THE NEW CLASS OF THE DIBORIDE NANOTUBES: STRUCTURE AND ELECTRONIC PROPERTIES

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Two types of materials in solid state physics and chemistry are of interest last time: high temperature superconductors and nanotubes (NT). Discovery of the superconductiv transition for MgB_2 [1] can become an important step in ideas about superconducting.

In present work we pay attention to possible new class of NT from diborid material [2]. NT atomic structures of MgB_2, CaB_2 and ZrB_2 have been modeled by means of molecular mechanics and *ab initio* methods. Contrary to the familiar carbon NT the dependence of the strain energy of MB_2 (M=Mg, Zr) tube on its diameter deviates from $1/D^2$ low because the MB_2 nanocrust is predominantly rolled up around the axis parallel to M-M bonds. Thus most stable "armchair" MgB_2 and ZrB_2 tubes are that with external hexagonal boron layers, since most favorable CaB_2 NTs have internal boron layers.

We used approach of calculation of electronic spectrum for single wall NT based on known spectrum of unfolded layer. This approach was proposed in work [3] and was used for prediction of main properties of carbon NT. Electronic spectrum of NT can be obtained by applying the periodic boundary conditions to the electronic wave functions of corresponding striplike fragment of plane layers. 1D dispersion curves of a NT in such case are sections of 2D layer spectrum [4] along certain direction in Brilliouin zone.

We calculated spectra for a number of MB_2 NTs: (4,4), (5,5), (6,6), (7,7), (8,8), (9,9), (9,0), (10,0), (19,0), (20,0), (21,0). It was found that in contrary of carbon NT all considered MB_2 nanotubes have high density of states near Fermi level (<0.2 eV). Furthermore for certain NTs there are high densities of states on the Fermi level can appear thus one can expect rather high temperature of transition into superconductive state (for bulk MgB_2 $T_c \approx 39$ K).

For example for (6,6), (20,0), and (21,0) MgB_2 nanotubes spectrum there were area where the derivation of energy to the wave vector was about zero that leads to the high density of states near the Fermi level, and so such tubes are candidates to superconductive NT.

We have also calculated electronic spectra of considered MB_2 NTs more accurately by Extended Huckel Theory approach and obtained qualitively the same behavior.

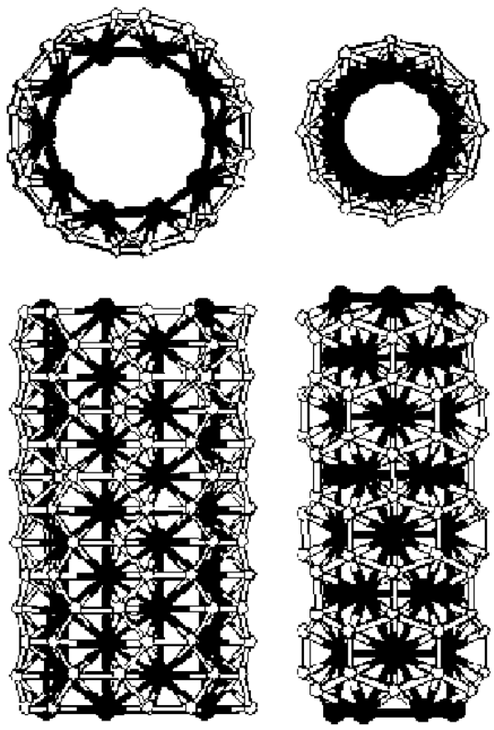

Fig. 1. Armchair (5,5) (left) and zigzag (6,0) (right) MB_2 bitubulenes. The M and B atoms are shown by the dark and light circles, respectively.

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