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THE EFFECTS OF DEFECTS ON ELECTRON TRANSPORT IN METALLIC SINGLE WALL CARBON NANOTUBES

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We report the transport behavior of an open-end metallic single wall carbon nanotube (SWCNT) with and without local structural defects using the non-equilibrium Green's functions approach together with the density functional theory (DFT). The transmission spectra and the projected density of states for the devices such as SWCNT (3, 3), (4, 4), (5, 5) and (6, 6) with and without defects were compared. In all cases, we found that the Stone-Wales defect had an almost negligible impact on the electrical performance compared to the monovacancy defect of the single wall carbon nanotubes at the Fermilevel. The Current-Voltage (I-V) characteristics of the devices were studied using the generalized Landauer - Buttiker formalism under low bias conditions. From our results, we concluded that our systems were suitable for use in various CNT based nano-electronic devices.

Keywords: Density functional theory, Single wall carbon nanotubes, Transport properties, I-V characteristics.

1. Introduction

In recent years, carbon nanotube (CNT) based electronics has received much attention because of its tremendous potential in applications such as active components, switches, memory devices, display devices and sensors. Single walled carbon nanotubes (SWCNT) exhibit metallic or semiconducting behaviour, depending on its diameter and chirality [1,2]. Single wall armchair carbon nanotubes are one dimensional conductors with only two open conduction channels. Hence, the conduction of electrons ultimately becomes localized owing to defects in the tube which is inevitable with increasing length due to the interactions between the tube and its environment. These transport properties have been studied extensively. Early theoretical and experimental work on SWCNT predicted that a special achiral subset of these structures known as armchair nanotubes should be metallic. That coherent electron transport can be maintained through the nanotubes was confirmed experimentally by Tans, et al. [3]. Recently, the ab-initio method [4] based on Non-equilibrium Green's Function(NEGF), in combination with Density Functional Theory(DFT), has allowed the determination of electronic transport properties of systems with hundreds of atoms in the presence of a finite voltage, which is more accurate. In this paper, we report a study on the effects of defects such as monovacancy and Stone-Wales on the electron transmission in metallic SWCNTs. The I-V characterizations were analyzed, and a negative Differential Resistance (NDR) effect was observed, which is a very useful property in nano devices such as switches, logic cells and memory storage.

2. Computational Formalism

To analyse the quantum transport through the ab-initio method, one must deal with open systems within the DFT formalism, as the system is either isolated or periodic and can be considered as two semi-infinite electrodes coupled via a contact region. Hence, the SWCNTs were divided into three regions, namely, the left electrode, right electrode and the scattering region in between the electrodes. The scattering region consisted of five unit cells and the length of the electrode was 0.492nm. For convergence, a tolerance of 1×10^{-5} of the total energy was used. Electron transport was performed on devices of metallic single wall nanotubes by a fully self-consistent NEGF combined with first-principles DFT, which is implemented in the Atomistic Tool kit (ATK) [5] package (Version 11.8.2). The generalized gradient approximation (GGA) with Perdev Zunger (PZ) pseudo potentials was used in the calculation. A double-ζ polarization (DZP) basis set was employed to describe the localized atomic orbitals and the multigrid poisson-solver must be set with the same boundary conditions. The K-point sampling is $1\times1\times100$.

In our calculations, the transmission function was calculated by

$$T(E,V) = \mathrm{Tr}\left[\Gamma_L(E,V)G(E,V)\Gamma_R(E,V)G^{+}(E,V)\}\right], \tag{1}$$

where $\Gamma_{L/R}$ stands for the coupling matrix between the left/right electrode and scattering region, G and G^{+} are the retarded and advanced Green's function.

The I-V characteristics were calculated by using Landauer-Buttiker [6] formula, which relates the conductance to the transmission probability $T(E,V)$

$$I(V) = G_0 \int_{\mu_L}^{\mu_R} dET(E,V)\{f(E-\mu_L) - f(E-\mu_R)\}, \tag{2}$$

where $G_0 = 2e^2/h$ is a quantum unit of conductance, μ_L and μ_R are the chemical potential of left and right electrodes respectively, $f(E-\mu_{L/R})$ is the Fermi-Dirac distribution function. The resistance was derived from the current-voltage relationship.

3. Results and Discussion

The electron transmission coefficients of metallic SWCNTs with and without defects are shown in Fig. 1. In all the cases, the electron transmission coefficient of the defect-free was equal to 2 around the Fermi level (0 eV), indicating that there are two transmission channels, π-bonding and π^*-antibonding state. But a sudden drop at 0 eV occurs in the (4, 4) nanotubes because of weak coupling. The transmission coefficient for Stone-Wales defect does not reduce at the Fermi level for all the nanotubes. Hence, the electrical conductance of all metallic nanotubes at the Fermi level is not affected. In the case of monovacancy, the transmission coefficient was significantly reduced due to the formation of dangling bonds where σ-bond states are perpendicular to the π-valence bond states. As a result of this, weak coupling occurs between them [7, 8].

Under bias condition, the transmission peaks were shifted from Higher Occupied Molecular orbitals (HOMO) to the Lower Unoccupied Molecular Orbitals (LUMO). Above 1 Volts, there is a formation of symmetric gap in the transmission channels for all the nanotubes, however, this appears at 0.2 Volts for the (4, 4) nanotube. Hence, the transmission channels are suppressed in that position.

Based on the calculated electron coefficient, the current-voltage (I-V) relationship of the systems can be determined as shown in Fig. 2. Ohmic behavior occurs at low bias voltages

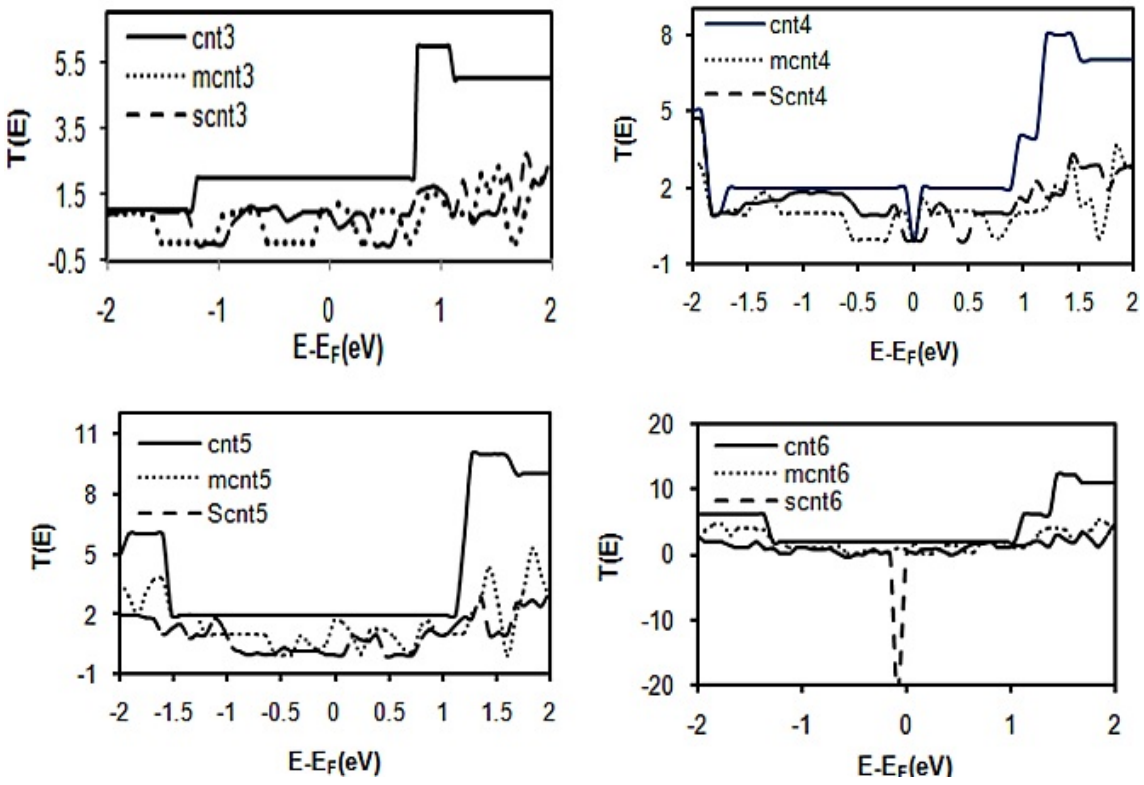

FIG. 1. Transmission spectra of metallic single wall nanotubes at zero voltage (a) (3, 3); (b) (4, 4); (c) (5, 5); (d) (6, 6)

(0-1 Volts). However, above 1-2 Volts, the current decreases as the bias voltage increases and the nanotubes exhibit a non-Ohmic behavior known as Negative Differential Resistance (NDR) [9, 10] in all the cases. The NDR occurs at 0.2 V for the (4, 4) nanotube. Hence, the I-V characteristics of the systems will depend on the leads and the radius of the nanotubes (i.e.) nature of the nanotubes. The monovacancy shows low current than the Stone-Wales defect in all the cases except (6, 6) nanotubes due to the monovacancy defect near the open ends of the nanotube. In other cases, the monovacancy and Stone-Wales defects are in the curvature. These are comparable with diode characteristics, indicating diode-like applications of nanotubes.

4. Conclusion

We have investigated the electron transport properties of metallic SWCNTs with or without defects using NEGF formalism combined with first-principles DFT. From our results, we concluded that all the metallic nanotubes had similar characteristics under low bias conditions and Stone-Wales defect had negligible effect on the electrical conductance of the SWCNTs at the Fermi level while monovacancy defect significantly reduced the electrical conductance by severely blocking one of the transmission channels. These conclusions demonstrate the effective application of our systems in various CNT-based nano-electronic devices such as memory devices, switches and sensors.

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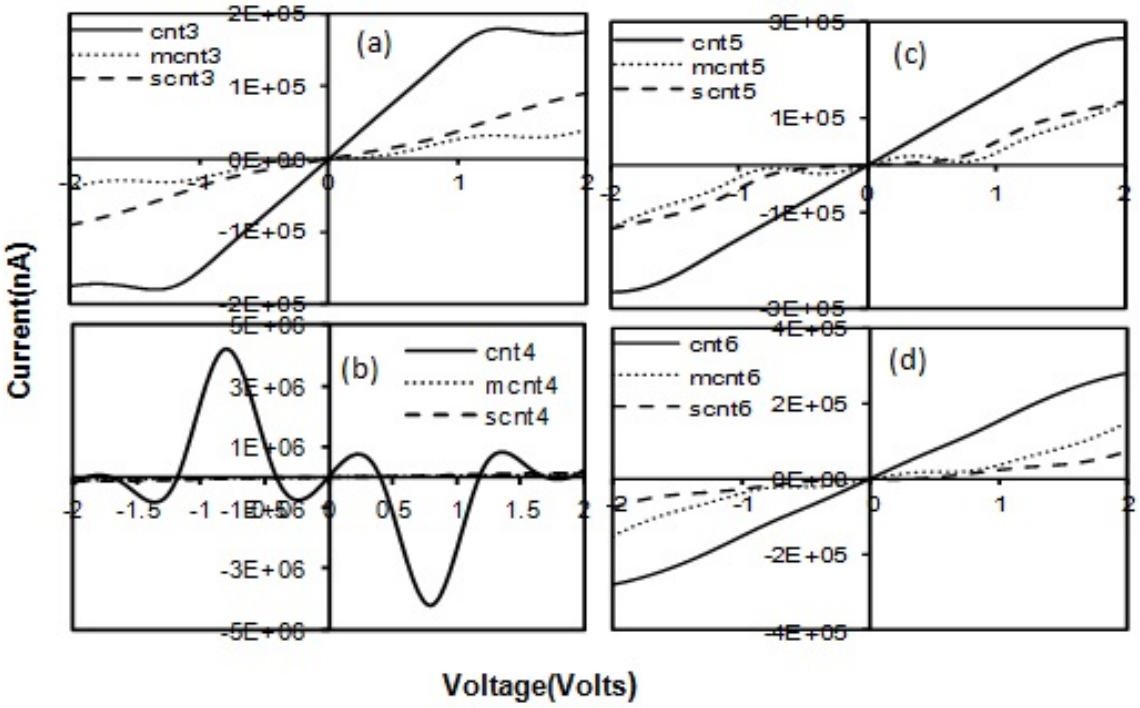

FIG. 2. The I–V characteristics of metallic nanotubes (a) (3, 3); (b) (4, 4); (c) (5, 5); (d) (6, 6)

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