Negative differential resistance in an (8, 0) carbon/boron nitride nanotube heterojunction*

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Abstract: Using the method combined non-equilibrium Green's function with density functional theory, the electronic transport properties of an (8, 0) carbon/boron nitride nanotube heterojunction coupled to Au electrodes were investigated. In the current voltage characteristic of the heterojunction, negative differential resistance was found under positive and negative bias, which is the variation of the localization for corresponding molecular orbital caused by the applied bias voltage. These results are meaningful to modeling and simulating on related electronic devices.

Key words: nanotube heterojunction; negative differential resistance; non-equilibrium Green's function
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1. Introduction

One-dimensional (1D) heterojunctions, especially nanotube heterojunctions, have attracted tremendous interest because of their distinctive structures and properties, which are of importance for both scientific fundamentals in nanoscience and potential application in nanoelectronics[1]. More important, nanotube heterojunctions have been fabricated recently, for instance, heterojunctions formed with different types of carbon nanotubes (CNTs)[2], heterojunctions between pure CNT and nitrogen doped CNT[3], and boron carbonitride/carbon nanotube heterojunctions[4]. CNT and boron nitride nanotube (BNNT) are the two deeply studied nanotube materials[5, 6]. Blase *et al*. investigated the electronic structures of the nanotube heterojunction formed with the above nanotubes[7]. The electronic transport properties of this heterojunction are rarely studied, which limits research on the working mechanism for related electronic devices.

The method combining non-equilibrium Green's function (NEGF) with density functional theory (DFT) has been used to explore the transport properties of molecular devices[8, 9], quantum wires[10] and SiCNT[11], in which some important properties of these devices were revealed. These studies indicate that this method is reasonable to determine the electronic transport properties of the CNT/BNNT heterojunction. In this paper, the electronic transport properties of a heterojunction formed between an (8, 0) CNT and BNNT coupled to Au electrodes were studied. Negative differential resistance was discovered. These results are helpful for the modeling and simulation of relevant devices.

2. Model and method

The structure of the heterojunction has an obvious influence on its electronic transport properties, which was optimized with the CASTEP package to achieve the geometry close to the synthesized geometry. In optimization, the maximal force, stress and displacement were set as 0.05 eV/Å, 0.05 GPa and 5×10^{-4} Å. The optimized heterojunction is shown in Fig. 1. There are 64 C atoms, 32 B atoms and 32 N atoms in the heterojunction. By comparing the difference between the diameters of the nanotube in the heterojunction and the isolated, its rearrangement can be achieved. The diameter of the (8, 0) CNT is 6.264 Å. The diameters of the nitrogen layers and the boron layers in the BNNT have a slight difference, they are 6.449 Å and 6.356 Å, respectively. The rearrangement mainly lies at the layers near its interface. Variations in the diameters of layer 8 and layer 9 are 0.084 Å and –0.032 Å, which are much larger than other layers. The changes in geometry for the fourth layers (layers 5 and 12) on both sides of the interface are –0.004 Å and –0.007 Å (about 0.11% and 0.06% compared with the corresponding diameters), which can be ignored. This indicates that in an investigation of the electronic transport properties,

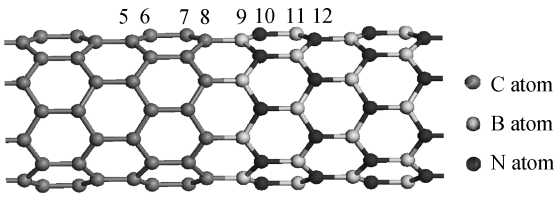

Fig. 1. An optimized (8, 0) CNT/BNNT heterojunction.

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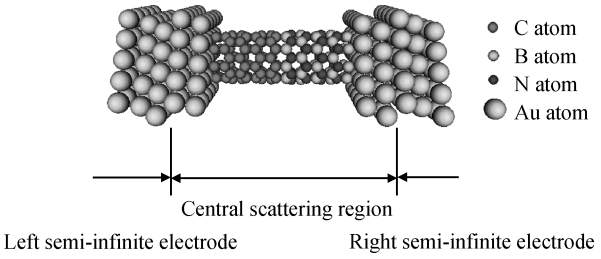

Fig. 2. A two-probe model for the heterojunction coupled to Au electrodes.

the heterojunction should not be shorter than eight layers. More details can be found in Ref. [12].

To investigate the electronic transport properties of the CNT/BNNT heterojunction coupled to Au electrodes, a two-probe model was established based on the optimized heterojunction shown in Fig. 2. The model can be divided into three parts: left semi-infinite electrode, central scattering region, and right semi-infinite electrode. The left and right electrodes are realized with three layers of Au (111) surfaces. Since the periodic boundary conditions are imposed on the plane parallel to the Au surfaces, electrodes are represented by a 5×5 supercell to eliminate the influence of the adjacent supercell. The central scattering region concludes the CNT/BNNT heterojunction and two surface layer Au atoms of each electrode. There are 9 C layers in the CNT section and 5 B layers and 4 N layers in the BNNT section. In calculations, the distance between the heterojunction and the electrodes is set to 1.6 Å.

Studies of the transport properties of the heterojunction with the above model were implemented in the TranSIESTA -C package and in a version of Atomistix ToolKit 2.3 (ATK 2.3). In calculations, the exchange-correlation energy was described by the local density approximation (LDA) proposed by Perdew and Zunger[13]. The valence electrons were expanded in a numerical atomic orbital with a basis set of single zeta (SZ). The core electrons were modeled using Troullier–Martins local pseudopotentials[14]. The physics parameters, such as the Hamiltonian and charge density, are set as 10^{-4}.

The transmission spectrum and the current-voltage characteristics are of great importance for the electronic transport properties of the heterojunction. The transmission spectrum describes the probability of an electron with an incident energy of E transferring from one electrode to another and is calculated by

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

where $G(E,V)$ is Green's function of the two-probe model and $\Gamma_{\mathrm{L/R}}$ is the coupling matrix. The integral of the transmission spectrum gains the current through the system

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

where $\mu_{\mathrm{L}} = -V/2$ and $\mu_{\mathrm{R}} = +V/2$ are the chemical potential of the left and right electrodes, respectively.

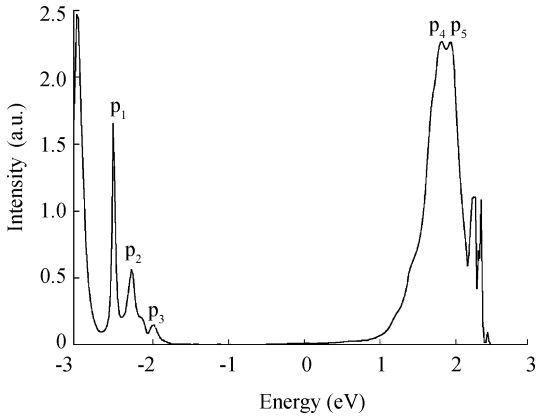

Fig. 3. Equilibrium transmission spectrum of the heterojunction.

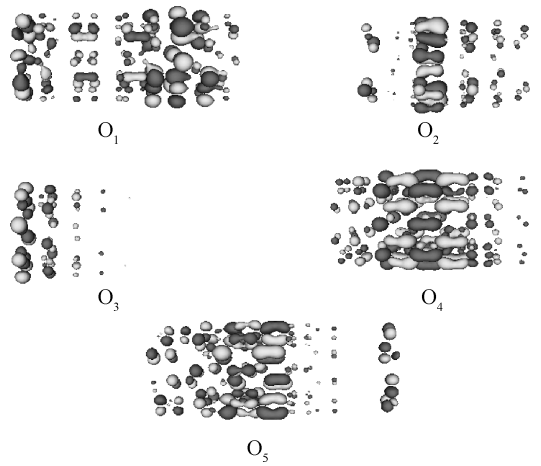

Fig. 4. Frontier orbitals of the MPSH for the heterojunction.

3. Results and analysis

The equilibrium transport properties (with no bias voltage applied) of the heterojunction are investigated first. The transmission spectrum $T(E,V)$ of the heterojunction is shown in Fig. 3, in which the Fermi energy is set as 0.0 eV. A distinct feature of the transmission spectrum is the existence of a transmission valley of about 2.34 eV, in which transmission coefficients are nearly zero. This indicates the existence of a band gap for the heterojunction. The equilibrium transport properties of the heterojunction are determined by transmission peaks near the Fermi energy. These five transmission peaks are labeled as p_1, p_2, p_3, p_4 and p_5. Their corresponding energies are –2.48, –2.24, –1.94, +1.98 and +2.02 eV.

The relationship between the eigenstates of the molecular projected self-consistent Hamiltonian (MPSH) and the poles of Green's function is close. The eigenenergies of the poles roughly correspond to the locations of the transmission peaks in the transmission spectrum[15]. To achieve the origin of the peaks in Fig. 2, five frontier molecular orbitals of the MPSH for the heterojunction were calculated.

In these molecular orbitals of the heterojunction (shown in Fig. 4), the location of the orbital O_3 is highest, which mainly concentrates on the interface between the CNT section and the left Au electrodes. This is the result of the gap states caused by

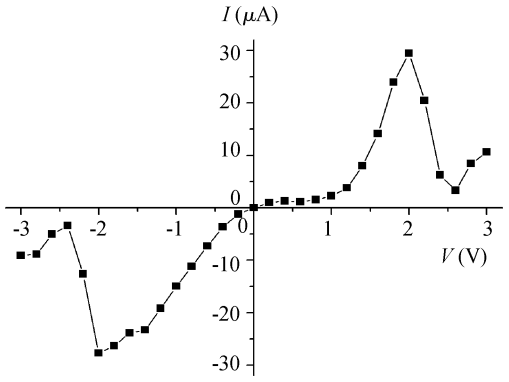

Fig. 5. I–V curve of the heterojunction.

the charge transferring between the heterojunction and the electrode, which was discovered in the electronic transport properties of CNTs. The highest location results in the lowest transmission peaks value p_3 in the five peaks. Orbitals O_2 and O_4 are the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). Their eigenenergies are –2.20 eV and +1.63 eV, which means that the band gap of the heterojunction is about 3.83 eV. The two orbitals have higher charge density near the interface of the heterojunction. The former orbital has a higher electron density in the BNNT section and the latter has a lower density in the same part of the heterojunction. As the localization of the orbital O_4 is lower than that of the orbital O_2, the transmission peak p_4 is higher than p_2. Orbitals O_1 and O_5 are HOMO-1 and LUMO+1, whose localization are low. Transmission peaks p_1 and p_5 are mainly formed by these two orbitals and their peak values are high.

The current–voltage (I–V) characteristic is one of the most important non-equilibrium transport properties of the heterojunction. As the calculation is a time-consuming work, the bias voltage was set from –3.0 to +3.0 V. The I–V curve of the heterojunction is plotted in Fig. 5.

Due to the high similarity of the variation trend for the I–V curve under positive bias and negative bias, it is analyzed with part under positive bias. This partial curve can be divided into three parts. In the bias range from 0.0 to +2.0 V, the current increases with the bias voltage with a near exponential relationship. In the bias range from +2.0 to +2.6 V, the current decreases with the increase in the voltage. This indicates the occurrence of negative differential resistance (NDR). While the bias voltage is greater than +2.6 V, the current increases again with the bias.

To obtain the origin of NDR for the heterojunction, its transmission spectra under +2.0 and +2.2 V are calculated and plotted in Fig. 6. The current is determined by the transmission coefficients $T(E, V)$ and the integral window of the current integral, which can be gained from Eq. (2). The Fermi energy being set to zero in calculations, the integral window is [$-V/2$, $+V/2$]. As the integral window widens with the increase in bias voltage, the most likely reason for NDR is the decrease in transmission peaks in the integral window. Comparing the transmission spectra under bias +2.0 and +2.2 V (Figs. 5(a) and 5(b)), it can be seen that the transmission peak p_6 and the two adjacent peaks (p_6, p_7 and p_8) are depressed with the increase in bias.

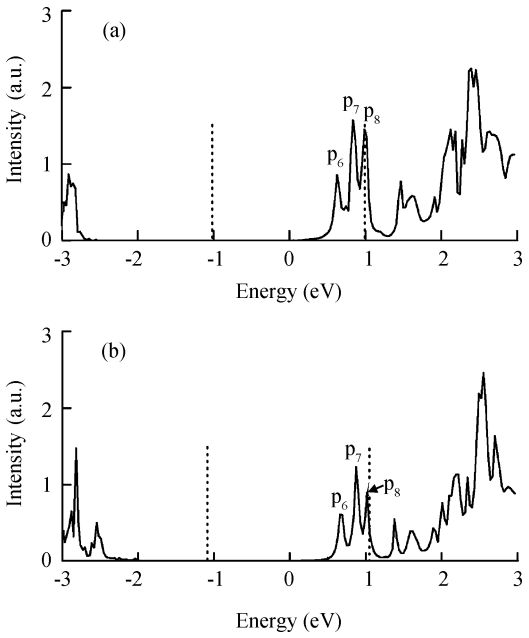

Fig. 6. Transmission spectra of the heterojunction under bias of (a) V = +2.0 V and (b) V = +2.2 V.

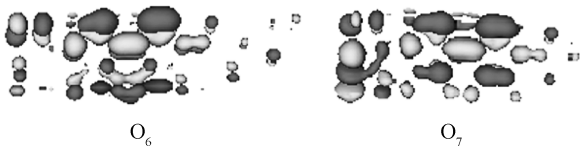

Fig. 7. Frontier orbitals of the MPSH for the heterojunction under different bias.

The depressions of transmission peaks indicate the lowering of the probability of electrons transferring from one electrode to another. This variation results in a decrease in the current with the increase in bias voltage.

As in the above analysis, the transmission peak has a close relation with the locality of the corresponding molecular orbital. This change in the transmission peaks may originate from the variation in the localization of the corresponding molecular orbital. To get the essential origin of the NDR, the molecular orbital of the MPSH is calculated under bias +2.0 and 2.2 V, which plays an important role in the formation of transmission peak p_8. From Fig. 7, it can be seen that the localization of orbital O_6 is higher than that of orbital O_7. This increase in the localization results in the depression of the transmission peak p_8. Furthermore, this leads to a decrease in the current. The reasons for the variations in transmission peaks p_6 and p_7 are similar to that of p_8. Briefly, the origin of the NDR is the increase in localization of molecular orbitals of the heterojunction caused by the applied bias voltage.

4. Conclusions

The transport properties of an (8, 0) CNT/BNNT heterojunction coupled to Au electrodes were investigated with a method combining NEGF with DFT. The gap state is found in the equilibrium transport properties of the heterojunction. In its I–V characteristic, negative differential resistance is dis-

covered under positive bias and negative bias, which is the increase in the localization of the heterojunction's molecular orbitals caused by the applied bias voltage. These results are of great significance for research on the modeling and simulation of electronic devices based on nanotube heterojunctions.

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