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A band structure study on inter-wall conductance of double-walled carbon nanotubes

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ABSTRACT

Recent advances in etching agents and techniques on the fabrication of double-walled carbon nanotubes (DWCNTs) have introduced various techniques and devices based on nanotube technology. The present study evaluates the inter-shell interaction of DWCNT through density functional theory (DFT) and charge transfer model. The results showed that the band structure of a DWCNT is determined by super positioning of the band structures of the two individual CNT constituting the DWCNT. In next step, interwall conductance the electronic properties of DWCNT were studied through the band-structure approach. Our assessments have shown that at lower potentials the amount of intershell leakage current is negligible.

1. Introduction

Since the discovery of carbon nanotubes(CNTs) in 1991, their unique properties have drawn a great deal of research attention in both experimental [1] and theoretical viewpoints [2]. The CNTs can be used to develop the next generation of nano-electronic components. CNTs can be divided into two main groups based on their capabilities for rolling graphene pages including single-walled CNT (SWCNT) and multi-walled CNT(MWCNT) [1–3]. The simplest form of MWCNT is DWCNT which consists of two interacting subsystems: an inner and an outer CNT. Peapod annealing produced DWCNT possess a number of unique properties such as very long phonon and optical excitation lifetimes [4,5]. The electronic properties of SWCNT can be fully determined by their (n,m) chiral indices [6]. However, the properties of DWCNT cannot be identified due to the inter-shell interactions. Experimental and theoretical studies conducted on the inner CNT shells have indicated a great potential of CNTs in devices such as quantum capacitor [7,8] or as the channel and gate of CNT field effect transistor (CNTFET) [9]. In such devices the interwall tunneling current is a leakage current and the bias should be chosen so that tunneling current is negligible. To our knowledge, few studies have focused on the MWCNT properties considering their potential applications in electronic devices. Resonant Raman measurements have previously determined experimental evidence for an orbital mixing related effect, the red shift of the Van Hove transition energies caused by the inner–outer layer interaction DWCNTs as well as the dependence of the red shift on the inter-shell distance. In addition, photoemission measurements have recently showed the charge transfer (CT) between the inner and outer layer of DWCNTs [10,11]. Etching some segments of the outer shell allows access to the inner shell while altering the electronic properties of such structures [12]. Previous studies on DWCNTs were usually complex with no practical contributions for the design of new nano-structured electronic devices. Therefore, the present study introduces a new easy-to-understand and simple method to calculate the electronic properties of DWCNTs. Using this method, the interwall conduction were studied. Zólyomi et al. [11], and Su et al. [10] studied the CT orbital mixing, and band structure of DWCNTs [10]. Cheung and Chan using an

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intuitive CT model, calculated the work function and the electronic band structure of their SWCNT [10]. Using these findings, we found that band structure of a DWCNT is a superposition of the band structures of the two individual CNT constituting the tube. Therefore, we investigated the interwall conductance from band-structure point of view. Findings of our study can be used for fabrication of new electronic devices containing separate electric current on each layer.

2. Methods

The present study was aimed to evaluate the inter-shell interaction of a DWCNT through DFT theory and CT model as well as electronic properties of the interwall conductance through band structure approach. We studied the band structure and charge transfer of 3 different DWCNTs with a standard ~3.4 Å adjacent layers separation distance as well as the interwall conductance of DWCNT using DFT and superposition method. To evaluate the band structure of the DWCNT, band structure of the two individual SWCNT forming the DWCNT was first investigated. Then, the DWCNT was studied using DFT and superposition model [10]. In DFT [13,14], we used the local density approximation (LDA) [10,11] as implemented in the Atomistix toolkit (ATK) software. In our calculations, a 4.26 Å length super cell model was used where an infinite-length DWCNT was placed in a cell with 12.2 Å from vacuum regions and each cell was arranged in a simple tetragonal lattice. The cut off energy was set to 2040 ev and the k-point sampling was set to $1 \times 1 \times 80$ for both SWCNT and DWCNT. Atomic positions were optimized under the zero-bias voltage.

3. Results and discussion

We found that the band structure of the DWCNT is determined by a superposition of the band structures of two individual CNTs constituting the DWCNT. It is noted that the band structure of the inner tube shifts up and the band structure of outer tube shifts down. This shift in the band structure can be attributed to the CT process [15]. A slight difference was observed in the band structures of a DWCNT and the one formed from two individual SWCNT (where charge transfer is also considered) [16–23]. This difference can be caused by orbital mixing which is negligible because of the large distance assumed between the inner and outer shells. The CT creates a depletion region on the inner surface of the outer shell and the outer surface of the inner shell(as shown in Figs. 1 and 2). The amount of CT between the two shells in DWCNT can be calculated by Eq. (1)

$$Q = Q_{DWCNT} - Q_{inner} - Q_{outer} \tag{1}$$

Where Q_{DWCNT} is the charge density of the DWCNT and Q_{inner}, Q_{outer} are the charge density distribution of individual inner and outer layer determined by DFT.

In the superposition model of the CT, shifting of band structure and electrical field between the inner and outer shells can be calculated as follows: in the band structure, the highest occupied (HO) state represents the direction of electrons transferred between the tubes. Therefore, the

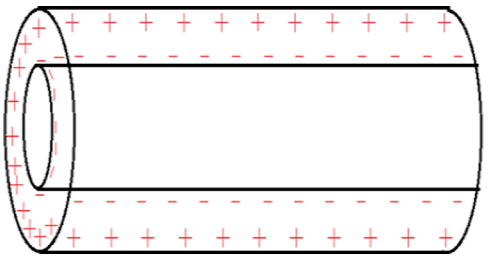

Fig. 1. Inter-shell charge transfer: CT creates the depletion region on the inner surface of the outer shell and the outer surface of the inner shell.

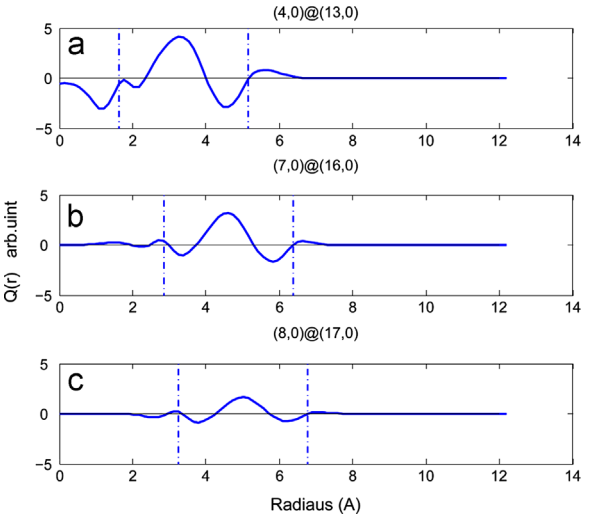

Fig. 2. Redistribution of charge density (a) (4,0)@(13,0), (b) (7,0)@(16,0) and (c) (8,0)@(17,0) calculated with the DFT method obtained from Eq. (1).

flow of electron is from the tube having HO (outer tube) to the other one (inner tube). Consequently, an electric field is formed from the outer tube towards the inner one which stops further transfer of charge between tubes. The amount of HO shifting down in the outer tube equals ΔE_d and the HO shifting up in the inner tube equals ΔE_U.

$$\varepsilon_{out}^{HO\oplus} = \varepsilon_{out}^{HO} - \Delta E_d \tag{2}$$

$$\varepsilon_{out}^{HO\oplus} = \varepsilon_{in}^{HO} - \Delta E_u \tag{3}$$

$$\varepsilon_{out}^{HO\oplus} = \varepsilon_{in}^{HO\oplus} + \Delta V \tag{4}$$

Where ε_{out}^{HO}, $\varepsilon_{out}^{HO\oplus}$, ε_{in}^{HO} and $\varepsilon_{in}^{HO\oplus}$ are the HO of the outer and inner tube before and after electron transfer, respectively. Electrostatic potential 'ΔV' between inner and outer tube is determined with the Eq. (4):

$$\Delta V = \frac{q}{2\pi\varepsilon_0 l} \ln \frac{R_{out}^{eff}}{R_{in}^{eff}} \tag{5}$$

Where Q, l, R_{out}^{eff}, and R_{in}^{eff} are the transfer charge, length of tubes and effective radius of outer and inner tube, respectively.