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Electronic and electrical properties of silicon nanowire-single wall carbon nanotube junction as a nanoelectronic switch

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ABSTRACT

In this work, we performed first principles calculations based on self-consistent charge density functional tight-binding to investigate how the overlapping length of two inter-shell structure effect on the electronic and electrical properties of silicon nanowire-single wall carbon nanotube junction. By computing of density of state, current–voltage curve, conductance and transmission probability, it is found that the binding energy, charge transferring between two structures and conductance changes with the overlapping length. Our results show that charge transferring between the two structures is not affected by overlapping length. Also, we found that the current increases by increasing the overlapping length. At finally, the conductance increase from the zero to the high amount of overlapping length as an off and on states of a nanometer switch.

1. Introduction

In nanometer scale electronic devices [1–4], research is currently being carried out on new structures of semiconductors such as nanoparticles, nanowires and nanotubes in order to find suitable components for future miniature electronic devices [5–11].

A new generation of nanoelectronic devices based on inter-shell electron transport in carbon nanotubes and semiconductor nanowires [12,13] is crucial for potential applications of nano scale switch [14]. In these systems, two inter-shell is assembled by a double wall carbon nanotube or a nanowire into the single layer carbon nanotube. The nature of the inter-shell interaction is important role in the structural stability and electronic property of the switches [15–18] in comparison with inter-layer connections [19,20]. Because in the inter-shell switches, the current can be controlled by modifying the inter-shell configuration.

The electrical properties of an inter-shell switch have been reported by different method of calculations. For example, Tamura [11] computed the conductance of telescoped double-wall nanotubes using the Landauer formula and a tight binding model. Yan et al. [21] studied a nanoelectronic switch based on telescoping double-walled carbon nanotubes (TDWCNT) by a method based on real-space nonequilibrium Green's function formalism and density-functional theory. They computed electronic transport of TDWCNTs. They found that the quantum conductance of switch periodically oscillates with the overlapping length of the two shells of the TDWCNT. Pomorski et al. [22] investigated capacitance and bound states of biased two and three carbon nanotube inter-shell systems based on a recently developed real-space nonequilibrium Green's-function approach. They found that the estimates of the capacitance coefficients are related to the overlapping density of state (DOS) of each junction element.

The present paper discusses the electronic properties and electron transport characteristics of inter-shell switch consists a silicon nanowire into single-wall carbon nanotube (NW–SWCNT) junction by ab initio calculations. Silicon nanowires appear to be an especially appealing choice, due to their ideal interface compatibility with conventional Si-based technology [23,24]. Moreover, it can be used as a part of the switch because of the metallic behavior of Si nanowires. We subsequently evaluate the possibility of using SiNW–SWCNT junction as nanoelectronic inter-shell switches based on the effect of overlapping length (L) on their electrical properties. In this work, we calculate the binding energy, transferred charge, current–voltage curves, conductance, transition probability and DOS based on density functional tight-binding (DFTB) method for different inter-shell overlapping length.

2. Simulation method

To compute the electronic and electrical properties of typical NW–SWCNT switch, we considered a [1 1 0] coaxial silicon nano-

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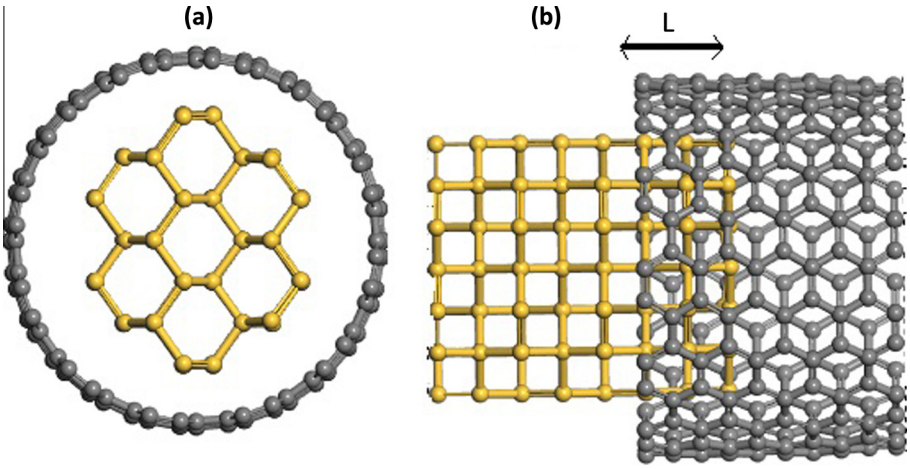

Fig. 1. The structure of silicon nanowire-single wall carbon nanotube junction.

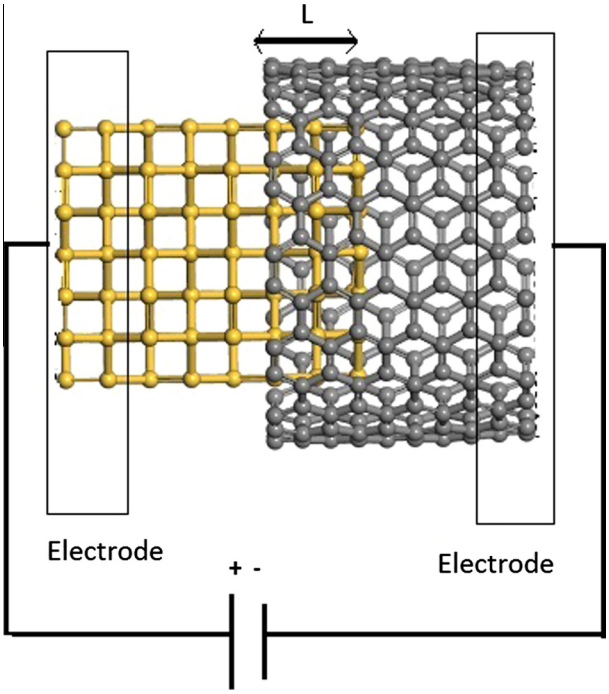

Fig. 2. The bias voltages along two electrodes of left and right.

wire with the diameter of 10.35 Å and a length of 13.44 Å into a single wall carbon nanotube with the chirality, diameter, length and number of atoms of (12, 12), 16.27 Å, 11.44 Å and 240, respectively (Fig. 1). One tip of each element at the junction is open, while the other is assumed to be connected to the external electrode.

An ab initio code package, DFTB+ based on self-consistent charge density functional tight-binding (SCC-DFTB) formalism based on the second-order expansion of the Kohn–Sham total energy in DFT with respect to charge density fluctuation within the tight-binding framework is employed to perform electronic transport calculations of NW–SWCNTs [25]. We used pbc parameters set which was developed for solids and surfaces [26].

To compute electron transport, nonequilibrium Green's function formalism (NEGF) was used with SCC-DFTB+. The current was calculated by Landauer–Büttiker formula

$$I = \frac{2e}{h}\int_{\mu_L}^{\mu_R} T(E, V_b)[f(E, \mu_L) - f(E, \mu_R)]dE \quad (1)$$

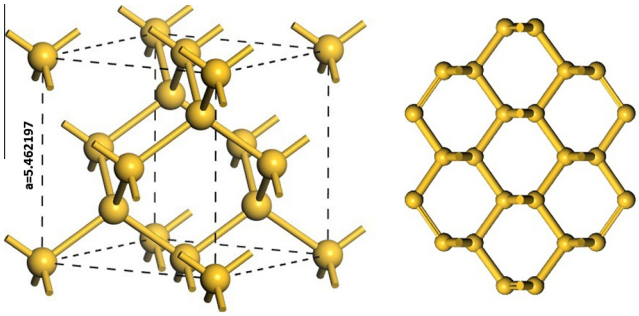

Fig. 3. The structure of (a) Si bulk and (b) cross section of Si nanowire.

where μ_R and μ_L are the chemical potentials of the right and left electrodes, e is the electron charge, h is Planck's constant, $f(E, \mu)$ is the Fermi–Dirac distribution, $T(E, V_b)$ represents the electronic transmission probability, and V_b is the applied bias voltage across the electrodes.

For the switch, k-points were used for the axes with a $1 * 1 * 100$ Monkhorst–Pack grid for the Brillouin zone integration. The mesh cutoff was chosen to be 200 Ry and also the convergence of total energy and Hellman–Feynman forces were 10^5 eV and 0.01 eV/Å, respectively.

The steps of our calculations were starting with optimizing the structure of the Si bulk and nanowire, single wall CNT and SiNW–SWCNT junction with minimizing the total energy for different inter-shell overlapping length (L = 0, 1.92, 3.84, 5.76 and 7.86 Å). Then in the next step, we calculated electronic properties of these structures. The final step was applying the bias voltage along the electrodes to compute the current and the transmission probability for SiNW–SWCNT junction. The applied bias voltage was increased from 0 to 0.5 V in steps of 0.1 V (Fig. 2).

3. Results and discussion

We first calculate the structural and electronic properties of the Si bulk and nanowire, in order to examine the accuracy of our calculations. Figs. 3 and 4 show the lattice structure and total density of states for bulk and nanowire Si after relaxation, respectively.

We obtain the value of the crystal lattice parameter a = 5.4621 Å and gap energy of 1.21 eV for the bulk Si. There are a good agreement between our results and experimental data and other calculations [27,28].