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Theoretical study on transport properties of a BN co-doped SiC nanotube

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ABSTRACT

We investigate the electronic transport properties of silicon carbide nanotubes (SiCNT) in presence of both boron (B) and nitrogen (N) impurities. The results show that co-doping BN impurities suppresses the important negative differential resistance (NDR) property. NDR suppression is attributed to the introduction of new electronic states near the Fermi level followed by weak orbital localization. BN co-doping results in exponential current–voltage (I–V) characteristics which is in contrast to linear I–V characteristics for individual boron and nitrogen doped SiCNTs. HOMO has no contribution from B impurity, whereas, LUMO has contribution from N impurity at low and high bias.

1. Introduction

Silicon carbide nanotubes have a great potential for application in chemical and biological sensors [1,2]. Recently, the scientists have suggested to make silicon carbide nanotubes (SiCNTs) as a possible alternative to carbon nanotubes (CNTs) for field emitting applications [3,4], which has boosted the interest for SiCNTs and several studies on the electronic properties of SiCNTs can be found in the literature [5,6]. It is well known that bulk silicon carbide (SiC) is commonly contaminated by nitrogen and boron impurities where nitrogen substitutes the carbon site making n-type conductivity and boron substitutes both carbon and silicon sites forming an acceptor region in bulk SiC [7].

The electron transport properties for individual boron and nitrogen doped SiCNTs could be found in previous research works [2,8,9]. Therefore, it is of interest to understand the transport properties in presence of both boron and nitrogen impurities in SiCNT. For this purpose, in Fig. 1, a silicon atom toward the left electrode is replaced by a boron atom forming a p-type (acceptor) region and a silicon atom toward the right electrode is replaced by a nitrogen atom making an n-type region. The whole geometry in Fig. 1 could be visualized as a p–n junction formed by a doped $(8, 0)$ SiCNT placed between the gold (Au) electrodes.

The traditional methods find difficulty in studying the transport properties of SiCNTs because of their small feature size. However, the method combined with density functional theory (DFT) and non-equilibrium Green's function (NEGF) has been applied successfully to investigate the electron transport and other properties [8,10]. In our previous research work, the transport properties of deformed SiCNTs and vacancy defected SiCNTs have been analyzed using DFT in combination with NEGF and the negative differential resistance (NDR) effect was observed [11,12]. In this Letter, transport properties of BN co-doped SiCNTs have been studied by combining DFT and NEGF. To the best of our knowledge, the effect of BN co-doping on electron transport in SiCNT has not been studied so far.

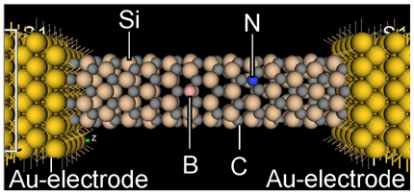

Fig. 1. Two-probe geometry of a BN-doped $(8, 0)$ SiCNT with Au electrodes.

2. Model and method

A two-probe geometry [8,11] that consists of a left semi-infinite electrode, right semi-infinite electrode and a central region (scattering region) was constructed using BN co-doped SiCNT and Au electrodes. Si–C bond length of 1.78 Å [4,13] and 1:1 Si–C ratio was considered. Both left and right electrodes are made up of $5 \times 5 \times 5$ Au layers perpendicular to the nanotube axis, distance between the SiCNT and Au electrode is set as 1.3 Å which was found by relaxing a five period (40 atoms) SiCNT and $5 \times 5 \times 3$ layer Au electrodes with C atom at the electrode contacts. In the previous research works, this distance was taken as 1.5 Å [14], 1.6 Å [8,15] and 1.7 Å [16] found by relaxing a diatomic Au–C dimer. We found stronger

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coupling between the electrodes and SiCNT on using 1.3 Å as this distance. Further, BN co-doped (8, 0) SiCNT and two Au layers of each electrode (left and right) consist of the central scattering region. The doped SiCNT was relaxed using quasi-Newton geometry optimization methods until all residual forces on each atom are smaller than 0.05 eV/Å.

The simulation parameters were selected to provide accurate measurements as reported for CNTs [11,12,17] and are following: mesh cut-off energy was 400 Ry, basis set was double zeta polarized with 0.001 Bohr radial sampling, exchange correlation functional was set to local density approximation (LDA) type with double zeta polarized (DZP) basis set, Brillouin zone integration parameters of three-dimensional electrodes are taken as $(3, 3, 500)$. Electrode temperature was set to 1000 K which makes the convergence easier; it has no effect on the overall measurement which was also verified at lower electrode temperatures. It is important to keep in mind about the uncertainty in the calculated LDA band gap as it is well known that the LDA underestimates the width of the band gap due to the self-interaction of the electrons. The above parameters were used by [17] to obtain accurate results using LDA.

To obtain transmission spectrum and I–V characteristics, self-consistent calculation are performed on an ab initio based simulator called Atomistix [18] which uses density functional theory (DFT) and non-equilibrium Green's functions formulations (NEGF) together for obtaining electronic transport properties of molecules and devices. More details about the method and software could be found in previous reports [19–21]. Same simulator was used by [8,9] for studying SiCNTs with individual boron and nitrogen doping.

The transmission spectrum describes the probability for electron with incident energy (E) to transfer from the left electrode to the right electrode under applied bias voltage (V). The analytical expression for calculating the transmission spectrum is given by [7,8,22]:

$$T(E, V) = \mathrm{Tr}\big[\Gamma_L(E, V)G^{\dagger}(E, V)\Gamma_R(E, V)G(E, V)\big]$$

where $\Gamma_{L/R}$ is the coupling matrix.

The integral of the transmission spectrum yields the current through the system [7,8,22], given by:

$$I(V) = \int_{\mu_L}^{\mu_R} T(E, V)\big(f(E-\mu_L) - f(E-\mu_R)\big)\,dE$$

where $\mu_L = -V/2$ $(\mu_R = V/2)$ is the chemical potential of the left (right) electrode.

3. Electron transport results and analysis

3.1. Equilibrium transport properties

The transmission spectrum $T(E)$ for various bias voltages is plotted in Fig. 2, here the Fermi energy is set as 0 eV. The equilibrium transport properties (no bias voltage applied, Fig. 2(a)) of the BN-doped SiCNTs are studied firstly. A (8, 0) SiCNT is semiconducting by nature, a BN doped (8, 0) SiCNT is also semiconducting which is confirmed by the transmission gap (transmission coefficient is zero) around Fermi level in Fig. 2(a). The eigenstates of molecular projected self-consistent Hamiltonian (MPSH) are closely related to the poles of Green's function, which roughly corresponds to the peaks (p1, p2, p3, p4, p5 and p6) of the transmission spectrum in Fig. 2(a) [22]. The frontier molecular orbitals of the MPSH are calculated and shown in Fig. 3 to study the physical origin of these peaks.

The highest occupied molecular orbital (HOMO) lies at −0.42 eV and has no contribution from BN atoms. The lowest unoccupied molecular orbital (LUMO) lies at 0.23 eV and is mainly contributed by N atom. The difference in HOMO–LUMO levels gives

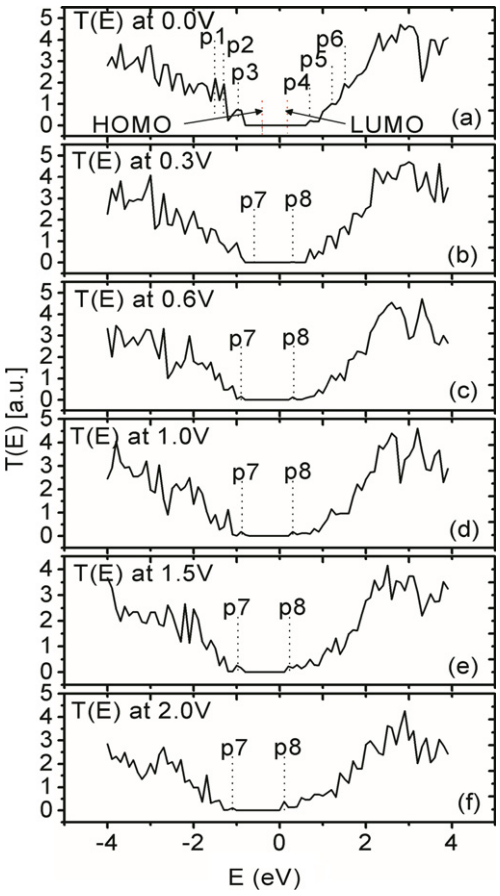

Fig. 2. Transmission spectrum $T(E)$ in the bias range 0 to +2.0 V. New peaks (p7 and p8) appear near the Fermi level at high bias voltages.

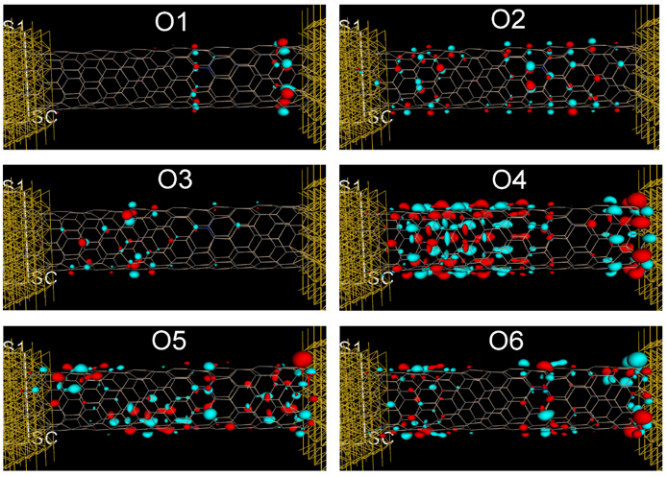

Fig. 3. Frontier orbitals of the MPSH for BN-doped SiCNT at zero bias; O1, O2, O3, O4, O5, O6 are the orbitals corresponding to the peaks p1, p2, p3, p4, p5, p6 of the transmission spectrum in Fig. 2.

the bandgap of BN co-doped SiCNT as ∼0.65 eV, which is comparable with the bandgap of individual B-doped SiCNT (∼0.7 eV) and N-doped SiCNT (∼0.5 eV) reported in [7]. The transmission peaks (p1, p2, p3) in Fig. 2(a) with lower values than Fermi level originate mainly from orbitals O1, O2 and O3 in Fig. 3, whose localization is high. The transmission peaks (p4, p5, p6) with higher values than Fermi level primarily come from O4, O5 and O6, which exhibit weaker localization.