Extended Abstracts of the 2008 International Conference on Solid State Devices and Materials, Tsukuba, 2008, pp. 674-675

P-13-1

First principle calculation of contact between Scandium and semiconducting carbon nanotube

Yu He[1,2], Jinyu Zhang[1], Mingzhi Gao[1], Qiushi Ran[1], Yan Wang[1] and Zhiping Yu[1]

[1]Institute of microelectronic, Tsinghua University, Beijing, China
[2]Phone:86- 010-62771394-122; E-mail:heyu07@mails.tsinghua.edu.cn

1. Introduction

Carbon nanotubes (CNTs)[1] are promising for future high performance electronics such as field effect transistors (FET) owing to their various unique properties[2][3]. Much has been done to achieve high performance p-type nanotube FETs but progress on n-FETs has been slow[3]. Various experimental and theoretical works have been done to investigate contact properties between different metal electrodes such as Ti, Al and Pd and CNTs[4]. Recent experiment shows that Scandium (Sc) can make a good performance contact with CNT to fabricate n-FETs[8]. In this paper, for the first time, we explore Sc and semiconducting CNT contact properties using first principle calculation.

2. Physical Model and Computational Methods

To demonstrate our calculation, we first calculate Pd and CNT contact (Pd-CNT) which has been studied by Zhu et al.[5]. Then we will calculate Scandium and CNT contact (Sc-CNT).

(8,0) single-wall CNTs(SWCNT) is used for both metal-CNT systems. The configuration of Pd-CNT is shown in Fig.1(a) and 1(b). The CNT is covered by Pd atoms [5].The whole system includes 160 C atoms and 32 Pd atoms. In Sc-CNT shown in Fig.1(c), the Sc (110) surface is chosen as the electrodes which end-contacted with a (8,0) single-wall CNT. The whole system includes 160 C atoms and 88 Sc atoms.

The structural optimization and the corresponding total energy calculations are performed by using VASP[9]. Plane-wave cutoffs from the PW91-GGA[10] ultrasoft-pseudopotential[11] are used for Pd, C and Sc. The optimized atomic geometries are obtained until all the forces are smaller than 0.03eV/Å. The Monkhorst-Pack[12] method is employed for Brillouin zone sampling.

3. Results and Discussion

The relaxed structures of metal-CNT contact systems are shown in Fig.1. The diameter of the optimized CNT is 6.28Å, which is consistent with Ref.[5] of 6.37Å. Fig.1(a) and 1(b) show the views of relaxed structures of Pd-covered (8,0) CNT along and perpendicular to the nanotube axis. Note that in Fig.1(c), interactions between Sc electrodes and the CNT are quite strong, resulting in the large distortion of the CNT at the interface of the contacts.

Fig.2 shows the self-consistent electrostatic potential distribution for metal-CNT contact systems. The Fermi level is about -2eV and 3.1eV in Pd-CNT and Sc-CNT, respectively. Contours shaded gray indicate that the electrostatic potential is lower than Fermi level. Contiguous gray areas extending from the CNT to Pd and Sc indicate that there is no electrostatic potential barrier between the CNT and metals for conduction electrons near the Fermi level in the region of contact.

Now we consider the possible formation of a Schottky barrier. A p-type Schottky barrier is defined as the energy difference between the Fermi level of the metal and the top of the valence band of the semiconductor. To align the energy levels, we follow the method of potential profile lineup[13]. In this approach, a C atom is chosen far away from the metal as the reference. The reference C atoms for the two systems are indicated by arrows in Fig.1(a) and 1(c).

Fig3.(b) and 3(c) show the local density of states (LDOS) of the reference C atoms for the two structures, respectively, in which the energy levels are aligned with the ideal (8,0)CNT. It can be seen that the Schottky barrier of Pd-covered CNT system is about 0.34eV, which is in

agreement with the experimental measurement of about 0.4eV[6]. The p-type Schottky barrier between Sc and (8,0)CNT is about 0.45eV. Note that the Fermi level of Sc is closer to the bottom of the conduction band of CNT, indicating that the Sc end-contacted with CNT system may form an n-type CNT-FETs[8].

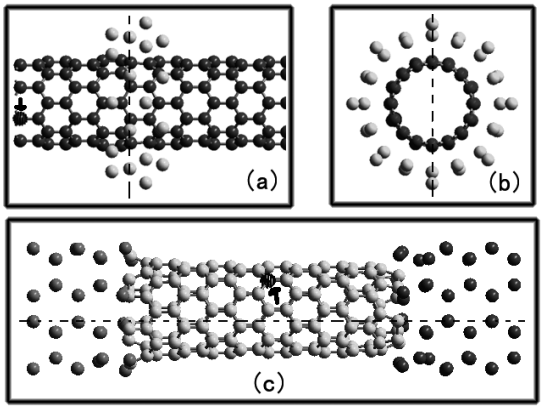

Fig.1 Views of relaxed structures of Pd-covered (8,0) CNT(a) along and (b) perpendicular to the nanotube axis are shown. In(c), the view of relaxed structure of Sc end-contacted with (8,0)CNT is shown.

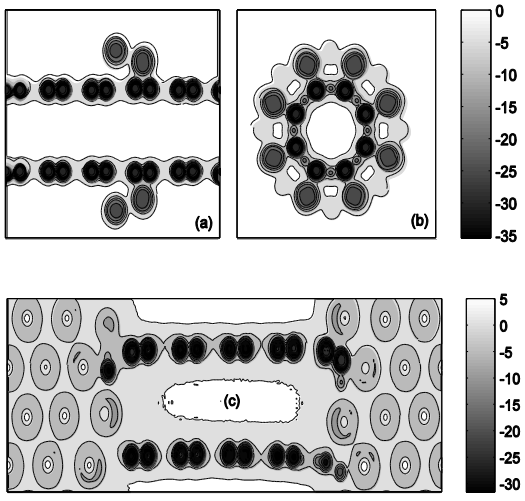

Fig.2 Self-consistent electrostatic potential distribution for Fig.1(a) and (b)Pd-covered (8,0) CNT system along two representative cross sections and (c)Sc end-contacted (8,0) CNT along the CNT axis, indicated by the dashed lines in Fig.1(a), (b) and (c).

4. Conclusion

We have studied the contact between Pd and (8,0)CNT, and Sc and (8,0)CNT. The p-type Schottky barrier of Pd-covered CNT system is 0.34eV, which is close to the experimental value of 0.4eV. The p-type Schottky barrier for end-contacting between Sc and (8,0)CNT is about 0.45eV. The Fermi level of Sc is close to bottom of the conduction band of CNT which may be responsible for forming n-type CNT-FETs.

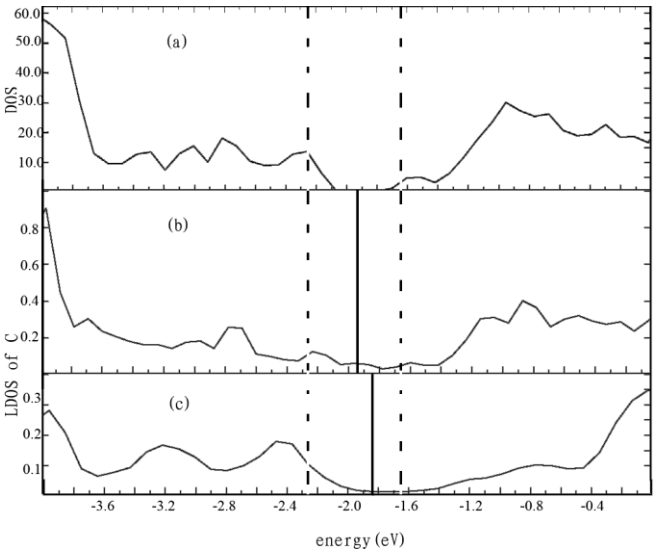

Fig.3 (a) Density of states of an ideal (8,0) CNT and Local density of states of the reference C atoms for (b)Pd-covered CNT and (c)Sc-contacted CNT. The area between the dash lines is the band gap of the ideal (8,0)CNT. The solid line shown in (b) and (c) is the Fermi level for the two systems, respectively.

References

[1] S. Iijima, Nature (London) **354**, 56 (1991)

[2] S. J. Tans et al., Nature (London) **393**, 49 (1998).

[3] A. Javey et al., Nature (London)**424**, 654 (2003).

[4] W. Kim et al., Appl. Phys. Lett.**87**, 173101 (2005).

[5] W. Zhu and E. Kaxira, Appl.Phys. Lett. **89**, 243107 (2006).

[6] Z. Chen et al., Nano Lett.**5**, 1497 (2005).

[7] T. Meng et al., J. Appl. Phys. **102**, 013709 (2007).

[8] Z. Zhang et al., Nano. Lett. 7, 3603(2007).

[9] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).

[10] J. P. Perdew and Y. Wang,Phys. Rev. B 45, 13244 (1992).

[11] D. Vanderbilt, Phys. Rev. B **41**, 7892(1990).

[12] H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).

[13] B. Shan and K. Cho, Phys. Rev. B **70**, 233405 (2004).