Nanocomposites and nanomaterials

Life time and stability of carbyne

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Creation of all-carbon-based nanodevices is currently one of the promising directions in development of nanoelectronics. The use of monatomic chains of carbon atoms (carbynes) is a characteristic feature of these devices. This will enable not only to employ the unusual functional properties of carbynes, but also to approach the maximum attainable level of miniaturization of these devices. At that, stability and service time of carbyne is one of the key challenges towards creating all-carbon-based nanodevices. The results of direct experimental tests of carbyne for tension [1], as well as *ab-initio* simulation findings [2] showed that carbyne is the strongest material in the world. However, break of only one atomic bond is enough for the failure of such nanodevices. This requires the development of methods of the lifetime prediction for carbyne chains.

The report proposes an approach to predicting the thermomechanical stability and lifetime of carbyne in a wide range of temperatures and the values of mechanical load. This approach is based on the fluctuation model of atomic bonds break developed by the authors. Unlike existing models, it contains no empirical constants. The data of DFT calculations are used as the initial data for the calculation. The quantum-mechanical nature of stability of the carbyne chain has been ascertained. It manifests itself in the dependence of lifetime on the number of atoms in the chain, as well as on whether this number is even or odd.

Possibility of synergistic effect of temperature and mechanical load on stability of carbyne chains is predicted. It is ascertained, that this synergism results in a significant decrease in the lifetime of carbyne chain. The atomic mechanism of this phenomenon is outlined. Conditions of thermo-force loading are predicted at which the use of carbyne chains in nanodevices is possible.

1. *Mikhailovskij I., Sadanov E., Kotrechko S., V. Ksenofontov V., and Mazilova T.* Measurement of the inherent strength of carbon atomic chains // Phys. Rev. -2013.- **87**.-P. 045410 -045418.

2. *Timoshevskii A., Kotrechko S., and Matviychuk Yu*. Atomic structure and mechanical properties of carbyne // Phys. Rev.-2015.- **91**.-P.- 245434-245442.