Nanotechnology and nanomaterials

Thermal stability of structures based on carbyne

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Linear monatomic chains or carbyne were intensively investigated due to their unique physical properties [1,2] and promising applications [3,4], however, the possibility of realization of their properties is limited by their strength and elasticity.

The aim of this work is to analyze the atomism of deformation and fracture of structures based on carbyne over the wide temperature range, and to ascertain, on this basis, the temperature dependence of their strength.

Findings on the structure and mechanical properties of carbyne chain, which contains 10 atoms and joints two graphene sheets, are obtained in this work as a result of MD-simulation. The temperature range for simulation was 4,2 - 2000K. It was established that the fracture occurred in the contact bond of chain with graphene sheet, thus, critical fracture stress is a stochastic value that with sufficient accuracy may be described by Weibull distribution. It is found that before break of the chain its length is increasing by unraveling. This effect increases with temperature growth. It is established that structures based on carbyne have high thermal stability up to temperatures 1000-1250K.

1. *L. Ravagnan, N. Manini, E. Cinquanta, G. Onida, D. Sangalli, C. Motta, M. Devetta, A. Bordoni, P. Piseri, and P. Milani //* Phys. Rev. Lett. **102**, 245502.
2. *E. Cinquanta, L. Ravagnan, I. E. Castelli, F. Cataldo, N. Manini, G. Onida, and P. Milani //* J. Chem. Phys. **135,** 194501.
3. *E. E. Durgun, R. T. Senger, H. Mehrez, S. Dag, and S. Ciraci //* Europhys. Lett. **73**, 642 (2006).
4. *Y. Wang, X.-J. Ning, Z.-Z. Lin, P. Li, and J. Zhuang //* Phys. Rev. B **76**, 165423 (2007).