

# Influence of vacancy defect density on electrical properties of armchair single wall carbon nanotube

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## Abstract

The relationship between the bandgap and the vacancy density is investigated from first principles. The range influence of a vacancy defect due to structural deformation is characterized and a microscopic explanation is proposed to relate the structural deformation to the bandgap variation. In order to investigate the effect of the defect density on carbon nanotube, 5 models of (5,5) armchair carbon nanotubes were built with the defect density as one vacancy per 79, 119, 159, 199 and 239 carbon atoms, respectively. The long range of influence of a MVD is characterized by structural deformation analysis and the strain caused by the MVD is the main reason to cause the strong fluctuation in bandgap of the defected armchair SWCNTs. However, no simple correlation between the MVD density and bandgap are found. Our results can shed some light on the instability of the defected armchair SWCNTs in electronic properties synthesized via ion-irradiation for future potential applications.

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**Keywords:** Armchair carbon nanotube; Vacancy defect density; Dangling bond

The design and reliability of the circuits made by carbon nanotubes (CNTs) have become important issues ever since CNTs demonstrate successfully as a working transistor [1]. Contrast to the prevailing conception of SWCNTs as perfectly crystalline wires, even high-quality SWCNTs on average contain one structural defect per 4  $\mu\text{m}$ . [2] Regardless of the location in the SWCNTs, a mono-vacancy defect (MVD) can reduce the drive current by about 28%. [3] Generally the armchair SWCNTs are predicted as metallic and no bandgap existed due to the symmetry consideration. [4] However, symmetry breaking can cause a bandgap opening in metallic SWCNTs as discussed by Li et al. [5]. Vacancy defect can also break the symmetry to open up the bandgap and this gap opening depends on the tube radius as shown by Ma et al. [6]. Gomez-Navarro et al. generated a uniform density of defects by employing consecutive Ar<sup>+</sup> irradiation doses to examine the dependence of the conductance on the vacancy defect density in SWCNTs. [7] Furthermore, the results of selected electrochemical deposition reveal that most of the electronic behaviours of a particular SWCNT transistor are caused by defects, and are not a

characteristic of the SWCNT itself. [2] Biel et al. examined the characteristics of the localization regime in terms of the length, temperature, and density of defects of SWCNTs by averaging over various random configurations of defects for a metallic (10,10) SWCNT. [8] Even though both experimental and theoretical findings are beginning to yield a general picture of the effects of vacancies on the electrical characteristics of SWCNTs, numerous critical issues remain unresolved. For example, how the structural changes due to vacancy defects influence the electronic structures of SWCNTs has not been determined yet. It is urgently needed to understand the effects of vacancy defect density. In this letter, the variation in the bandgap of an armchair SWCNT due to the MVD density is investigated by employing density functional theory (DFT) calculations.

To facilitate computation, a single-walled (5,5) nanotube with one or two MVDs was modelled by various number of unit cells (20 carbon atoms per unit cell) with one carbon atom missing, to represent vacancy defects. The simulated nanotube was placed in a tetragonal supercell with lattice constants  $a$ ,  $b$  and  $c$ . The lattice constants  $a$  and  $c$  were 20 Å, preventing interaction between adjacent nanotubes. The lattice constant  $b$  along the tube axis was taken to be equal to the one-dimensional lattice parameter of nanotubes. DFT calculations were

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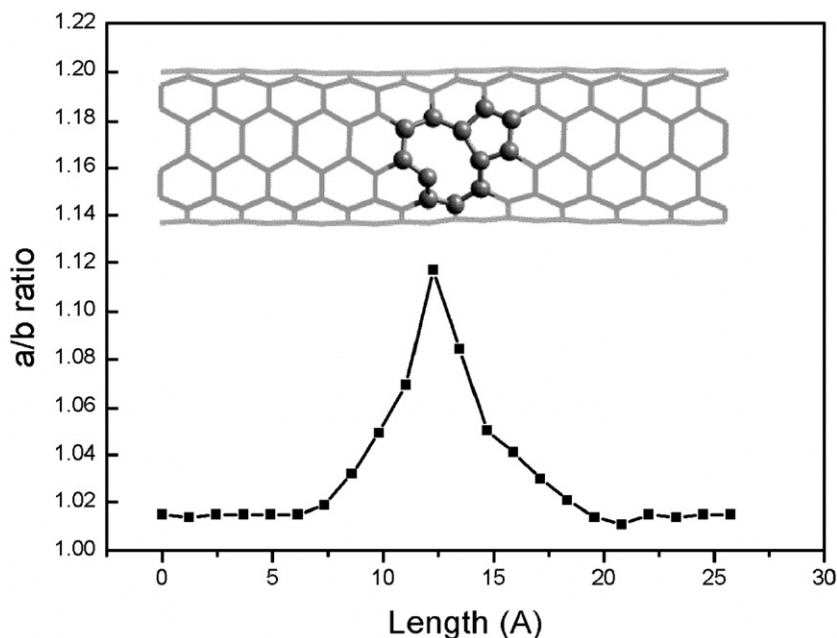


Fig. 1. The oblateness variation along the tube axis for the single mono-vacancy defected (5,5) armchair carbon nanotube with 239 carbon atoms. The inset plot is its optimized structure. The length unit is Å.

performed with CASTEP code [9]. The typical calculation is as follows. The calculations were done using geometric optimization with the generalized gradient approximation (GGA) [10,11]. The structure of the defective nanotube was fully optimized when the force on each atom during relaxation was under  $0.005 \text{ eV } \text{\AA}^{-1}$ . The nuclei and core electrons were represented by ultrasoft pseudopotentials [12]. The summation was performed over a 1D Brillouin zone with wavevectors' varying only along the tube axis, using  $k$ -point sampling and a Monkhorst–Pack grid [13]. A kinetic energy cut-off of 240 eV and 20  $k$  points were used along the tube axis to ensure the convergence in the calculations. The fast-fourier-transform (FFT) grid is chosen according to the number of carbon atoms in the particular model. For example, the FFT grid for the model with 79 carbon atoms is set to be  $90 \times 45 \times 90$ .

Five models were used with defect densities of one MVD per 4, 6, 8, 10 and 12 unit cells, corresponding to 79, 119, 159, 199 and 239 carbon atoms, respectively, to elucidate the effect of MVD density on the electrical characteristics of armchair

SWCNTs. After structural optimization, each MVD in all models becomes a so-called 5-1DB defect with two of its three adjacent dangling bonds (DB) in an ideal MVD, recombining with each other to yield a pentagon ring with the remaining DB unchanged [14]. In all our models, the newly formed carbon–carbon bond is tilt about the tube axis and this is the same as found by Lu et al. [14]. The structural deformation associated with variation in MVD densities is analyzed by calculating the oblateness, which is measured by dividing the largest diameter with the shortest one in the same ring of the defected SWCNTs.

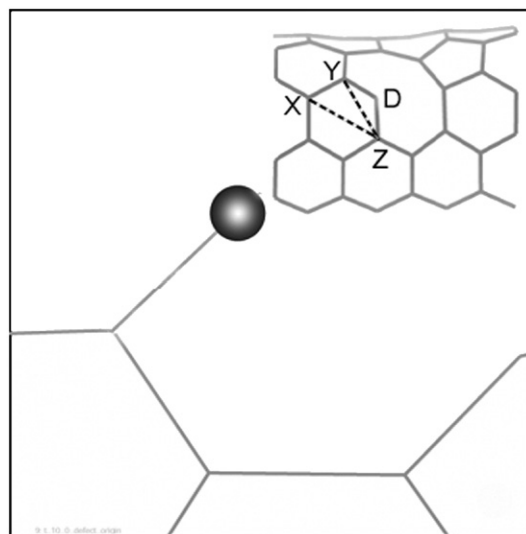


Fig. 2. The schematic plot for the protruding angle, which is defined by the twist angle between the two planes constructed by YDZ and XYZ, respectively, as shown in the inset. The schematic plot is viewed from ZY direction and  $D$  is the twofold coordinated carbon.

Table 1  
Oblateness and bandgap of SWCNT with single mono-vacancy defect

| Number <sup>a</sup> | Oblateness <sup>b</sup> | Length variation <sup>c</sup> | Protruding angle | Bandgap (eV)           |
|---------------------|-------------------------|-------------------------------|------------------|------------------------|
| 79                  | 1.150                   | 0.023                         | 28.5             | 0.098(D <sup>d</sup> ) |
| 119                 | 1.122                   | −0.001                        | 38.5             | 0.145(I <sup>e</sup> ) |
| 159                 | 1.115                   | −0.006                        | 38.5             | 0.000                  |
| 199                 | 1.112                   | 0.008                         | 37.5             | 0.065(I <sup>e</sup> ) |
| 239                 | 1.117                   | −0.011                        | 37.6             | 0.073(D <sup>d</sup> ) |

<sup>a</sup> Number of carbon atoms per one mono-vacancy defect.

<sup>b</sup> Oblateness measured around the vacancy site.

<sup>c</sup> The difference in the lattice constant  $c$  of the defected SWCNTs before and after the structural optimization.

<sup>d</sup> Direct bandgap.

<sup>e</sup> Indirect bandgap.

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