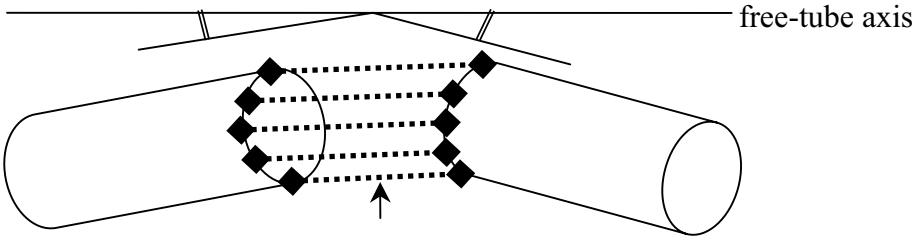
Stone–Wales defect generation in carbon nanotube being fractured

Moliver S.S.

State University Ulyanovsk, 432970, Ulyanovsk, Russia
e-mail: moliver@sv.uven.ru

Quantum-chemistry modelling of small-radii nanotubes, was fulfilled in frame of INDO parametrization, the same one had been applied previously to other condensed states of carbon. These total-electron calculations of the supercell models reveal some properties of the Stone–Wales defect (SW), i.e. a topo-chemical turning of a C–C bond, providing 5-7-7-5 cycling within graphene net. It was found, that rolling of the plane graphene into (8,0) nanotube decreases SW defect formation energy by 0.6 eV. The electronic spectrum obtains resonant levels when SW defect appears in the tube. Under the fracture-type loading (see figure below) of the tube, SW position at the compressed side has an advantage over stretched-bond side. Critical value of the zigzag (8,0) tube fracture was found to be 1.7 degree (this angle is marked on figure below): it is a ductility barrier, at which SW defect generation reduces the total energy [1].

Recently it was proved by many-electron calculations, that SW defects and their complexes may be generated in carbon nanotubes under tensile strain [2-3]. To compare our semi-empirical calculations with *ab initio* level [3], one should note the similarity of the above mentioned difference of SW defect formation energy in graphene and nanotubes.



Supercell model of (8,0) tube of 192 atoms is divided on 2 cylinders, whose axes make a fracture. 5 of 3 C–C bonds between undistorted half-tubes are shown by dashed lines.

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[2] Orlikowski D., Buongiorno Nardelli M., Bernholc J., Roland C. *Phys.Rev.Lett.* **83**, 4132 (1999); *Phys.Rev.B.* **61**, 14194 (2000).
[3] Zhao Q., Buongiorno Nardelli M., Bernholc J. *Phys.Rev.B.* **65**, 144105 (2002).