Research of dependence of SWCNTs dipole moment on its length

Belolipetskii A.A., Lebedev N.G.

Volgograd State University, 400062 Volgograd, Russia

For the purpose of studying possibility of use carbon nanotubes [1] as gauges research of dependence of SWCNT's dipole moment on their length has been carried out. In this work the polarized carbon nanotubes of two structure modifications: (n, n) and (n, 0) are used as a research object. Boundary broken bonds are isolated on one side by hydrogen atoms and on another by fluorine atoms. The length of tubes has been varied.

To determine the mentioned above dependence the electronic structure and the power characteristics were calculated with use of semi-empirical methods of quantum chemistry [2]. The dependence of the dipole moment on the number of elementary cells along nanotube's axis is computed. The obtained data show, that dependence of the nanotube's dipole moment on the length has a nonlinear character. It makes possible the application of carbon nanotubes as the sensor controls reacting even on weak electromagnetic signals. Dependences of charges on boundary atoms of fluorine and hydrogen have a similar character.

These values have some oscillations. We can see it in even and odd lengths (elementary cells). In tubes (n, 0) does we have not same results.

- [1] Harris P. Carbon nanotubes and related structures. New materials of the XXI-st century. - M: the Technosphere, 2003.
- [2] Stepanov N.F. Quantum of the mechanic and quantum chemistry. M: the World, 2001.