Electronic transport properties of the armchair silicon carbide nanotube*

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Abstract: The electronic transport properties of the armchair silicon carbide nanotube (SiCNT) are investigated by using the combined nonequilibrium Green's function method with density functional theory. In the equilibrium transmission spectrum of the nanotube, a transmission valley of about 2.12 eV is discovered around Fermi energy, which means that the nanotube is a wide band gap semiconductor and consistent with results of first principle calculations. More important, negative differential resistance is found in its current voltage characteristic. This phenomenon originates from the variation of density of states caused by applied bias voltage. These investigations are meaningful to modeling and simulation in silicon carbide nanotube electronic devices.

Key words: electronic transport properties; armchair silicon carbide nanotube; negative differential resistance; nonequilibrium Green's function
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1. Introduction

Since the discovery of the carbon nanotube (CNT)[1], massive effort has focused on nanotube materials, in which the silicon carbide nanotube (SiCNT) is one of the typical nanotubes and has been synthesized with different methods[2−6]. Theoretical investigations into this nanotube show that it is a wide band gap material and its electronic structures are nearly independent of its structure[7]. This nanotube is an ideal candidate for the fabrication of nanometer electronic devices and sensors.

The electronic transport properties of the silicon carbide nanotube are the foundation for exploring the working mechanism of related electronic devices. It is rarely studied and limits studies on the applications of this nanotube. The method used here combined the nonequilibrium Green's function (NEGF) with density functional theory (DFT) has been applied to explore the transport properties of molecular devices and the CNT, in which some properties are discovered[8−11]. This method is appropriate to study the transport properties of the armchair SiCNT.

In this work, the electronic transport properties of a (4, 4) armchair SiCNT are investigated with a method combining the NEGF with DFT. Negative differential resistance (NDR) is found in the current voltage characteristic of the nanotube, which originated from the variation of density of states caused by the applied bias.

2. Model and method

To investigate the electronic transport properties of the (4, 4) armchair SiCNT, a two-probe model is established (see Fig. 1). There is a finite (4, 4) SiCNT with 16 layers of atoms in the central scattering region of the model. In each layer, four carbon atoms and four silicon atoms are included. More details of the SiCNT in structure can be found in Ref. [12]. The structure of the left and right electrodes is ABC. The structure of the left two layer Au atoms in the central scattering region is AB and the right is BC. An ABC–AB–BC–ABC structure is established, which has the minimum electrode defects in a stack. The distance between the nanotube and the electrodes has a certain effect on its transport properties. In the calculations, the distance is set to be 1.7 Å, which is usually used in studies of the transport properties of carbon nanotube devices.

The transport properties of the SiCNT are explored with the method based on NEGF in combination with DFT implemented in the TranSIESTA-C package and in version 2.3 of Atomistix ToolKit (ATK 2.3). This method has been applied to study the transport properties of carbon nanotubes. The exchange-correlation energy is described by the local density approximation (LDA) proposed by Perdew and Zunger[13]. The valence electrons are expanded in a numerical atomic-

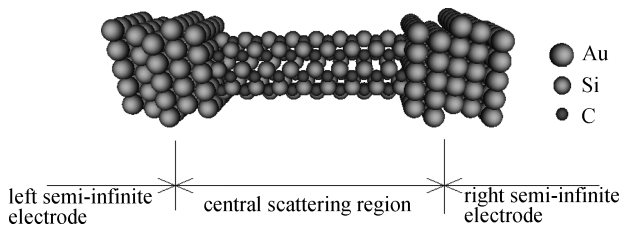

Fig. 1. A two-probe model for a finite (4, 4) SiCNT.

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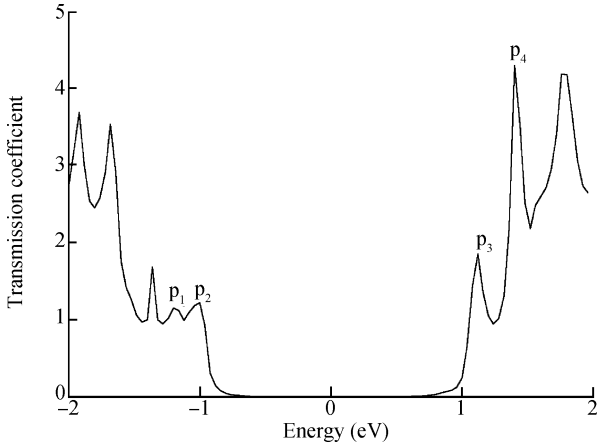

Fig. 2. Transmission spectrum of the SiCNT with no bias applied.

orbital basis set of single zeta (SZ). The core electrons are modeled using Troullier-Martins local pseudopotentials[14]. The parameters for convergence, such as the Hamiltonian and the charge density, are set as 10^{-4}.

The transmission coefficient describes the probability of electrons with incident energy E transferring between the electrodes and reflects the electronic transport property of the nanotube. This can be calculated by

$$T(E,V) = T_{\rm r}[\Gamma_{\rm L}(E,V)G(E,V)\Gamma_{\rm R}(E,V)G^{\dagger}(E,V)], \quad (1)$$

where $G(E,V)$ is Green's function of the two-probe model and $\Gamma_{\rm L/R}$ is the coupling matrix. The current following through the two-probe system can be achieved by integration of the transmission coefficients,

$$I(V) = \frac{2e}{h}\int_{\mu_{\rm L}}^{\mu_{\rm R}} T(E,V)[f(E-\mu_{\rm L}) - f(E-\mu_{\rm R})]{\rm d}E, \quad (2)$$

where $\mu_{\rm L} = -V/2(\mu_{\rm R} = +V/2)$ is the chemical potential of the left (right) electrode.

3. Results and analysis

3.1. Equilibrium electronic transport properties

The transmission coefficient means the probability for electrons with certain energy transferring from one electrode to another. The transmission spectrum $T(E)$ of the nanotube with no bias applied is shown in Fig. 2, in which the Fermi energy is set as 0 eV. The most important feature for the transmission spectrum is the existence of a transmission valley about 2.12 eV around the Fermi energy, in which the transmission coefficients are nearly zero. This means that the armchair SiCNT is a wide band gap semiconductor and is consistent with the results of first principles calculations. The transmission peaks on both sides of the valley play an important role in its transport properties. Four transmission peaks are labeled in Fig. 2. The two peaks (p_2, p_1) lower Fermi energy located at –1.00 eV and –1.20 eV and their peak values are 1.22 and 1.15. The other two (p_3, p_4) higher than Fermi energy lie at +1.12 eV and +1.40 eV.

To further investigate the transmission spectrum, the frontier molecular orbitals of the molecular projected self-consistent Hamiltonian (MPSH) for the nanotube are calculated. The MPSH can be achieved by projecting the self-consistent Hamiltonian onto the Hilbert space spanned by the basis functions of the atoms in the central scattering region. The eigenstates of the MPSH are associated with the poles of the Green function and roughly correspond to the transmission peaks in the transmission spectrum[11].

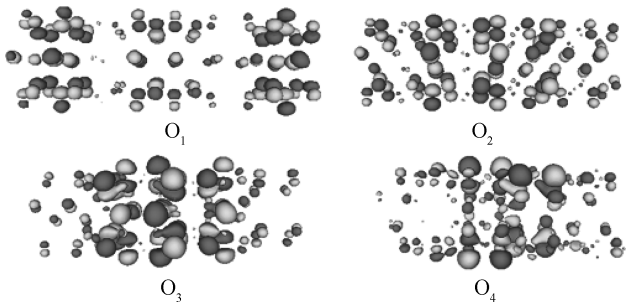

Fig. 3. Frontier molecular orbitals of the MPSH for the SiCNT.

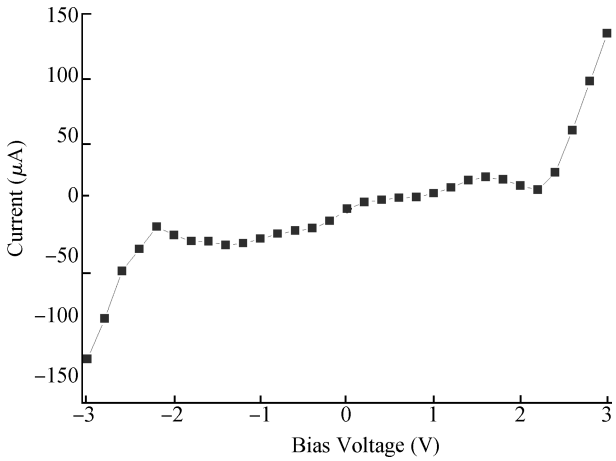

Fig. 4. I–V curve of the SiCNT.

Four frontier molecular orbitals for the silicon carbide nanotube are shown in Fig. 3. The orbital O_2 is the highest occupied molecular orbital (HOMO) of the nanotube, and the orbital O_3 is the lowest unoccupied molecular orbital (LUMO). Their eigenvalues are –0.97 eV and +1.15 eV. Orbital O_1 with an eigenvalue of –1.26 eV has a higher electron density on the central and the two terminal of the nanotube, which results in the transmission peak p_1. Orbital O_4 mainly concentrates on the central of the nanotube and forms the transmission peak p_4.

3.2. Nonequilibrium electronic transport properties

The voltage current (I–V) characteristic of the nanotube is one of the important properties, which is calculated and shown in Fig. 4. As the calculation of the I–V curve for the nanotube is time-consuming, the bias voltage is set from –3.0 to +3.0 V.

As the high symmetry of the I–V curve for the nanotube, it can be studied with that under positive bias. The I–V curve under positive in Fig. 4 can be divided into three parts. In bias range from 0.0 to +1.6 V and +2.2 to +3.0 V, the current following through the SiCNT increases with the increase in the bias. In bias from +1.6 to +2.2 V, the current decreases with

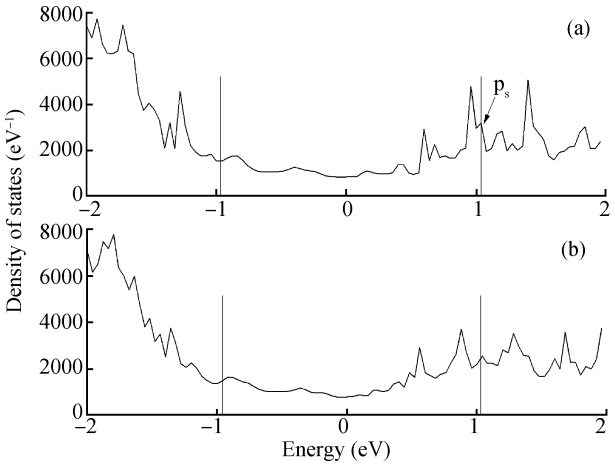

Fig. 5. The DOS for the nanotube under the biases (a) +1.8 V and (b) +2.0 V.

the increase in the bias. This means the occurrence of the negative differential resistance (NDR). The NDR is an important property widely used in molecular switches and other devices. To achieve the origin of the NDR, the density of states (DOS) under +1.8 and +2.0 V are calculated and shown in Fig. 5, in which the solid lines indicate the energy positions for the two discrete levels of the HOMO and the LUMO.

The DOS of the two Au electrodes shifts up and down according to the applied bias voltage, while the positions of the two levels are relative stable to the Fermi level, which is not obviously influenced by the applied bias voltage. As +1.8 V biased voltage is applied to the probe model, the energy levels LUMO matches well with the density of states peak p_5. This means that the electrons can transfer easily from one electrode to another through tunneling and it results in a higher current following through the SiCNT. While the bias voltage reaches +2.0 V, the DOS peak p_5 is seriously depressed (from 2710 to 2142) and the difficult degree of tunneling for electrons is raised, which leads to the current decreasing with the increase in the bias voltage. From the above analysis, it can be seen that the variation in the density of the states is the origin of the NDR for the SiCNT.

4. Conclusions

The electronic transport properties of the (4, 4) armchair SiCNT are investigated with the method combining the NEGF with DFT. In the transmission spectrum with no bias applied, a transmission valley about 2.12 eV is discovered, which is consistent with the result of the first principles calculations. More important, negative differential resistance is found in the I–V curve of the SiCNT. This comes from the variation in DOS for the two probe model caused by applied bias voltage. These results are helpful for the modeling and design of SiCNT electron devices.

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