

Investigation of the effect of bending on the polymerization of fullerenes inside carbon nanotubes

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The aim of this work is to investigate theoretically the influence of peapod bending on the process of C₆₀ fullerenes polymerization with the help of the model that effectively combines molecular and quantum techniques and is well recommended to study the mechanical properties of carbon nanostructures [1-3].

The process of peapod bending formed from nanotube (10,10) with the length of 0.244 nm, filled with twenty-seven C₆₀. C₆₀ is distanced from the tube walls at a distance equal to 0.338 nm. Fullerenes are on the tube axis at the distance between their centers equal to 0.815 nm. The polymerization of fullerenes and partial connection with the walls of the tube were observed at the bending of 270 degrees.

It was established that at such a bending:

1. The atomic structure of peapod is not destroyed.
2. The nanotubes surface of smaller radius is becomes wave-like and in some places of trough is connected with the fullerenes.
3. The fullerenes come to the distance of 0.14 nm between the atoms of the cell and are polymerized.
4. The hybrid compound of the nanotube, which was formed, retains the atomic structure unchanged even when there is no external load.

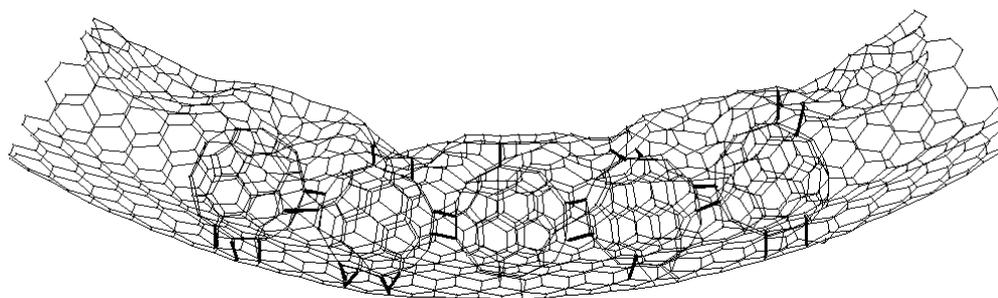


Figure. Fragment of peapod at bending of 270 degrees. The thick lines show the connections formed during the polymerization of fullerenes with neighboring fullerenes and a nanotube.

- [1] O.E. Glukhova, I.N. Saliy, R.Y. Zhnichkov, I.A. Khvatov, A.S. Kolesnikova, M.M. Slepchenkov. *Journal of Physics: Conference series*, **248**, 012004 (2010).
- [2] O.E. Glukhova, I.V. Kirillova, I.N. Saliy, A.S. Kolesnikova, M.M. Slepchenkov. *Proc. of SPIE* **7910**, 79101 (2011)