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Structural feature and electronic property of an (8, 0) carbon–silicon carbide nanotube heterojunction*

Liu Hong-Xia(刘红霞)†, Zhang He-Ming(张鹤鸣),
Hu Hui-Yong(胡辉勇), and Song Jiu-Xu(宋久旭)

Key Lab of Ministry of Education for Wide Band Gap Semiconductor Materials and Devices, School of Microelectronics, Xidian University, Xi'an 710071, China

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A supercell of a nanotube heterojunction formed by an (8, 0) carbon nanotube (CNT) and an (8, 0) silicon carbide nanotube (SiCNT) is established, in which 96 C atoms and 32 Si atoms are included. The geometry optimization and the electronic property of the heterojunction are implemented through the first-principles calculation based on the density functional theory (DFT). The results indicate that the structural rearrangement takes place mainly on the interface and the energy gap of the heterojunction is 0.31 eV, which is narrower than those of the isolated CNT and the isolated SiCNT. By using the average bond energy method, the valence band offset and the conduction band offset are obtained as 0.71 and –0.03 eV, respectively.

Keywords: carbon nanotube/silicon carbide nanotube heterojunction, electronic properties, average-bond-energy method, band offsets

PACC: 7115M, 3640B, 7125

1. Introduction

Nanotube heterojunctions have attracted a great interest because of their distinctive structures and properties, which are of importance for both scientific fundamentals in nanoscience and potential applications in nano-electronic devices.[1] Most of the fabricated nanotube heterojunctions are formed between bulk material and nanotube, for example Si/CNT heterojunction and CNT/TiC heterojunction.[2−6] Owing to the existence of great difficulty in fabrication, the heterojunctions formed by nanotubes are rarely studied. The boron carbon-nitride nanotube/CNT heterojunction was realized by using the bias-assisted hot-filament chemical vapour deposition (CVD) method and its rectification behaviour has been found.[7] By using the chosen synthesis method, multiwall CNx/CNT junctions have been successfully fabricated.[8] The lack of the study on structural and electronic properties of the nanotube heterojunctions restricts their fabrication and application in nano-electronic devices.

The first principles calculation has been applied to the study of the stability and the properties of the nanotube materials, and satisfactory results are achieved. Yu *et al* studied the B/N substitutional doped zigzag single-walled nanotube.[9] The influence of the uniaxial strain on the band structure of single-walled carbon nanotube has also been found from the first principles calculations.[10] Other properties of CNT, such as oxygenation, static dielectric properties, are also investigated. Similar studies on the SiCNT have been performed by using the same method.[11−13]

In the present paper, the structural feature and the electronic property of a nanotube heterojunction formed by an (8, 0) CNT and an (8, 0) SiCNT are studied through the first-principles calculation based on the density functional theory (DFT). The results show that the structural rearrangement takes place mainly on the interface. The energy gap of the heterojunction is obtained through the analysis of its density of states, and the band offsets are also achieved based on the average-bond-energy method.

2. Model and method

To study the structural feature and the electronic property of the heterojunction formed by an (8, 0) CNT and an (8, 0) SiCNT, a supercell is established,

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†E-mail: liuhongxia_xidian@126.com

in which 96 C atoms and 32 Si atoms are included. This supercell is large enough for calculation.[14]

The geometry optimization and the electronic property investigation are performed by using the CASTEP package. In calculation, the interaction between electron and ion is represented by the ultrasoft pseudo-potential, the exchange-correlation potential is described in the generalized gradient approximation. The electron wave function is expanded in plane waves with a cutoff energy of 300 eV. The Brillouin zone integrations are realized in the special k-point scheme of Monkhorst–Pack, with a $1\times1\times10$ k-point grid used.

3. Results and discussion

It is known that the geometry of the isolated nanotube and the nanotube heterojunction can seriously influence its electronic properties. The isolated (8, 0) CNT and the SiCNT are optimized in geometry. The bond length of Si–C in SiCNT is 1.78 Å(1Å=0.1 nm), which is agreed with the result given by Gali.[11] The diameters of silicon layers and carbon layers of the SiCNT section are 7.805 Å and 7.905 Å, respectively. The diameter of the (8, 0) CNT is 6.264 Å, which is similar to the result of 6.26 Å presented by Song *et al.*[15] These results imply that our method is applicable for the study of the structure of heterojunction.

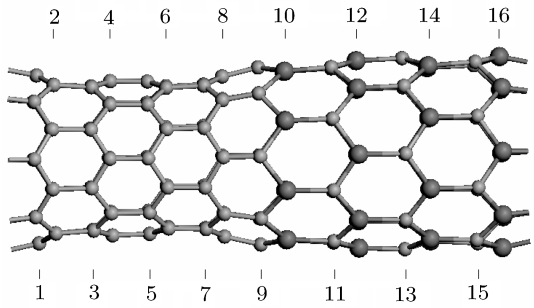


Fig.1. Structure of CNT/SiCNT heterojunction where the small light grey balls represent C atoms while the big dark grey balls refer to Si atoms.

The optimized structure of the CNT/SiCNT heterojunction is shown in Fig.1. The difference in diameter between (8, 0) CNT and SiCNT leads to the structural rearrangement at the interface. The rearrangement in the heterojunction can be studied by comparing the diameter of C layer with that of Si layer near the interface as presented in Table 1. The maximal change in diameter of the CNT section is 1.088 Å in layer 9. With the increase of the distance from the C layer to the interface of the junction, the deviation of the diameter decreases sharply. The deviation of the third C layer (layer 7) from the interface is 0.010 Å (about 0.16%), which can be ignored. In the SiCNT section, the SiCNT is slightly narrowed and the maximum change in diameter is about 3.268%, occurring in layer 10. From the above analysis, it is obvious that the structural rearrangement takes place mainly at the interface.

Table 1. Diameters and their variations of the CNT/SiCNT heterojunction.

	Layer number	Diam/Å	ΔD
C	7	6.364	0.010
C	8	6.630	0.366
C	9	7.352	1.088
Si	10	7.558	–0.247
C	11	7.855	–0.050
Si	12	7.756	–0.049

The electronic properties of the heterojunction are studied based on its optimized structure. First, the densities of states (DOSs) of the CNT/SiCNT heterojunction, the isolated CNT and SiCNT are examined as shown in Fig.2. The energy gaps of the isolated CNT and the isolated SiCNT are found to be about 0.42 and 1.10 eV, respectively. The energy gap of the heterojunction is about 0.31 eV, narrower than those of the isolated CNT and the isolated SiCNT, which is reasonable. The bottom of the conduction band of the heterojunction is at –0.33 eV, while the top of the valence band is at –0.64 eV.

To further study the electronic structure of the heterojunction, the partial densities of states (PDOSs) of C atoms in the CNT section and the SiCNT section are investigated (in Fig.3). From the curves for PDOSs, we can see that the bottom of the conduction band for the heterojunction is occupied by the C 2p orbit in the CNT section and the top of the valence band is occupied predominantly by the C 2p orbit in the SiCNT section.

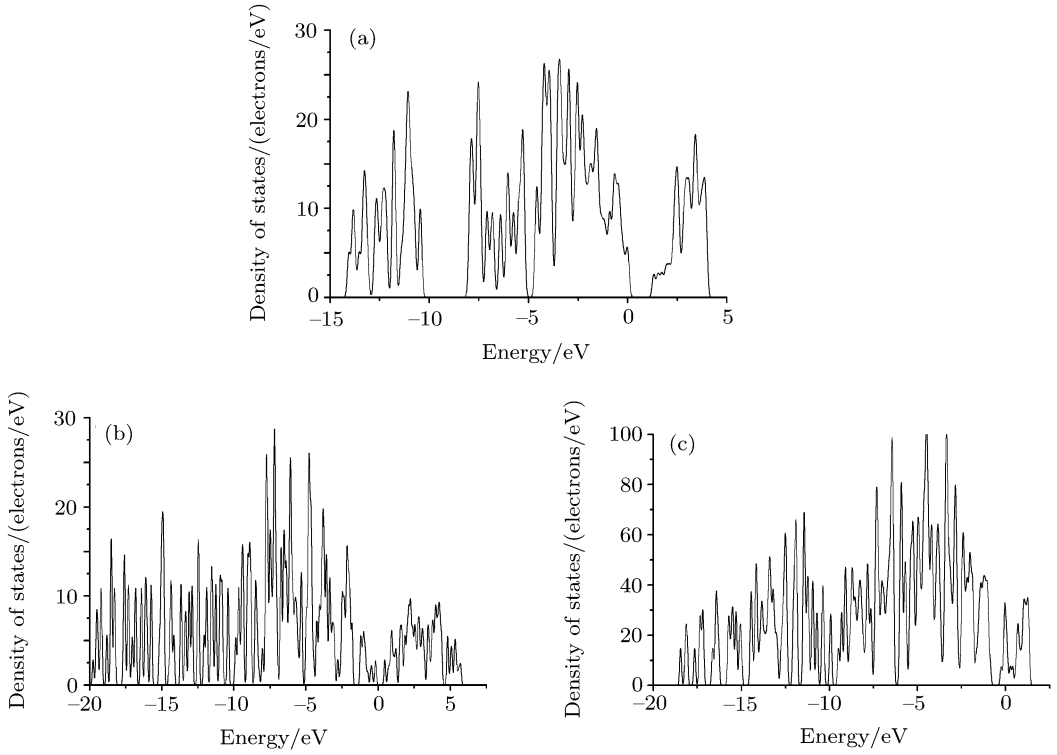


Fig.2. DOSs of the SiCNT (a), CNT (b) and the heterojunction (c).

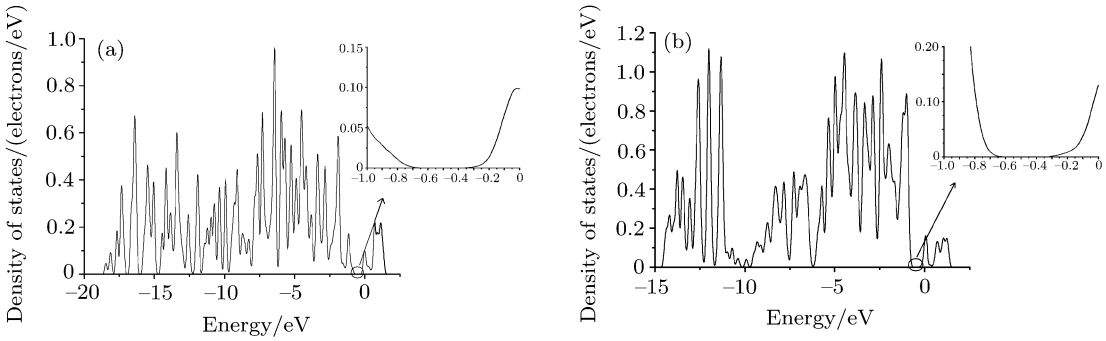


Fig.3. PDOSs of the C atoms of CNT section (a) and SiCNT section (b).

The highest occupied states and the lowest unoccupied states of the CNT/SiCNT heterojunction are investigated, as plotted in Fig.4. The highest occupied states are mainly localized at the SiCNT section and the lowest unoccupied states concentrate on the CNT section, which is consistent with the results of the PDOSs of the C atoms. The electronic distribution of the highest occupied states, shown in Fig.4(a), presents a concentration in the internal layers of the SiCNT part, while the electronic distribution of the lowest unoccupied states concentrates in the CNT section (Fig.4(b)).

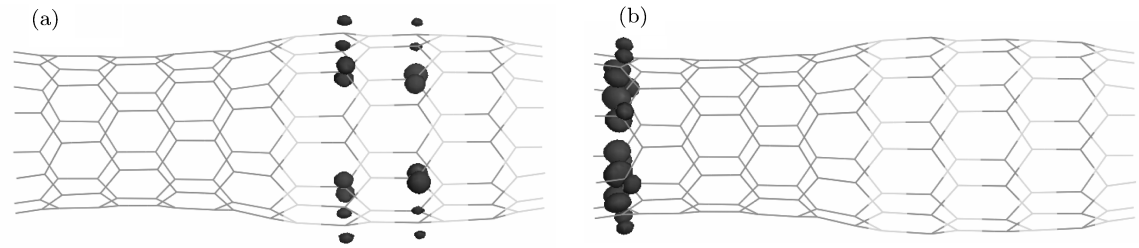


Fig.4. The charge densities for the states at the top of the valence band (a) and bottom of the conduction band of the heterojunction (b).

The so-called 'band offset' refers to the discontinuity between the valence band edge and the conduction band edge of the heterojunction junctions.[16] As the electronic property and the optical property of a heterojunction device are seriously influenced by the band offset, the band offset is one of the most important features of the heterojunction.[17] The band offsets of the CNT/SiCNT heterojunction has been calculated by using the average-bond-energy method,[18,19] which is based on the energy band structures of the materials forming the heterojunction ((8, 0) CNT and SiCNT). The average bond energy, E_m, can be achieved by calculating the average values of the eigenvalue of the $E_n(k)$ of the four highest valence bands and those of the four lowest energy conduction bands in the whole Brillouin zone, which is represented as follows:

$$E_m = \frac{1}{8N} \sum_{n=1}^{8} \sum_{k} E_n(k). \tag{1}$$

The band offset parameter, E_{mv}, can be obtained by subtracting E_v from E_m

$$E_{mv} = E_m - E_v, \tag{2}$$

where E_v is the energy of the top of the valence band. The valence band offset of the heterojunction is determined by

$$\Delta E_v = E_{mv\,\mathrm{SiC}} - E_{mv\,\mathrm{C}}, \tag{3}$$

where $E_{mv\,\mathrm{C}}$ and $E_{mv\,\mathrm{SiC}}$ are the band offset parameters of CNT and SiCNT, respectively. The conduction band offset of the heterojunction is achieved from

$$\Delta E_c = \Delta E_g - \Delta E_v, \tag{4}$$

in which ΔE_g is the difference between the energy gaps of the materials forming the heterojunction.

From expression (2), $E_{mv\,\mathrm{C}}$ and $E_{mv\,\mathrm{SiC}}$ are calculated as 0.08 and 0.79 eV, respectively. Substituting the obtained results into expression (3), the valence band offset is obtained as 0.71 eV. Then the conduction band offset is –0.03 eV. This discontinuous band configuration causes the electrons to be confined in the CNT section and the holes to be trapped in the SiCNT section.

4. Conclusion

The structural feature and the electronic property of a heterojunction formed by an (8, 0) CNT and an (8, 0) SiCNT are studied through the first-principles calculation. From the optimized structure of the heterojunction, it can be seen that the structural rearrangement takes place mainly on the interface. The energy gap of the heterojunction is about 0.31 eV, which is narrower than those of the isolated CNT and the isolated SiCNT. By using the average-bond-energy method, the band offsets are also calculated. The valence band offset and the conduction band offset are 0.71 and –0.03 eV, respectively. Our results are helpful for the fabricating and the applying of the nanotube heterojunction in nano-electronics.

References

[1] Qi X, Bao Q L, Li C M, Gan Y, Song Q L, Pan C X and Tang D Y 2008 *Appl. Phys. Lett.* **92** 113113

[2] Hu J T, Ouyang M, Yang P D and Lieber C M 1999 *Nature* **399** 48

[3] Zhang Y, Ichihashi T, Landree E, Nihey F and Iijima S 1999 *Science* **285** 1719

[4] Wu Y Y, Fan R and Yang P D 2002 *Nano Lett.* **2** 83

[5] Björk M T, Ohlsson B J, Sass T, Persson A I, Thelander C, Magnusson M H, Deppert K, Wallenberg L R and Samuelson L 2002 *Nano Lett.* **2** 87

[6] Gudiksen M S, Lauhon L J, Wang J F, Smith D C and Lieber C M 2002 *Nature* **415** 617

[7] Liao L, Liu K H, Wang W L, Bai X D, Wang E G, Liu Y L, Li J C and Liu C 2007 *J. Am. Chem. Soc.* **129** 9562

[8] Chai Y, Zhou X L, Li P J, Zhang W J, Zhang Q F and Wu J L 2005 *Nanotechnology* **16** 2134

[9] Yu S S, Zheng W T, Wen Q B, Zheng B, Tian H W and Jiang Q 2006 *Nanotechnology* **5** 595

[10] Ito T, Nishidate K, Baba M and Hasegawa M 2002 *Surf. Sci.* **514** 222

[11] Gali A 2006 *Phys. Rev.* B **73** 245415

[12] Menon M, Richter E, Mavrandonakis A, Froudakis G and Andriotis A N 2004 *Phys. Rev.* B **69** 115322

[13] Zhao M W, Xia Y Y, Li F, Zhang R Q and Lee S T 2005 *Phys. Rev.* B **71** 085312

[14] Thesing L A, Piquini P and Kar T 2006 *Nanotechnology* **17** 1637

[15] Song C, Xia Y Y, Zhao M W, Liu X D, Li F and Huang B D 2005 *Chem. Phys. Lett.* **415** 183

[16] Van de Walle C G 2003 *J. Vac. Sci. Technol.* A **25** 5182

[17] Kroemer H 2001 *Rev. Mod. Phys.* **73** 783

[18] Wang R Z, Huang M C 1992 *Science in China* A **10** 1073 (in Chinese)

[19] Li S P, Wang R Z, Zheng Y M, Cai S H and He G M 2000 *Acta Phys. Sin.* **49** 1441 (in Chinese)