구두발표 II-3

Magnetic properties of Fe, Co, and Ni atoms doped in the infinite Si nanotubes

Y.-R. Jang*[1], Chulsu Jo[2], and J. I. Lee[2]
[1]Department of Physics, University of Incheon, Incheon 402-749, Korea
[2]Department of Physics, Inha University, Incheon 402-751, Korea

인천대학교 물리학과 장영록*
인하대학교 물리학과 조철수, 이재일

1. Introduction

The metal-doped Si nanotubes have attracted much attention due to their usefulness for spintronics and other magnetic device applications [1]. It has been reported that very long Si nanotubes stabilized by metal doping have very small diameters and are metallic [2, 3] while the finite nanotubes were found to be semiconducting. It is well known that the transition metals are suitable for doping elements in Si nanotubes considering the relative atomic sizes of Si and the transition metals.

There have been investigations such as the stabilization of pentagonal Si rings with Ni doping [2] and hexagonal nanotube with V doping [4] while significant distortions in the finite Si nanotubes with Cr doping [5]. Recently, a theoretical calculation [6] on the stability of finite and infinite Si nanotubes with the 3d transition metals (Mn, Fe, Co, Ni) using the ultrasoft pseudopotential plane wave method were carried out.

In the present work, using the localized basis calculational method, we have investigated magnetic properties of magnetic transition metals doped in the infinite hexagonal Si nanotubes (infinite $Si_{12}M_n$, M=Fe, Co, Ni) for two different (n=1, 2) number of dopants.

2. Method

We considered the hexagonal prism structure for Si nanotube and transition metal doping between these prisms as shown in Fig. 1. The stable geometries are determined by minimizing the total energies of doped nanotubes.

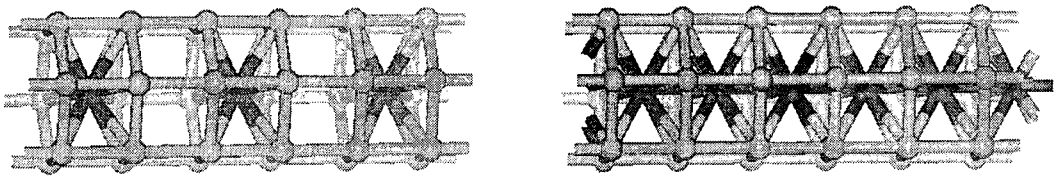

Fig. 1. Schematic structures of infinite Si nanotubes with transition metal doping.

We have performed *ab initio* spin-polarized total energy calculations within the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof 1996 (PBE96) [7] for the exchange-correlation energy. We solved the self-consistent Kohn-Sham equations by direct diagonalization of the Hamiltonian in atomic orbitals basis set consisting of finite-range numerical pseudoatomic wave functions. Norm-conserving Troullier-Martins pseudopotentials factorized in the Kleinman-Bylander form were used to consider core electrons. For Brillouin zone integrations 14 k-points are considered . The geometry is optimized until the atomic force is less than 0.04 eV/Å using the conjugate gradient method.

3. Results and discussion

We have firstly determined equilibrium stacking distance for infinite hexagonal Si nanotubes without doping by calculation of total energy, and inserted the transition metals at the middle of

two hexagonal prims as shown in Fig. 1 and optimized the equilibrium positions of Si and transition metals. We found that the transition metals attract neighboring hexagonal prisms for alternate doping system.

The calculated magnetic moments per atom for transition metal in infinite Si nanotubes with two different doping systems are summarized in Table 1. The value of magnetic moment per dopant Fe atom (2.39 μ_B) is slightly higher than that of previous calculations [6] for finite (1.7 μ_B) and nearly same as infinite (2.4 μ_B) doped nanotubes, and is also higher than that of bulk Fe. However, the magnetic moments for transition metals are calculated to be very small for the alternate doping system. For Co and Ni, the magnetic moments are smaller than those of bulk metals.

Table 1. Calculated magnetic moments per atom in μ_B at the transition metals for infinite Si nanotubes with transition metal dopings.

system \ M	Fe	Co	Ni
$Si_{12}M_1$	1.215	0.005	0.050
$Si_{12}M_2$	2.389	1.382	0.008

The atom- and angular momentum-projected density of states (DOS) and total DOS for the alternate Fe doping system are presented in Fig. 2. The DOS feature below the Fermi energy indicates that there is hybridization between Si p and Fe d electrons.

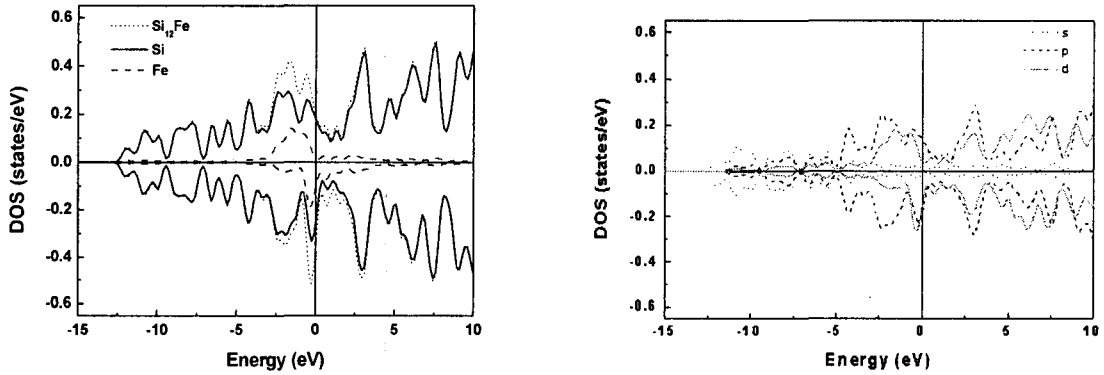

Fig. 2. Density of states (DOS) for infinite hexagonal Si nanotubes with alternate Fe doping.

4. Summary

In conclusion, we have investigated the magnetic properties of magnetic transition metals such as Fe, Co, and Si doped in the infinite hexagonal Si nanotubes for two different number of dopants. The Fe- (Co- and Ni-) doped nanotube shows larger (smaller) magnetic moments than those of bulk ones, respectively.

5. References

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