Nanocomposites and nanomaterials

Ab-initio design of 3D-carbyne based materials

S. Kotrechko, A. Timoshevskij, Yu. Matviychuk, N. Stetsenko

G. V. Kurdyumov Institute for Metal Physics, Nat. Acad. of Sci. of Ukraine, Vernadsky Blvd.,36, Kyiv 03680, Ukraine

Carbyne is linear allotrope of carbon that has unique properties, and it is very promising for several applications. Work [1] has presented the high-field technique for obtaining carbyne in the form of monatomic linear chains of carbon on the surface of carbon fibers as a result of the high-field treatment of carbon nano-fibers. Besides, the lower experimental estimation of breaking strength of carbyne was obtained, which equals 270 Gpa, and it is the upper limit of materials' strength on the whole [2]. Findings of *ab-initio* simulation have shown that carbyne strength depends on both number of atoms in chain and whether this number is even or odd. Thus, chains containing five atoms have the maximum strength (417 GPa) [3].

This report is aimed at substantiation on the basis of *ab-initio* calculations of possibility to use carbyne for creation of bulk material with unique properties.

The material was modeled that is composed of graphene sheets joined by five-atom carbon chains. When modeling, the distance between chains was varied as well as how a chain is anchored on graphene sheet. The enthalpies of formation of such systems were calculated for all configurations. It is exhibited that type of bond of the edge atom in chain with atoms of graphene sheet has the key effect on the value of enthalpy. Equilibrium configurations of such 3D-material are found. It is ascertained that strength of these material may reach ultimately high levels: 16 - 32 GPa at relatively low values of elasticity modulus 100 - 175 GPa.

1. *Mikhailovskij, I.M., Wanderka N., Ksenofontov V.A., et. al*. Preparation and characterization of monoatomic C-chains: unraveling and field emission // Nanotechnology-2007-18.- P.475705 -.

2. *I. M. Mikhailovskij, E. V. Sadanov, S. Kotrechko,et. al.* Measurement of the inherent strength of carbon atomic chains // Physical Review – 2013.- B **87.-P.** 045410-045417.

3. *S. Kotrechko, I Mikhailovskij, T Mazilova, et al.* Mechanical properties of carbyne: experiment and simulations // Nanoscale research letters-2015.- 10 (1).-P. 1-6.