Nanocomposites and nanomaterials

Influence of carbyne chain length on its lifetime

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Recently, much attention is paid to investigation of carbyne (a monatomic chain of carbon). This is due, first of all, to the fact that carbyne is one of the key elements of all-carbon-based nanodevices. The possibility to use carbyne in such devices is limited by it lifetime. Specific feature of carbine, as a monatomic carbon chain, is that it strength and mechanical stability are *directly* pre-determined by the atomic interaction. This property was used in the fluctuation model of instability of one-dimensional crystals developed by the authors. Unlike existing models, it doesn't contain empirical constants. To obtain the initial information on the interatomic interaction, the results of the DFT calculations are used. Unlike molecular dynamics, which enables to predict the lifetime for a period not exceeding tens of nanoseconds, in this model, there are no restrictions on the time interval length. This report presents the results of investigation of the effect of temperature and mechanical loading on the time to break for carbyne chains containing from 3 to 12 atoms. The existence of a quantum-mechanical size effect is predicted, which manifests itself in the dependence of a time before carbyne break on the total number of atoms in the chain, and whether this number is even or odd. It is found that chains with an odd number of atoms have the maximum values of lifetime. "Even" chains are shorter-lived; however, their lifetime increases with the number of atoms in the chain. For "odd" chains, the number of atoms practically does not affect the time to failure. In addition, calculations predict the existence of a synergy of temperature and the applied load, which manifests itself in a steep (by many orders of magnitude) decrease in the time to failure in a certain range of loads. The value of the critical load of the beginning of synergism manifestation, F_f, depends on the number of atoms in the chain, and increases from $F_f = 0.7F_C$ (F_C is the bond strength) for a chain with 10 atoms to $F_f = 0.9F_C$ for a 4-atom chain. The nature of this effect consists in the fluctuation-induced explosive release of accumulated potential energy. In the range of loads where synergy is observed, parity effects do not appear. The report provides a map to predict the service life of carbyne chain depending on the number of atoms, temperature and applied load. The results obtained enable to choose the thermo-force conditions of load of carbyne, which ensure the reliability and durability of nanodevices based on it.

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