Electronic structures of double-walled armchair SiC nanotube under transverse electric fields

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A B S T R A C T

By using first-principle calculations based on density functional theory (DFT), the electronic structures of a double-walled armchair (5,5)@(9,9) SiC nanotube (SiCNT) under transverse electric fields are investigated. The band gap of the SiCNT has a decreasing tendency as increasing the intensity of the applied electric field. The mechanism of narrowing in the band gap of the SiCNT is the charge redistribution caused by the electric field. Furthermore, an empirical model for the dependence of the band gap on the electric field is proposed. These results are meaningful for investigations on SiCNTs electronic devices.

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1. Introduction

Since the discovery of carbon nanotubes (CNTs) [1], one dimensional nanometer materials have attracted tremendous interests due to their unique physical properties and potential applications in novel devices. Boron nitride nanotubes (BNNTs) [2–4], SiC nanotubes (SiCNTs) [5–7] and other nanometer semiconductors in tubular form have been successfully synthesized. SiCNTs widen the application range of SiC crystals, especially in nanometer electronic devices and sensors operating in high temperature and high power harsh environments.

The electronic structures of SiCNTs in an applied electric field are the foundations for some applications, such as field-effect transistors (FETs) and field emission devices. Investigations on CNTs, BNNTs and zinc oxide nanotubes (ZnONTs) indicate that their band gaps can be modified by a transverse electric field [8–12]. The band gaps of these nanotubes decrease with the enhancement of the applied electric field and the influence of the electric field is weaker on large diameter nanotubes than on small diameter nanotubes. Nevertheless, the electronic structures of SiCNTs under external electric fields are rarely studied. Alfieri studied band gap modifications on single-walled SiCNTs with transverse electric fields [13]. The band gaps of SiCNTs decrease with the increases of the electric field intensities. Most synthesized SiCNTs have a multi-walled structure. Interwall interactions in multi-walled CNTs and BNNTs seriously influence their properties. Because of the complexity in studies on multi-walled SiCNTs, structural and electronic properties of these nanotubes are rarely studied. In Adhikari studies on stability of double-walled SiCNTs [14], interwall interaction is founded, which indicates a high similarity in the properties of multi-walled SiCNTs and double-walled nanotubes. Studies on double-walled SiCNTs are more valuable than investigations on single-walled nanotubes. It is regrettable that no research on the electronic structures of double-walled or multi-walled SiCNTs under transverse electric fields is reported. In this paper, the electronic structures of a double-walled (5,5)@(9,9) SiCNT in transverse electric fields are calculated and the influence of the applied electric field on the band gap of the nanotube is analyzed. More importantly, the mechanism for the decrease in the band gap of the nanotube is achieved. These results are meaningful for studies on novel SiCNTs electronic devices.

2. Model and method

In geometry, a double-walled nanotube can be regarded as being formed with two coaxial single-walled nanotubes. Under the reference of Adhikari's studies on double-walled SiCNTs [14],

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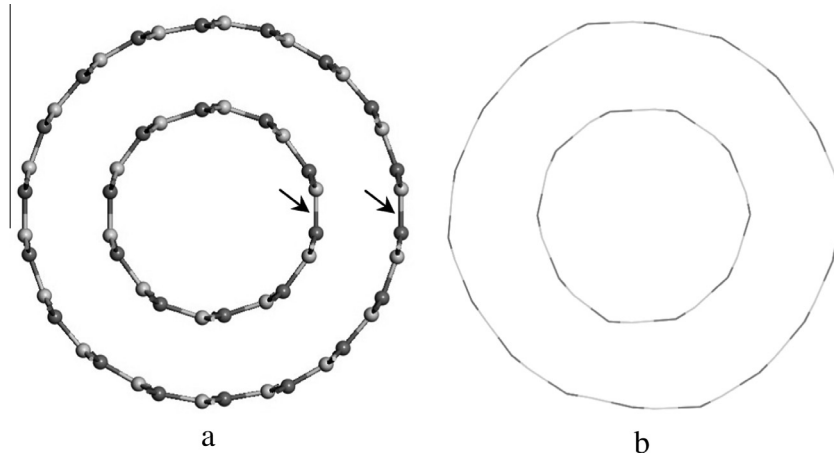*E-mail address:* sonx@mail.xidian.edu.cn (J. Song).

Fig. 1. Model for (5,5)@(9,9) SiCNT with a 0° rotational angle (a) and the optimized SiCNT with 60° rotational angle (b).

models for (5,5)@(9,9) SiCNTs with different rotational angles between its two layers are established. The rotational angle is defined by two Si–C bonds in the outer layer and inner layer (labeled out in Fig. 1a), which have the same coordinate along its axis. The rotational angle is the angle between these Si–C bonds. Due to the symmetry of the (5,5)@(9,9) double-walled SiCNT, the rotational angle varies in the range from 0° to 72° with an increment of 12°. The model for the (5,5)@(9,9) SiCNT with a 0° rotational angle is presented in Fig. 1a. The distance between the two layers of the SiCNTs is about 3.40 Å. To release stress in these models, geometry optimizations on SiCNTs are realized with Broyden–Fletcher–Goldfard–Shanno (BGFS) method. In calculations, convergence standards are determined by the force, stress and displacement of each atom, which are set as less than 0.05 eV/Å, 0.05 GPa and 5×10^{-4} Å.

Formation energy has been successfully applied to explore the stable structure of the double-walled boron nitride nanotubes [15]. The formation energy for the (5,5)@(9,9) SiCNT is defined as:

$$E_{form} = (E_{inner} + E_{outer}) - E_{double} \qquad (1)$$

where E_{double} is the energy for the optimized double-walled nanotube, E_{inner} and E_{outer} indicate energies for the inner and outer layer of the nanotube. Formation energies for (5,5)@(9,9) SiCNTs are calculated and listed in Table 1.

Although the formation energies of the double-walled SiCNTs are similar, the nanotube with the rotational angle of 60° has the highest formation energy, which indicates that this nanotube has the most stable structure. The optimized SiCNT is shown in Fig. 1b. Its inner nanotube and outer nanotube are not ideal cylinders. Si–C bond distances in the inner layer vary from 1.770 Å to 1.782 Å, while bond distances in the outer layer lie in range from 1.781 Å to 1.796 Å.

The electronic structures of the double-walled SiCNT have been achieved with first-principle calculations based on density functional theory. In investigations, the exchange–correlation potential is realized with the generalized gradient approximation (GGA) provided by Perdew, Burke and Ernzerhof (PBE) [16]. Double numerical plus d-function is used as atomic orbital basis set throughout the calculations. The Brillouin zone sampling is performed using special k points generated by the Monkhorst–Pack grid with a

value of $1 \times 1 \times 8$, which is suitable to one dimensional materials [17].

3. Results and discussions

3.1. Electronic structures of the (5,5)@(9,9) SiCNT

The band structure of the double-walled (5,5)@(9,9) SiCNT with a rotational angle of 60° is calculated and presented in Fig. 2a. Partial density of states (PDOS) for C atoms and Si atoms in the nanotube are also achieved (Fig. 2b).

The (5,5)@(9,9) SiCNT posses an indirect gap of about 1.74 eV. The bottom of the conduction band for the double-walled nanotube locates at the Z point of the first Brillouin zone. The top of the valence band lies at the point T labeled out in Fig. 2a. The conduction band mainly consists of Si $3p$ states (Fig. 2b). The upper valence band is mainly originated from C $2p$ states and Si $3p$ states. The lower valence band is formed primarily with C $2s$ states and Si $3s$ states. The bottom of the conduction band and the top of the valence band are occupied by Si $3p$ states and C $2p$ states. These are similar to PDOS distribution of Si toms and C atoms in single-walled (9,0) SiCNT [18].

The band gap of the (5,5)@(9,9) SiCNT is narrower than that of the (5,5) nanotube (about 2.17 eV). Curvature effect plays an important role in this difference. When a SiC sheet is rolled up to form a single-walled SiCNT, the π and σ orbitals are not orthogonal to each other and hybridized [19]. The hybridization of the π and σ orbitals shifts the π^* and π bands to lower energy. The π^* and π bands form the bottom of the conduction band and the top of the valence band of the SiCNT. Their shifts seriously depend on the nanotube diameter. The shifts of the π states of the inner tube are smaller than that of the outer tube. Thus, the top of the valence band for the double-walled SiCNT is determined by π state of the inner tube. The bottom of the conduction band mainly originates from the π^* state of the outer tube. These leads to the narrow in the band gap of the double-walled SiCNTs. More important, its electronic structures near the energy gap may have richer variations than that of the single-walled SiCNTs.

3.2. Electronic structures under transverse electric fields

The band gaps for the (5,5)@(9,9) SiCNT under transverse electric fields are calculated. The electric field intensity is set from 0.00 V/Å to 0.10 V/Å and its increment is set as 0.01 V/Å. Some achieved band gaps are given in Table 2. The band gaps of the SiCNT under transverse electric fields decrease with the increase

Table 1
Formation energies of double-walled SiCNTs.

Angle (°)	0	12	24	36	48	60
E_{form} (eV)	0.250	0.255	0.327	0.297	0.296	0.337