Graphene-like autointercalated Niobium Diselenide nanoparticles: new possibility of 2D nanomaterials design

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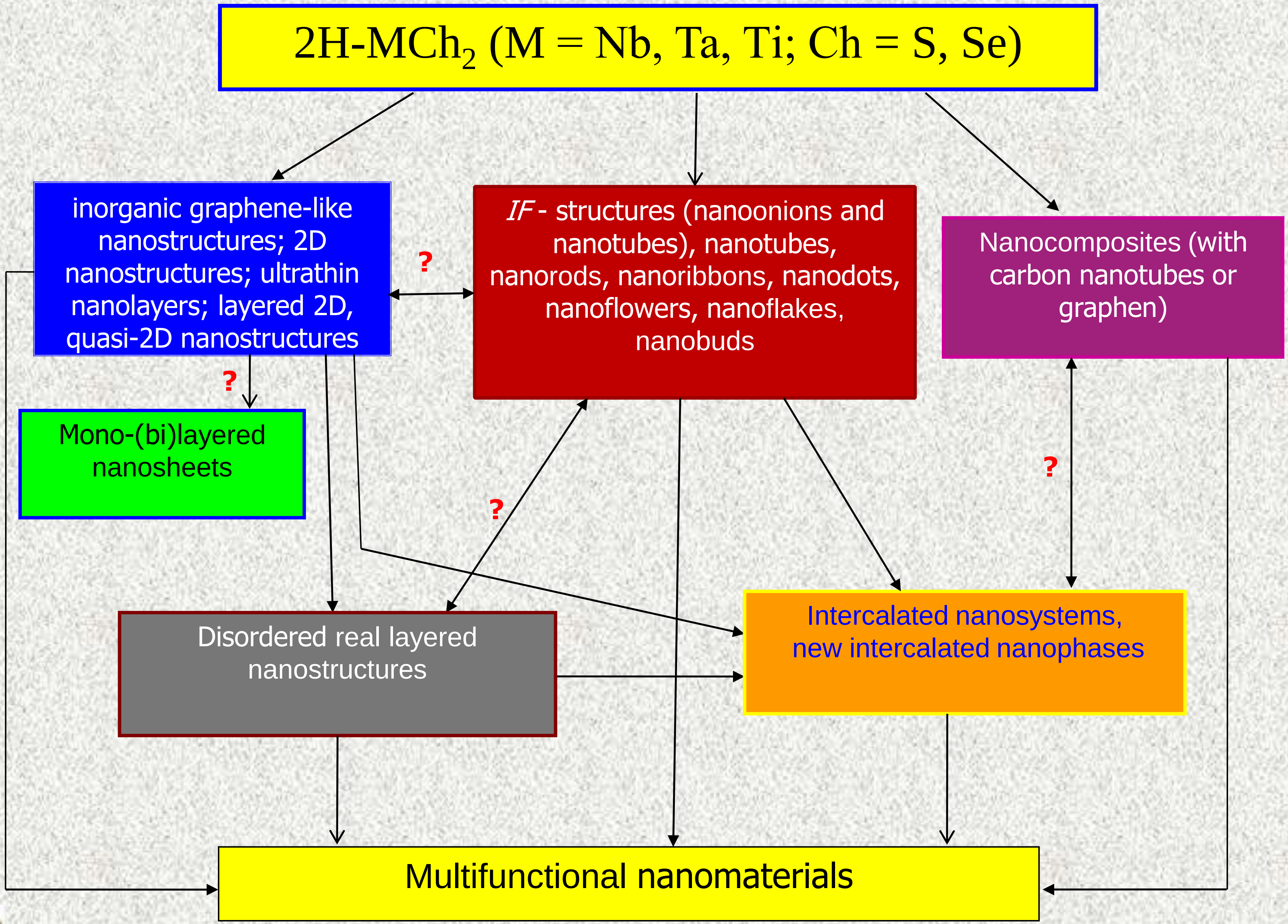

2H-MCh_2 (M = Nb, Ta, Ti; Ch = S, Se)
inorganic graphene-like nanostructures; 2D nanostructures; ultrathin nanolayers; layered 2D, quasi-2D nanostructures
IF - structures (nanoonions and nanotubes), nanotubes, nanorods, nanoribbons, nanodots, nanoflowers, nanoflakes, nanobuds
Nanocomposites (with carbon nanotubes or graphen)
?
?
Mono-(bi)layered nanosheets
?
?
Disordered real layered nanostructures
Intercalated nanosystems, new intercalated nanophases
Multifunctional nanomaterials

APPLICATION OF 2D NANOMATERIALS ON THE BASE OF GRAPHENE-LIKE 2H-$Nb_{1+y}Se_2$, $0 \le y \le 0{,}29$

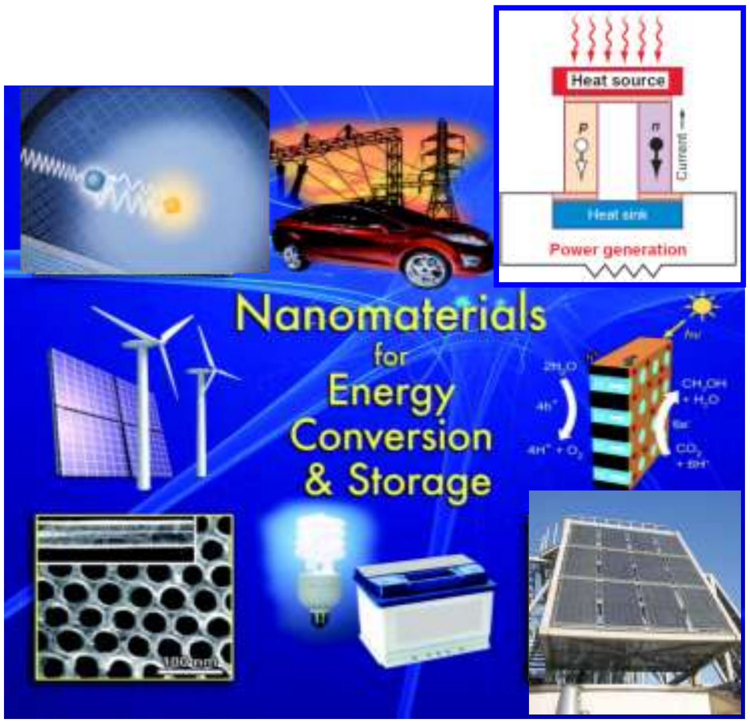
1. Nanomaterials for energy converters:

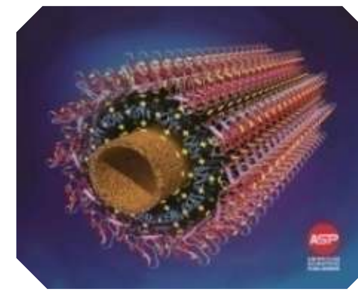
○ Lithium chemical current sources

○ photointercalation solar energy converters

2. Hydrogenous nano-materials and sensors:

Hydrogen energetic





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3. Nanolubricants:

- multifunctional solid nanolubricant additives for the tribotechnical parameters improvement of industrial machine oils and greases

- solid, radiation-resistant, electro-conductive nanolubricants (anti-friction composition nanomaterials, multifunctional nanostructured coatings) for space and ground based operation conditions at high and low temperatures, for hydrogen atmosphere and medical equipment

- ○ aerospace engineering,
- ○ mechanical engineering,
- ○ oil and gas complex,
- ○ transport,
- ○ military equipment,
- ○ metallurgy, etc.

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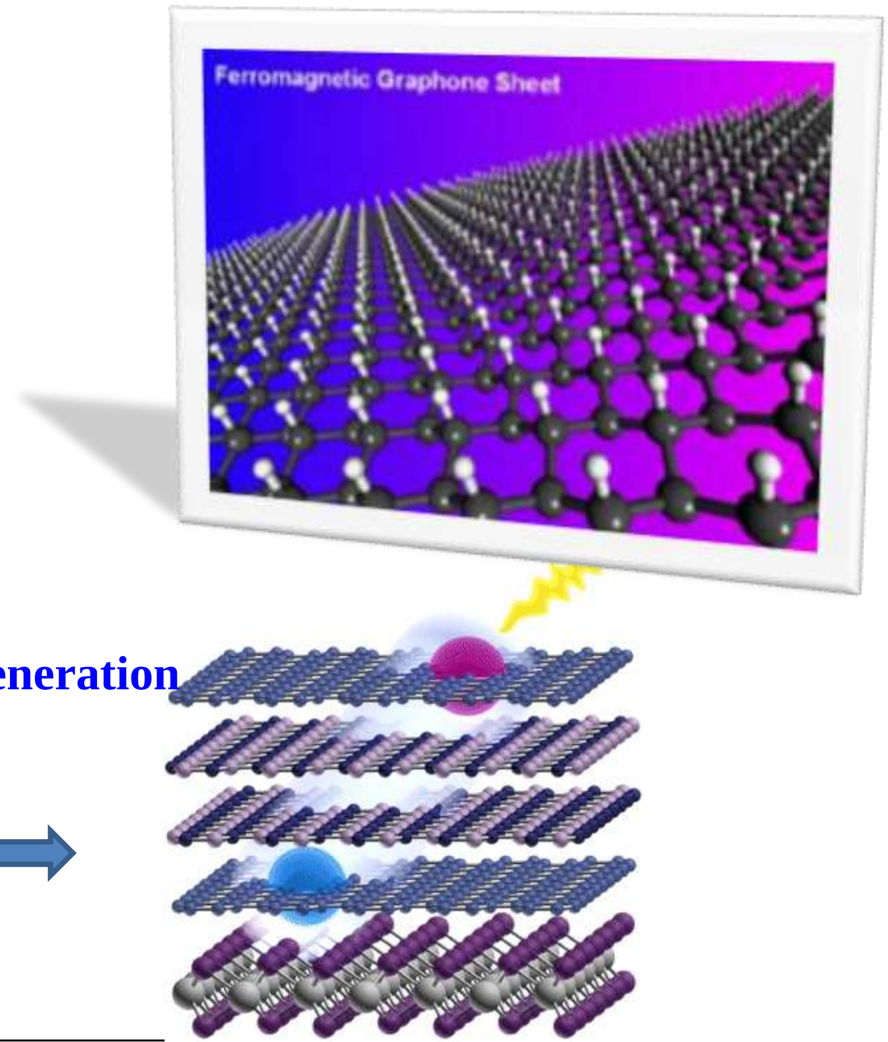
4. "Nanoarmor":

nanomaterials as super shock absorbers at very high pressures (to 40 GPa).

5. Magnetic 2D nanomaterials:



6. Nanoelectronics:

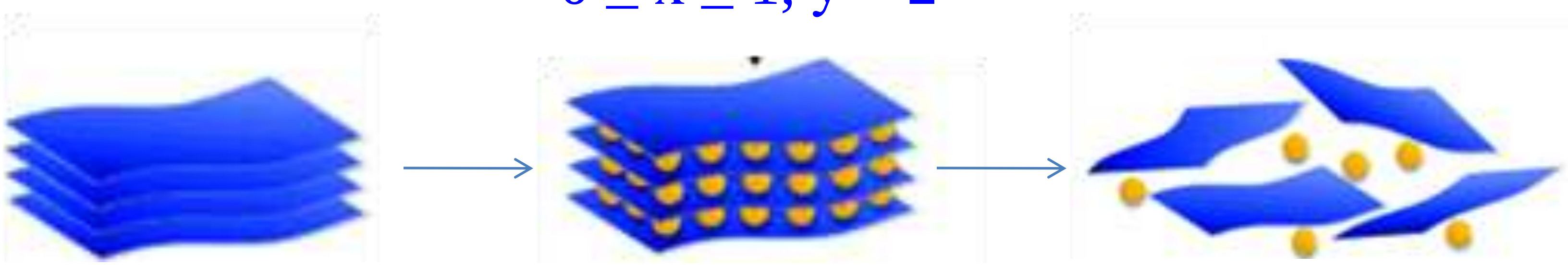
2D nanolayers ⇒ 3D nanocomposites of new generation

Optically active nanocomposite: graphene, BN and $NbSe_2$ layers

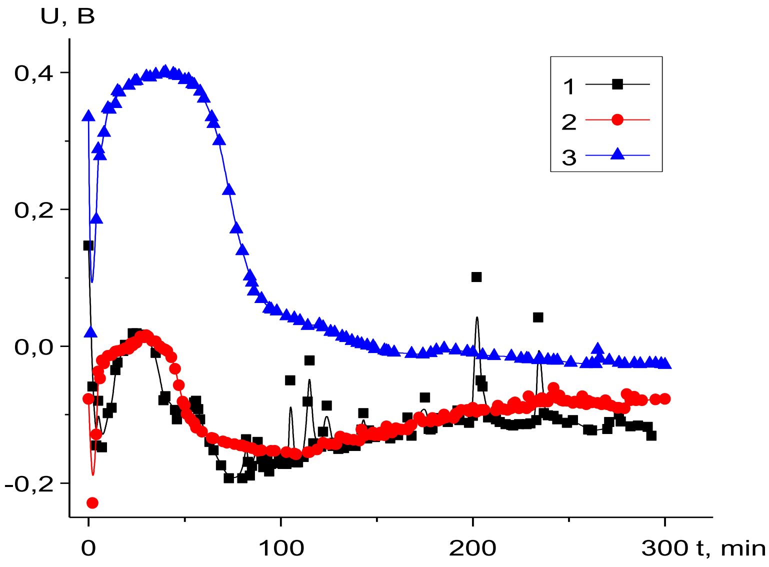
NANOSYNTHESIS OF GRAPHENE-LIKE 2H-$Nb_{1+y}Se_2$, $0 \le y \le 0,29$

- The nanosynthesis was carried out by “up-bottom” activated processes of intercalation (Li^+/H_2O) of autointercalated 2H-$Nb_{1.02(1)\div1.29(1)}Se_2$ micron powders. We studied the timing data of galvanostatic processes of intercalation with the potentiostat (PI-50-1, reference electrode – AgCl). The structural properties of dispersed powders were investigated by X-ray studies, SEM.
- The activated processes of intercalation (Li^+/H_2O) lead to substantial dispersion of 2H-$Nb_{1.02(1)\div1.29(1)}Se_2$ micron particles along cleavage plane where weak Van der Waals forces act.

$$xLi^+ + NbSe_2 + xe^- + H_2O \rightarrow Li^+_x(H_2O)_y\ [\ NbSe_2]^{x-}$$
$$0 \le x \le 1,\ y = 2$$



Layered bulk material | Li-intercalated compound | Isolated 2D nanosheets



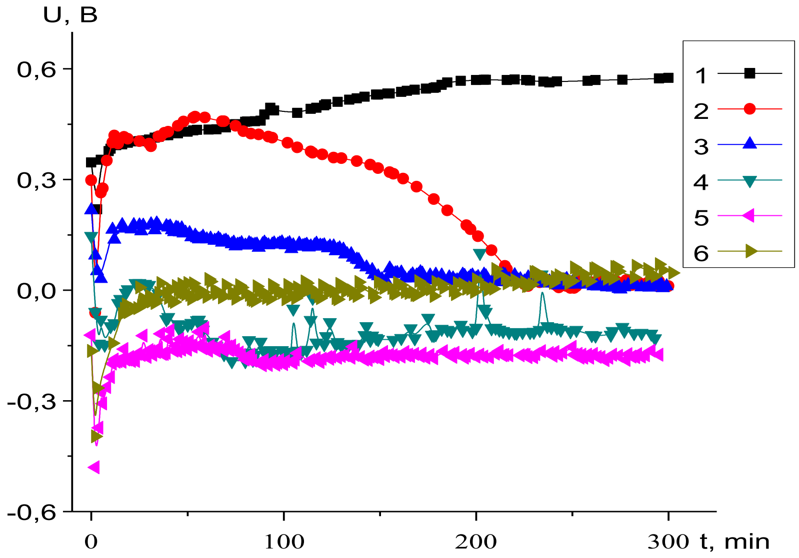


Fig. 1. Dependences of potential for 2H-$Nb_{1+y}Se_2$ powders, U, vs. time, t: 1 – 2H-$Nb_{1.02(1)}Se_2$, 2 – 2H-$Nb_{1.09(1)}Se_2$, 3 – 2H-$Nb_{1.12(1)}Se_2$ (I=10 mA).

Fig. 2. Dependences of potential for 2H-$Nb_{1.02}Se_2$ powders, U, vs. time, t, at current, I: 1 – 10 mA, 2 – 30 mA, 3 – 50 mA (single crystals), 4 – 10 mA, 5 – 30 mA, 6 – 50 mA (micron particles).

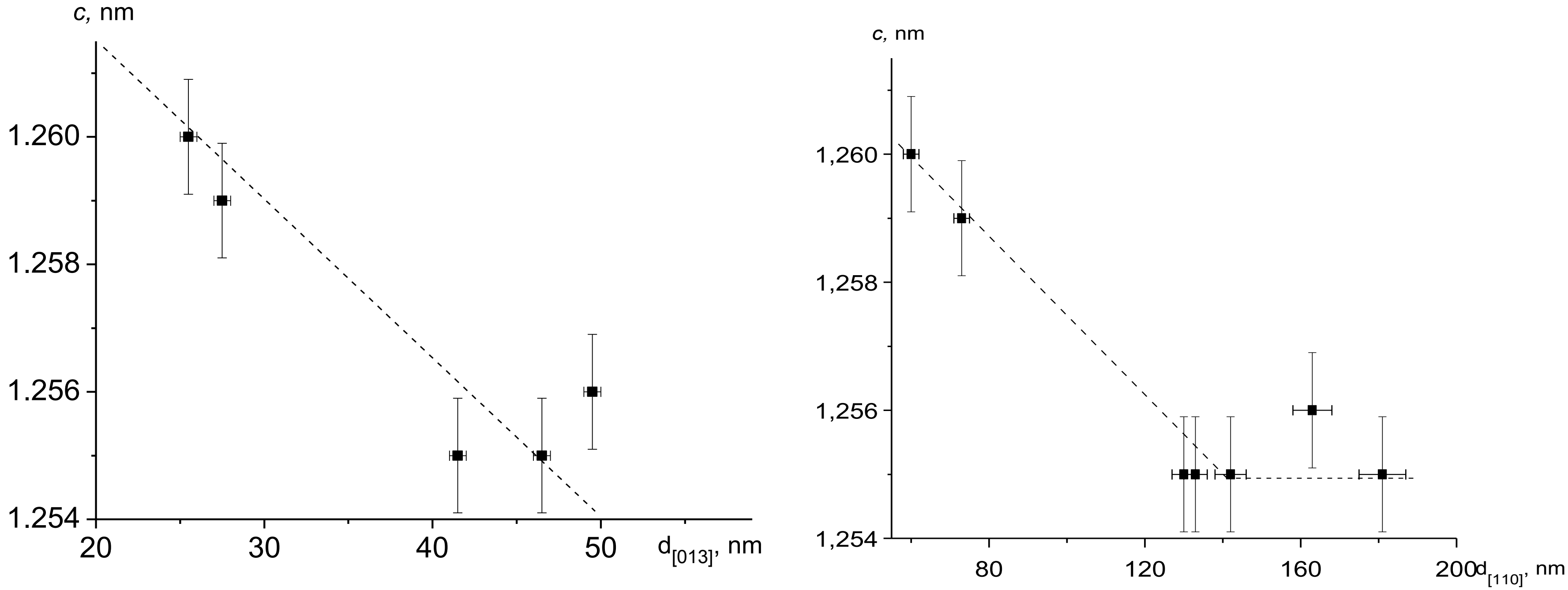
- The average sizes (XRD) of homogeneous, anisotropic graphen-like 2H-$Nb_{1.02(1)}Se_2$ nanoparticles (2H-TaS_2 structural type) are :

22.7(7) – 46.4(1.4) nm for [013] crystallographic direction and
61.9(1.7) – 144(7) nm for [110] direction.

Table 1 - Results of X-ray studies 2H-$Nb_{1.02(1)}Se_2$ after electrochemical intercalation (Li^+/H_2O) and dispersion

Compound	Parameters of unit cells of initial particles, nm		Data for the powders after electrochemical processing					
			Parameters of unit cells, nm		Average size of particles, nm, in the crystallographic directions [013] and [110].		Amount nanolayers, n	Relation $d_{[110]}/d_{[013]}$
	a	*c*	*a*	*c*	$d_{[013]}$	$d_{[110]}$		
2H-$Nb_{1.02(1)}Se_2$	0.34449(2)	1.2554(1)	0.3447(2)	1.2597(9)	27.4(9)	75.0(1.9)	43	2.74
			0.3447(2)	1.2550(9)	41.6(1,4)	143.5(7.0)≈144(7)	66	3.46
			0.3447(2)	1.2558(8)	46.4(1,6)	183.4(9.6)≈180(10)	73	3.95
			0.3446(2)	1.2607(9)	25.4(8)	61.9(1.7)	40	2.44
			0.3444(2)	1.2563(9)	49.7(1,4)	164.8(7.4)≈165(7)	79	3.32
			0.3447(2)	1.2550(9)	28.1(8)	135.0(6.4)≈135(6)	44	4.80
			0.3448(2)	1.2551(9)	22.7(7)	132.4(4.2)≈132(4)	36	5.81

Elementary cells parameters (*a*, *c*) of 2H-MCh_2 nanostructure correlate with average sizes of nanoparticles in the crystallographic directions [013] and [110] (**fig. 3**).



a **b**

Fig. 3. Dependences of unit cell parameter *c* of graphene-like 2H-$Nb_{1.02(1)}Se_2$ nanoparticles on their average size, d, in the crystallographic directions [013] (a) and [110] (b).

a b

c d

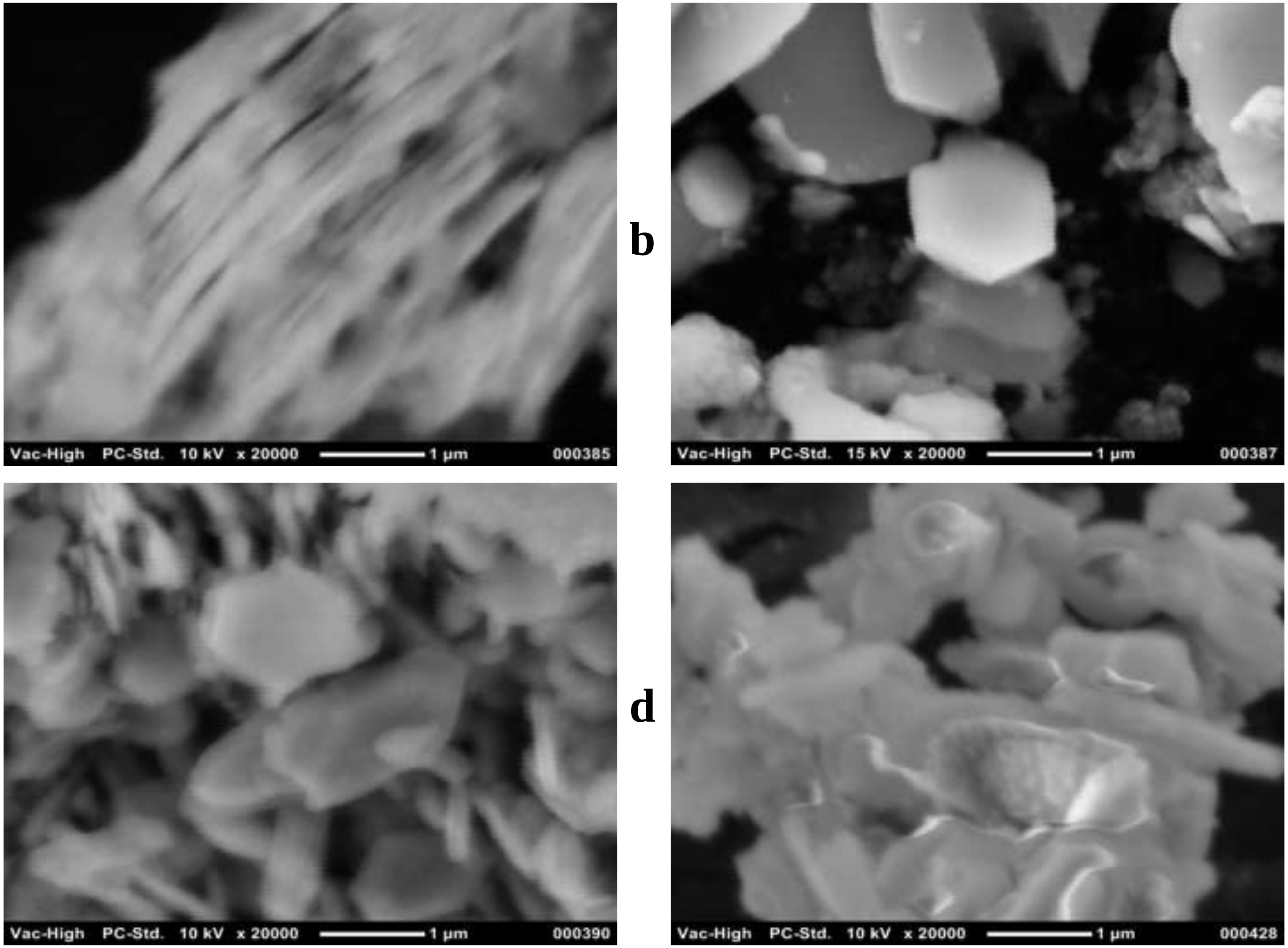


Fig. 4. The results of scanning electron microscopy of graphene-like 2H-$Nb_{1.02(1)\div1.29(1)}Se_2$ nanoparticles, the values of a current I=30 mA (magnification – x20000): a – 2H-$Nb_{1.02(1)}Se_2$, b – 2H-$Nb_{1.09(1)}Se_2$, c – 2H-$Nb_{1.12(1)}Se_2$, d – 2H-$Nb_{1.22(1)}Se_2$.

Conclusions

- The activated processes of intercalation (Li^+/H_2O) lead to substantial dispersion of 2H-$Nb_{1.02(1)\div1.29(1)}Se_2$ micron particles.
- The nanoparticles size is controlled efficiently by kinetic parameters of intercalation processes.
- The average sizes (XRD) of homogeneous, anisotropic graphen-like 2H-$Nb_{1.02(1)}Se_2$ nanoparticles (2H-TaS_2 structural type) are 22.7(7)–46.4(1.4) nm for [013] crystallographic direction and 61.9(1.7)–144(7) nm for [110] direction.

Thanks for your attention