A density functional theory study of the electronic structures and magnetic properties of $Fe_{(1-x)}Co_x$ alloy nanowires encapsulated in (10,0) carbon nanotubes*

Xie You(解 忧)[a)b)] and Zhang Jian-Min(张建民)[a)†]

[a)] College of Physics and Information Technology, Shaanxi Normal University, Xi'an 710062, China
[b)] College of Science, Xi'an University of Science and Technology, Xi'an 710054, China

(Received 6 July 2011; revised manuscript received 11 August 2011)

Under the generalized gradient approximation, the electronic structures and magnetic properties of $Fe_{(1-x)}Co_x$ alloy nanowires encapsulated inside zigzag (10,0) carbon nanotubes (CNTs) are investigated systematically using first-principle density functional theory calculations. For the fully relaxed $Fe_{(1-x)}Co_x$/CNT structures, all the C atoms relax outwards, and thus the diameters of the CNTs are slightly increased. Formation energy analysis shows that the combining processes of all $Fe_{(1-x)}Co_x$/CNT systems are exothermic, and therefore the $Fe_{(1-x)}Co_x$ alloy nanowires can be encapsulated into semiconducting zigzag (10,0) CNTs and form stable hybrid structures. The charges are transferred from the $Fe_{(1-x)}Co_x$ nanowires to the more electronegative CNTs, and the Fe–C/Co–C bonds formed have polar covalent bond characteristics. Both the spin polarization and total magnetic moment of the $Fe_{(1-x)}Co_x$/CNT system are smaller than those of the corresponding freestanding $Fe_{(1-x)}Co_x$ nanowire, and the magnetic moment of the $Fe_{(1-x)}Co_x$/CNT system decreases monotonously with increasing Co concentration, but the $Fe_{(1-x)}Co_x$/CNT systems still have a large magnetic moment, implying that they can be utilized in high-density magnetic recording devices.

Keywords: Fe–Co alloy, carbon nanotube, electronic structure, magnetic property

PACS: 73.22.–f, 75.75.–c, 71.15.Mb **DOI:** 10.1088/1674-1056/20/12/127302

1. Introduction

Fe–Co alloys are important soft magnetic materials due to their low magnetic anisotropy, relatively low coercive field and large magnetic moment per atom among various binary alloys of 3d transition metals. So Fe–Co alloys are promising materials in a wide and important range of technological applications such as magnetic recording media, high-performance transformers and sensors.[1,2] With the rapid development of nanofabrication techniques, opportunities to observe some of the fascinating magnetic properties in nanostructures made from these alloys that were previously thought impossible could arise. For example, the in-plane arrangements of Fe–Co alloy nanowires exhibit high coercivity and large shape anisotropy with the easy magnetization direction along the nanowire axis, in contrast to the respective bulk material.[3] The magnetic moment of the Fe–Co alloy, one of the most technologically important features, is also expected to be enhanced at the nanoscale due to finite size effects.

In experiments, the Fe–Co alloy nanowires encapsulated in carbon nanotubes (CNTs) have been realized.[4–7] The CNT has a hollow tubular channel, high thermal and electronic conductivity, and extremely high mechanical strength. The tube shell not only provides structural stability, but also effectively protects a nanowire inside its cavity. CNTs have attracted much attention and extensive investigations.[8–25] However, there are seldom systematical and theoretical studies about Fe–Co nanowires encapsulated in CNT. Theoretically, only Jo[26] has carried out first-principle calculations on Fe–Co alloy nanowires encapsulated in metallic (6,6) CNT with varying Co concentrations. His binding energy analysis showed that polar covalent bonds between Fe–Co nanowires and C atoms contributed to higher stability. He found that CNT encapsulation provoked a reduction in magnetic moment, spin polarization and coercivity, in comparison with the counterparts of freestanding nanowires. However, the electronic and magnetic properties of Fe–Co nanowires

*Project supported by the State Key Development for Basic Research of China (Grant No. 2010CB631002) and the National Natural Science Foundation of China (Grant No. 51071098).

†Corresponding author. E-mail: jianm_zhang@yahoo.com

© 2011 Chinese Physical Society and IOP Publishing Ltd

inside semiconducting CNTs have not been systematically and theoretically explored yet. Consequently, such an investigation is done in this paper. Our first-principle calculations demonstrate that $Fe_{(1-x)}Co_x$ alloy nanowires can be encapsulated into semiconducting zigzag (10,0) CNTs and form stable hybrid structures. Therefore, $Fe_{(1-x)}Co_x$/CNT systems can be expected to have potential applications in building nanodevices.

2. Calculation method and model

All the calculations are performed within the framework of density functional theory (DFT) using the plane-wave basis implemented with the Vienna *ab initio* simulation package (VASP).[27–29] The electron–ionic core interaction is represented by the projector-augmented-wave (PAW) potentials,[30] which are more accurate than the ultrasoft pseudopotentials. The electron exchange and correlation is treated with the Perdew–Burke–Ernzerhof formulation of generalized gradient approximation,[31] which can yield the correct ground state of the combined systems. The energy cutoff of the plane wave basis set is taken to be 400 eV. A one-dimensional Brillouin zone integration is performed using the Monkhorst–Pack scheme with $1\times1\times13$ k-points.[32] All the calculations are done for tetragonal supercells with a tube–tube distance of 16 Å (1 Å=0.1 nm) to prevent any tube–tube interaction. In order to find the ground state of the combined systems, the conjugate-gradient minimization scheme is utilized. The Gaussian broadening scheme with a width of 0.2 eV is used to calculate the density of states (DOS). Finally the force on each ion is converged to less than 0.02 eV/Å, and all the geometric structures are fully relaxed to minimize the total energy of the system until a precision of 10^{-4} eV is reached.

For the structural model of $Fe_{(1-x)}Co_x$/CNT hybrid systems, the $Fe_{(1-x)}Co_x$ nanowire and (10,0) CNT repeat periodically along a coincident tube axis. The $Fe_{(1-x)}Co_x$ nanowires are constructed by the body centered cubic (0 0 1) type staggered structure composed of 10 atoms in a unit cell. The justifications of the alloy nanowire models used in this study have been detailed elsewhere.[26,33,34] The unit cell length for freestanding $Fe_{(1-x)}Co_x$ nanowires is about 4.30 Å, whereas the periodicity length of (10,0) CNTs is 4.26 Å. In order to match the zigzag CNT periodicity length, the $Fe_{(1-x)}Co_x$ nanowires are compressed by 0.93% along the tube axis. The compressed degree is much less than that of $Fe_{(1-x)}Co_x$ alloy nanowires encapsulated in (6,6) CNT, where the Fe–Co nanowires are extended by 14%.[26]

The initial geometric structure of the $Fe_{0.5}Co_{0.5}$ nanowire encapsulated in a (10,0) CNT is given in Fig. 1 as an example. The black, white and gray balls denote Fe, Co and C atoms, respectively. The coplanar four Fe (or Co) atoms are located in the middle of the axial C–C bonds, while the single Fe (or Co) atom on the tube axis lies in the middle of zigzag C–C bonds. Moreover, the corresponding freestanding Fe–Co nanowires are also investigated for comparison with the $Fe_{(1-x)}Co_x$/CNT systems. To vary the Co concentration, a centered Fe atom is first substituted by a Co atom, because that substitution is energetically preferred to other arrangements.

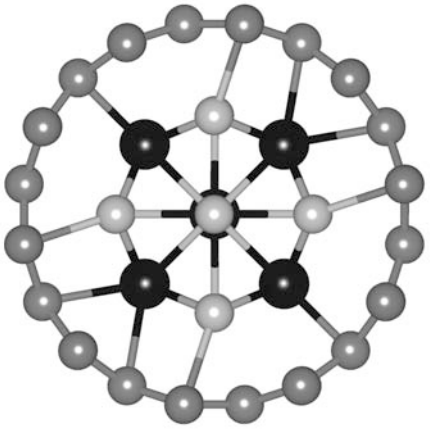


Fig. 1. The initial geometric structure of an $Fe_{0.5}Co_{0.5}$ nanowire encapsulated inside a (10,0) CNT. The black, white and gray balls denote Fe, Co and C atoms, respectively.

3. Results and discussion

3.1. Structural stability and difference charge density

The geometric structures are relaxed fully for all the $Fe_{(1-x)}Co_x$ nanowires and $Fe_{(1-x)}Co_x$/CNT systems. We allow the positions of all atoms in the $Fe_{(1-x)}Co_x$/CNT systems to move in three directions during the relaxation process until the optimal configuration, and thus the lowest total energy, is reached. As an example, the positions of the C (circles), Fe (squares) and Co (triangles) atoms before (open symbols) and after (closed symbols) relaxation are displayed in Fig. 2 for the $Fe_{0.5}Co_{0.5}$/CNT system. After relaxation, all C atoms relax outwards and therefore the diameter of the CNT is slightly increased. For the layer with coplanar four Fe atoms, as shown in Fig. 2(a), the interior Fe_1 and Fe_3 atoms relax in-

wards, while the Fe_2 and Fe_4 atoms rotate in a somewhat clockwise direction around the common axis of the nanowire and nanotube. For the layer with coplanar four Co atoms on it, Fig. 2(c), the interior four Co atoms relax outwards, simultaneously, and the Co_1 and Co_3 atoms rotate in an anticlockwise direction around the common axis of the nanowire and nanotube, while the Co_2 and Co_4 atoms rotate in a clockwise direction. So the Co_1 (Co_3) and Co_2 (Co_4) atoms move away from their initial positions and get close to each other. The Fe_1–C_1 (or C_2), Fe_2–C_4, and average Co–C bond lengths are 2.19 (2.16), 2.10, and 2.13 Å, respectively. The bond lengths are similar to those of the same structural Fe–Co nanowires inside the (6,6) CNT,[26] in which the nearest-neighbor distances between the Fe–Co nanowires and the CNTs are in the range 2.0 Å–2.3 Å.

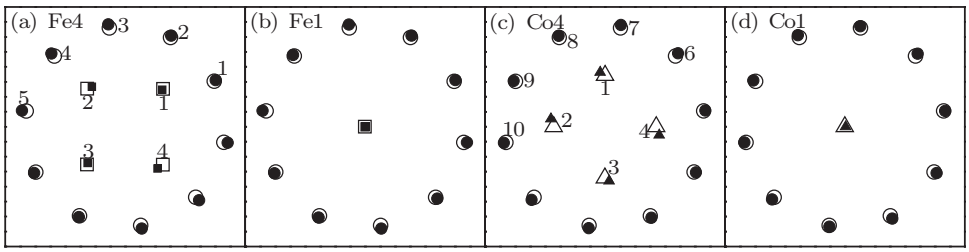


Fig. 2. The positions of the C (circles), Fe (squares) and Co (triangles) atoms before (open symbols) and after (closed symbols) relaxation of the $Fe_{0.5}Co_{0.5}$ nanowire encapsulated inside the (10,0) CNT. Panels (a), (b), (c) and (d) represent the planes through the coplanar four Fe atoms, one Fe atom, coplanar four Co atoms and one Co atom, respectively.

To quantitatively investigate the composition dependence of stability, the calculated formation energy of the $Fe_{(1-x)}Co_x$/CNT systems is illustrated in Fig. 3 as a function of Co concentration x. Here, the formation energy $E_{\rm form}$ is defined as $E_{\rm form} = (E_{\rm tot} - E_{\rm NW} - E_{\rm NT})$, where $E_{\rm tot}$, $E_{\rm NW}$ and $E_{\rm NT}$ represent the total energies of the $Fe_{(1-x)}Co_x$/CNT systems, freestanding $Fe_{(1-x)}Co_x$ nanowires and pure (10,0) CNTs, respectively. The negative (positive) values of the formation energy indicates an attractive (repulsive) interaction between the Fe–Co nanowires and CNT, and also indicates that the combining processes of the hybrid systems are exothermic (endothermic). It can be seen from Fig. 3 that the combining processes of all $Fe_{(1-x)}Co_x$/CNT systems are exothermic. Therefore, the $Fe_{(1-x)}Co_x$ alloy nanowires can be encapsulated into semiconducting zigzag (10,0) CNTs and form stable hybrid structures. Comparing the relative values of formation energies, we can see that the stability of the $Fe_{(1-x)}Co_x$/CNT system is sensitively dependent on Co concentration, and the most stable $Fe_{(1-x)}Co_x$/CNT system is at Co concentration $x = 0.9$. The absolute values of our formation energies are much less than those of the $Fe_{(1-x)}Co_x$ nanowires encapsulated in (6,6) CNT,[26] and this difference is mainly caused by the fact that they used the energy difference between the $Fe_{(1-x)}Co_x$/CNT structures and the CNT and isolated metal atoms.

Although the most stable $Fe_{(1-x)}Co_x$/CNT system is at Co concentration $x = 0.9$, in the following discussion we pay more attention to the $Fe_{0.5}Co_{0.5}$/CNT system. This is because the $Fe_{0.5}Co_{0.5}$ alloy is a highly favorable material in the field of spin electronics and is actively applied in the ferromagnetic layer of a magnetoresistive head.[6,35–40] Furthermore, the experiments found that the $Fe_{0.5}Co_{0.5}$ nanowire has an approximate maximum coercivity of 2150 Oe (1 Oe=79.5755 A/m) in all $Fe_{(1-x)}Co_x$ nanowires,[35] and Fe–Co nanowires inside multi-walled CNTs with Fe:Co ratios of 1:1 show a large coercivity of 928 Oe at room temperature compared with the bulk phase of Fe–Co (0.68 Oe).[4,7]

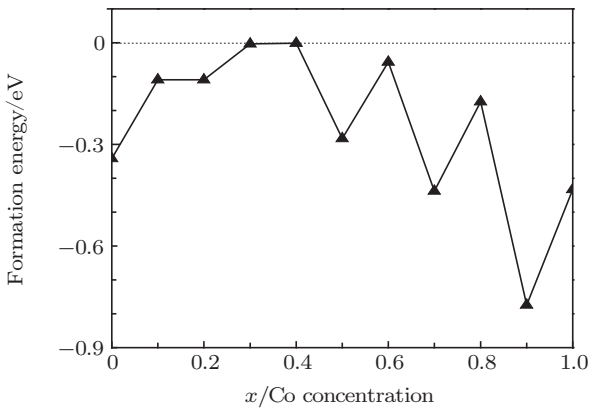


Fig. 3. The formation energies of $Fe_{(1-x)}Co_x$/CNT systems.

The chemical bond character between Fe–Co nanowires and CNTs is worth considering in order to understand the properties of $Fe_{(1-x)}Co_x$/CNT

systems. The difference charge density of the stable $Fe_{0.5}Co_{0.5}$/CNT system is displayed in Fig. 4(a) and (b) for the coplanar four-Fe atoms layer and the coplanar four-Co atoms layer, respectively. Black solid and gray dashed contour lines depict charge accumulation and depletion, respectively. From Fig. 4 we can draw the following two conclusions. First, an electron accumulation in the region between the $Fe_{0.5}Co_{0.5}$ nanowire and the CNT is observed, which indicates a strong interaction between Fe (or Co) atoms and their nearest neighbor C atoms, and that the formed Fe–C (Co–C) bonds have a covalent bond character. Second, the electron density of the C atoms represented by gray dots is accumulated, while that of the Fe (or Co) atoms described by white dots is obviously depleted, showing a charge transfer from the $Fe_{0.5}Co_{0.5}$ nanowire to the more electronegative CNT, and thus the polar bond character of the Fe–C (Co–C) bonds. Such a polar covalent bond character is also observed in $Fe_{(1-x)}Co_x$ nanowires encapsulated in (6,6) CNT.[26]

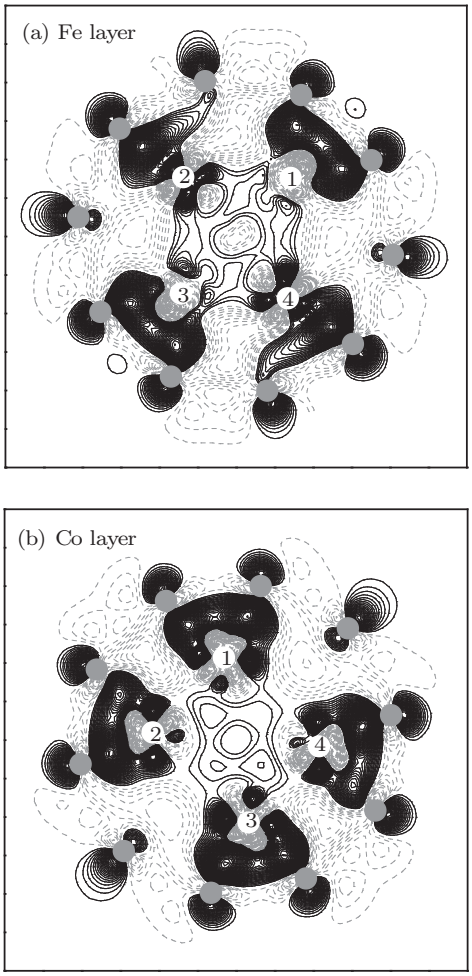


Fig. 4. Difference charge density contours of the $Fe_{0.5}Co_{0.5}$/CNT system; (a) coplanar four-Fe atoms layer and (b) coplanar four-Co atoms layer. The isodensity curves are drawn from −0.17 (−0.15) to 0.12 (0.13) e/Å^3, with an increment of 0.003 e/Å^3 for the Fe (Co) atoms layer, and the black solid and gray dashed contours lines denoting charge accumulation and depletion, respectively. The gray and white dots designate C and Fe (or Co) atoms, respectively.

3.2. Electronic structure properties

The stability of $Fe_{(1-x)}Co_x$/CNT systems is attributed to the charge rearrangement effect. The Bader charge analysis[41] is employed to obtain the quantitative amount of charge transfer. We find that overall charges are transferred from the $Fe_{(1-x)}Co_x$ nanowires to the (10,0) CNT. It is 3.09 e per unit cell from the $Fe_{0.5}Co_{0.5}$ nanowire to the CNT in the $Fe_{0.5}Co_{0.5}$/CNT system. The direction of charge transfer is identical to the $Fe_{(1-x)}Co_x$ nanowires encapsulated in (6,6) CNT.[26]

The curves of the total DOS of pure (10,0) CNT and the freestanding $Fe_{0.5}Co_{0.5}$ nanowire are depicted in Fig. 5(a) and (b), respectively. The total DOS of the $Fe_{0.5}Co_{0.5}$/CNT system, and the partial DOS projected onto the outer CNT and inner $Fe_{0.5}Co_{0.5}$ nanowire are displayed in Fig. 5(c) simultaneously. The vertical dotted lines denote the Fermi levels shifted to zero energy in the three figures. From Fig. 5(a) we find the symmetric DOS between majority and minority spins, which shows that the pure (10,0) CNT is nonmagnetic. However, asymmetric DOS between majority and minority spins in Fig. 5(b) reflects that the freestanding $Fe_{0.5}Co_{0.5}$ nanowire is ferromagnetic.

Furthermore, the following features can be obtained by comparing Fig. 5(c) with Fig. 5(a) and (b). First, the energy states near the Fermi level of the $Fe_{0.5}Co_{0.5}$/CNT system mainly stem from the $Fe_{0.5}Co_{0.5}$ nanowire. Moreover, the asymmetric partial DOS of the $Fe_{0.5}Co_{0.5}$ nanowire, and thus the total DOS of the $Fe_{0.5}Co_{0.5}$/CNT system near the Fermi level, imply that the $Fe_{0.5}Co_{0.5}$ nanowire and thus the $Fe_{0.5}Co_{0.5}$/CNT system have strong ferromagnetism. Lastly, the total DOS of the $Fe_{0.5}Co_{0.5}$/CNT system shown in Fig. 5(c) is not a simple superposition of the total DOS of the pure (10,0) CNT and the freestanding $Fe_{0.5}Co_{0.5}$ nanowire shown in Fig. 5(a) and (b), respectively, also indicating that a strong interaction between the inner $Fe_{0.5}Co_{0.5}$ nanowire and outer CNT exists. This interaction can also be seen from the differences between the partial DOS projected onto the inner $Fe_{0.5}Co_{0.5}$ nanowire and the outer (10,0) CNT shown in Fig. 5(c), and the total DOS of the pure (10,0) CNT and the freestanding

$Fe_{0.5}Co_{0.5}$ nanowire shown in Fig. 5(a) and (b), respectively. The $Fe_{0.5}Co_{0.5}$ alloy nanowire not only transforms its outside CNT from semiconductor to conductor, but also shifts the total DOS of the pure (10,0) CNT down to the lower energy region.

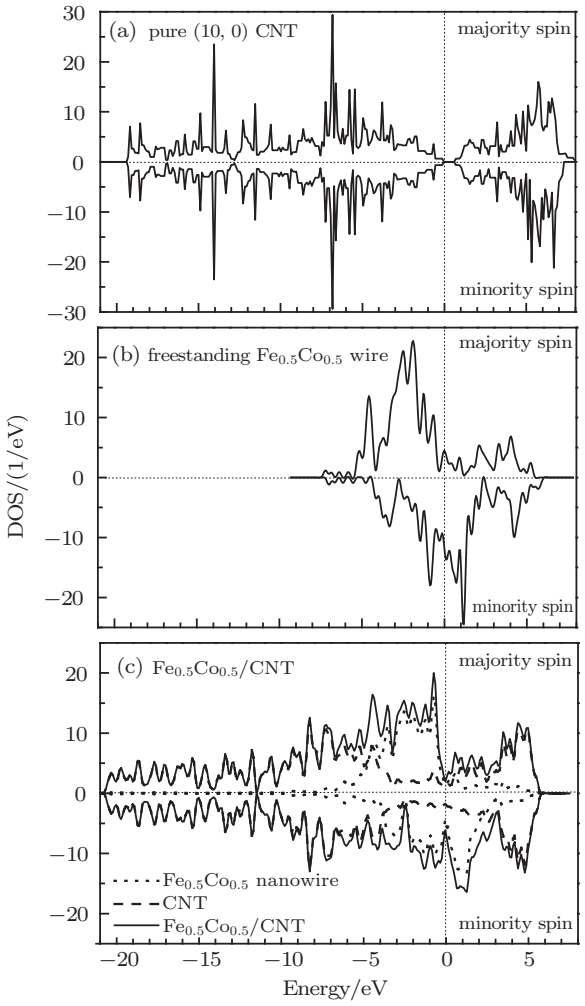


Fig. 5. (a) The total DOS of the pure (10,0) CNT, (b) the total DOS of the freestanding $Fe_{0.5}Co_{0.5}$ nanowire, and (c) the total DOS of the $Fe_{0.5}Co_{0.5}$/CNT system and the partial DOS projected onto the inner $Fe_{0.5}Co_{0.5}$ nanowire, as well as onto the outer (10,0) CNT. The vertical dotted lines denote the Fermi level.

3.3. Spin polarizations and magnetic moments

Spin polarization (P) is one of the important parameters for spin-dependent electronic transport. P is defined as

$$P = [N_{\downarrow}(E_{\rm F}) - N_{\uparrow}(E_{\rm F})]/[N_{\downarrow}(E_{\rm F}) + N_{\uparrow}(E_{\rm F})],$$

where $N_{\downarrow}(E_{\rm F})$ and $N_{\uparrow}(E_{\rm F})$ represent the DOS amplitudes of minority spin and majority spin at the Fermi level, respectively. The calculated spin polarizations and total magnetic moments of the $Fe_{(1-x)}Co_x$/CNT systems and the corresponding freestanding $Fe_{(1-x)}Co_x$ nanowires are illustrated in Fig. 6(a) and (b), respectively. Owing to the restriction of the outer CNT, the spin polarization of the $Fe_{(1-x)}Co_x$/CNT system is smaller than that of the corresponding freestanding $Fe_{(1-x)}Co_x$ nanowire. This is also the reason why the total magnetic moment of the $Fe_{(1-x)}Co_x$/CNT system is smaller than that of the corresponding freestanding $Fe_{(1-x)}Co_x$ nanowire. However, the $Fe_{(1-x)}Co_x$/CNT systems with larger magnetic moments imply that they still have potential applications in high-density magnetic recording devices. The magnetic moment of either the $Fe_{(1-x)}Co_x$/CNT system or the corresponding freestanding $Fe_{(1-x)}Co_x$ nanowire decreases monotonously with increasing Co concentration, due to the fact that the magnetic moment of the Fe atom is larger than that of the Co atom. In addition, both the magnetic moment values of the $Fe_{(1-x)}Co_x$/CNT system and their variation with Co concentration are very close to those of the $Fe_{(1-x)}Co_x$ alloy encapsulated in (6,6) CNT.[26]

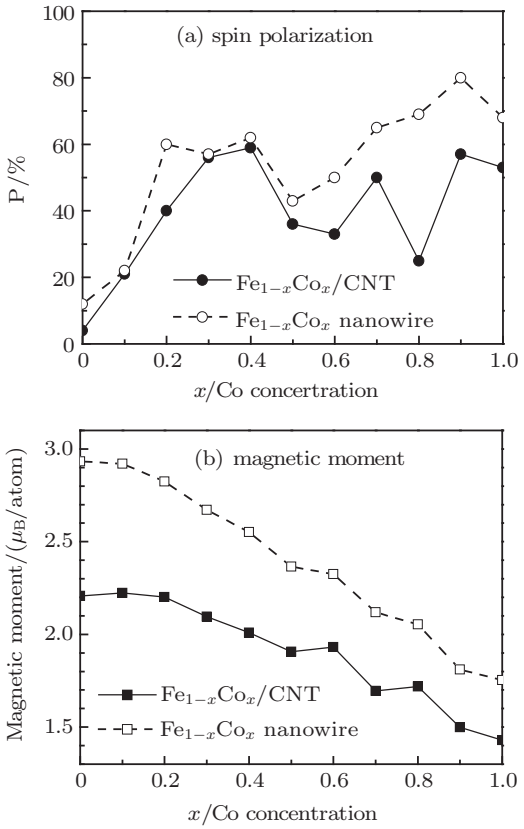


Fig. 6. Comparison of (a) spin polarization and (b) magnetic moments between the $Fe_{(1-x)}Co_x$/CNT systems and the corresponding freestanding $Fe_{(1-x)}Co_x$ nanowires.

The spin charge density (the difference between the majority spin and minority spin) of the stable

$Fe_{0.5}Co_{0.5}$/CNT system is illustrated in Fig. 7(a) and (b) for the coplanar four-Fe atoms layer and the coplanar four-Co atoms layer, respectively. The black solid (gray dashed) lines show there is more majority (minority) spin. It can be seen that the magnetism is mainly confined within the $Fe_{0.5}Co_{0.5}$ nanowire because the pure (10,0) CNT is nonmagnetic while the freestanding Fe–Co nanowires are ferromagnetic. Moreover, the roughly circularly distributed positive spin densities at Fe (Co) sites are due to the Fe/Co atom having six (seven) 3d electrons. The 2p electrons of the C_1, C_2 and C_4 atoms bonding to the nearest Fe atoms in Fig. 7(a), and the 2p electrons of all C atoms in Fig. 7(b), are antiferromagnetic couplings with 3d electrons of the Fe and Co atoms, respectively, while the 2p electrons of un-bonding C_3 and C_5 atoms in Fig. 7(a) are ferromagnetic couplings with 3d electrons of the Fe atoms. Therefore, the magnetism is also presented at C atoms with slightly more majority or minority spin. The magnetic moments of the corresponding C_1, C_2, C_3, C_4, C_5, Fe_1, and Fe_2 atoms in Fig. 7(a) are −0.028, −0.029, 0.011, −0.028, 0.011, 2.580, and 2.606 μ_B, respectively, and those of the C_6, C_7, C_8, C_9, C_{10}, Co_1, and Co_2 atoms in Fig. 7(b) are −0.001, −0.017, −0.011, −0.004, −0.015, 1.451, and 1.410 μ_B, respectively.

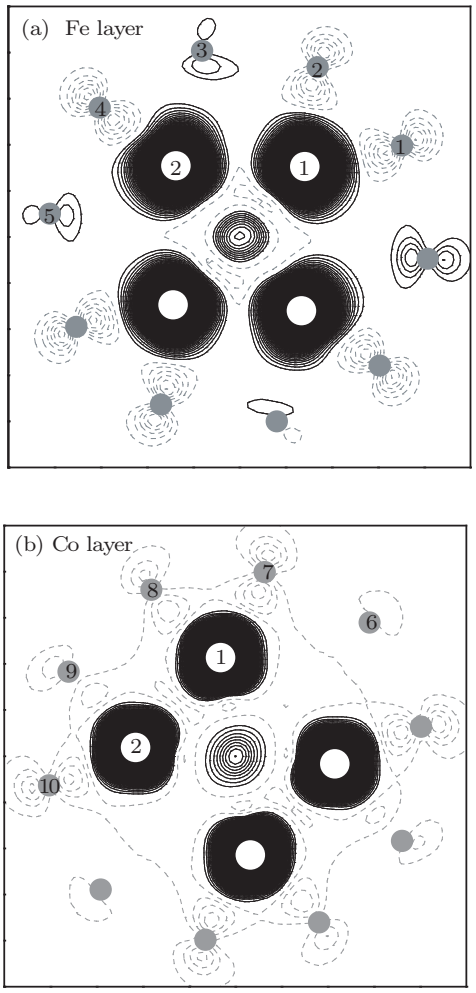


Fig. 7. The spin charge density contours of the $Fe_{0.5}Co_{0.5}$/CNT system for (a) the coplanar four-Fe atoms layer and (b) the coplanar four-Co atoms layer. The isodensity curves are drawn from −0.07 (−0.04) to 3.23 (2.02) e/Å^3, with an increment of 0.01 e/Å^3 for the Fe (Co) atoms layer, and the black solid and gray dashed lines show that there are more majority and minority spins, respectively. The gray and white dots designate C and Fe (Co) atoms, respectively.

4. Conclusions

In conclusion, the structures, electronic and magnetic properties of the $Fe_{(1-x)}Co_x$ alloy nanowires encapsulated in zigzag (10,0) CNTs are systematically investigated by the first-principles PAW potential within the DFT framework. The following conclusions are obtained.

(i) For the fully relaxed $Fe_{(1-x)}Co_x$/CNT structures, all C atoms relax outwards, and thus the diameters of the CNTs are slightly increased.

(ii) The negative values of the formation energies for the $Fe_{(1-x)}Co_x$/CNT hybrid systems indicate that the combining processes of all the $Fe_{(1-x)}Co_x$/CNT systems are exothermic. Therefore, the $Fe_{(1-x)}Co_x$ alloy nanowires can be encapsulated into the semiconducting zigzag (10,0) CNT and form stable hybrid structures. So the stable $Fe_{(1-x)}Co_x$/CNT systems can be expected to have potential applications in building nanodevices.

(iii) The charge is transferred from the Fe–Co nanowire to the (10,0) CNT, and the formed Fe–C (Co–C) bonds have polar covalent bond characteristics.

(iv) After the $Fe_{(1-x)}Co_x$ nanowires are encapsulated into the (10,0) CNT, the spin polarization and total magnetic moment of the $Fe_{(1-x)}Co_x$/CNT system are smaller than those of the corresponding freestanding $Fe_{(1-x)}Co_x$ nanowire. However, the $Fe_{(1-x)}Co_x$/CNT systems still have a large magnetic moment, implying that they can be utilized in high-density magnetic recording devices.

References

[1] Sourmail T 2005 *Prog. Mater. Sci.* **50** 816
[2] Sunder R S and Deevi S C 2005 *Int. Mater. Rev.* **50** 157
[3] Qin D H, Cao L, Sun Q Y, Huang Y and Li H L 2002 *Chem. Phys. Lett.* **358** 484
[4] Terrones H, López-Urías F, Muñoz-Sandoval E, Rodríguez-Manzo J A, Zamudio A, Elías A L and Terrones M 2006 *Solid State Sci.* **8** 303

[5] Kozhuharova R, Ritschel M, Elefant D, Graff A, Mönch I, Mühl T, Schneider C M and Leonhardt A 2005 *J. Magn. Magn. Mater.* **290–291** 250

[6] Turgut Z, Scott J H, Huang M Q, Majetich S A and McHenry M E 1998 *J. Appl. Phys.* **83** 6468

[7] Elías A L, Rodríguez-Manzo J A, McCartney M R, Golberg D, Zamudio A, Baltazar S E, López-Urías F, Muñoz-Sandoval E, Gu L, Tang C C, Smith D J, Bando Y, Terrones H and Terrones M 2005 *Nano Lett.* **5** 467

[8] Yang C, Zhao J and Lu J P 2003 *Phys. Rev. Lett.* **90** 257203

[9] Cao J X, Yan X H, Xiao Y and Ding J W 2003 *Chin. Phys.* **12** 1440

[10] Fan B B, Wang L N, Wen H J, Guan L, Wang H L and Zhang R 2011 *Acta Phys. Sin.* **60** 012101 (in Chinese)

[11] Kang Y J, Choi J, Moon C Y and Chang K J 2005 *Phys. Rev.* B **71** 115441

[12] Peng G W, Huan A C H and Feng Y P 2006 *Appl. Phys. Lett.* **88** 193117

[13] Li S L and Zhang J M 2011 *Acta Phys. Sin.* **60** 078801 (in Chinese)

[14] Ivanovskaya V V, Köhler C and Seifert G 2007 *Phys. Rev.* B **75** 075410

[15] Zhang Y, Cao J X and Yang W 2008 *Chin. Phys.* B **17** 1881

[16] Yuan S and Li F 2009 *J. Appl. Phys.* **106** 014307

[17] Du X J, Zhang J M, Wang S F, Xu K W and Ji V 2009 *Eur. Phys. J.* B **72** 119

[18] Zhang J M, Du X J, Wang S F and Xu K W 2009 *Chin. Phys.* B **18** 5468

[19] Ni M Y, Wang X L and Zeng Z 2009 *Chin. Phys.* B **18** 357

[20] Liu H X, Zhang H M, Hu H Y and Song J X 2009 *Chin. Phys.* B **18** 734

[21] Zhang L J, Hu H F, Wang Z Y, Wei Y and Jia J F 2010 *Acta Phys. Sin.* **59** 527 (in Chinese)

[22] Wang L G, Zhang H Y, Wang C and Terence K S W 2010 *Acta Phys. Sin.* **59** 536 (in Chinese)

[23] Yang P F, Wu F M, Teng B T, Liu S and Jiang J Z 2010 *Chin. Phys.* B **19** 097104

[24] Chen L N, Ma S S, OuYang F P, Xiao J and Xu H 2011 *Chin. Phys.* B **20** 017103

[25] Xie Y, Zhang J M and Huo Y P 2011 *Eur. Phys. J.* B **81** 459

[26] Jo C 2009 *J. Phys.* D: *Appl. Phys.* **42** 105008

[27] Kresse G and Furthmüller J 1996 *Comput. Mater. Sci.* **6** 15

[28] Kresse G and Furthmüller 1996 *Phys. Rev.* B **54** 11169

[29] Kresse G and Hafner J 1993 *Phys. Rev.* B **47** 558

[30] Kresse G and Joubert D 1999 *Phys. Rev.* B **59** 1758

[31] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865

[32] Monkhorst H J and Pack J D 1976 *Phys. Rev.* B **13** 5188

[33] Drautz R, Díaz-Ortiz A, Fähnle M and Dosch H 2004 *Phys. Rev. Lett.* **93** 067202

[34] Jo C, Lee J I and Jang Y 2005 *Chem. Mater.* **17** 2667

[35] Fodor P S, Tsoi G M and Wenger L E 2002 *J. Appl. Phys.* **91** 8186

[36] Kota Y, Takahashi T, Tsuchiura H and Sakuma A 2009 *J. Appl. Phys.* **105** 07B716

[37] Yildiz F, Przybylski M and Kirschner J 2009 *J. Appl. Phys.* **105** 07E129

[38] Chermahini M D, Zandrahimi M, Shokrollahi H and Sharafi S 2009 *J. Alloy Compd.* **477** 45

[39] Chermahini M D, Sharafi S, Shokrollahi H, Zandrahimi M and Shafyei A 2009 *J. Alloy Compd.* **484** 54

[40] Chermahini M D, Sharafi S, Shokrollahi H and Zandrahimi M 2009 *J. Alloy Compd.* **474** 18

[41] Bader R 1990 *Atoms in Molecules: A Quantum Theory* (New York: Oxford University Press)