and transition metal ions, are studied during a long time as physical objects with pronounced quantum properties of their thermodynamical behavior. Currently, it became clear that these compounds have good perspectives for applications in ultrafast spin switching devices, sensors, high-frequency generators due to their unique characteristics associated with the presence of magnetoelectric coupling, negative magnetization, spin flips, and exchange bias.

In this work, in the framework of quantum mechanical theory with anisotropic Hamiltonian an expression for the free energy $F(\alpha)$ as a function of antiferromagnetic axis direction was obtained. The detailed $F(\alpha)$ analysis for $ErFeO_3$ shows availability of two minima with $\alpha = \pm\pi/2$ and a potential barrier near the compensation temperature Tcomp. The anisotropy of the R-M exchange interaction plays an important role in realization of spin-reorientation phase transition at temperature $T = T_{SR} = -d^2\sigma(\sigma+1)(J_x^2-J_z^2)/(bJ^2)$, where d, J_i and b are Dzyaloshinskii–Moriya parameters, Er^{3+}-Fe^{3+} and Fe^{3+}-Fe^{3+} anisotropic parts of exchange interactions, respectively, with an isotropic part J for Fe^{3+} - Fe^{3+} exchange and effective spin σ. Therefore, orthoferrites with low T_{SR} point out on a weak anisotropy of the *R-M* exchange interaction.

Using the experimental data for magnetization, T_{comp}, T_{SR} and the Neel temperature, microscopic parameters of interactions in $ErFeO_3$ have been determined. One can say that the studied othoferrites are related to systems with competing interactions. The Neel-Brown model for magnetic nanoparticles is used to explain the experimentally observed effects of the irreversibility, spin overturns and exchange bias in the hysteresis phenomena.

Investigation of nanoscale core-shell structure of silicon microcrystal doped by boron and nickel: properties and application

Druzhinin A., Ostrovskii I., Khoverko Yu., Liakh-Kaguy N., Medvid A.

Department of Semiconductor Electronics, Institute of Telecommunications,
Radioelectronics and Electronic Engineering, Lviv Polytechnic National
University, Kotliarevskyi Str., 1, Lviv-79013, Ukraine.
E-mail: druzh@polynet.lviv.ua.

The p-type silicon microcrystals doped with boron impurity and modified with nickel transition metal impurity were investigated. According to the results of Hall studies, the concentration of impurities of electrically active charge carriers corresponds to the metal-dielectric transition in silicon (5.5×10^{18} см$^{-3}$). The electrical conductivity of crystals was studied in a wide temperature range from 4.2 K to 300 K. Due to the specific "core-shell" structure of the crystal, the magnetoresistance of the crystal in magnetic fields up to 14 T was studied. The level of doping of silicon microcrystals doped with boron impurities doped to concentrations is substantiated: Boron impurities doped to concentrations of 5×10^{18} см$^{-3}$, which directly corresponds to the metal-dielectric transition in silicon on the dielectric side for use in microelectronic magnetic field sensors with magnetoresistive principle of operation.

The use of Si <B, Ni> microcrystals allows to create high-precision sensitive elements of the microelectronic sensor that can operate in liquid helium temperatures under strong magnetic fields up to 14 T with the ability to integrate sensitive elements with information processing schemes and low cost.

As a result of magnetic field studies, it was found that the proposed sensitive element of the microelectronic sensor has a extremely high sensitivity to the magnetic field, and the simplicity of construction provides low inertia and high speed.

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Quantum wells delta-doped to the center with background doping in barriers

Demediuk R.[1]***, Tulupenko V.***[1,4]***, Akimov V.***[1,2]***, Tiutiunnyk A.***[3]***,***
Duque C.[1,4]***, Sushchenko D.***[1]***, Fomina O.***[1]***, Laroze D.***[3]

[1] *Physics Department, Donbas State Engineering Academy,*
Academichna str., 72, Kramatorsk-84313, Donetsk reg., Ukraine.
E-mail: demediuk.roman@gmail.com

[2] *Facultad de Ciencias Basicas, Universidad de Medellín, Grupo de Materia Condensada-UdeA, Universidad de Antioquia, Medellín, Colombia.*

[3] *Instituto de Alta Investigación, CEDENNA, Universidad de Tarapacá, Arica, Chile.*

[4] *Grupo de Materia Condensada-UdeA, Universidad de Antioquia, Medellin, Colombia.*

Previously we proposed the idea of a novel design of tunable optical device based on intersubband transitions within quantum well and grounded it numerically for Si/Ge heterostructure [1]. The tunability is provided by altering the ionization degree of the Phosphorus delta-layer within the well and subsequent distortion of potential profile of the well that leads to the change of transition energies and working frequencies of the device. To calculate energy characteristics of the structure we elaborated a numerical method based on the self-consistent scheme by including impurity binding energy with a Vinter technique [2] as a part of iteration.

Here we verify the viability of the proposed design by including sparce background impurity to the barriers of the structure in the approximation of a single well with infinite barriers. We have modified the numerical procedure to account for the infinite barriers and altered calculation of Fermi energy.

Calculations for the background impurity up to 10^{16} cm^{-3} showed that the tuning effect remains stable qualitatively with some notable quantitative changes for higher concentrations. The binding energy of impurity within the well demonstrated changes about two times depending on the ionization degree of the delta level.

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Kinetic theory of magnetic absorption of laser irradiation by a metallic nanoparticles

Biliuk A.A., Semchuk O.Yu., Havriliuk O.O.

Chuiko Institute of Surface Chemistry NAS of Ukraine
17 General Naumov Str., Kyiv 03164 Ukraine.
E-mail: philosoph.tb@gmail.com

The kinetic theory is constructed and the dependence of the magnetic absorption on the ratio of the radii of curvature of spheroidal metal nanoparticles is theoretically investigated $\rho = R\perp/R\|$, as well as the dependence of the angle between the axis of symmetry of the spheroid and the vector of the magnetic field of the electromagnetic wave θ. The magnetic absorption of electromagnetic waves by a small metallic particle of ellipsoidal form is investigated in frequency regions both higher and lower than the characteristic frequency of the free passage of an electron between walls of the particle. The boundary conditions chosen are diffuse reflection of the electron from the inner surface of the particle. For the case when the thickness of the skin layer is large compared to the characteristic size of the particle, analytical expressions are obtained which permit determination of the dependence of the energy absorbed by a particle on its shape and orientation with respect to the direction of incidence of the radiation. The low-frequency absorption by small metallic particles is analyzed in detail for the first time. For particles in the form of oblate or prolate ellipsoids of revolution it is shown at particle sizes and what initial polarizations of the incident wave that the magnetic absorption becomes dominant over electric absorption. We have found that when the shape of the particle deviates from spherical to the oblate side, one can obtain growth of the magnetic absorption if electric field E_0 is directed along the major axis of the ellipsoid. If E_0 is directed along the minor axis, then for particles of prolate shape significant growth of the magnetic absorption in comparison with the spherical particle! can be achieved in the MT- polarization and a small amount of growth in the ML- polarization. For oblate particles the electric absorption is dominant in these polarizations. The work also contains the results of computational experiments. The most interesting result of the latter is the growth of the energy absorption by the spheroidal nanoparticle with the growth of (its disk-like character) at an arbitrary value of the angle. Of much greater interest is thespatial distribution of the ratio between the energies absorbed by spheroidal nanoparticles $W_m(\rho,\ \theta)W^0_m$. The only value, at which the curve $W(\theta=\pi/2)/\ W(0)\ m$ asymptotically approaches zero, is $\theta = \pi/2$.

Electrical conductivity, mechanical and optical properties of polyamide 6 composites with methylene blue dye

Popruzhko V. M.[1], Pinchuk-Rugal T.M.[1], Dmytrenko O.P.[1], Kulish M.P.[1], Onanko A. P.[1], Strelchuk V.V.[2], Kolomys O.F.[2], Alieksandrov M.A.[2]

[1] Taras Shevchenko Kyiv National University, Kyiv, Ukraine.
64/13, Volodymyrska Street, City of Kyiv, Ukraine, 01601.
E-mail: pvm13031997@gmail.com

[2] National Academy of Science of Ukraine,
V.E. Lashkaryova Institute of Semiconductor Physics NAS of Ukraine.
03028 Ukraine, Kyiv, 45, Nauky pr.

Polyamide 6 (PA6) has an excellent properties such as hydrogen bone in molecular chains of the polyamide which makes it one of the major engineering and high performance plastic [1]. Methylene blue (MB) is a heterocyclic aromatic compound containing a thiazine ring, and has many applications in microbiology, medicine and diagnostic fields [2].

Physically-mechanical properties of polyamide can be improved by creating composites filled with methylene blue.

In this work the electrical conductivity, shear modulus, Young's modulus, Raman and photoluminescence spectra of PA-MB nanocomposites were investigated. It is shown that for nanocomposites PA/MB with the increasing concentration of the modifier, the electrical conductivity of composites increases by almost an order of magnitude, contact phenomena are dominant. Mechanical characteristics are nonmonotonic. There is a change in the intramolecular structure. Emission centers in the photoluminescence spectra are shifted, fig.1.

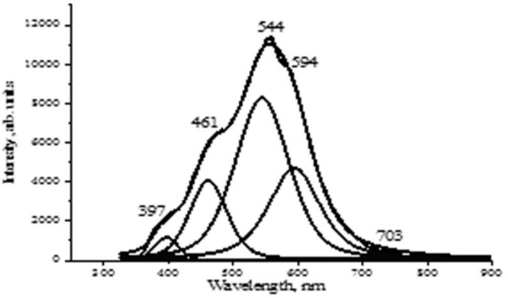

Fig.1. *Photoluminescence of PA 6 (λex=325 nm, T=293 K).*

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ZnO “seed” layers deposited by magnetron sputtering: the effect of the nanoscale morphology on the morphological and optical properties of ZnO aligned nanorods layer grown on it

Vasin A.V. **[1, 2], *Rusavskya A.V., Yatskiv R.*[3], *Nazarov A.N.*[1, 2]**

[1] *Lashkaryov Institute of Semiconductor Physics NAS of Ukraine, Kyiv, Ukraine*

[2] *National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”, Kyiv, Ukraine*

[3] *Institute of Photonics and Electronics of the Czech Academy of Sciences Chaberska 1014/57, 182 51, Prague, Czech Republic*

The research is concerned with the growth of ZnO aligned nanorods (NRs) layers as antireflection layers on the top of transparent n^+-ZnO thin films to reduce optical reflection from the ZnO surface. In the solar cells, the antireflection layer plays an important role in the improvement in the conversion efficiency by increasing the light transmission and suppressing the Fresnel refraction. It has been demonstrated earlier that the arrays of vertically aligned ZnO nanorods grown via hydrothermal processing can be effectively used as antireflection surface layer through increased light coupling [1,2]. It has been reported that nanoscale morphology, controlled through synthetic chemistry, has a great effect on the macroscopic antireflection performance. Calculations suggested that the highly tapered ZnO NRs on Si reduced the reflectance wavelength dependence due to the nanoscale morphology, because the tapering produces impedance matching between Si and air through a gradual reduction of the effective refractive index away from the surface, resulting in low reflection particularly at longer wavelengths and eliminating interference fringes through roughening of the air-ZnO interface. Variation in the nanorod length, presence of a fused ZnO base layer, and introduction of tip tapering all contributed to the decrease in reflectance and the elimination of interference fringes, in good qualitative agreement with experimental results.

In present work we suggest to develop similar approach for the synthesis of ZnO NRs antireflection layers on the top of conductive n^+-ZnO window for thin film solar cells. Conductive “seed” layers have been deposited on Si wafers and glass substrates by RF magnetron sputtering. It has been demonstrated by SEM examinations that morphology of the ZnO NRs is determined not only by hydrothermal synthesis conditions but by morphology of the “seed” layer as well. For example, diameter of ZnO NRs was found to be strongly correlated with average size of the grains in “seed” layer, while grain size in the seed layers was found to be strongly correlated with ZnO film thickness. The finest ZnO grains were observed in very thin “seed”. The thicker “seed” layer the larger grain size. Typical diameter of ZnO NRs of few tens of nanometers were successfully grown on the “seed” layer with smallest thickness of few tens of nanometers. It has been demonstrated that such morphology strongly reduced optical reflectance of the surface. However the effect of the NRs layer in the optical transmittance was more complicated. The effects of ZnO NRs layer on optical properties of the surface will be analyzed and discussed in the presentation.

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RF-dynamics of vortex kinks in the mixed state of nanostructured superconductors with columnar defects

Boliasova O.O.[1], ***Kasatkin A.L.***[2], ***Pokusinskii A.O.***[3],
Shapovalov A.P.[4], ***Tsvitkovskyi V.P.***[2]

[1] *Donetsk Institute for Physics and Engineering Named after O. O. Galkin,*
NAS of Ukraine, Nauky Ave., 46, Kyiv-03028, Ukraine.
E-mail: ol.boliasova@gmail.com

[2] *G. V. Kurdyumov Institute for Metal Physics, NAS of Ukraine,*
36 Academician Vernadsky Blvd., Kyiv-03142, Ukraine.

[3] *Taras Shevchenko National University of Kyiv,*
Volodymyrska St, 60, Kyiv-01033, Ukraine.

[4] *Kyiv Academic University, 36 Academician Vernadsky Blvd.,*
Kyiv-03142, Ukraine.

We suggest a theoretical model for the microwave response of Abrikosov vortices in nanostructured superconductors with columnar defects which serve as effective pinning sites for vortices that are considered as the elastic strings [1]. For this case, we suppose that microwave losses related to the vortex oscillations in a microwave field arise caused by viscous oscillations of vortex kinks, which connect different parts of the vortex line pinned on adjacent columnar defects. In what follows it is supposed that there is rigid pinning of vortex parts settled on columnar defects while vortex kinks can viscously move along the columnar defect axis under the Lorentz force action. At high enough temperatures vortex kinks arise as thermal excitations of the whole vortex lines settled in potential wells produced by columnar defects. In this case, the kinks attract to the flat specimen surface and their concentration inside the superconductor should obey the barometric law. For the case of inclined magnetic field $\boldsymbol{H}$, *rf* losses due to viscous kinks oscillations under the microwave current action arise even at $T=0$ if the inclination angle θ_H concerning the columnar pinning site axis (z-axis) exceeds some locking angle value θ_L [2].

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Magneto-optical visualization of the mechano-thermal effect on the pinning structure in the NbTi

Rusakov V.F.[1]***, Chabanenko V.***[2]***, Kuchuk O.I.***[2]***, Chumak O.M.***[3]***, Abaloszewa I.***[3]***, Abaloszew O.***[3]***, Nabiałek A.***[3]***, and Puźniak R.***[3]

[1] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv 03056 Ukraine*
E-mail: vladimir.rusakov26@gmail.com

[2] *O. Galkin Donetsk Institute for Physics and Engineering, NAS of Ukraine, Kyiv 03028 Ukraine*

[3] *Institute of Physics, Polish Academy of Sciences,*
Warsaw 02-668, Poland

The paper considers the effect of magnetic flux pinning centers that arise in the Nb50%Ti superconducting alloy obtained as a result of thermo-mechanical cycling, consisting of a series of material drawing and heat treatment on the front of the magnetic flux penetrating the superconductor in an external magnetic field. A magneto-optical technique was used to determine the structure of the flux front of both the hydroextruded sample, which is determined by the pinning centers that appear during the flow of the material under the action of external pressure during extrusion, and the heat-treated sample. As a result, successive positions of the flux fronts in the samples obtained with different processing methods and different temperatures were plotted. The scaling analysis of the flux profile behind the front using fast Fourier transform method was carried out of the roughness exponent [1] of both the methods of processing the sample and the temperature was studied. It is shown that the depth of flux penetration into the sample after annealing decreased significantly, which indicates an increase in the critical current density, which in turn indicates a change in the pinning structure. The dependence of the roughness exponent on the external field is nonmonotonic. Other features of magnetic field penetration into SC are discussed.

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Viscoelastic properties of starches measured by the ferrofluid droplet deformation method

Azarkh D., Schnakenberg U.

Institute of Materials in Electrical Engineering
1, RWTH Aachen, Aachen, 52074, Germany.
E-mail: azarkh@iwe1.rwth-aachen.de

The viscoelastic properties of starches of different concentrations from normal corn (NC) and waxy corn (WC) were investigated. Ferrofluid droplets were injected into the starches by micropipettes. After applying constant magnetic stress, the time-dependent strain was calculated from measuring the minor and major radius of the elliptically deformed droplet. The obtained creep curves are shown in Fig 1. The creep behaviour of starch can be well described by an appropriate mechanical equivalent circuit, for example, the generalized Kelvin-Voigt model (GKV) or generalized Maxwell model (GM) [1]. While the GM model describes viscoelastic liquids, it would be better suited for a precise physical description of the experiment. However, GKV is easier to calculate and can be analytically described by following equation [1],

$$\varepsilon(t) = \frac{\sigma}{E_0}\left(1+\frac{E_0}{E_1}\left(1+e^{\frac{tE_1}{\eta_1}}\right)+\frac{E_0}{E_2}\left(1+e^{\frac{tE_2}{\eta_2}}\right)\right)$$

The extracted coefficients $(E_0, E_1, \eta_1, E_2, \eta_2)$ from the upper fitted function can be transformed to the respective coefficients in GM $(E_0^m, E_1^m, \eta_1^m, E_2^m, \eta_2^m)$ according to the known relations between the two models [1]. Values of elasticity and viscosity at two retardation time constants are presented in Fig. 1 A comparison with oscillatory tests [2] allows us to consider the delayed elasticity E_2^m and the viscosity η_2^m as the Young's modulus and the viscosity of the starch.

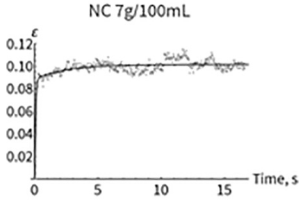

Fig.1 *Creep curve of NC 7 g/100 mL (dots) and fitted function (line).* E_0^m *is the capillary stress from the ferrofluid droplet,* E_1^m *and* η_1^m *describe the instantaneous elasticity and viscosity, respectively, while* E_2^m *and* η_2^m *denote the delayed elasticity and viscosity*

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Method of reducing cmos inverter switching energy

Druzhinin A.A.*, Kogut I.T., Holota V.I.,
Nichkalo S.I.*, Khoverko Y.M.*, Benko T.G.

Vasyl Stefanyk Precarpathian National University,
57 Shevchenko St., Ivano-Frankivsk, Ukraine, 76018,
taras.benko@pnu.edu.ua

**Lviv Politechnic National University,*
12 Bandery St. Lviv, Ukraine, 79013, druzh@polynet.lviv.ua

Abstract – A method for reducing the switching energy of the CMOS inverter by using additional transistors that are switched to triode mode when the switching transistors are saturated is proposed.

Keyword – CMOS inverter, power consumption, state switching, peak current

One of the important aspects when designing CMOS inverters is to reduce power consumption. The energy consumption of CMOS inverters is determined by an expression that contains static and dynamic components:

$$P = I_{DDQ}V_{DD} + (C_{Dn} + C_{Dp} + C_{OUT})V_{DD}^2 f,$$

where I_{DDQ} – quiescent leakage current; V_{DD} – power supply; C_{Dn}, C_{dp}, C_{OUT} – drains and output capicitance; f – frequency of signal change.

When switching the inverter Fig. 1a between the states of log.1 and log.0 there is an area in which $V_{out} = V_{in} = V_M$ and both CMOS transistors are in a state of saturation, Fig. 1b.

The middle of this region $VM = V_{DD}/2$ is taken as the switching threshold if the conditions $\beta_n \approx \beta_p$, $V_{thn} = |V_{thp}|$, $W_p/W_n = \mu_n/\mu_p$ are met. In the middle of the switching

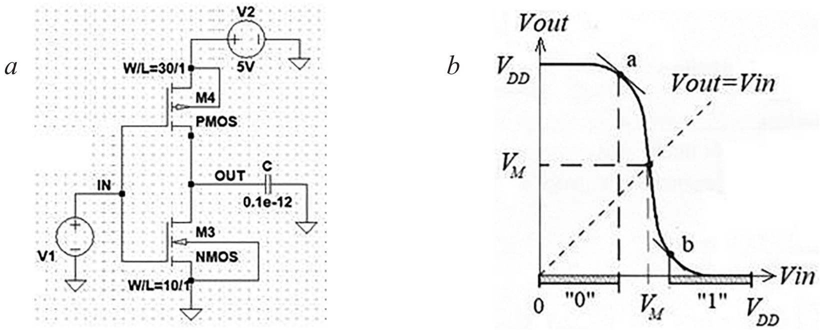

***Fig. 1**. Switching threshold of CMOS inverter*

area corresponds the maximum value of the leakage current $I_{DDQ}=I_{peak}$ from the power supply to the grounded substrate, Fig. 1c.

To reduce the leakage current, and hence the static component of the switching energy, it is proposed to connect additional CMOS transistors and their control circuit to the leakage current flow paths. The Ipeak current control circuit will switch additional CMOS transistors to triode mode, thereby limiting peak currents.

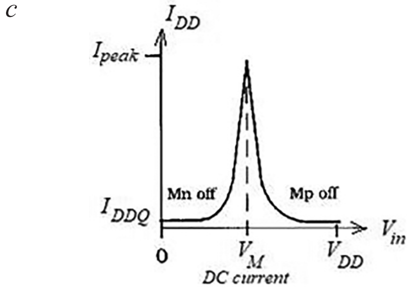

***Fig. 1**. Switching threshold of CMOS inverter*

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Short-scale scattering effects in critical fluids and heterogeneous media

***Sushko M.Ya*, Krychun T.V., Vorobel A.V.**

Department of Theoretical Physics and Astronomy,
Odesa I.I.Mechnikov National University.
2 Dvoryans'ka St., Odesa 65026, Ukraine.
E-mail: mrs@onu.edu.ua

Multiple scattering theory is a traditional technique for study of optical properties of systems incorporating various local inhomogeneities, such as order-parameter fluctuations in critical fluids, dispersed particles in solutions, or filler inclusions in composite materials. Since, in most cases, the higher-order correlation functions of a system are unknown, the pertinent iterative series for the scattered field is truncated to include several corrections to the first Born approximation, and the higher correlation functions involved are replaced by model expressions.

We argue that such an approach leads to overlooking significant effects caused by multiple reemissions and correlations among inhomogeneities spaced by distances much shorter than the wavelengths of probing radiation in the system. Using a special representation fot the inner propagators, these "short-scale" scattering contributions can be singled out from the entire iterative series and then summed up without employing uncontrolled assumptions.

To exemplify one of these effects, we present our latest results of processing critical opalescence data for xenon [1]. They reveal the significance of so-called molecular light scattering of multiplicity 1.5 [2] near the liquid-vapor critical point. In particular, this scattering may noticeably affect the width of the overall spectra, causing its multiplicative renormalization and altering its temperature dependence.

The other example demonstrates the effect of short-scale scatterings on the parameters of photon transport in concentrated suspensions of nanoparticles [3].

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Tunneling of the ultrarelativistic dirac quasielectrons through the structure based on the dice lattice

Korol A.M.[1,2]***, Medvid N.V.***[1]***, Shevchenko O.***[1]

[1] *National University of Food Technologies,*
Volodymyrska str., 68, Kyiv,

[2] *Laboratory on Quantum Theory in Linkoping, International Society*
for Independent Research (ISIR), box 8017, Linkoping, 58080 Sweden

The ballistic motion of the ultrarelativistic quasi-electrons in a structure based on a dice lattice is considered and studied. It is assumed that the barrier has a rectangular shape and is created by the external electrostatic potential. The transmission coefficient T is calculated in the continuous model by matching of the eigenfunctions at the interface of the barrier and out-of-barrier areas. The eigenfunctions, in turn, are found as a solution of the Dirac-type equation with the Hamiltonian, which takes into account the presence of a flat energy band. The difference in the values of the Fermi velocity in the barrier and out-of-barrier regions (v_1 and v_2 respectively) is taken into account. It is also believed that the flat band is located halfway between the valence band and the conduction band and is separated from each of them by the energy gap Δ. The detailed analysis of the tunneling spectra (dependences of the transmission coefficient Ton the quasielectron energy, incidence angle, Fermi velocity, electrostatic potential, energy gap Δ) is provided. Depending on the values of the parameters of the considered structure, it is possible to implement a large number of different spectra. In particular, it is shown that: 1. Tunneling spectra have a pronounced angular dependence, i.e. the transmission coefficient T varies greatly when the angle of incidence of quasielectrons on the structure changes. 2. Spectra are highly sensitive to changes in the Fermi velocity (in the parameter $\beta = v_2/v_1$). 3. At certain combinations of the parameter values, the phenomenon of supertunnelling is observed, which is that the transmission coefficient is equal to unity regardless of the angle of incidence of quasi-electrons on the structure. 4. The Klein tunneling can also be manifested in this structure. 5. For many parameter values the Klein tunneling can be suppressed. 6. For certain values of the parameters, there may be a wide plateau of incidence angles for which T is close to unity. This phenomenon can be called the limited supertunnelling. 7. For most parameter values, the spectra are characterized by three regions with T values that differ significantly. This is due to the possibility of both intra and inter tunneling between the conduction and the valence bands of the considered structure.

Gate tunable electron interaction in atomically thin dielectric films

***Kostrobii P.P.*, Ryzha I.A.**

Lviv Polytechnic National University,
12 Bandera Street, Lviv, Ukraine, 79013.
E-mail:Petro.P.Kostrobii@lpnu.ua

High dielectric constant (high ε – 2D systems) enjoy an intense experimental and theoretical attention [1, 2]. The interest is motivated by a high technological promise of such systems for fabrication of nanoscale capacitors components.

In this paper we present the results of the theoretical investigation of the electrostatic potential φ in a dielectric film with a high dielectric permittivity ε_1 that is sprayed over a substrate with a dielectric constant ε_2 ($\varepsilon_1 >> \varepsilon_2$). In contrast to [2] here we considered the influence of polarization effects that emerge on the interface between dielectrics.

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Modeling of thermodynamic characteristics of 2D electronic layers near the surface of an atomically thin dielectric

Kostrobii P.P.**, **Markovych B.M.**, **Ryzha I.A.**, **Polovyi V.Ye.

Lviv Polytechnic National University,
12 Bandera Street, Lviv, Ukraine, 79013, Ukraine.
E-mail: Vitalii.Y.Polovyi@lpnu.ua

Over the past 50 years transport, optical and thermodynamics properties of two-dimensional electrons have been extensively studied in the metal-oxide-semiconductor [1] and semiconductor [2] heterostructures. During last years an atomically thin dielectric (ATD) films, such as mono- and a few-layer hexagonal boron nitride or transition-metal dichalcogenides, have substantially studied [2].

In this paper we proposed and investigated a model of inversion layer of electrons near ATD. Unlike an approach proposed in [2] we investigated degenerated inversion layer of electrons with a correct taking into account of the electroneutrality condition. Carried out a comparative analysis of the obtained results with an experimental data for inversion layers in the metal-dielectric-semiconductor structures.

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CFD-simulation and analyses of cavitation and dispersion processes for globulated multilayer graphene obtaining

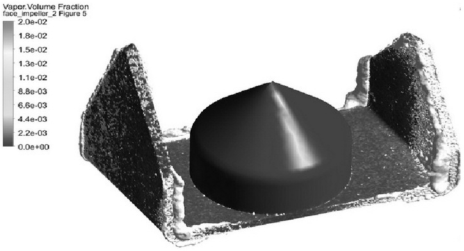
Strativnov E.V.[1], Khovavko A.I.[1], Nie Guochao[2], Pu-Guang Ji[3]

[1] Nano-technologies department of Gas Institution of the NAS of Ukraine.
Gegtarevska, 39, Kyiv-03131, Ukraine.
E-mail: estrativnov@gmail.com

[2] School of Physics and Telecommunication Engineering (China).

[3] School of Materials Science & Engineering and Tianjin Key
Laboratory of Materials Laminating Fabrication and Interface
Control Technology (China).

Globulated multilayer graphene has recently been introduced as an electron-conductive additive in lithium-ion batteries. When optimally mixed with the base, it forms a three-dimensional electron-conducting network of cathode material. This increases the conductivity of the material and the charging speed of the battery [1]. Given the advantage of electronically conductive graphene additive over other types of carbon, it can be expected to be widely used in commercially available high-performance lithium-ion batteries.



Multilayer globular graphene [2] can produce from thermally expanded graphite [3]. Cavitation (centrifugal mechanical cavitator) is one of the stages of its mechanical processing.

In this paper, the CFD-simulation of a real cavitation machine will be considered. The analysis of the obtained data was carry out with the aim of its technological and energy optimization.

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Plasmon resonance in the prism structure with sinusoidal grating

Vernyhor O.L.

Department of Electronic Engineering,
Lviv Polytechnic National University,
S.Bandery str.12, Lviv, 71013, Ukraine.
E-mail: oleksandr.l.vernyhor@lpnu.ua

Nowadays, there is an increasing interest in optimizing plasmon sensors based on prisms by forming periodic structures on them [1,2]. Plasmon resonance in the prism structure, on the surface of which a sinusoidal relief profile with silver film, has been researched by the finite element method (FEM). The angular sensitivity was calculated for the wavelength 1064 nm. At this wavelength for silver, the refractive index is 0.087829 and the extinction coefficient is 7.6761 [3]. The refractive index of the prism is 1.76. The period of the sinusoidal grating is 150 nm. Resonance angles for two refractive indices of the research medium n1 = 1.333 and n2 = 1.334 were determined. The angular dependence of absorption and reflection is obtained in the structure heights ranging from 0 to 100 nm.

It was determined that the sensitivity increases from 1 to 2.8 rad with increasing structure height. However, increasing the height leads to a degradation of the resonant properties of the structure, which is expressed in a reduction in resonant absorption. Also, with the increasing height of the structure, there is an expansion of the resonance curve from 0.0018 to 0.0161 rad. This suggests that the optimal selection of the height of the structure can improve sensitivity.

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Structural anisotropy of ethylene vinyl acetate film

Kislyuk V.V.[1]***, Vorona I.P.***[2]***, Trachevskij V.V.***[3]***, Kotrechko S.O.***[1]

[1] *G.V.Kurdyumov Institute of Metal Physics, NAS of Ukraine,*
36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine.
E-mail: viktor.kislyuk@gmail.com

[2] *V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine,*
41 pr. Nauki, 03028, Kyiv, Ukraine.

[3] *Technical Center, NAS of Ukraine,*
Pokrovs'ka St., 13, UA-04070, Kyiv, Ukraine.

Eethylene vinyl acetate (EVA) film used widely as encapsulant for photovoltaic modules [1] was found to demonstrate rather strong anisotropy (as to the axis of its rolling) both at macrolevel (mechanical tensile creep testing) and nanolevel (paramagnetic resonance spectra - EPR).

Tensile testing. The film oriented parallel to the rolling direction have several orders of magnitude longer time of creep than that of the sample oriented perpendicularly at the same conditions of the.

EPR spectra (Fig. 1) contain wide bands and narrow triplet series (with a suppressed component) attributed to hindered amine stabilizer. The former is sensitive to the orientation of samples as to the constant magnetic field and to their line of rolling while production. The series of the stabilizer resonances remains almost unchanged and used for quantitative analysis.

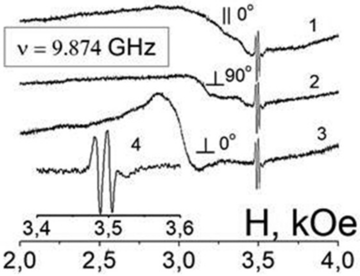

Fig 1. *EPR of the EVA film cut parallel (1) and perpendicular (2,3) to the rolling direction and placed in the resonator with* ***H*** *in-plane (2) and out of plane of the film (1,2) (with 90 and 0 angle between H and normal, respectively);*
(4) – zoomed-in fragment corresponding to triplet of hindered amine stabilizer.

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New reversible photothermoplastic oligomer recording media and its application in the holographic method of determination of refractive index of liquid objects

***Studzinsky S.L.**, **Solodukha H.A.**, **Pavlov V.A.**,*
Iukhymenko N.M.**, **Mokrinskaya E.V.

Kyiv Taras Shevchenko National University,
Volodymyrs'ka Str., 64, Kyiv, Ukraine, 01601
E-mail: studzs@ukr.net

The photothermoplastic medium based on the films of photosensitive polymeric composites with semiconductor properties is developed for application in optical information recording and storage, in holographic interferometry as well as for medical purposes. The present work is aimed at creation of new cooligomer providing higher diffraction efficiency when it is used as the holographic recording media (HRM) base for photothermoplastic (PTP) holographic recording as well as at employing these HRM for determination of the refractive index of the liquid and gaseous objects. Cuvette without diffuser and reversible holographic medium without "wet" development of the holograms were used. With the aim to increase the precision of measurements of the refractive index, the method of phase steps (Phase Shifting Interferometry) of analysis of the interferograms was applied. This medium was used in the modified holographic device for determination of the refractive index of homogeneous and inhomogeneous liquid and gaseous objects. To reach the aim of the present work, above described HRM were used for determination of the refractive index *(n)* of liquid objects by using Phase Shifting Interferometry. Experimentally demonstrated precision of the measurements is not less than 10^{-5}.

Transition from order to chaos of incommensurate superstructure described by the Lifshitz invariance under conditions *n* = 3

Sveleba S.A.[1], Katerynchuk I.M.[1], Kuno I.M.[1], Velgosh A.S.[1], Shmygelsky J.A.[1], Semotyuk O.V.[2], Kuno V.M.[3]

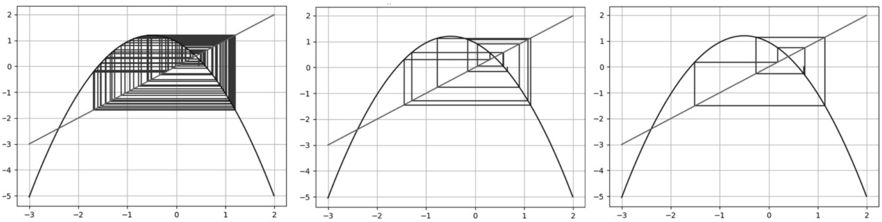
[1]National Ivan Franko University of Lviv 107 Tarnavskogo st., Ukraine
E-mail: incomlviv@gmail.com

[2] Ukrainian Academy of Printing of Lviv 19 Pid Goloskom st., Ukraine

[3] Lviv Politechnic National University 12 St. Bandera st., Ukraine

The goal of this work is to construct bifurcation diagrams that illustrate the occurrence of chaos by the method of doubling the period for ferroelectric crystals with multiplication of the unit cell *n* = 3. To do this, we calculated the amplitude function of an incommensurate (IC) superstructure described by two second-order differential equations. This system of two second-order differential equations was solved by the numerical BDF method. The calculations were performed in the Python software environment, using the JiTCODE library.

Based on the studies of the branching diagram and the mapping function diagram for IC superstructure occurring in ferroelastic crystals with elementary cell multiplication n = 3, it can be stated that due to frequency doubling bifurcations the system goes into a chaotic state. The parameters *T* and *K*, which are responsible for long-range and anisotropic interactions, respectively, in the first approximation well describe the behavior of IC modulation, and its modes. It is established that at small values of long - range interaction (*T* <0.1) there is an undeveloped chaotic state which is characterized by blurred processes of frequency doubling and their breaks. According to the diagrams of logistics functions, the influence of surface energy on IC superstructure causes an increase in the magnitude of the anisotropic interaction, which leads to the removal of the degeneracy of the system Fig.1.



n=3, T=1.0, K=0.95, E=0.07 n=3, T=1.0, K=0.95, E=0.7 n=3, T=1.0, K=0.95, E=2

Fig.1. *Diagram of the logistic function under influence of the surface energy of E.*

Transitional processes in a incommensurate superstructure in the surface energy field

Sveleba S.A.[1], Katerynchuk I.M.[1], Kuno I.M.[1], Velgosh A.S.[1], Shmygelsky J.A.[1], Semotyuk O.V.[2], Kuno V.M.[3]

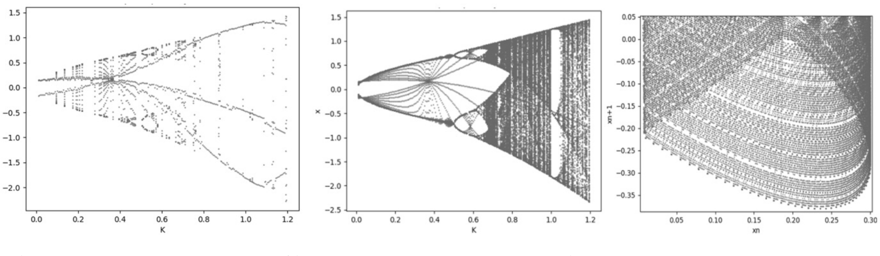
[1]*National Ivan Franko University of Lviv 107 Tarnavskogo st., Ukraine*
E-mail: incomlviv@gmail.com

[2] *Ukrainian Academy of Printing of Lviv 19 Pid Goloskom st., Ukraine*

[3] *Lviv Politechnic National University 12 St. Bandera st., Ukraine*

In this work, we construct bifurcation diagrams that illustrate the occurrence of chaos by the method of doubling the period for ferroelectric crystals with multiplication of the unit cell $n = 5$. To do this, we calculated the amplitude function of the incommensurate (IC) superstructure described by two differential equations.

It is established that at small values of long-range interaction ($T < 0.05$) there is an undeveloped chaotic state characterized by blurred processes of frequency doubling (Fig. 1). According to the diagrams of logistics functions, the influence of surface energy on the incommensurate superstructure causes an increase in the magnitude of the anisotropic interaction, which leads to the removal of the degeneracy of the system.



a) $n=5$, $T=0.01$, $K=0.01\div1.1$ b) $n=5$, $T=0.05$, $K=0.01\div1.1$ c) $n=5$, $T=0.05$, $K=0.01\div1.1$

Fig.1. *Branching diagram a-b); diagram of the mapping function c), when the parameter K describes, which describes the anisotropic interaction, and is determined by the Dzialoshinsky invariant at a constant value of the long-range interaction (parameter T).*

Therefore, the surface energy for the IC superstructure arising in ferroelectric crystals with the multiplication of the unit cell $n = 5$ removes the degeneracy of this system.

Electronic structure of Ni, Pd and Pt ultrathin films

Romansky A.A., Karbivska L.I., Karbivskyy V.L.

Department of Nanostructures Physics,
G.V. Kurdyumov Institute for Metal Physics of the NAS of Ukraine.
Academician Vernadsky Boulevard, 36, Kyiv-03142, Ukraine.
E-mail: anromansky@gmail.com

Today, studying the properties and possibilities of using both layered nanostructures and thin films of metals is extremely important, particularly in electronics, energetics, plasmonics, and the creation of metamaterials. In turn, theoretical study of the electronic structure of metal monolayers is the necessary step to studying the patterns of layer-by-layer growth of metallic nanostructures.

Within the framework of the density functional theory using the Wien2k package [1], the total and partial densities of the electronic states (DOS) of Ni, Pd, and Pt slabs with a thickness of 1–9 atoms, as well as bulk samples of the corresponding metals (for the correct analysis), were calculated.

A comparative analysis of the obtained curves is carried out: a) between each other, b) with experimental data (in particular UPS spectra), c) with the results of previous studies for Cu, Ag and Au [2].

It was found that the greatest similarity with the experimental UPS spectra is shown by nickel curves calculated with "up" spin-polarization.

It is shown that the Ni, Pd, Pt set shows the tendencies of changes in the DOS curve shape with increasing slab thickness, as well as with the transition from one metal to another, similar to the tendencies for the Cu, Ag, Au set. The main difference between the sets is a more pronounced separation of the peaks on the curve in the Ni, Pd, Pt set, while the Cu, Ag, Au set is characterized by the same basic tendencies of curve formation, but the width of the band is smaller and the peaks are more "blurred".

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Theoretical study of the interactions inside the system of N nanoparticles

Rusinchuk N.[1]***, Lozovski V.***[1,2]

[1] Institute of High Technologies, Taras Shevchenko National University of Kyiv, Glushkova ave., 4g, Kyiv-03187, Ukraine.
E-mail: n.m.rusinchuk@gmail.com

[2] V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine

Adsorption of one nanoparticle onto another or onto some configuration of the nanoparticle is an important problem of modern nanoscience. Furthermore, the studies of the interaction between nanoparticles of different nature are part of wide investigations of the systems of nanoparticles and bio-objects – viruses [1], microbes [2], and biomolecules. Theoretical models are mainly constructed for pair interactions between two nanoparticles. However, dispersion interactions are not additive, so it is impossible to model interactions in the many-particles system just via summation of pair interactions. Hence, the study of mutual adsorption in the system of nanoparticles is the actual problem that is considered in the present work. In the work we consider the system consisting of N nanoparticles and study the interactions inside the system. We suppose the reason for the interactions is the fluctuating field (vacuum fluctuations) and fluctuating dipole moments inside the nanoparticles caused by temperature oscillations of the atoms and electron densities inside the particles. In the work, we propose an equation for the interaction potential of three nanoparticles, based on the model for two nanoparticles [3], and present results of numerical calculations for different systems, demonstrating the non-additivity of such interactions.

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The deformation effects in isovalent doping of CdSe quantum dots with a multilayer shell for their biomedical applications

Kuzyk O.V.[1]***, Dan'kiv O.O.***[1]***, Stolyarchuk I.D.***[1]***, Peleshchak R.M.***[1,2]

[1] Drohobych Ivan Franko State Pedagogical University,
24, Ivan Franko Str., Drohobych, Ukraine.
E-mail: olehkuzyk74@gmail.com

[2] Lviv Polytechnic National University,
12, Stepan Bandera Str., Lviv, Ukraine.

Surface passivation of quantum dot (QD) due to the use of shell of different materials, proved to be an effective approach to reduce surface defects, which can expand the spectrum of absorption, accelerate the transfer of current carriers and reduce recombination losses. A special positive effect can be achieved if you use the multilayer shell [1].

Recently, a new approach has been developed tocontrol the properties of semiconductor heterostructures with QDs. It is based on the introduction of a single impurity atom into the QD. The exclusive properties of the structures with QDs reveal themselves only in the case where the QDs are uniform enough by their shapes and dimensions. Therefore, the main task at the QD growing is the control over their morphology: the average size, density, uniformity, and so on [2]. Isovalent impurity is not an electrically active impurity, i.e. it does not increase the charge carrier concentration. However, it substantially changes the conditions of QD formation owing to the induced diffusion-deformation flux. The investigation of deformation effects in QD with a multicomponent shell doped with an isovalent impurity is an urgent task associated with their use in medicine.

In this work, the investigations of deformation effects in CdSe / ZnS/CdS/ZnS QDs, which are doped with an isovalent impurity and interact with human serum albumin molecules, have been conducted.

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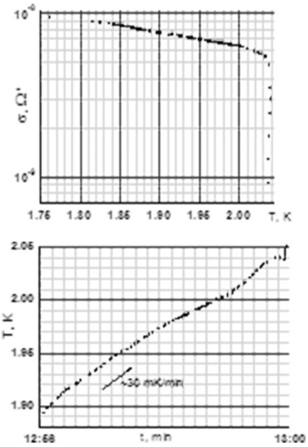
Thermo-Effect at Transition Surface Electron to Surface Polaron over Superfluid Helium Film on Structured Substrate

Nikolaenko V.A., Sokolov S.S.

B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkov - 61103, Ukraine
E-mail: nikolaenko@ilt.kharkov.ua

The exchange interaction of electrons with a neutral matter is study now. The surface electrons on helium (SEs) can use as a research tool. SE mobility along is limited by interaction with the helium atoms in vapor and with ripplons. At large electric field and/or at enough vapor density the SE forms a surface polaron (SP) [1]. The large mass of the complex leads to drop its mobility caused hydrodynamic. A mono-crystalline Si substrate 1 cm^2 in square by 0.3 mm in thickness with pores of 2 μm is used for study transition. The substrate is covered the superfluid helium film ~ 20 nm. The Sommer-Tanner measurement transport method is applied.

The mobility of SE in gas region is $\mu_g = 8\cdot e / (3\cdot\pi\cdot\hbar\cdot\sigma s\cdot ng\cdot\gamma)$ and the mobility of SP is $\mu_{sp} = 2\cdot\pi\cdot\hbar\cdot\alpha^{5/2/} (\eta\cdot m^{1/2}\cdot e^2\cdot E_{eff}^3)$ (here σs is the electron scattering section on helium atom at density ng, γ^{-1} is the effective Bohr's radius of SE, α and η is the surface tension and the viscosity of liquid helium accordingly. The value E_{eff} was ~ $7\cdot10^5$ V/m. In this work (left figure), the σ vs T smoothly decreases from value of ~ 10^{-8} sim at 1.75 K to $5.3\cdot10^{-9}$ sim at 2.03K and at T = 2.04 K take a place SE-SP transition with drop of σ on 2 orders. The monitoring T vs t, (right) shows a temperature dip at transition. From the energy balance of the SE-SP transition energy and of the helium heat capacity change, as $e\cdot\Delta V\cdot N=CHe\cdot m\cdot\Delta T$, the value ΔT- dip is ~ 5 mK about ~ 10 s in time. Here $\Delta V \sim 10^2$ V is the SE-SP potential [2]; $N \sim 10^{10}$ is number electrons on substrate with developed square 25cm^2; CHe and m are the specific heat capacity (~1 J/g·K) and mass of He film (~$2.5\cdot10^{-5}$ g) accordingly. Notice, the magnitude of C the Cu (chamber and cell) or Si (substrate) is 5 – 7 orders lower helium one. The effect can be related to effects like the electro-caloric or the magneto-caloric one.



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Electric transport properties of a Ni-Mn-In alloy subjected to external stimuli

Konoplyuk S.M.[1], **Kolomiets A.V.**[2]

[1] *Institute of magnetism of NASU and MESU,*
Vernadsky blvd. 36-b, Kyiv-03142, Ukraine.
E-mail: ksm@imag.kiev.ua

[2] *Department of Physics, Lviv Polytechnic National University,*
St. Bandery str. 12, Lviv, Ukraine.

The polycrystalline $Ni_{45.4}Mn_{40}In_{14.6}$ Heusler alloy was studied to find dominant factors affecting its electric transport behavior in austenitic and martensitic phases. Analysis of three main contributions into temperature dependent resistivity has shown that prevalent mechanisms of carrier scattering in the austenitic phase are scattering on structural and magnetic disorders rather than on thermal fluctuations. In spite of the small transformation volume effect of 0.09 %, application of hydrostatic pressure of 2 GPa results in almost threefold rise in the longitudinal resistivity and twofold rise in the Hall resistivity due to the pressure-induced martensitic transformation. The measurements of the ordinary Hall resistivity have shown that main charge carriers in both phases are holes whose mobility is ten times as high in the austenitic phase as in the martensitic one. The anomalous Hall resistivity (AHE) of the $Ni_{45.4}Mn_{40}In_{14.6}$ reaches significant magnitude of 20 $\mu\Omega\cdot$cm in the martensitic phase. Unusual scaling relation between AHE and the longitudinal resistivity is discussed.

Quantum Cone - Nano Source of Light with Dispersive Spectrum, Separated in Time and Space

Medvid A.

Riga Technical University, Lab Semiconductor Physics,
P. Valdena 3/7, Riga, Latvia
E-mail:medvids@latnet.lv

Nanostructures (NSs) are the most investigated object in solid-state physics, especially the Quantum confinement effect in quantum dots – 0D, quantum wires - 1D, and quantum wells – 2D systems. Because of these conditions constructing new electronic and optical devices is possible. Twenty years ago we have found a new quantum system, the so-called Quantum cone in Ge single crystal [1, 2] possesses unique optical properties: a huge “blue shift” of photoluminescence (PL) spectrum on 1.1 eV with increased intensity of more than a million times, with period 1 μ of pattern C_{6i} point group symmetry and “redshift” of LO phonon line frequency on 6 cm^{-1} in Raman spectrum. The symmetry of PL band and sharp LO phonon line in Raman spectrum is evidence present of OD quantum cone. The appearance of a new band in the PL spectrum of CdZnTe slid solution is explained by the exciton quantum confinement effect in quantum cones [3]. Irradiation of SiO_2/Si structure by Nd:YAG laser has led to the formation of nanocones which possesses a unique PL spectrum: “blue shift” on 1.1 eV, an asymmetric wide band from 1.1 eV till 2.2 eV with gradually decreases intensity in the red part of the spectrum, rainbow-like spectrum, and maximum of PL intensity increase more than million times [4]. These properties of the system of PL spectrum are typical for graded bandgap semiconductors. It means that the quantum cone with the solid angle at top of the cone less than 60° is a 1D system with a gradually decreasing diameter from the base to the top of the cone. Therefore, where the cone diameter is equal to or less than Bohr’s radius of an electron or exciton quantum confinement effect takes place [5]. Colossal increase intensity of PL and shift of maximum in the blue part of the spectrum takes place due to transformation of Si and Ge crystal from indirect to quasi direct and confinement of electron-hole pair in the quantum cone. These facts speak forward to the possibility of a gradual decrease in the lifetime of electron-hole pairs or excitons from base to top of a cone. The aim of this study is to determine the change of electron-hole pair's lifetime depending on height in a cone using the kinetics of the PL method. PL kinetic of diamond-like carbon sample with nanocones diameters on the base 100 nm and top 2 nm and hight 60 nm is investigated. The kinetic is described by a stretched exponent of PL intensity $I_{PL}= I_0 \exp(-(t/\tau^0)^\beta)$, where $\tau^0= 5x10^2$ ps, $\beta= 0.5$. It means, τ decreases from base to top of cone monotonously from 1 ns to 50 ps.

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The effect of the pressure on electronic structure of the doped solid solutions ZnSeTe:T (T=Cr, Mn, Fe)

***Syrotyuk S.V.*[1], *Malyk O.P.*[1], *Klysko Yu.V.*[1]**

[1] Semiconductor Electronics Department, Lviv Polytechnic National University,
S. Bandera str., 12, Lviv-79013, Ukraine.
E-mail: svsnpe@gmail.com

Here we evaluate the electronic structure taking into account the strong correlated 3d electrons of the Cr atom. The strong correlations are treated by means of the exchange-correlation functional PBE0. The obtained results are shown in Fig. 1. The calculations were done in the 64-atom supercell by means of ABINIT code [1].

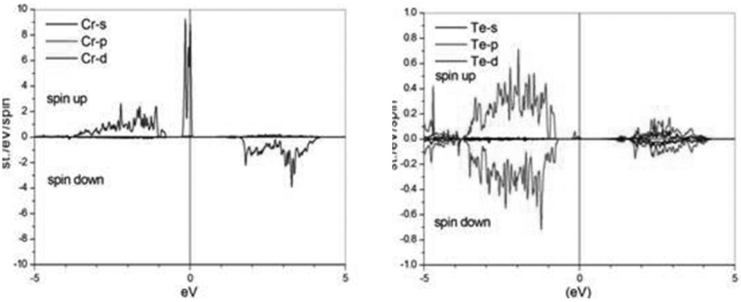

Fig. 1. *Spin-resolved partial density of states of the solid solutions ZnSeTe:Cr, evaluated at ambient conditions. Fermi level is set at zero energy.*

As can be seen from Fig. 1 the material ZnSeTe:Cr shows the metallic properties for the spin up and for the opposite spin it is the semiconductor. The magnetic moment of a supercell equals to 4.00 Bohr magnetons.

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Effect of the electric field and the acceptor impurity on the energy spectrum of spherical quantum dot

Bilynskyi I.V.[2], Leshko R.Ya.[1], Metsan Kh.O.[1]

[1] *Drohobych Ivan Franko State Pedagogical University,*
3 Stryiska Str., 82100 Drohobych, Ukraine.
E-mail: kristik98@gmail.com

[2] *Kryvyi Rih State Pedagogical University,*
54 Gagarin av., 50086 Kryvyi Rih, Ukraine

Modern nanotechnologies give the opportunity to get various nanoscale objects with different properties. Every time, the use of those nanoobjects leads to improving the operation parameters of different devices. It is very important to control the mentioned properties with high accuracy. Ways to solve this range of problems include the change of the QD size, doping, and applying external fields.

In this work we propose a model for determining the hole spectrum in the multiband model in the electric field with the presence of acceptor impurity. We investigate a heterosystem where the dielectric permittivity of each layer does not differ. That is why we do not consider the polarization and deformations effects, and we use the average value of dielectric permittivity.

For the hole and acceptor states we use the multiband effective mass models. For considered nanosystem $GaAs/Al_xGa_{1-x}As$ the Luttinger model with spherical approximation comfortably can be used.

We place the hydrogen impurity at a distance D from the center of the QD. The external electric field Fel is applied to the heterosystem and we considered three cases of electric field directions.

We consider the case of the quantum dot (QD) with the central and off-central acceptor impurities in the electric field. The shift of the impurity from the center also causes the shift of the absorption band into the low-energy region when we applied electric field to a quantum dot. The presence of the impurity in the QD center decreases the energy levels in compare with the case of the impurity absence.

As a result of research, the spectrum of holes in a multiband model in an electric field in different directions is determined. The dependence of the hole energy spectrum on the radius of the quantum dot and the location of the impurity from the center of the quantum dot is shown. The dependence of the energy spectrum of central and non-central acceptor impurity in the electric field and without it is obtained.

Quantum size effects and transport properties of $Bi_2(Te_{1-x}Se_x)_3$ 3D-topological insulators thin films

Rogachova O.I.**, **Doroshenko G.M.,
Sipatov O.Yu., Nashchekina O.M.

National Technical University “Kharkiv Polytechnic Institute”,
2, Kyrpychova St., Kharkiv 61002, Ukraine
E-mail: rogachova.olena@gmail.com

The V_2VI_3 compounds and their solid solutions are among the best low-temperature thermoelectric (TE) materials. Today they are increasingly being used in thin-film TE converters. Recently it has been discovered that V_2VI_3 compounds belong to a new type of objects of nanophysics - 3D topological insulators (TI) with spin-polarized surface states, protected by time reversal symmetry, and unique properties, which can be more clearly observed in thin films. All this stimulates studying these materials in the thin film state.

Electron confinement in low-dimensional structures leads to quantum size effects, which are manifested in thin films through an oscillatory behavior of the thickness dependences of kinetic coefficients. We observed such size-dependent oscillations in Bi_2Te_3 and Bi_2Se_3 thin films in [1,2]. The goal of the present work is to find out how the anion substitution in Bi_2 $(Te_{1-x}$ $Se_x)$ alloys and the presence of a topological layer affect the manifestation of quantum size oscillations.

Thin films with thicknesses d=15-85 nm were prepared by thermal evaporation in vacuum of the Bi_2 $(Te_{0.9}$ $Se_{0.1})$ crystal and subsequent deposition onto glass substrates. It was established that the dependences of electrical conductivity, the Seebeck coefficient and the Hall coefficient on d exhibit an oscillatory behavior with a certain period. The experimental results were interpreted within the framework of notions about size quantization of the electron spectrum and taking into account the presence of the topological metallic surface layer in the films.

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On spintronic torque effect in multilayer magnetic nanostructures

***Korostil A.A.*, Krupa M.M.**

Department of Physics of Meso- and Nanocrystalline Magnetic Structures,
Institute of Magnetism NAS and MES of Ukraine.
Vernadsky av., 36b, Kyiv, Ukraine.
E-mail: amand@rambler.ru

Spintronics of multilayer magnetic nanostructures is based on the electric control and detection of localized magnetic states via the exchange interaction of the electric-induced spin current with localized magnetic moments. Regardless of the type of the magnetic exchange interaction (ferromagnetic (FM) or antiferromagnetic (AFM)), the impact on the localized magnetic states occurs via the spin torques exerting on the localized magnetic moments. In the FM and AFM cases, these spin torques can result in the FM and AFM order dynamics and switching, respectively. In the case of FM nanostructures it exhibits in the known giant magnetoresistance effect, which was applied for new kinds of field-sensing and magnetic memory devices [1, 2]. The spin torque effectiveness is determined by threshold spin current density for excitation of localized spins due to the nature of spin polarization. The spin polarization can be induced by the effective field of magnetic exchange interaction and magnetic field of spin-orbit interaction related and unrelated to spin polarized electron transport through interface to the localized magnetic states, respectively. The origin of the spin polarization and magnetic exchange interaction between localized magnetic states determines the time and spatial scales of the spin torque effects. The lasts are described in the framework of the microscopic tight-binding model involving the spin-orbit interaction, the interaction between free and localized magnetic states.

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Magnetic Field-Controlled Light Transmission in Ferronematic Liquid Crystals

Korostil A.A., Krupa M.M.

Department of Physics of Meso- and Nanocrystalline Magnetic Structures,
Institute of Magnetism NAS and MES of Ukraine.
Vernadsky av., 36b, Kyiv, Ukraine.
E-mail: amand@rambler.ru

Ferronematic liquid crystals (FNLQ) are characterized by combination of the orientation structural ordering of the anisotropic (nematic) molecules (characterized by a so-called nematic vector) with the magnetic ordering of magnetic nanoparticles, arched by interphase interaction with the nematic molecules. The strong effect of an external magnetic field on an orientation ordering molecular structure occurs indirectly via its interaction with magnetic nanoparticle moments. The impact of the magnetic field on the molecular orientation is orders of magnitude larger than the direct magnetic influence due to the molecular diamagnetism [1-2]. The magnetic field-induced change of the nematic director is accompanied by the corresponding change of the optical axis, and the effect of the polarization twisting and birefringence of linear polarized light transmitted through the FNLC (the so-called magneto-optical effect). The transmission of the linearly polarized light through the FNLC sandwiched by two crossed polarized is characterized by the strong dependence of the transmitted light intensity on the applied magnetic field, that may have important applications in displays and photonics. Investigation of the magneto-optic effect is based on the macroscopic FNLC model and the Jones matrix description of light transmission.

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Electrical excitation of magnetic waves in nanoheterostructures

Korostil A.A.

Department of Physics of Meso- and Nanocrystalline Magnetic Structures,
Institute of Magnetism NAS and MES of Ukraine.
Vernadsky av., 36b, Kyiv, Ukraine.
E-mail: amand@rambler.ru

Spintronic effect of electric-controlled local spin dynamics under the spin current-induced torque in magnetic nanostructures is the basis for the controlled excitation of the coherent spin waves of given amplitude and phase. The electrically insulating magnetic materials provide their exceptionally low magnetic damping and relative large distances of propagation. The coherent ratio, frequency and possibility of the electrical manipulation of the spin waves are depend on the origin of the spin polarization and spin torque exerting on the localized spin that results in the spin wave propagation. The electric-induced spin torque can be exhibited as the spin transfer torque related to conversation of electric current into spin polarized current [1], the spin-orbit torque related to the spin Hall effect of electric current conversation into spin current and spin-orbit torque related to the electric field-induced surface spin polarization in the effective Rashba field [2]. The latter results in the voltage controlled magnetic anisotropy (VCMA) which is characterized as an efficient mechanism for low-energy excitation and propagation of coherent spin waves with given amplitude and phase [3]. In the case of antiferromagnetic nanostructures, VCMA-induced spin waves possess low susceptibility, lack of stray fields, and THz dynamics. The proposed self-consist description of the electric controlled excitation and propagation of spin waves is based on first-principle density functional theory in a tight-binding model realized with second quantization accounting for features of electron and magnetic structures and interface exchange interactions.

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Positron spectroscopy of nanoscale regions of homogeneous atomic and magnetic orderings in strongly correlated alloys

Len E.G.[1,2], Shatnii T.D.[1], Len T.S.[3],
Galstian I.Ye.[1], Tsapko Ye.A.[1], Lizunov V.V.[1]

[1] G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine,
36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine.
E-mail: len@imp.kiev.ua

[2] Kyiv Academic University, NAS and MES of Ukraine,
36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine.

[3] National Aviation University, 1 Kosmonavt Komarov Ave.,
UA-03058 Kyiv, Ukraine.

Today, the most promising materials of electronic, energy, and aerospace industries are developed not only taking into account quantum effects due to the nanometer level of the element base of devices, but also complex collective phenomena in the electrons' subsystem, which strongly interact with each other and other excitations (phonons, magnons, etc.) in solids. A very limited number of methods allows an experimental observation of these effects in the electronic structure. Such methods reproduce the Fermi surface in strong magnetic fields or permit a direct observation of the band structure (using angle-resolved photoemission spectroscopy (ARPES)) and require the magnetic fields, low temperatures and ultra-high vacuum (ARPES). They are applicable to systems with a well-defined band structure and Fermi surface only. All these experimental complexities and natural limitations are absent in the method of positron spectroscopy, namely, in the method of angular correlation of electron positron annihilation radiation (ACAR). In addition, this method allows to determine the size and concentration of defects in crystalline or non-crystalline matter and to study their electronic properties. Thus, the theoretical consideration of the influence of some many-particle effects on the momentum distributions of conduction electrons recorded by the ACAR method is actual.

At the framework of the single-band Hubbard model for binary substitutional alloys with strong electron correlations, the changes in momentum distributions of electrons are investigated depending on the presence and magnitude of pair correlations in the arrangement of atoms of different types and/or in the orientation of electron magnetic moments at nearest sites. These correlations determine the size of regions of homogeneous atomic and/or magnetic short-range (nanoscale) ordering. As shown at temperature of 0 K, the effects of pair correlations on these distributions are clearly defined, which allows the use ACAR for their experimental identification in the studied systems.

Description of electrostatic semiconductor quantum dot based swap gate interacting perturbatively with Josephson junction

Pomorski K.[1,2]

[1] *Cracow University of Technology,*
Faculty of Computer Science and Telecommunications,
Department of Computer Science, Cracow, Poland

[2] *Quantum Hardware Systems company, Lodz, Poland*
[www.quantumhardwaresystems.com +QHS YouTube channel]

Single-electron semiconductor devices [1-3] present big potential in implementation of CMOS based scalable, compact and highly integrated quantum computer. On another hand Josephson junctions have already shown potential in implementation of quantum computer [4], but are limited in further downscaling due to value of superconducting coherence lenght and non-scalable sources of vector potential. One can use advantages of very recent compact cryogenic CMOS technologies [3], [5] having from 3 to 22 nm of field-effect transistor channel lenght that can be combined with medium integrated Josephson junction quantum circuits and leading to proposed hybrid semiconductor-superconductor quantum computer architecture [6-7]. The essence of such solution relies on the usage of quantum swap gate made from two electrostatically coupled semiconductor single-electron lines coupled electrostatically to Josephson junction(s) [6-7]. Such system is described in semi-analytical way by Schroedinger-Bogoliubov-de Gennes integro-differential equations expressing perturbative interaction between semiconductor and superconducting qubits. Alternative and simplified picture using tight-binding Bogoliubov-de Gennes model is also given [7]. Various technological and fundamental research perspectives of pointed physical system are presented. One characteristic feature is expressed by ability of continous tunning of quantum phase transition both by electric and magnetic field present in hybrid semiconductor-

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superconducting structures [7]. The presented scheme also broadens tunnability scheme of semiconductor and electrostatic position-based Wannier qubits of any geometry [8].

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Vapor-condensed composite materials $Ni-Al_2O_3$, $NiCr-Al_2O_3$ with oxide nanophase

***Grechanyuk V.,* Grechanyuk M., Chornovol V., Kozyrev A., Kovalchuk Yu.**

Department of Chemistry, Kyiv National University of Construction and Architecture.
Povitroflotsky Ave., 31, Kyiv-03037, Ukraine.
E-mail: missvik@ukr.net

High-speed electron-beam evaporation of metals and non-metals in vacuum (the deposition rate of atomic or molecular flows on a substrate can reach 150 μm/min) is a relatively new direction in materials science. These processes are currently widely used mainly for the application of protective coatings to gas turbine parts. New materials obtained by condensing vapor flows on a substrate heated to a certain temperature include dispersion-strengthened, layered, and porous materials [1-3].

The structure and physico-mechanical properties of bulk composite materials condensed from the vapor phase with a dispersed oxide nanophase: $Ni – Al_2O_3$, $NiCr-Al_2O_3$ in a wide (up to 40% wt.) range of Al_2O_3 concentrations are studied in this work. The dependences of the physico-mechanical properties of composites on the temperature of the substrate on which vapor flows are deposited are established. It is shown that in the above range of oxide nanophase concentrations, there is a smooth transition from dispersion-strengthened to microporous materials. The influence of the deposition temperature and vacuum annealing time on the morphology, micropore volume, and mechanical properties of the composites has been studied.

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Optimization of photoelectric converters

Beliak Ie.V., Kryuchyn A.A., Manko D.Yu.

Institute for Information Recording of the NAS of Ukraine.
M. Shpak, str 2, Kyiv-03113, Ukraine.
E-mail: beliak1312@gmail.com

The improvement of the efficiency of photovoltaic converters (Power Electronic Transformer, PET) which absorbs solar radiation in the visible and near infrared ranges of the spectrum is relevant for the creation of a new generation of solar photovoltaic systems and optical channels energy transmission optoelectronic systems [1-2]. It should be also noticed that optimization of the characteristics of optoelectronic systems is one of the most important areas in the field of organization of optical monitoring and data transmissions systems. Compact camera units, which today are actively included in the composition of general-purpose electronic devices and, in particular, mobile devices due to the simplification of the optical photo-registration system are characterized by relatively low photosensitivity and imbalance of color rendering scheme. The concept of the luminescent solar concentrator has emerged as an efficient approach to harvesting sunlight economically, able to overcome the factors that limit the conversion efficiency of photovoltaic systems. LSCs (luminescent solar concentrator) consist of a layer containing optically active centers applied to a transparent substrate, which, when exposed to light, converts part of the absorbing radiation corresponding to the short-wave visible and ultraviolet part of the solar spectrum into radiation of a certain wavelength corresponding to the PET absorption spectrum. While part of the emitted signal will be lost at the surface (through the so-called exit cone), the rest will be trapped inside the layer and substrate and directed towards the edges (through total internal reflection) where it can be collected by the photovoltaic cell. Various optically active centers have been tested in LSC, including organic dyes, quantum dots, and trivalent lanthanide ions [3].

An effective way to optimize the characteristics of PET can be the application of photoluminescent layers based on nanostructured photoluminescent dyes with fixed Stokes shear and photoluminescence range, selected according to the absorption spectra of photovoltaic components of triad and tetrads of the photoelectric transducers. Conventional dyes often suffer from a low photoluminescence quantum yield, insufficient photostability, and a insufficient Stokes shift. In other hand the use of organic dye nanoparticles provides efficient luminescence’s resonance energy transfer with markedly improved imaging performance. Currently, the most widely used organic dyes, which are usually encapsulated in various nanoparticles to overcome the internal limitations of conventional dyes, including poor hydrophilicity, low photostability, low quantum yield. Compared to pure dyes, organic dye nanoparticles have an almost 50-fold increased quantum yield, large Stokes shifts (~250 nm), and significantly increased photostability [3]. The general principle of optimizing the photoelectric conversion process by applying a photoluminescent layer to the elements of the photo matrix is to transfer radiation to the absorption region of the photoelectric converter — thus, the Stocks shift of the photoluminescent dye should be equal to the difference between the main peak of solar spectrum and the photoelectric converter absorption spectrum.

Obtaining the characteristics of the luminescent converter determined as a result of mathematical modeling is carried out through the use of the procedure of nanostructuring the organic photoluminescent dyes with zeolite pores, laser annealing, and the inclusion of impurities of polymeric materials (polymethyl methacrylate, polystyrene and others). Based on the study, the effectiveness of improving the photosensitivity and color rendering of photodetection systems by expanding the absorption spectrum of photocells was proved and the value of Stokes shift of photoluminescent materials of the coating layer for color channels was calculated.

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Quantum –chemical portrait of the π-stacked complex of thiochrome and tryptophane

Gaponov A.M.[1]***, Dmytrenko O.P.***[1]***, Kulish M.P.***[1]***,***
Pavlenko O.L.[1]***, Neimash V.B.***[1]***, Kachkovsky O.D.***[2]

Taras Shevchenko National University of Kyiv,
64/13 Volodymyrska Str. Kyiv,
E-mail: antongaponov@ukr.net

[1] V.E. Lashkarev Institute of Semiconductors Physics, National Academy of Sciences, 45 Nauky Ave, Kyiv, Ukraine

[2] Institute of Bioorganic Chemistry and Petrochemistry, National Academy of Sciences, 1 Murmanska Str., Kyiv, Ukraine

The aim of the work is to determine peculiarities of tryptophane -tiochrome interaction for case of their closest distance (so called π-π stacking, that equals 3,4 A for pure aromatic rings) that can be realized in protein-dye complexes.

The characteristics of the tryptophane -tiochrome complex compared to its independent constituents parts were studied by DFT method (basis set 3-21g, functional B3LYP) quantum-chemical methods in Gaussian -09 package. Obtained data (table 1) were compared to experimental absorption of films, prepared by vacuum evaporation (fig.1). The energies of the electron transitions were calculated with TD-SCF methods.

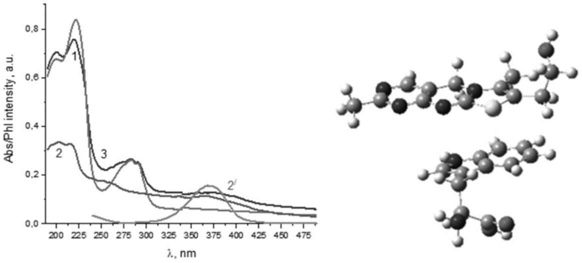

***Fig.1**. Absorption spectra of films, prepared by vacuum evaporation on quarts substrate of pure powders of: 1 – tryptophan, 2 –thiochrome, ($2^{/}$ - absorption of water dissolved thiochrome), 3 – thiochrome, tryptophan, layer by layer.*

Maxima of the absorption,in nm ***Table 1.***

	Trp	Thio	Complex
Experimental	283	370	384
TD SCF	260	325	345

The red shift, observed experimentally for the complex clearly shows TD SCF, therefore, this method can be used for further analysis of the system.

Slowed magnetic relaxation in the Er^{3+} single ion magnet in the absence of external magnetic field

Koplak O.[1]***, Dvoretskaya E.***[2]***, Kunitsyna E.I.***[2]***, Bazhenova T.A.***[2]***,***
Yagubskii E.B.[2]***, Calloni A.***[1]***, Goto F.***[1]***, Bussetti G.***[1]***, Morgunov R.***[2]

[1] *Politecnico di Milano, Piazza Leonardo da Vinci,*
32, 20133 Milano
E-mail: o.koplak@gmail.com

[2] *Institute of Problems of Chemical Physics,*
142432 Chernogolovka, Russia

Single-molecule magnets (SMMs) attract great interest of specialists in the view of development of platforms for quantum computation and information storage [1, 2]. Typical SMM involves a magnetic ion incorporated in organic structure chemically designed to satisfy desirable symmetry of the ligand field. More or less strong coupling between an ionic spin and organic environment is provided due to spin-orbital interaction within the complex. The Er^{3+} based complexes demonstrate relaxation typical for single ionic magnets (SIMs). Magnetic relaxation in Er^{3+} SIM in the presence of the ferromagnetic environment is analyzed. Incorporation of the $[Er(HL)(L)]4CHCl_3H_2O$ complexes (L = DAPBH = 2,6-bis(phenylhydrazone) pyridine) to the ferromagnetic matrix consisting of PrDyFeCoB microparticles significantly changes magnetic relaxation in the Er^{3+} ions. Internal magnetic field of the magnetized ferromagnetic matrix delays spin relaxation in the Er^{3+} complexes in the absence of the external magnetic field. Compaction of the Er^{3+} complexes with ferromagnetic microparticles results in a composite material, in which magnetic relaxation is governed by Zeeman interaction of Er^{3+} spin with ferromagnetic microparticles possessing remnant magnetization at zero external field. Additional channel of microparticles effect on the magnetic relaxation is chemical interaction of the complexes with metallic surface of microparticles and corresponding orbital hybridization accelerating magnetic relaxation.

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Formation of Composite Layers by Ultrasonic Impact Treatment of Cu–39Zn–1Pb Brass Using Silicon Carbide Reinforcing Particles

Burmak A.P.[1]***, Mordyuk B. N.***[2,1]***, Sidorenko S. I.***[1]***,***
Voloshko S. M.[1]***, Mohylko V. V.***[1]

[1] *National Technical University of Ukraine 'Igor Sikorsky Kyiv Polytechnic Institute', 37 Peremohy Ave., UA-03056 Kyiv, Ukraine*

[2] *G. V. Kurdyumov Institute for Metal Physics, NAS of Ukraine,*
36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine

The structure, phase composition and mechanical properties of composite coatings synthesized by ultrasonic impact treatment (UIT) of the surface layers of two-phase Cu–39Zn–1Pb brass with the addition of reinforcing SiC particles of different fractions, *i.e*. 3–5 μm, 14–20 μm, 40–50 μm, 80–100 μm, 160–200 μm, are studied. Owing to severe plastic deformation caused by UIT, there is a partial grinding and embodiment of the SiC powders into the near-surface layers of brass. The proposed approach allows synthesizing the high-strength composite coatings with a thickness of ~ 50 μm.

The maximum hardening effect due to the maximum crystallites refinement of the phase components of brass is achieved under conditions of reinforcement with the SiC powder with a particle size of 160–200 μm. Application of the SiC powder fraction of 40–50 μm gives the best result in terms of the minimum of coherent-scattering regions size of the SiC powder and its higher volume fraction and more uniform distribution in the surface layer (EDX analysis shows minimum contents of Zn and Cu, and maximum contents of Si and C). Despite the fact that the microhardness of such a coating is slightly lower than those for the UIT-produced composites with the powders of larger size, the integrity, homogeneity, and uniformity of the formed composite coating are maximal in this case.

Effect of high Ni Doping on the properties of ZnO Nanopowders

Amari R.[1,2]***, Benrzgua E.***[1,3]***, Allali D.***[4,6]***,***
Deghfel B.[1,4]***, Boukhari A.***[1,5]

[1] *Laboratory of Materials and Renewable Energy, Faculty of Sciences, University of M'sila, Algeria.*

[2] *Department of Civil Engineering, Faculty of Technology, University of M'sila, Algeria.*
E-mail address: rabie.amari@univ-msila.dz

[3] *Department of natural and life sciences, Faculty of Sciences, University of M'sila, Algeria.*

[4] *Department of Physics, Faculty of Sciences, University of M'sila, Algeria.*

[5] *Department of Mechanical Engineering, Faculty of Technology, University of M'sila, Algeria.*

[6] *Physics and Chemistry of Materials Lab, Department of Physics, University of M'sila, 28000, M'sila, Algeria.*

Pure and Ni-doped ZnO nanoparticles (NPs) with concentration of Ni (12.5%) were successfully prepared by using co-precipitation method [1]. Among TM, nickel is very significant element which has a similar ionic radius as that of Zn. Literature studies show that Ni doping into ZnO matrix can enhance its various properties [2, 3]. The prepared samples in powder form were characterized by X-ray diffraction spectroscopy (XRD), Scanning Electron Microscopy (SEM), Ultraviolet–visible spectroscopy (UV-Vis), Photoluminescence (PL) and Fourier transform infrared spectroscopy (FTIR). The obtained results have been discussed and compared with those from other sources whatever possible.

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Phonon bottleneck in emission of rare earth ions embedded into nanocrystal structures

Francini R.[1], De Matteis F.[1], Zhuchenko Z.Ya.2,
Zolotovsky A.[2], Bacherikov Yu.[2], Tarasov G.[2]

[1] *Dipartimento di Ingegneria Industriale, Università di Roma "Tor Vergata", Via del Politecnico, 00133 Roma, Italy*

[2] *Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, Prospect Nauki 45, 03028 Kiev, Ukraine*
E-mail: zhuchenko@isp.kiev.ua

Recently, rare earth doped nanocrystals and structures are widely used for numerous photonic applications. In this report we consider different nanostructures doped with Er^{3+} ions. These systems have been structurally studied by the TEM, EDX, and XRD techniques, and optically investigated by means of photoluminescence and up-conversion technique. In such structures, the certain structural stabilization is expected. Indeed, we have found from TEM, EDX, and XRD studies that the structures with a fully determined crystalline (mono-phase) structure can be realized. The low-temperature spectra ascribed the ${}^4I_{13/2} \rightarrow {}^4I_{15/2}$ transitions in Er^{3+} reveal some peculiarities which cannot be understand without knowledge of the crystal- field splitting of ${}^4I_{13/2}$ and ${}^4I_{15/2}$ manifolds. These manifolds are especially important while they are the working levels for Er-based lasers. The simulation has been performed using multi-electron molecular orbitals cluster model developed for the case of nanocrystal structures. Both energy levels and the probabilities of transitions between the split levels have been calculated, thus allowing to reproduce the PL line shape for the ${}^4I_{13/2} \rightarrow {}^4I_{15/2}$ transitions. It has been found the existence of peculiar energy gap in level distribution of split ${}^4I_{13/2}$ states. Taking into account possible absence of low-energy phonons in the phonon spectrum of spatially confined structures, the energy restricted relaxation (so called phonon bottleneck) is expected for ${}^4I_{13/2}$ manifold. This mechanism is an origin of appearance of the "hot PL bands" in the low-temperature PL spectra in the range of the ${}^4I_{13/2} \rightarrow {}^4I_{15/2}$ erbium transitions. The consequences of this restricted relaxation can be also revealed by means of time-resolved luminescence.

Annealing effect in ZnO/Si heterostructures doped with rare earth ions (Eu and Tb)

Leroux C.[1], Pelloquin D.[1], Portier X.[2], Zhuchenko Z.[3],
Zolotovsky A.[3], Tarasov G.G.[3]

[1] CRISMAT, UMR CNRS 6508, ENSICAEN, Normandie Université,
6 Boulevard du Maréchal Juin, 14050 Caen Cedex 04, France

[2] CIMAP, CEA, UMR CNRS 6252, ENSICAEN, Normandie Université,
6 Boulevard du Maréchal Juin, 14050 Caen Cedex 04, France

[3] V. Lashkaryov Institute of Semiconductor Physics of the NAS of Ukraine,
45 Prospect Nauky, 03028 Kyiv, Ukraine
E-mail:tarasov@isp.kiev.ua

ZnO belongs to II-VI semiconductors with an electrical conductivities of about 7x10^{-7} S.cm^{-1} at room temperature in case of a nanostructured thin film growing up to 10^{-4} S.cm^{-1} for higher temperatures. If this film is doped with Al, its electrical conductivity significantly increases. As a result, thin film ZnO structures are widely used for the PL and photovoltaic applications. The doping of ZnO thin films with rare earth (RE) ions allows to get original and alternative white LEDs structures or to enhance the efficiency of a solar cell. Here we present the result of detailed structural analysis of Eu/Tb codoped ZnO thin films annealed at different temperatures. Analysis was performed using PEDT data combined with atomic STEM-HAADF imaging and spectroscopic approaches (EDX, EELS). The theoretical calculations (PL modeling) based on the method of multielectron molecular orbitals are applied. This method allows, in fact, to reproduce to spectral lineshape of rare earth emission for different crystalline surrounding, thus facilitating understanding the observed changes in the PL experimental data.

Voltage generation in hydrated calcium structures

Kidalov V.[4], Sadigov A.[3], Tarasov G.G., Okhrimenko O.B.[1],
Lyubchyk A.[2], Liubchenko O.1, Gudimenko O. Y.[1],
Maksimenko Z.V.[1], Ponomarenko V.V.[1], Bacherikov Y.Y.[1]

[1] V. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine,
45 Nauky Ave., Kyiv 03028, Ukraine

[2] Lusófona University, Lisbon, Portugal

[3] National Nuclear Research Center, Baku, Azerbaijan

[4] Tavria State Agrotechnological University
18, Bohdan Khmelnytskii Avenue Melitopol,
Zaporizhzhia oblast,Ukraine, 72310
E-mail: yuyuodessa@gmail.com

Rapid industrial development significantly deteriorates natural surrounding. As a result, the necessity of green and environmental protection is extremely needed. In part, it can be can be formulated as: the full usage of ecological building materials to save energy and improve the validity of environmental protection on the basis of reducing environmental pollution and resource waste in the process of realizing ecological architecture. Many semiconductor materials do not satisfied these requirements being nevertheless the basic materials for modern electronic, optoelectronic and intellectual systems. Some fresh ideas arise with usage of, so called, conductors of type II, which reproduces to some extent the functions of semiconductor structures and nanostructures. Special sorts of calcite seems to satisfy the requirements outlined above for the materials needed in ecological architecture. In this report we have studied some peculiarities of calcite powder structure hydrolyzed with water. This hybrid structure which combines the membrane properties (due to nanoscale porous) and water (which is considered as an electrolyte) specific dynamics at the interface solid/liquid present rather complicated structure and appearance time threshold for voltage generation can be related with initial formation of nanostructures which facilitate the charge carrier transfer and local polarization.

Temperature range of deuterium retention from ferritic-martensitic steel implanted deuterium at elevated temperatures

Morozov O., Zhurba V.I., Progolaeva V.O., Seliukova V.V.

NSC-Kharkiv Institute of Physics and Technology of the NAS of Ukraine.
1, Akademichna St., Kharkiv-61108, Ukraine.
E-mail: morozov@kipt.kharkov.ua; morozovtds@gmail.com

Deuterium thermal desorption spectra were investigated on the samples of ferritic-martensitic steel (16Cr12W2VTiAB) implanted deuterium at temperatures 100 K, 300 or 600 K with deuterium ions in the dose range from 5×10^{16} to 4×10^{18} D/cm^2. It has been determined that for low implantation doses, the thermal desorption spectrum of ion-implanted deuterium is a wide temperature range of deuterium desorption in the temperature range of 400–1000 K. As the dose increases, this temperature range of deuterium desorption expands in the direction of decreasing temperature and at a dose of 1.6×10^{17} D/cm^2, a wide peak with a maximum temperature of 400 K appears. A further increase in the implantation dose of deuterium is accompanied by the appearance of a lower temperature region of deuterium desorption with a maximum temperature in the temperature range of 200–250 K. At doses above 8×10^{17} D/cm^2, a qualitative change in the deuterium thermal desorption spectrum occurs, which manifests itself in the appearance of a lower temperature region of deuterium desorption in the form of a clearly pronounced peak with a maximum temperature of ~180 K.

A further increase in the dose of implanted deuterium leads to an increase in the intensity of the lowest temperature peak of the deuterium thermal desorption spectrum, and it becomes dominant. The formation of a low-temperature intense peak in the deuterium thermal desorption spectrum may indicate the appearance of a new phase state, which can be considered as the formation of a hydride. The conclusion about the formation of a hydride was made on the basis of the data obtained by us in the study of the thermal desorption spectra of deuterium from Pd, Ti and ASS steel. These works show that the formation of hydrides is reflected in the deuterium thermal desorption spectrum by the appearance of lower temperature peaks. It is important that the formation of low-temperature deuterium desorption regions is accompanied by the appearance of a deuterium desorption region extended along the temperature scale in the temperature range of 200–1000 K.

Deuterium implantation at temperatures of 300 and 600 K leads to a significant decrease in both the temperature range of deuterium desorption and the amount of retained deuterium.

The role of nanotechnology in sustainable agriculture

Pruntseva G.O.

PO "Institutional reforms",
Tsitadelna str, 4/7, 51. Kiev-01015, Ukraine.
E-mail: gelenaprunceva@gmail.com

The loss of biodiversity, soil degradation, water pollution, irresponsible waste disposal, and the use of fossil fuels lead to catastrophic consequences in agriculture. Nanotechnology is gradually becoming a universal platform that provides an economically efficient, socially responsible and ecological solution to global problems of sustainable development. Instead of incremental improvements to existing technologies, nanotechnology offers disruptive, game-changing breakthroughs and innovations that can provide immediate answers and solutions to help our society, environment, and the planet [1]. Nanotechnology is used in the development of intelligent systems for the controlled release of nutrients, the production of highly effective fertilizers, increasing the fertility of soils, processing and storage of food products. Convergence between existing tools and nanotechnologies in the field of providing clean water is leading to revolutionary advances in water desalination, purification and reuse technologies. However, it is critical to make sure that any potential adverse effects of nanotechnology on human health and the environment are effectively assessed and addressed before the large-scale deployment of nanotechnology-based solutions and products for the global sustainability challenges facing the world in the next 10–20 years [2].

Thus, nanotechnology plays an important role in the sustainable development of agriculture, providing increased efficiency in agricultural production and increasing the possibility of overcoming world hunger.

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Nanoparticles of rhamnolipids with thiosulfonates

Prokopalo A.M.[1]***, Shcheglova N.S.***[1]***,***
Karpenko O.V.[1,2]***, Volianiuk K.A.***[2]***, Lubenets V.I.***[2]

[1] *Department of Physical Chemistry of Fossil Fuels of the Institute*
of Physical-Organic Chemistry and Coal Chemistry named after
L. M. Lytvynenko of the National Academy of Sciences of Ukraine,
Naukova street, 3A, Lviv-79060, Ukraine.
E-mail: zayarnyuka@gmail.com

[2] *Lviv Polytechnic National University,*
Bandera street, 12, Lviv-79013, Ukraine.

The development of new effective and low-toxic pharmaceuticals is an urgent task. Among the promising compounds, thiosulfonates are noteworthy - synthetic analogues of natural allicins with a wide range of biological activity. They are more resistant than natural substances, have low toxicity, antimicrobial, antiviral, antitumor, antithrombotic, anthelmintic action [1]. However, their use is limited by low solubility. The use of biogenic surfactants in compositions with thiosulfonates makes it possible to increase their solubility in water and bioavailability of drugs. The ability of rhamnolipids to enhance the action of various biologically active substances to stabilize pH-sensitive liposomes is known. [2] In addition, rhamnolipids are used to obtain microemulsions as solubilizers. The size of nanoparticles, their unique physicochemical properties, the ability to penetrate into tissues and cells open up new possibilities for use in pharmacy. In this regard, nanoparticles based on rhamnolipid biosurfactants of bacteria Pseudomonas sp PS-17 with thiosulfonates have been developed. The work uses: ATS – S-allyl ester of p-aminobenzenethiosulfonic acid; ETS – S-ethyl ester of p-aminobenzenethiosulfonic acid; MTS – S-methyl ester of p-aminobenzenethiosulfonic acid. Nanoparticles of rhamnolipids / thioethers were obtained to increase their solubility by the appropriate procedure. [3]. Hydrodynamic size difference of obtained particles in aqueous solution to determine were measured by dynamic light scattering on the DynaProNanoStar device (Wyatt Technology, USA) using noninvasive back scatter technology at 298 K (Fig.1,2,3) at the National Technical University "Lviv Polytechnic".

It was determined that rhamnolipids form spherical nanoparticles with sizes from 5 to 100 nm, with low polydispersity and stability in a wide range of concentrations. The obtained results show (Table 1) that the sizes of nanoparticles decrease when using rhamnolipids. This can be explained by the reduction of particle agglomeration due to the formation of rhamnolipid / thioether micellar structures and the stabilizing effect of surfactant rhamnolipids.

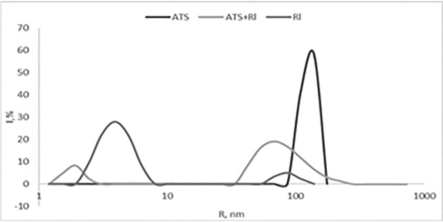

Fig 1. *Dynamic light scattering of solutions: ATS, ATS + Rl, Rl*

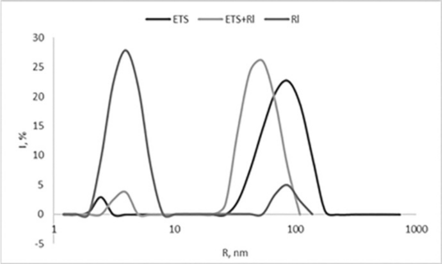

Fig 2. *Dynamic light scattering of solutions: ETS, ETS +Rl, Rl.*

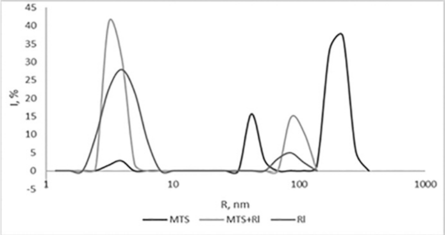

Fig 3. *Dynamic light scattering of solutions: MTS, MTS +Rl, Rl.*

Notes:
- *RL - rhamnolipids;*
- *ATS - S-allyl ester of p-aminobenzene thiosulfonic acid;*
- *ETS -S-ethyl ester of p-aminobenzene thiosulfonic acid;*
- *MTS - S-methyl ester of n-aminobenzene thiosulfonic acid.*

The antimicrobial activity of ETS / RL nanoparticles against test-culture S. aureus was established. The minimum inhibitory and bactericidal concentrations are 0.018 g / l and 0.009 g / l, respectively.

Thus, low-toxicity and tolerance of rhamnolipids to human cells, biosurfactants

Table 1

The size of the obtained nanoparticle

Nanoparticles	R, nm
ATS	140
ATS+RL	70
ETS	100
ETS+RL	55
MTS	40 and 225
MTS+RL	90
RL	4 and 85
ATS	140

may be promising tools for drug delivery. Further research will focus on the benefits of rhamnolipid carriers of drugs over existing or alternative delivery systems.

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Structure and physical properties changes of Fe-based amorphous alloys at annealing by electrical current.

***Prunitsa V.*, Mudry S.I., Kulyk Y.O., Nykyruy Y.S.**

Metal Physics Department, Ivan Franko National University of Lviv,
Kyrylo and Mephodiy, 8, 79005 Lviv, Ukraine
E-mail: yuliya.nykyruy@lnu.edu.ua

Amorphous and nanocrystalline metal alloys have attracted interest for a long time due to the combination of their unique properties like strength and elasticity, soft magnetic and giant magnetoimpedance effects, etc. The properties of this kind of materials are very sensitive to their structure, so by changing the structure, one can control properties changes, achieving optimal values. Different methods for structure transformation from amorphous to a nanocrystalline state like thermal annealing, heat, and laser treatments were used in the research and demonstrated various effects on the structure [1-3]. The method of electrical current annealing is based on the Joule heating effect of the material through which an electric current flows. Changing current parameters allows effect on the crystallization process of the amorphous phase achieving optimal parameters of structure and properties improving.

Amorphous ribbons under investigation were produced by the melt quenching method in the form of a 25 μm thick ribbon. Structure changes were investigated by the X-ray method. FE SEM method was used to study the surface topology.

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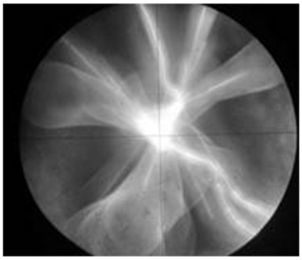
Laser-induced white-light emission from an organic/rGO-flake-mixed Au nanoparticle film

Fesenko O., Budnyk O., Rallev M.

SES laboratory, Institute of Physics of the NAS of Ukraine,
prospect Nauki, 46, Kyiv-03680, Ukraine
E-mail: fesenko.olena@gmail.com

Graphene is one of the attractive materials because of its superior electronic and photonic properties, thermal/chemical stability, and mechanical properties, which has been utilized for various applications including sensors, and nano/micro electrooptical devices. Especially, its high photo-thermal conversion property enables graphene to be employed in novel optical devices. In addition to the interest in pristine graphene, considerable scientific attention has also been devoted to the chemically derived hybrid known as graphene oxide, which exhibits unusual and tunable properties.



Laser-induced white-light emission

We studied organic/r GO-flake-mixed Au nanoparticle film by Raman and luminescence spectroscopy. Raman spectra have been measured using a Renishaw InVia Raman spectrometer equipped with a confocal DM2500 Leica optical microscope, a thermoelectrically cooled CCD as a detector, and a laser operating at a wavelength $\lambda = 633$ nm.

We demonstrate random lasing with star-shaped gold nanoparticles (“nanostars”) as scattering centers embedded in organic/rGO flakes nanostructures. The nanoparticles are randomly distributed within a thin film of organic/graphene-flakes films, forming resonators which support coherent laser modes. It can be explain by characteristic of graphene flakes (large negative thermal expansion and high absorption rate) by which random lasing modes could be modified by the structural change based on the elastic expansion and contraction of graphene flakes induced by light absorption/emission. Laser-induced white-light emission from an organic/rGO-flake-mixed Au nanoparticle film can be also connected with photoinduced, transient, domain-like $sp2 \rightarrow sp3$ phase transitions.

Detection of Vesicular Stomatitis Virus and Betacoronavirus by SERS spectroscopy

***Fesenko O. M.*[1], *Klochek A.V.*[1], *Zholobak N.M.*[2]**

[1] *Institute of Physics, National Academy of Sciences of Ukraine,*
46, pr. Nauky, 03028 Kyiv, Ukraine

[2] *D.K. Zabolotny Institute of Microbiology and Virology, National Academy of Sciences of Ukraine,*
154 , Akademika Zabolotnoho Str., 03680 Kyiv, Ukraine

Recently, Surface enhanced Raman spectroscopy (SERS) only started to enter into the biological and medical fields. It's enables non-destructive analysis of structural details at the molecular level and is uses to study viruses and their constituents. Here, we used SERS spectroscopy to study Vesicular Stomatitis Virus (VSV), virus family Rhabdoviridae and Betacoronavirus. VSV has been extensively studied as a prototype of the nonsegmented negative-strand RNA viruses. The relative safety of the virus combined with its abundant replication in a broad range of cultured cells have favored the use of VSV in research laboratories. Raman studies of VSV will have led to understanding of fundamental host cell processes, molecular details of viral gene expression, and the pathogenesis of viral infection. Advantageously, Raman spectroscopy can identify specific protein signals in relatively impure samples. Thus, this proof-of-principle technological development has implications for the rapid identification and biostability characterization of viruses in medical, veterinary, and food samples and for the analysis of virion glycoprotein conformational changes in situ during viral entry.

VSV from the collection of the viruses D.K.Zabolotny IMV NAS of Ukraine was cultured in epithelial cell line MA104 (ATCC CRL-2378.1). The virus-containing suspension was purified by ultracentrifugation. "Minisart® High Flow" polyester sulfone filters with a pore size of 0.22 µm (Sartorius, Germany), which is commonly used for sterile filtration, was used to remove the liquid phase and fixation the virions on the filter surface.

We measured and compared the Raman spectra of the virions of VSV and Betacoronavirus. Raman spectra have been measured using a Renishaw InVia Raman spectrometer equipped with a confocal DM2500 Leica optical microscope, a thermoelectrically cooled CCD as a detector, and a laser operating at a wavelength λ = 633 nm. The direct identification is based on trapping the viruses with Au nanostrucure and recording the SERS signal from RNA fragments or membrane proteins.

Challenges for Modern Science in Ukraine

Fesenko O., Tkachenko V., Kifiuk Ye.

The International Science and Innovation Cooperation, Technology Transfer and Intellectual Property Department, Institute of Physics of the NAS of Ukraine. 46, Nauky Ave., Kyiv-03039, Ukraine.
E-mail: fesenko.olena@gmail.com

After partial recovery from lock downs and quarantine measures regarding recent COVID-2019 pandemic Ukrainians scientists faced new challenge. Russia's unprovoked and unjustified invasion of Ukraine produced a number of new negative factors that lead to further regress of science in Ukraine.

Thus in a frame of Ukrainian Science Reload project representatives of Ukrainian and foreign universities, National Research Foundation of Ukraine and National Erasmus+ Office in Ukraine & HERE team conducted a poll among 2173 scientists of Ukraine.

Results of this poll show that science in Ukraine goes through grievous times:

- more than 67% respondents can not conduct scientific activities at the same level as before Russia aggression;
- since the war beginning 83.8% respondents observe worsening financial situation;
- due to lack of science funding almost 30% scientists stated that projects they were involved in were put on hold.

Now we face two possible scenarios. Either number of researchers will be reduced by 4.6 times by 2035. This will lead to completion of the final liquidation of Ukrainian science. Or in order to get closer to European scientific personnel indicators Ukraine has to double number of young scientists every 5 years without losing more than 1% of scientists aged from 30 to 59 years and 5% for scientists older than 60 years.

Main steps in achieving second scenario should be:

- increasing funding for science from 0.41 to 2% of GDP;
- increasing the number of young people in science;
- increase the salary of scientists, especially young ones, to a level higher than the average salary in the country;
- increasing funding for the purchase of research equipment.

Failing to break negative trend in Ukrainian science will lead to further “brain drain” to European countries and total decline of research activities of Ukraine.

Radiation of gallium phosphide LEDs in a state of negative differential resistance

Vernydub R.M.[1], Kyrylenko O.I.[1], Petrenko I.V.[2], Radkevych O.I.[3], Tartachnyk V.P.[2], Shlapatska V.V.[4], Stratilat D.P.[2], Poliakova I.O.[5], Budnyk O.P.[6]

[1] National Pedagogical Dragomanov University,
Pyrogova St. 9, Kyiv-01601, Ukraine

[2] Institute for Nuclear Research of the NAS of Ukraine,
Nauki Ave., 47, Kyiv-03680, Ukraine, reactor_104@ukr.net

[3] SE "SRI of Microdevices" STC "Institute for Single Crystals" of the NAS of Ukraine, Nauki Ave., 60, Kharkiv - 61072, Ukraine

[4] L.V. Pisarzhevski Physical Chemistry Institute of the NAS of Ukraine, Nauki Ave., 31, Kyiv-03028, Ukraine

[5] SSE "Radon Association",
Pyrogovsky Shlyach St., 50, Kyiv- 03083, Ukraine

[6] SES laboratory, Institute of Physics of the NAS of Ukraine,
Nauki Ave., 46, Kyiv-03680, Ukraine

The region of negative slope on the current-voltage characteristics (CVCs) of diodes is the result of the existence of positive feedback in current and voltage. In the first case (current-controlled connection), an S-like dependence I(U) is formed; in the second (voltage-controlled connection), an N-like section of the CVCs appears.

Due to the negative value of dU/dI, resistance losses can be compensated and, in particular, inextinguishable electromagnetic oscillations can exist in the oscillatory circuit. In light-emitting diodes (LEDs) GaP at temperatures below T = 120 K, a region of negative differential resistance (NDR) S - type (main) arises; in addition to it, there are also sections of the N - type on the forward and reverse branches of the CVCs, where the amplitude values ΔU and ΔI are much less than the voltage and current fluctuations in the main region of NDR.

The emission spectrum of green LEDs in the NDR mode consists of two main lines $\lambda_1 = 546$ nm, $\lambda_2 = 575$ nm, and their phonon repeats; an increase in the diode temperature from 77 K to 120 K entails an increase in the intensity of the glow of both lines. Irradiation by electrons with E = 2 MeV leads to a decrease in the intensity of radiative recombination in the entire spectral range under study as a result of the introduction of nonradiative levels of radiation defects.

It was found that when the "breakdown" voltage UBR is reached, the diode jumps into a low-resistance state, while the current value can sharply increase several times. The brightness of the glow also increases due to an increase in the emission intensity of the band λ_2 = 546 nm and a decrease in the emission intensity of the band λ_1 = 575 nm. The mechanism of NDR formation in different solid objects, as a rule, is different. The authors of [1] came to the conclusion that in GaP diodes, as well as in GaAs diodes, the materials of which belong to the same crystal group, it is possible to implement the mechanism of intervalley scattering of carriers, when, when a sufficient electric field strength is reached, carriers flow from the lower valley of the conduction band, where their effective mass is large towards the upper valley with a larger curvature and, accordingly, a smaller effective mass.

In our case, this means the accumulation of carriers in the upper valley of the C - band and their recombination through a system of levels within 2.27–2.16 eV located near the V - band.

Areas of NDR found in GaP LEDs N-type are most likely associated with the zone-defect-zone tunneling-recombination mechanism.

The application of the effect of NDR is quite diverse, the flow of current in the area of NDR, with the exception of the effect of intervalley scattering, is provided by a quantum-mechanical tunneling mechanism that is insensitive to the magnitude of electron mobility; this feature may be useful in determining ways to use semiconductor materials with low carrier mobility.

The combination of the effect of NDR with a change in the spectral composition of the radiation is promising from the point of view of using LEDs as a high-speed photoswitch. There is the possibility of forming memory cells, logic circuits, various communication devices, and so on.

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Special session of the TransFerr Project - ID: 778070

MSCA-RISE - Marie Skłodowska-Curie Research and Innovation Staff Exchange (RISE)

The influence of annealing temperature on various properties of $Bi_{1-x}Gd_xFe_{0.85}Mn_{0.15}O_3$ solid solutions prepared via sol-gel synthesis

Karoblis D.[1]***, Diliautas R.***[1]***, Beganskiene A.***[1]***, Mazeika K.***[2]***,***
Baltrunas D.[2]***, Niaura G.***[3]***, Talaikis M.***[4]***, Lukowiak A.***[5]***,***
Strek W.[5]***, Zarkov A.***[1]***, Kareiva A.***[1]

[1] *Institute of Chemistry, Vilnius University,*
Naugarduko 24, LT-03225, Vilnius, Lithuania
E-mail: Dovydas.karoblis@chgf.vu.lt

[2] *Center of Physical Sciences and Technology, Vilnius, LT-02300, Lithuania*

[3] *Institute of Chemical Physics, Faculty of Physics, Vilnius University,*
Sauletekio Ave. 3, Vilnius, LT-10257, Lithuania

[4] *Department of Bioelectrochemistry and Biospectroscopy,*
Institute of Biochemistry, Life Sciences Center,
Vilnius University, LT-10257, Vilnius, Lithuania

[5] *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okolna 2, PL-50422 Wroclaw, Poland*

Bismuth ferrite ($BiFeO_3$) and gadolinium ferrite ($GdFeO_3$) are perovskite-type materials with known multiferroic properties. Substitution of Bi^{3+} ions with Gd^{3+} can lead to improvement in ferroelectric and magnetic properties [1], while intercalation of 15% of Mn^{3+} causes enhanced magnetoelectric coupling [2].

This work focuses on the chemical composition as well as annealing temperature influence on structural, morphological, and magnetic properties of novel sol-gel derived $Bi_{1-x}Gd_xFe_{0.85}Mn_{0.15}O_3$ solid solutions. Gd^{3+} introduction led to few structural changes, which were investigated by X-ray diffraction analysis, Raman and FT-IR spectroscopies. Furthermore, scanning electron microscopy revealed that particle size is dependent upon the annealing temperature. Lastly, magnetic measurements at room temperature were performed.

Acknowledgments: The work has been done in frame of the project TransFerr. This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska-Curie grant agreement no. 778070.

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High-Pressure effects on Sm doped $BiFeO_3$

Pakalniškis A.[1]***, Skaudžius R.***[1]***, Karpinsky D.***[2]***,***
Niaura G.[3]***, Kareiva A.***[1]

[1] *Institute of Chemistry, Vilnius University,*
Naugarduko 24, Vilnius, Lithuania
E-mail: andrius.pakalniskis@chgf.vu.lt

[2] *Namangan Engineering-Construction Institute, Namangan, Uzbekistan.*

[3] *Department of Organic Chemistry, Center for Physical Sciences and Technology (FTMC), Sauletekio Ave. 3, Vilnius, Lithuania*

$BiFeO_3$, a lead free multiferroic compound with perovskite type structure, was found to have a polar to non-polar morphotropic phase boundary. Substitution of bismuth ions by rare-earth elements causes the structural transition from the polar rhombohedral phase to the non-polar orthorhombic phase via stabilization of $PbZrO_3$-like anti-polar orthorhombic phase [1]. The concentration ranges of the structural stability of the different phases strongly depend on the type of rare-earth element and the reduction in the ionic radius of the dopant ions leads to a shrinkage of the mentioned ranges [1]. The concentration range attributed to the anti-polar orthorhombic phase reduces to 1% in the system $Bi_{1-x}Sm_xFeO_3$ [2]. In the case of Sm-doping the concentration range ascribed to structural stability of the antipolar orthorhombic phase becomes extremely dependent on the preparation conditions and post synthesis treatment of the samples. The characterization of the MPB region performed based on microscopic measurements can give different results as compared to local measurements which poses a problem for scientific research.

In the present study, we report on the correlation between the type of structural distortions, morphology of crystallites and an onset of remanent magnetization for Sm-doped $BiFeO_3$ compounds prepared by different methods. As well the effects of high pressure on the structural and magnetic properties.

Acknowledgements. This work was supported by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 778070.

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Effect of Nb cationic substitution on the microstructure and Raman spectra of $SrBi_2(Ta,Nb)_2O_9$ thin films

Fesenko O.M.[1], ***Yaremkevich A.D.***[1], ***Tsebrienko T.V.***[1],
Budnyk O.P.[1], ***Morozovska A.N.***[1]

[1] *Institute of Physics, National Academy of Sciences of Ukraine,*
46, pr. Nauky, 03028 Kyiv, Ukraine

[2] *Francisk Skorina Gomel State University,*
Belarus, 246019, Gomel, 104, Sovetskaya str.

In the present work micro-Raman spectroscopy has been used to understand the lattice dynamics of Nb cation substituted $SrBi_2(Ta_xNb_{1-x})_2O_9$ (SBTN) thin films modified by crystallization annealing under 700 °C. Different concentrations of Nb were introduced into SBT lattices. Incorporation of Nb ion at Ta-site was confirmed by decrease in the lattice parameters and x-ray diffraction data. Substitution of Nb at Ta-site of SBT did not influence the low frequency Raman modes of SBTN. However, it showed a pronounced influence on the O-Ta-O stretching modes by shifting and splitting the mode frequency at 810-8 cm^{-1}. The relative intensity of (115), (006) and (200) peaks in x-ray diffraction increased with the increase of the Nb concentration. Landau approach was used to explain the experimentally observed fraction of perovskite phase in SBTN allowing possible appearance of finite size effects related with nanogranular structure of the studied SBTN films.

Raman spectroscopy was successfully used to study the lattice vibrational modes and structural transition of SBTN thin films with various Nb ions concentration (x=10, 20, 30, 40 and 50%) at Ta-sites. The blue shift of the Raman band from 810 to 830 cm^{-1} is associated with the amount of Nb concentration and defects present in the film, which in turn is related to the crystallization degree of the SBTN material. The substitution of Nb at Ta-site showed a significant splitting of O-Ta-O octahedral stretching mode.

Could the negative capacitance effect be used in FETs with a ferroelectric gate?

Strikha M.V. [1,2]***, Eliseev E.A.***[3]***, and Morozovska A.N.***[4]

[1] Taras Shevchenko Kyiv National University, Faculty of Radiophysics,
Electronics and Computer Systems,
Pr. Akademika Hlushkova 4g, 03022 Kyiv, Ukraine,
E-mail: maksym.strikha@gmail.com

[2] V.Lashkariov Institute of Semiconductor Physics, National Academy
of Sciences of Ukraine, Pr. Nauky 41, 03028 Kyiv, Ukraine

[3] Institute for Problems of Materials Science, National Academy of Sciences
of Ukraine, Krjijanovskogo 3, 03142 Kyiv, Ukraine

4 Institute of Physics, National Academy of Sciences of Ukraine,
Pr. Nauky 46, 03028 Kyiv, Ukraine,

Abstract

We consider a silicon MOSFET, in which the gate insulator is formed from thin layers of a dielectric SiO_2 and a weak ferroelectric HfO_2. We study the possibility of implementing a stable negative capacitance of the insulator in such a system, which would open the principal possibility to reduce the subthreshold swing to the values below the threshold, 60 mV/decade at room temperature, and supply voltage to the values below the fundamental Boltzmann limit, 0.5 V, which would be an important step towards further miniaturization of MOSFETs. It is shown theoretically that it is possible to achieve a transient negative capacitance of a ferroelectric in the situation when the charge at the capacitor plates increases more slowly than the ferroelectric polarization. Its temporal stabilization in the system composed from the thin dielectric and ferroelectric layers requires stable positive free energy and capacity of the whole system. Therefore, the effect of the negative capacitance of a ferroelectric itself cannot be manifested "outside" the system mentioned above, including the transistor applications and it is unrealistic to hope that the negative capacitance effect will help reduce the subthreshold swing below the critical value, and thus contribute to further miniaturization of the MOSFET.

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Raman scattering study of rare earth manganites $RMnO_3$ (R=Yb, Sm, Tb and Tm)

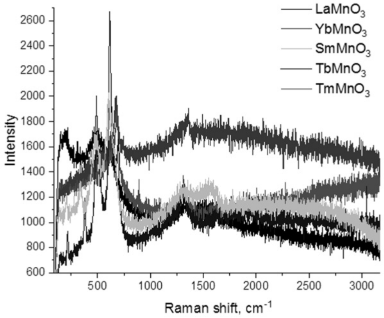
<u>Fesenko O.</u>[1], Yaremkevich A.[1], Morozovska A.[1], Tomala R.[2], Strek W.[2]

[1] SES laboratory, Institute of Physics of the NAS of Ukraine,
prospect Nauki, 46, Kyiv-03680, Ukraine
.E-mail: fesenko.olena@gmail.com

[2] Institute of Low Temperatures and Structural Research,
Polish Academy of Science, Wroclaw, 50-422, Poland

Now is very actual task to develop complex transition metal oxides with perovskite-like structure having improved and controllable (multi)ferroic properties. The mentioned materials are manganites and ferrites with optimal composition having distinct magnetization, polarization, (magneto)transport properties or magnetoelectric coupling. Improved functional properties of these oxides can be controlled via modification of the chemical bond character, structural parameters, stoichiometry, defects etc. The reduced stability is associated with the metastable structural state formed in the vicinity of the phase boundaries, while this state presumably consists of coexistent nanoscale regions of the adjacent structural phases. There is known two main way to create metastable state to design ceramics via chemical substitution asynthesis treatment by high pressure and/or thermal cycling in gases to induce nanoscale regions, or the second one assumes chemical routes synthesis of films and ceramics.

Here we presented the result which was observed by Raman spectroscopy of the rare earth manganites $RMnO_3$ (R=Yb, Sm, Tb and Tm) prepared at 900 °C. Raman spectra have been measured using a Renishaw InVia Raman spectrometer equipped with a confocal DM2500 Leica optical microscope, a thermoelectrically cooled CCD as a detector, and a laser operating at a wavelength λ = 633 nm. It was showed that shifts of some Raman bands depends of radius of the rare-earth R and local environment of the Mn^{3+} ions. The dependence can be explained by the electro-elastic coupling between the elastic dipole determined by the ionic radius and Raman modes.



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Nanocomposites based on porous III-V semiconductors

Barlas T.[1,2], Kotova N.[1], Mamykin S.[1], Romanyuk V.[1], Semtsiv M.[2]

[1] *V. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine.*
Prospect Nauki, 41, Kyiv-03028, Ukraine.
E-mail: barlas@academ.kiev.com

[2] *Department of Physics, Humboldt University Berlin,*
Newton str. 15, D-12489, Berlin, Germany.

Porous media are widespread in nature (bones, for example) and used in industry. In particular porous III-V semiconductors [1] and nanocomposite based on them are promising for optoelectronics [2], sensorics, laser technique etc. In our work porous semiconductors were obtained by cheep and effective electrochemical etching of n-type InP, GaP, GaAs single crystals with surface orientation (100) and (111). The etching was carried out in the galvanostatic regime in water solutions of HF, H_2SO_4 and HNO_1. With the correct choice of anodic etching conditions, self-organized phenomena take place that lead to the formation of quasi-ordered array of pore with possibility to control pore shape and size. Two types of pores were generated: oriented along the <111> crystallographic direction and oriented along the current line. In the latter case, it is possible to obtain more perfect porous structures. The possibility of freely choosing the direction of the pores opens up wider application. To produce nanocomposites with plasmon-active component, metal inclusions have been incorporated into the pores by electrochemical deposition from the solution of the Au salt. Diameter of pores was 100-200 nm and metal particle size was 10-40 nm. Hybrid heterostructures based on porous gallium phosphide and charge selective organic layer PEDOT:PSS were fabricated by spin coating method. Optical properties were studied mainly in far-IR spectral region, in plasmon-phonon range of the semiconductors, by micro-Raman mapping, specular reflection and ATR methods and also photoluminescence was analyzed. Phonon band intensities are significantly increased in the porous region especially near gold nanoinclusions and porosity significantly affects IR spectra.

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Hydride-nanosilica as an effective reinforcing additive for epoxy polymer composites.

Starokadomsky D.*[1,2], Reshetnyk M.*[3]

[1] *Chuiko Institute of Surface Chemistry, National Academy of Sciences (NAS) of Ukraina, Gen.Naumova 17, Kyiv, E-mail: epoxidian@gmail.com*

[2] *M.P.Semenenko Institute of Geochemistry, Mineralogy and Ore Formation, Acad.Palladina Ave.34, NAS, Kyiv*

[3] *National Nature-Historical Museum NAS, B.Hmelnytskogo 1, Kyiv*

Pyrogenic nanosized silica is an effective thickener and additive to coatings and polymer compositions, including epoxy ones. Chuiko ISC NAS has established industrial production of silica, and its modification is the direction of a number of scientific teams of the institute [1]. In this work, we synthesized nanosilica with a hydride coating (the concentration of grafted SiH groups was approximately 0.5 mmol/g), which, in an amount of 2 wt %, are relatively homogeneously distributed in epoxy resin. The good compatibility and distribution of silica hydrides in the epoxide enhances the important strength properties of the polymer. In particular, an increase in the modulus of elasticity in compression and by 30-40%, in bending - by 1.2-1.5 times, an increase in bending strength by 1.5-2 times, and adhesion to steel - by 2.5-2.8 times.

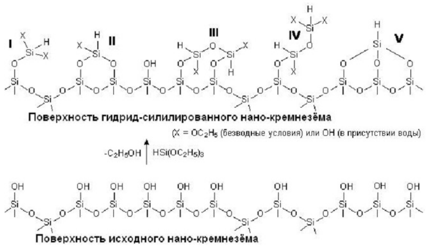

Fig.1. Scheme: the process of hydride-silylation of the surface of silica [1]

The reinforcing effect of hydride-silica is also manifested in an increase in resistance in aggressive solvents. Thus, in acetone, a sample of an unfilled polymer quickly swells and disintegrates into fragments already after 1 day of exposure. A little longer (up to 2 days) a sample with A-300 withstands. At the same time, samples with both types of silica hydride (SiH_8 and SiH_9) after a noticeable (by 20-30%) swelling remain in the solvent for an indefinitely long time (Fig. 2). Also, silica hydride significantly enhances the durability of composites in concentrated (50-60%) H_2O_2.

It has been shown by SEM microscopy that SiH8 samples with the SiO_2 surface completely covered with hydride groups form a nonporous uniform composition. In contrast, SiH_9 samples with a surface partially covered with hydride groups give a porous composite.

P.Kuzema, D.Starokadomsky,..V.Tertykh, Reinforcement of epoxy polymers with hydride-silylated fumed silica// Chem.,Phys. and Techn. of Surface, 2020, V.11, N4, p.484-491.

Development and characteristics research of ALT-sensitive biosensor

Mruga D., Soldatkin O., Dzyadevych S., Soldatkin A.

Department of Biomolecular electronics, Institute of Molecular biology and genetics of the NAS of Ukraine.
Zabolotnogo street, 150, Kyiv-03143, Ukraine.
E-mail: darynamruga@gmail.com

Alanine aminotransferase is a specific intracellular liver enzyme. Its content in the blood is a constant value (up to 35 unitsL-1). ALT activity in the blood serves as a diagnostic marker of liver and myocardial diseases. There-fore, the development of new fast, accurate and easy-to-use devices for ALT monitoring (in addition to existing various methods) is a very important task of biotechnology.

This paper describes the development of a highly selective am-perometric biosensor based on glutamate oxidase to determine the activity of ALT in multicomponent biological fluids. A platinum disk electrode (working surface diameter 0.4 mm) was used as an electrochemical transducer. The bi-oselective element was formed by the formation of glutaric aldehyde cross-linking between BSA and glumatoxidase. The membrane thickness is about 120 nm. The optimal concentrations of reactives were selected (alanine - 4 mM and α-ketoglutarate - 50 μM, pyridoxal phosphate - 50 μM).The selectivi-ty of the biosensor proposed in the work with respect to various components of biological fluids (ions, amino acids, other organic substances) and electro-active substances was also analyzed. The selectivity of the amperometric transducer with respect to electroactive substances was improved by the use of an additional semipermeable polyphenylenediamine membrane. The fun-damental ability of this biosensor to measure ACT activity was also demon-strated. The selectivity of the developed sensor for transaminases was tested: changes in the system under the presence of both enzymes were studied. Dur-ing the study of the analytical characteristics of the biosensor, a calibrated graph of the dependence of the magnitude of the biosensor response on the ALT concentration was obtained. Using the calibration curve, the linear range of the biosensor (10-500 units / l), the minimum limit of detection (5 units / l), noise, drift, sensitivity of the biosensor to the substrate (0.5 nA / min 100 Units) were determined. / l ALT) and others. In addition, the parameters of the biosensor were studied, such as signal reproducibility (92.4%), stability of functioning (88.5% in 3 days), signal duration (60 s) and the total duration of one analysis, taking into account the preparation (approximately 10 min).

Thus, the obtained characteristics of the biosensor allow us to pro-ceed to testing the operation of the developed ALT-sensitive biosensor based on glutamate oxidase in blood serum. It was also found that the development of a two-enzyme biosensor system is needed to simultaneously determine AST, ALT and their ratios.

Ultrafast dynamics of carrier relaxation in PdO thin films

Rudenko V.I.[1], Styopkin V.I.[2], Liakhovetskyi V.I.[1,3],
Brodyn O.M.[3], Brodyn M.S.[1]

[1] Nonlinear Optics Department, Institute of Physics of the NAS of Ukraine.
Prospect Nauky, 46, Kyiv-03039, Ukraine.
E-mail: val@iop.kiev.ua

[2] Department Of Physical Electronics, Institute of Physics of the NAS of Ukraine. Prospect Nauky, 46, Kyiv-03039, Ukraine.

[3] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37, Prospekt Peremohy, Solomyanskyi district, Kyiv, 03056, Ukraine

Nanoscale semiconductor structures are an active field of research due to their spesific posibilities to change physical properties their bulk counterparts. PdO is a p-type semiconductors with a band gap that can couple efficiently to the solar spectrum are of interest for energy conversion applications either as photovoltaics, photocatalysts or as electrodes for photoelectrolytic cells semiconductor with rather narrow bandgap energy and for optoelectronic applications because of the high nonlinear optical properties found [1].Although the nonlinear optical properties of PdO thin films have been investigated [1], it appears that poorly researched ultrafast carrier dynamics, despite their potential for using in optoelectronic devices.

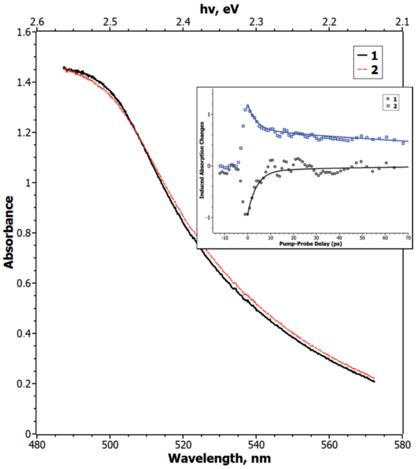

Fig.1. *Absorption spectrum of PdO film (curve 1) and its evolution after femtosecond laser irradiation at 800 nm (curve 2).*

In our work we have used the pump-probe method to detect changes in the 2.5 eV absorption band of 120 nm films when exposed to, 180 fs, 10 μJ pulsed excitations at 800 nm and 400 nm. Fig.1, and 2 show the absorption band edge spectra before (spectrum 1) and during (spectrum 2, zero time delay) the excitation pulse at 800 nm and 400 nm, respectively. At 800 nm excitation (Fig.1), subtle changes in absorption can be noticed, especially in the spectral range of 487-505 nm. It can be seen that while the absorption around 500 nm decreases after excitation, on the contrary, it increases at longer wavelengths above 510 nm. These changes, although subtle, were reproducible and much larger than the spectral noise. The maximum decrease in absorption is observed at 498 nm (2.49 eV), i.e., close to the absorption band maximum of 2.5 eV. At the same time, when excited at a wavelength of 400 nm, we have the opposite effect (Fig. 2). In the region of 500 nm the absorption increases and in the region >510 nm it decreases.

Fig.1 and 2 (insets) show the time dependences of the occurrence and relaxation (fited by biexponentials curves) of induced absorption changes in the 2.5 eV band. In the inset, the lower data set corresponds to the averaged differential absorption in the 495-500 nm interval, while the upper data set corresponds to 518-523 nm. At 800 nm excitation (Fig.1), we observe a fast relaxation with a characteristic time τ1 ≈ 2 ps, which must be related to the dynamics of nonequilibrium carriers mainly in the valence band, and an additional slow relaxation with τ2 ≈ 1 ns, possibly due to carrier diffusion. At the same time, the increased absorption in the region of 2.5 eV with 400 nm excitation can be caused by interband single-photon transitions, because the energy of the excitation quantum (h = 3.1 eV) is greater than the bandgap width (~2.5 eV).

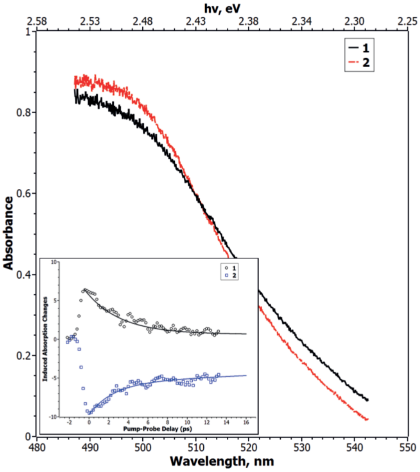

Fig.2. *Absorption spectrum of PdO film (curve 1) and its evolution after femtosecond laser irradiation at 400 nm (curve 2).*

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Effect of gold nanocomposites and Quercetin treatment on male reproductive function

Kaleynikova O.N.*[1]*, Ukrainska S.I.1, Blashkiv O.T.*[2]*, Muzychenko A.S.*[2]*,
Sribna V.A.*[1]*, Velykiy V.Y.*[1]*, Vinogradova-Anyk A.A.*[2]*, Tarasova K.V.*[2]*,
***Lagodich T.S.*[2]*, Karvatskiy I.M.*[2]*, Kuziv Y.I.*[3]*, Voznesenska T.Y.*[1]*, Kutsevol N.V.*[3]

[1] *Bogomoletz Institute of Physiology, NAS of Ukraine, Kyiv, Ukraine*

[2] *Bogomoletz National Medical University, Kyiv, Ukraine*

[3] *Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
E-mail:tblashkiv@gmail.com

Due to the peculiarities of structure and control of intramolecular structure, branched polymer systems are interesting objects of basic research, as well as promising functional materials of the new generation. Polymers with a dextran core and grafted polyacrylamide chains dextran-polyacrylamide (D-PAA) in the anionic form of D-*g*-PAA(PE), as a polymer matrix carrier, in particular gold nanoparticles (AuNPs) - are being actively studied.

The aim is to evaluate the effect of five treatment of gold nanosystems (D-*g*-PAA(PE)/AuNPs) and Ouercetin on male reproductive function in mice in experimental chronic kidney disease (EChKD).

The study was performed in two series of experiments on male and female mice with EChKD, a model of which was created by immunizing animals with kidney homogenate.

Introduction of substances: according to TEM, AuNPs loaded (synthesized, retained) in D-g-PA (PE) are spherical in shape, size 4-11 nm. D-*g*-PAA(PE) (2.00 mg/kg), D-*g*-PAA(PE)/AuNPs (1.96 mg/kg), saline was administered intravenously (in a tail vein of 0.3 ml) once a day, five times according to the immunization schedule after the fourth immunization (the last, 3 weeks after the start of the experiment). Quercetin (Quercetin, Sigma, USA) (50 mg/kg) was administered intraperitoneally once daily, five times according to the immunization schedule after the fourth immunization (last, 3 weeks after the start of the experiment) and after the introduction of gold in the group where they were injected together.

Estimated: sperm viability; the number of sperm (sperm concentration (thousand/ml)) and the number of abnormal forms of sperm (%); the ratio of cells of different generations of spermatogenic epithelium; pathways of cell death of testicular cells (spermatocytes (primary)) and sperm cells of testicular appendages (epididymis); embryonic mortality in mice; the number of live pups per female.

Under conditions of EChKD, the treatment of D-*g*-PAA(PE)/AuNPs in comparison with the following values under conditions of EChKD decreased: 1) the number of abnormal sperm (%) (1.41 times); 2) the number of necrotic cells

(1.69 times) of the testes (sperm cells (primary)); 3) the number of necrotic cells (1.71 times) of the epididymis (sperm) and 4) preimplantation mortality of embryos (1.61 times). Under conditions of EChKD+D-*g*-PAA(PE)/AuNPs+Quercetin found: 1) decrease in the number of abnormal sperm (%) (1.88 times); 2) increase (1.17 times) in the number of spermatids in the testes; 3) increase (1.18 times) of living cells and decrease (2.43 times) of necrotic cells of the epididymis (sperm); 4) reduction (1.84 times) of preimplantation mortality of embryos; 5) increase (1.64 times) in the number of live newborns (pups) compared to such values under the conditions of EChKD.

Our data suggest that Quercetin has a positive effect on spermatogenesis in EChKD, in the early stages of chronic kidney disease, when there is already kidney damage, accompanied by impaired filtration and manifested by proteinuria (the appearance of protein in the urine); gold nanosystems (gold nanoparticles in the polymer matrix D-*g*-PAA(PE)) are of particular interest for possible therapeutic applications to improve reproductive function.

The effect of such gold nanosystems may be manifested in the reduction of oxidative stress and improved repair (restoration of the integrity of fragmented DNA) of spermatocytes, which requires further study.

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Autor Index

The **Enterprise Europe Network** is a service that provides support for Small and Medium-sized Enterprises (SMEs) with international ambitions. Co-funded by the European Union's COSME and Horizon 2020 programmes, the Network's aim is to help businesses innovate and grow internationally.

The Enterprise Europe Network was launched on 7 February 2008 by former EU Commissioner Günter Verheugen. The Enterprise Europe Network combines the previous Euro Info Centres and the Innovation Relay Centres. From 2008 to 2014, the Network was co-financed by the EU's Competitiveness and Innovation Framework Programme (CIP), in cooperation with institutions at national and regional levels. From 2015-2020, the Network is co-financed under the European Union's programme for the competitiveness of SMEs [6] (COSME) and Horizon 2020[7].

Under the responsibility of the European Commission's Directorate-General for Internal Market, Industry, Entrepreneurship and SMEs, the Enterprise Europe Network is managed by the Executive Agency for Small and Medium-sized Enterprises (EASME).

The Network is active in more than 60 countries worldwide. It brings together 3,000 experts from more than 600 member organisations, including:

- chambers of commerce and industry
- technology poles
- innovation support organisations
- universities and research institutes
- regional development organisations

Enterprise Europe Network advisory services support businesses seeking to expand into international markets. The services cover a wide range of regulatory areas and market intelligence:

- Compliance with EU regulations and standards (e.g. CE marking)
- Access to international markets – market intelligence and capacity building
- International public contracts –access to cross-border procurement and EU tender opportunities
- National and regional finance and funding – identification of sources of finance and investor-readiness training
- EU funding schemes and application support
- Intellectual property rights (IPR) – patents and IPR applications and exploitation strategies
- Energy and resource efficiency – identification of technologies and finance opportunities
- Management improvement – capacity building

Enterprise Europe Network innovation support services[4] are available based on an assessment of the needs and development phase of the business.

At an entry level, Network services include:

- information on innovation-related policies, legislation and support programmes
- links with local innovation stakeholders
- information about access to local sources of funding/support

Network experts can provide one-to-one services to support innovation capacity building. Services include innovation audits, advice on intellectual property, marketing and access to finance.

Finally, the Network provides key account management services to businesses benefitting from the Horizon 2020 SME instrument programme[5], part of the European Innovation Council (EIC) pilot.

In 2017, Ukraine joined the European Enterprise Entrepreneurship Network (EEN) within the framework of the COSME program, which promotes the competitiveness and innovative development of small and medium-sized enterprises, innovation organizations and institutes / universities. For this purpose in Ukraine was created a Consortium EEN-Ukraine , which included representatives of business and government agencies, as well as scientific organizations

To contact EEN-Ukraine please follow the website

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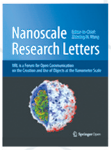

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