Nanocomposites and nanomaterials

An approach to prediction of stability and durability of carbon-based nanodevices

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Development of nanotechnologies has resulted in the creation of subminiature devices with unusual functional properties. However, lifetime and reliability of these devices are the main factors determining their competitiveness. Solution of this problem requires development of fundamentally new approaches, since the reliability of nanodevices is pre-determined by atomic rearrangements on the nanoscale. One-dimensional nanocrystals are defect-free, so, their strength is close to theoretical strength. For instance, carbyne strength is more than twice higher than graphene strength, and is equal to 270-400GPa [1, 2]. However, in many cases, breaking of a *single* atomic bond is enough for the failure of the entire nanodevice.

This report considers the key element of future all-carbon-based nanoelectronic, which is composed of two graphene sheets connected by a carbyne chain.

Stability and operating time of such nanoelement is determined by the probability of breaking of a contact bond. The approach to describe stability of such systems is formulated and the atomistic model of their strength and durability is presented. Unlike the conventional models, which are based on the theory of reaction rates, the model proposed enables to predict the lifetime of carbyne-based nanodevice accounting for not only the temperature, but also for force loading. Besides, it is exhibited that classic models overestimate the lifetime of such devices.

Characteristics of the thermo-mechanic stability of the considered carbon-based nanoelement are obtained.

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

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