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Competition and Cooperation between External and Internal Electric Fields for Carrier Injection in Carbon Nanotubes with Defects

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Abstract

We report the electronic properties of carbon nanotubes (CNTs) with defects under an electric field, based on density functional theory. The defects intrinsically induce an internal electric field in CNTs because of the modulation of the electrostatic potential arising from the defects. According to the internal electric field induced by the defects, the threshold gate voltage required to accumulate electron and holes strongly depends on the defect species and their relative positions in the CNTs with respect to the electrode.

1. Introduction

Carbon nanotubes (CNTs) are attracting much attention because of it unique geometric and electronic structures those allow them being an emerging material for semiconductor electronic devices in the next generation. It has been shown experimentally that CNTs can work as a conducting channel of field-effect transistors (FETs). In the electronic devices, external electric field is essential for operating the CNT based devices properly. However, the fundamental properties of CNTs under an electric field are not fully understood yet. In particular, it is still unclear how the defects introduced into CNTs affect the electronic properties and charge accumulation into CNT under an electric field. In this work, we aim to elucidate the fundamental electronic properties of CNT with various defects under the external electric field that injects electrons/holes into CNTs using density functional theory combining with effective screening medium method [1-3].

2. Calculation Method and Model

All of the calculations were performed using in the framework of the density functional theory (DFT) with the Simulation Tool for Atom Technology (STATE) package. To express the exchange correlation potential among the interacting electrons, the local density approximation is applied with the Perdew–Zunger functional generated by the homogeneous electron gas. We use an ultrasoft pseudopotential to describe the interactions between the valence electrons and ions generated by the Vanderbilt scheme. The valence wavefunctions and charge density were expanded with a plane-wave basis set with cutoff energies of 25 and 225 Ry, respectively. To integrate the Brillouin zone, four k-points were sampled along the direction of the CNT.

The effective screening medium method is applied to investigate the electronic properties of the CNTs with various defects with the carriers accumulating under an electric field using DFT. In this work, (10,0), (11,0), and (12,0) CNTs were considered with monovacancy, divacancy, C_2 adatom, and Stone-wales defects were embedded with triple periodicities in the CNTs along their axis. To simulate the CNT-FET device structure, we consider the structural model shown in Fig. 1, in which the CNT is located above the planar gate electrode simulated by an effective screening medium to mimic an ideal metal electrode. An electric field is applied between the electrode and the CNT up to about V_G = ±4 V, which injected 0.5 carriers into CNTs. The atomic structures were fully optimized under zero electric field with the lattice parameters for the direction of the tube axis, the direction of the electrode, and the lateral direction fixed at 12.71, 17.00, and 26.00 Å, respectively. During the calculations under the conditions with a finite electric field, the geometries were kept the same as those with a zero electric field.

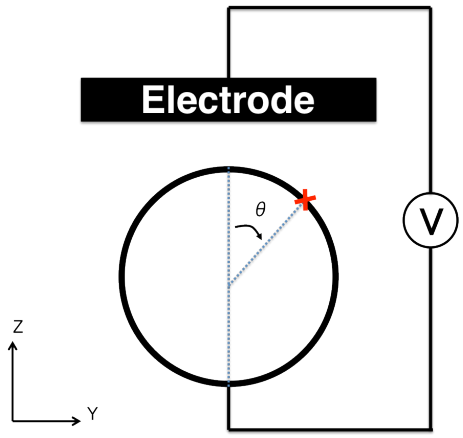

Fig. 1 A structural model of a CNT under an electric field. A cross indicates the position of the defects. The angle (θ) denotes the mutual angle of the defect with respect to the electrode.

3. Results and Discussion

Figure 2 shows the plane-averaged electrostatic potential of CNTs with defects along the z-direction under a zero electric field. Electrostatic potentials in Fig. 2 are averages in x–y plane for each z coordinate. In the calculation, we

impose an open boundary condition along the z-direction to elucidate the electrostatic potential modulation arising from these defects. In all cases, the defects are located at the topmost region of the CNTs (corresponding to the arrangement with θ = 0°) and lead to a higher vacuum level than that for the opposite side of the CNTs. Thus, all defects cause a potential difference between the topmost and bottommost regions of CNTs, indicating that the internal electric field is induced by the defects. The internal electric field affects carrier accumulation in CNTs by the external electric field caused by the electrode, because the internal electric field either competes with or cooperates with the external electric field for carrier injections.

Figure 3 shows gate voltages that are required for carrier injection in CNTs with defects. The gate voltage for requiring each carrier accumulation strongly depends on the position of the defects in CNTs relative to the electrode as well as on the defect species. This orientation dependence of gate voltages for carrier accumulation is caused by the competition and cooperation between internal and external electric fields. Furthermore, the variation in the gate voltage for carrier accumulation also exhibits a correlation with the internal electric field. The variation increases with increasing internal electric field. Thus, the defects and their mutual arrangement with respect to the electrode decisively affect the properties of CNT-based FETs.

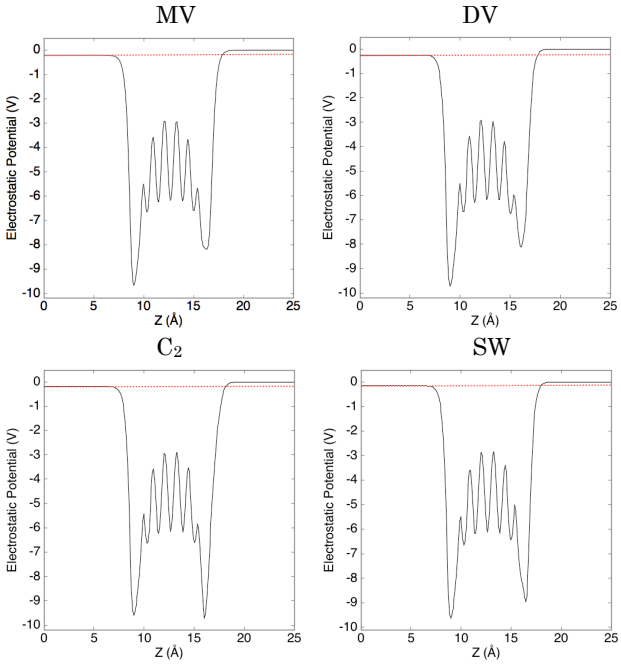

Fig 2 Plane averaged electrostatic potentials of CNTs with monovacancy (MV), divacancy (DV), C_2 adatom (C_2), and Stone-Wales defect (SW) normal to the z-direction under a zero electric field. The electrode is on the right end of the panel. Horizontal dotted lines denote vacuum level at the left end of the unit cell.

4. Conclusions

The electronic structure of CNTs with monovacancy, divacancy, C_2 adatom, and Stone–Wales defects was studied under a vertical electric field in terms of the defect species and their mutual arrangement relative to the gate electrode based on density functional theory combined with the effective medium screening method. Calculations showed that the internal electric field induced by the defects strongly depends on the defect species. The external electric field either cooperates with or competes with the internal field, leading to large variations in the gate voltage used to accumulate charge carriers. Therefore, the defect species and their position in the CNT are important factors when fabricating CNT-based electronic devices based on electric fields.

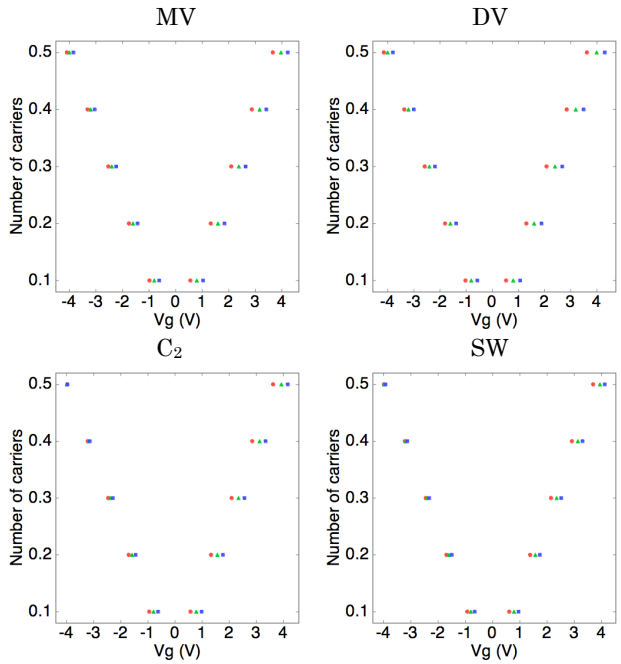

Fig 3 The number of accumulated carriers in CNT as a function of the external electric field. Circles, triangles, and squares denote the CNTs with the defects of which mutual angles are 0, 90, and180 degree, respectively.

References

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