The effect of the orientation of the Stone-Wales defects on the bands structure of carbon nanotubes

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Abstract. We have studied the effect of orientation of Stone-Wales (SW) defects formed on the armchair single-wall carbon nanotubes (SWCNTs) on their metal-semiconductor behaviour by means of the density functional formalism. It has been shown that two third of possible orientations of SW defects, at high concentrations, open a ≈ 40 meV gap at Fermi level while in the other one third orientations tube remains metallic.

A single-wall carbon nanotube (SWCNT), a graphene sheet warped around a specific axis, is supposed to be the building block for future nano-electronic technologies [1, 2]. The surprising feature of a perfect SWCNT, as a cluster of carbon atoms, is the dependence of its electrical conductivity on its geometrical structure alone: almost one third of these structures depending on their warping (chiral) vector are conductors, while the others are semiconductors [3]. However, presence of any kind of imperfection, may change the conductivity of a SWCNT drastically [4]. Now it has been a decade since the first proposition that addition of impurity atoms, like Nitrogen or Boron, on metallic SWCNTs, may reduce their conductance up to 50 percents [5]. An important class of imperfections on SWCNT, are the structural disorders. A common structural disorder, so-called Stone-Wales (SW) defect [6], appears when a carbon-carbon bond rotates 90 degrees, and consequently four hexagons around that reconstruct to form two pentagon-heptagon pairs. Usually a SW defect is formed on nanotubes under high tensile strain [7]. The existence of a SW defect alters many mechanical and electrical properties of CNTs [8, 9, 10, 11].

Here we have focused on possible metal-semiconductor transition in armchair nanotubes, which are believed to be metallic, in the presence of a high concentration of the SW defects. Depending on the mentioned rotating carbon bond, two types of SW defects are recognized on an armchair SWCNT.

Each carbon atom on the surface of a SWCNT has three bonds with three neighbors. In armchair tubes, when a SW defect occurs, rotating bond forms a 60 degree angle or it lies parallel to the tube axis. As such, there are two distinct orientation for a SW defect on a SWCNT (figure 1). Hereafter we call these two types 60 degree and parallel types respectively.

We have used a density functional formalism based on Troullier-Martins [12] norm-conserving pseudo-potentials using pseudo-atomic orbitals as implemented in SIESTA code [13]. Real space mesh grid is chosen in such a way that there is a mesh point approximately at each 0.15 Å on
Figure 1. Relaxed positions of carbon atoms in a SW defected (5, 5) tube. Rotated bond in SW defect form a 60 angle with tube axis in (a) and its parallel to tube axis in (b). Samples contain 100 carbon atoms.

three lattice vectors. We have used the generalized gradient approximation for the exchange-correlation functional and the structure is relaxed until we reach a maximum force per atom less than 0.04 eV/Å. Histograms of the tube radius and the C-C bond-length in a (5, 5) SWCNT are shown in figure 2 (a) and (b) for two types of SW defects, respectively. The range and the standard deviation, σ, in both (a) and (b) for the case of parallel rotating bond in the SW defect is broader. Moreover, radius and bond-length tend to higher values in comparison with the assumed value in a clean sample.

Figure 2. Histogram of (a) radius and (b) bond-length in a relaxed sample of a (5, 5) SWCNT with two types of SW defects (solid and dashed lines). Vertical dashed lines in (a) and (b) are the tube diameter and C-C bond-length in a clean sample, respectively.

Figure 3 shows the band structure of the above sample with two type of the SW defects. The results do not show a gap opening due to the SW defect in (a), while there is an ≈ 40 meV gap in (b) – predicting a semiconducting behaviour for the SWCNT. The K point in the figure is the point at which the two bands are closest to one another. Figure 3 shows a strong dependence of the electronic structure on the orientation of the SW defect at high concentrations. Figure 4 shows the total density of states (DOS) for two samples studied in figures 1 to 3 near the Fermi level.

In figure 4 (a) there is no gap at the Fermi level, while in (b), which corresponds to the 60 degree SW defect, there is a gap opening of about 40 meV.
In summary, the effect of orientation of Stone-Wales defect on the electronic structure of the armchair single-wall carbon nanotubes is studied at high concentrations using a density functional formalism. Results show a strong dependence of the electronic structure on the orientation of the Stone-Wales defect. In two third of the orientations of the defect, the armchair tube, which in its clean form is believed to be a metal, undergoes a metal-semiconductor transition as a gap in energy opens near the Fermi level.

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