Extended Abstracts of the 2009 International Conference on Solid State Devices and Materials, Sendai, 2009, pp715-716

First Principles Study of Metals Coating on Single Wall Carbon Nanotube

Yu He[1,2], Jinyu Zhang[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 employed as the channel to fabricate CNT field effect transistors (CNTFETs). The source and drain electrodes are made up of metals thus enabling low resistance Ohmic contacts to CNTs is critical in fabricating CNTFETs. Various experiments [2] [3] have been carried out to investigate the contact between different metals and CNTs. Metals such as Ti coating lead to the formation of continuous and uniform nanowires on the CNT, indicating firm coating and low resistance [2]. While other metals such as Fe lead to isolated particles, indicating weak interaction with the CNT and large resistance [2]. Molecular dynamics simulation[4] of such experimental process seems not to give correct Fe coating as experiment observed, while more fundamental study based on density functional theory is in lack. In this paper, we study the coating of different metals including Ti, Ni, Pd, Fe and Al on CNT using first principles calculation.

2. Physical Model and Computational Details

Fig.1(a) schematically shows a zigzag CNT surface. There are four types of high symmetrical points at the CNT as shown in Fig.1(a), with the meanings of which are: the H site above the hexagon, the Z and A sites above the zigzag and axial C-C bonds, and the T site above the carbon atom. Previous theoretical study shows that for the adsorption of individual metal atoms, the most favorable sites for each metal species are quite different, indicated by binding energies[5]. Noting that the side length of the triangles in Fig.1(b) is 2.5Å, comparable to the equilibrium bond lengths of the metals (2.48Å~2.88Å) under consideration, we suppose that when metals are coated on the CNT surface, they may adsorb in the vertex of the equilateral triangles shown in Fig.1(b) thus form symmetrical and stable structures. In this paper, we first investigate the adsorption of metals including Ti, Ni, Pd, Fe, and Al on an (8,0) single wall CNT (SWCNT) with three metal atoms positioned at such triangular vertices and obtain the most stable position of each metal species. Next, we put one more metal atom to the system to examine the trend of coating. The CNT in our study contains 64 atoms. All calculations are performed by VASP[6]. Ultrasoft-pseudopotential[7] and plane waves up to an energy cutoff of 400eV are used. The PW91[8] exchange correlation functional within generalized gradient approximation (GGA) is taken into account.

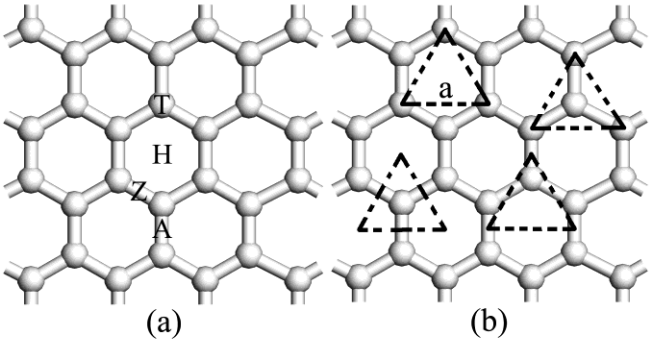

Fig.1 (a) Schematic of an SWCNT with four high symmetrical points. H: hollow; A: axial; Z: zigzag; T: top sites. (b) Possible positions of triangular structures of metal atoms coated on the CNT surface, with 'a' indicating the side length of the trangles.

3. Results and Discussions

We calculate the binding energies of all the relaxed structures. The binding energy is defined as

$$Eb = E[CNT] + n \cdot E[M] - E[n \cdot M + CNT] \quad (1)$$

Where E[CNT] and E[M] indicate the energy of an isolated CNT and metal atom, respectively. E[NM+CNT] denotes the energy of metal-absorbed CNT and n denotes the number of metal atoms. The binding energies of the metal-CNT structures with three metal atoms are shown in Table I. Since the Z site shares similar feature with the A site, the only difference between which is the slightly stretched

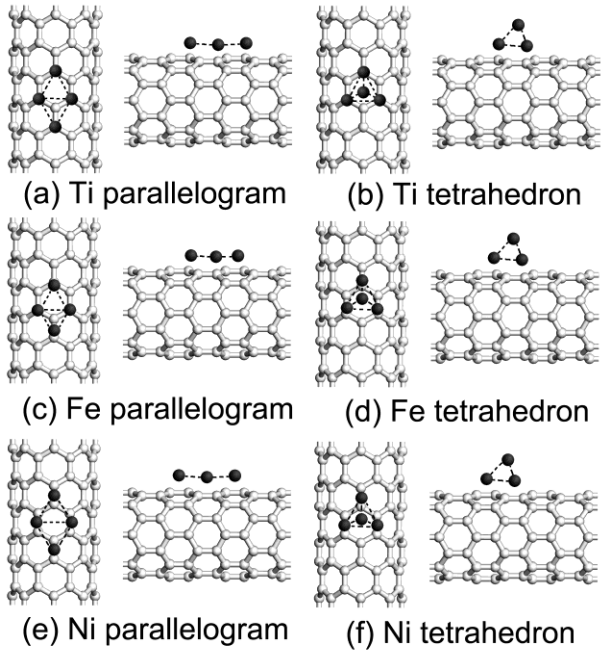

Fig.2 Coating with four metal atoms in both top and side view.

C-C bond of the Z site because of the curvature of the CNT, we have not collected the results of the Z site in Table I. The largest binding energy indicates the most favorable position of each metal species coating on the CNT surface.

After we obtain the most stable triangles of three metal atoms, we add another metal atom to the system in order to examine whether the metals will form continuous nanowires or isolated particles on the CNT surface as experiment claims[2]. To achieve this goal, we study two structures as indicated by Fig.2. In Group I we put the metal atom on the surface of the CNT to form a parallelogram with the metal triangle, while in Group II we put the metal atom on top of the metal triangle to form a tetrahedron. Metals including Ti, Fe and Ni are used as representatives of three different absorption types indicated by experiment[2]. The binding energies are shown in Table II. For Ti, Group I and II share similar binding energies, indicating that Ti has a potential trend to form a continuous layer on the CNT. However, for Fe and Ni, the binding energy of Group II is apparently larger than Group I, indicating that Fe and Ni tend to form isolated particles on the CNT. This result agrees with the experimental observation, which claims that Ti coating can always form continuous nanowires[2], while Fe and Ni will form discontinuous particles as the deposited thickness reduces[2]. The uniform coating of Ni with a thicker deposition [2] may be due to the bulk properties of metal as deposited thickness increases, which our small structure cannot exhibit. Further work is required on this issue.

4. Conclusion

We studied the coating of different metals including Ti, Ni, Pd, Fe and Al on an (8,0) SWCNT. The metal atoms will form an equilateral triangle on the CNT surface, and the most favorable triangular position of each metal species is indicated by the binding energy. Then we study the coating of four metal atoms to examine whether the metals will form continuous nanowires or isolated particles on the CNT. Our results are consistent with experimental observations.

Table I Binding energies of the metal triangles coating on the CNT surface at the H, T, A sites as shown in Fig.1. Units: eV.

	Ti	Al	Fe	Pd	Ni
H	12.52	→T(T)[a]	→T(H)	X[b]	→T(H)
T(H)	12.52	5.44	13.15	X	8.76
T(T)	X	5.59	X	X	→A
A	X	→T(T)	X	5.87	8.95

[a] For the T site, two structures are studied: T(H) and T(T) mean the center of the metal triangles is at the H site and T site, respectively. →T(T) means the metal triangles will move to the T(T) site.

[b] X means the metal triangles are not stable at that site.

Table II Binding energies of four metal atoms coating on the CNT as shown in Fig.2. Units: eV.

	Ti	Fe	Ni
I[a]	17.43	18.7	12.41
II	17.44	19.4	13.37

[a] I and II indicate two groups: parallelogram and tetrahedron structure of metal atoms, respectively.

References

[1] S. Iijima, Nature (London) **354** (1991) 56.
[2] Y. Zhang et al, Chem. Phys. Lett **331** (2000) 35.
[3] Z. Liu et al, *Interconnect Technology Conference* (2008) 144.
[4] S. Inoue, Y. Matsumura, Chem. Phys. Lett **464** (2008) 160.
[5] E. Durgun et al, J. Phys. Chem. B **108** (2004) 575.
[6] G. Kresse, J. Furthmüller, Phys. Rev. B **54** (1996) 11169.
[7] D. Vanderbilt, Phys. Rev. B **41** (1990) 7892.
[8] J. P. Perdew and Y. Wang, Phys. Rev. B **45** (1992) 13244.