Nanocomposites and nanomaterials

Atomic structure and mechanical properties of carbyne

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Carbon-based materials are among the most promising objects of modern nanotechnology. Carbyne - the linear allotrope of carbon - takes a notable place among such objects. To date, carbyne, as an object of research, leaves behind graphene by the number of works, due to its unique physical, mechanical and chemical properties. In particular, its strength is almost twice higher than the strength of graphene [1], which was considered six years ago as the strongest material in the world. It also has unique magnetic and electrical properties.

This work presents the fundamentals of 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 at the electric field strength of the order of 10^{11}V/m [2]. The results of comprehensive *ab-initio* analysis of atomic structure and properties of carbine and their dependences on both number of atoms in carbyne and parity of this number are discussed. Basen on these findings, it is exhibited that infinite atomic linear chain with cumulune or polyyne structures can't be used as physical model of carbyne.
On the basis of results of MD-modeling, the analysis of thernmal stability of carbyne is executed, and the temperature dependences of it strength are obtained.

1. *I. M. Mikhailovskij, E. V. Sadanov, S. Kotrechko, V. A. Ksenofontov, and T. I. Mazilova*. Measurement of the inherent strength of carbon atomic chains. Physical Review B **87**, 045410 (2013).
2. *Mikhailovskij, I.M., Wanderka N., Ksenofontov V.A., Mazilova T.I., Sadanov E.V. and Velicodnaja O.A. Nanotechnology*. Preparation and characterization of monoatomic C-chains: unraveling and field emission. Nanotechnology, 18, 475705 (2007).