Influence of Boron Nitrogen pairs codoping on transport properties of Carbon nanotubes

Zoubkoff Rémi, Latil Sylvain

CEA/IRAMIS/SPCSI/LNOSC, 91191 Gif-sur-Yvette, France
remi.zoubkoff@cea.fr

In order to tune the electronic properties of carbon nanotube (CNT), a chemical doping by Boron or Nitrogen has been proposed. It appears that the Boron or Nitrogen atoms impact the transport properties and specially for injection energy corresponding to the quasi-bound states induced by the dopant [1,2]. However, these theoretical works were only considering the case of a single defect. Later different authors reported the influence of a random distribution of Boron or Nitrogen substitutive dopant [3,4]. They extracted mesoscopic informations such the mean free path and predicted rules dependence as a function of the dopant concentration or the nanotube radius.

More recentlty, Kalfoun et al [5] have investigated the effect of the BN codoping and have found that the effect of the two dopants was annealing each other when they are nearest neighbors and was cumulated when they are distant. This study was limited to a single defect thus our aim is to study the effect of the BN codoping on CNT for more realistic systems. We proposed to study the influence of BN codoping for mesoscopic system, and to investigate the effect of disorder induced by the B-N relative positions.

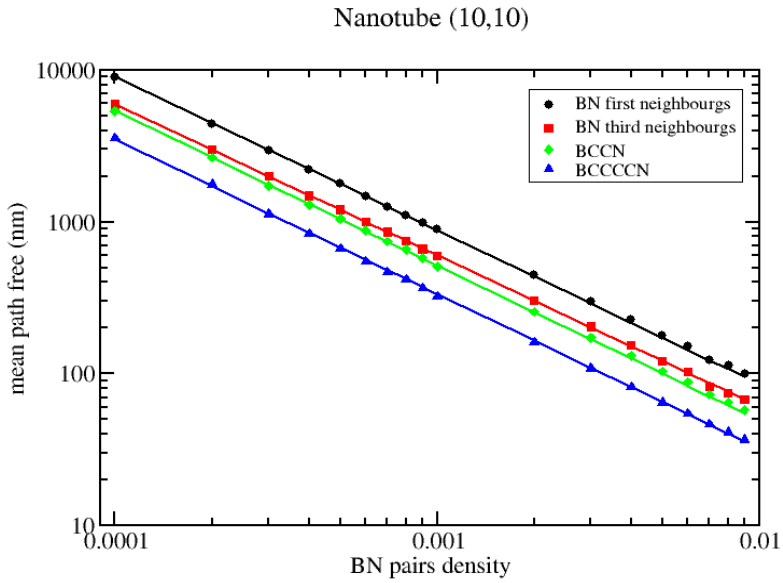
In order to compute the electronic properties of systems with a length scale as long as the µm, we adopt a Tight Binding formalism in a minimal basis formed by a single p orbital, that is known to give a good description of the electronic properties of CNT around the Fermi level. The influence of the N or B dopant was obtain by considering the electrostatic potential induced by a B or N on the one site element. It appears that the correction created by a BN pair is quite well described by the sum of the isolated dopant contribution. These corrections have been determined from DFT calculation performed with the SIESTA code.

We have computed the transport properties for random distribution of dopant. We consider different defects, with various distance between the B and N dopants. It appears that the mean free path behaves as an inverse of the dopant ratio, and evolves linearly with the nanotube radius. The distance between the B and N has significant effects as presented on the Figure 1. The mean free path decreases when the BN distance increases, as expected by considering results obtains for one BN pair default, the scattering potential created by the BN pair is attenuated by the proximity of the two species.

References

[1] H.J. Choi, J. Ihm, S. G. Louie, M. L. Cohen PRL, **84** (2000) 2917.
[2] C. Adessi, S. Roche, X. Blase, PRB, **73** (2006) .
[3] S. Latil,S. Roche, D.Mayou, J.C Charlier, PRL, **92** (2004) 256805.
[4] R. Avriller, S. Latil, F. Triozon, X. Blase, S. Roche, PRB, **74** (2006) 121406.
[5] H. Khalfoun, P Hermet, L. Henrad, S. Latil, PRB, **81** (2010) 193411

Figure 1



Evolution of the mean free path as a function of the dopant concentration for a metallic (10,10) nanotube. The different curves are obtained for various BN pairs configuration, in a first neighbors (black), third neighbors(red), separated by two carbon atoms (green) or four atoms (blue).