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Surface and Interface Magnetism in CoTi/FeTi/CoTi(110)

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We investigated the electronic structures and the magnetic properties of Ti-based intermetallic system of CoTi/FeTi/CoTi(110) surface and interface by using the all-electron full potential linearized augmented plane wave (FLAPW) method within the generalized gradient approximation (GGA). The calculated magnetic moments of interface Co and Fe atoms are 0.65 and 0.15 μ_B, respectively. Surface and interface magnetism of CoTi/FeTi/CoTi(110) are discussed using the calculated density of states (DOS) and the spin densities.

Key words : electronic structure, magnetism, FeTi, CoTi

1. Introduction

The intermetallic compounds FeTi and CoTi have many useful properties such as the high hardness and high melting temperature. These compounds are also promising materials for hydrogen storages [1]. Kellou *et al.* [2] investigated the electronic structures of bulk FeTi, CoTi, and NiTi as well as for the (001) surface and interface of these compounds by the full-potential linearized augmented plane waves (FP-LAPW) method. They reported that the bulk FeTi, CoTi, and NiTi are paramagnetic, while it is ferromagnetic at the (001) surface and interface. The magnetic moments of surface Ti atom and subsurface Fe atom in the FeTi(001) film are 0.40 and 0.23 μ_B, respectively. For the CoTi(001) film, the values of surface Ti atom and subsurface Co atom are 0.62 and 0.93 μ_B, respectively. The magnetic moments of subsurface Fe atom and Co atom in the FeTi/CoTi(001) film are 0.65 and 0.94 μ_B, respectively. They also found from the calculated density of states (DOS) that the interface electronic structure is a mixture of (Fe, Co) *d*-states and Ti *d*-states. Kulkova *et al.* [3] investigated the Fe-terminated FeTi(001) and Co-terminated CoTi(001) films. The surface magnetic moment of Fe atom is 2.27 μ_B in FeTi(001) and that of Co atom is 0.87 μ_B in the CoTi(001). Koroteev *et al.* [4] investigated the electronic structures for the (110) surface of FeTi, CoTi, and NiTi only in the paramagnetic state.

Recently, multi-layered structures have attracted much attention due to the interesting physical properties [5] and the applications for the high-storage magnetic recording media and devices [6]. In this study, we investigated the surface and interface electronic structures and the magnetic properties of CoTi /FeTi/CoTi(110) system by using the all-electron full potential linearized augmented plane wave (FLAPW) method [7] within the generalized gradient approximation (GGA). In Sec. 2, we briefly describe our model and the calculational method. The results of the electronic and magnetic properties of the surface and interface are presented in Sec. 3. A brief summary is given in Sec. 4.

2. Model and Calculational Method

In order to investigate the surface and interface properties of CoTi/FeTi/CoTi(110) film, we considered a thirteen-layer single slab which consists of three layers of CoTi attached on each side of seven-layers of FeTi as shown in Fig. 1. The lattice constant of the two-dimensional (2D) unit cell is set to 5.62 a.u. The spacing between the layers in the FeTi is chosen to be 3.98 a.u. and that of the CoTi is chosen to be 4.03 a.u. which is evaluated by keeping the volume of CoTi layer per formula unit same as that of the bulk CoTi.

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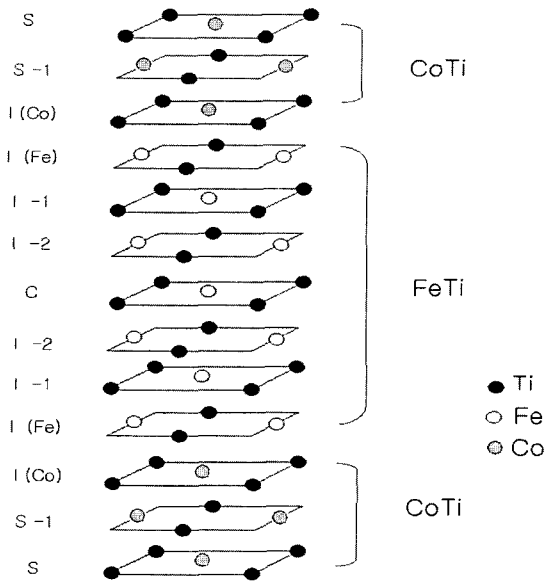

Fig. 1. The thirteen-layer single slab of CoTi/FeTi/CoTi(110) which consists of three layers of CoTi attached on each side of seven layers of FeTi.

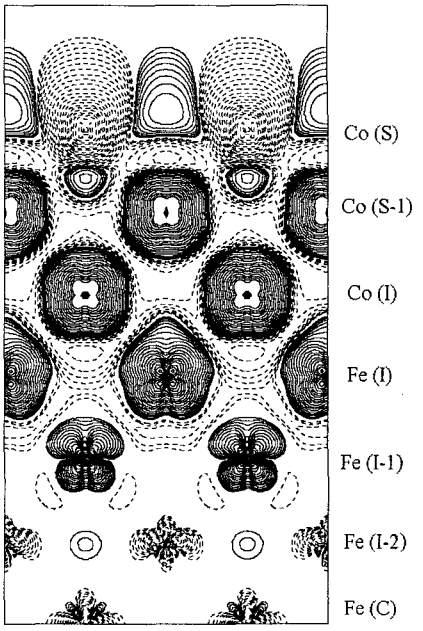

Fig. 2. Spin-density contour plots in the (020) plane of the CoTi/FeTi/CoTi(110). The lowest contour starts from 1.0×10^{-4} electrons/(a.u.)^3 and the subsequent lines differ by a factor of $\sqrt{2}$.

The FLAPW method is an all-electron calculation with no shape approximations for charge densities, potentials, and wave functions. The core (valence) electrons are treated fully (scalar) relativistically. The muffin-tin (MT) radii are taken to be 2.2 a.u. for Fe and Co, and 2.4 a.u. for Ti. Inside the MT spheres, the charge density and potential are expanded in lattice harmonics up to $l_{max} = 8$. We used about 2300 variational basis functions and the integrations over k-space in irreducible Brillouin zone is substituted by summation over 9 special k-points. We assumed self-consistent calculation when the root-mean-square difference between the input and output charge and spin densities are less than 1×10^{-4} electrons/(a.u.)^3.

3. Results and Discussion

The calculated spin-density contour plots in the (020) plane of the CoTi/FeTi/CoTi(110) are presented in Fig. 2. The solid and broken lines represent the majority spin and minority spin, respectively The lowest contour starts from 1.0×10^{-4} electrons/a.u.^{3} and subsequent lines differ by a factor of $\sqrt{2}$.

Table 1. Spin- and l-decomposed number of electrons within muffin-tin (MT) sphere for atoms in each layer, and magnetic moment in μ_B. Other symbols are the same as those in Fig. 1

	s (↑/↓)	p (↑/↓)	d (↑/↓)	Total (↑/↓)	Magnetic moment (μ_B)
Co (S)	0.20 / 0.21	0.11 / 0.11	3.41 / 3.74	3.72 / 4.07	–0.34
Co (S-1)	0.21 / 0.21	0.15 / 0.15	3.91 / 3.23	4.28 / 3.59	0.67
Co (I)	0.21 / 0.20	0.15 / 0.15	3.90 / 3.25	4.26 / 3.61	0.65
Fe (I)	0.19 / 0.18	0.14 / 0.14	3.13 / 2.98	3.47 / 3.31	0.15
Fe (I-1)	0.19 / 0.19	0.14 / 0.14	3.06 / 3.05	3.39 / 3.39	0.01
Fe (I-2)	0.19 / 0.19	0.14 / 0.14	3.06 / 3.06	3.39 / 3.39	–0.01
Fe (C)	0.19/ 0.19	0.15/ 0.15	3.06/ 3.06	3.39 / 3.40	–0.01
Ti (S)	0.14 / 0.14	3.01 / 3.02	1.04 / 0.96	4.21/ 4.12	0.08
Ti (S-1)	0.14 / 0.14	3.03 / 3.04	1.02 / 1.01	4.22 / 4.21	0.01
Ti (I:Co)	0.14 / 0.15	3.03 / 3.04	1.02 / 1.03	4.21 / 4.23	–0.02
Ti (I :Fe)	0.15 / 0.15	3.04 / 3.04	1.02 / 1.04	4.22 / 4.25	–0.03
Ti (I-1)	0.15 / 0.15	3.04 / 3.04	1.03 / 1.04	4.24 / 4.25	–0.01
Ti (I-2)	0.15 / 0.15	3.04 / 3.04	1.04 / 1.03	4.25 / 4.24	0.01
Ti (C)	0.15 / 0.15	3.04 / 3.04	1.04 / 1.03	4.25 / 4.24	0.01

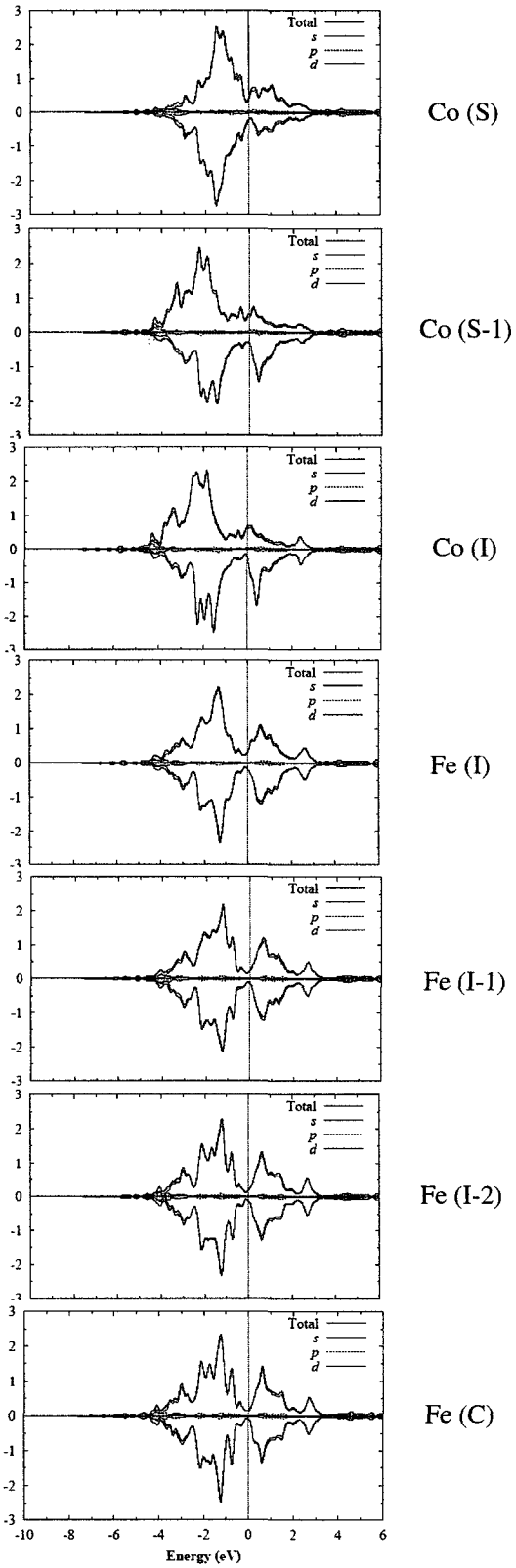

Fig. 3. The calculated layer-, atom-, and spin-projected DOS for CoTi/FeTi/CoTi(110) film. From the comparison of DOS for CoTi interface layer and FeTi interface layer, we see a hybridization between Co(I) atom and Fe(I) atom.

In the FeTi layers, we can see that the Fe(I-2), and Fe(C) atom sites are negatively spin-polarized while the Fe(I) is positively spin-polarized with compared to the inner layers. In the CoTi layers, the Co(I) and Co(S-1) atom sites are positively spin polarized and the Co(S) atom site is negatively spin-polarized.

More details of the magnetic properties can be explained by the number of electrons and magnetic moment of each atom. The calculated numbers of majority- and minority-electrons for each atom within the muffin-tin (MT) spheres are given in Table 1. In the FeTi layers, each magnetic moment of Fe atom in the inner layers is almost zero, which is consistent with the fact that the bulk phase is paramagnetic. But the magnetic moment for Fe atom of Fe(I) layer is much enhanced (0.15 μ_B) compared to the inner layers. This is due to the hybridization of Fe(I) and Co(I) as we can see from Fig. 3.

In the CoTi layer, the magnetic moment of Co atom is 0.65 μ_B in Co(I) layer and 0.67 μ_B in Co(S-1) layer. On the other hand, the calculated magnetic moment for Co(S) is –0.34 μ_B and antiferromagnetically coupled to that of Co(S-1). In the FeTi layer, Ti atoms have very small magnetic moment with the order of 10^{-2} μ_B.

The surface effect can be seen from the local density of states (DOS). The calculated layer-, atom-, and spin-projected DOS for CoTi/FeTi/CoTi(110) film are presented in Fig. 3. The difference between the DOS for surface and subsurface layer is significant. For the surface DOS, the majority states are shifted toward higher energy region and the minority states are shifted toward low energy region. For the minority states of Co atom, the peak which is seen above the Fermi level in DOS of Co(S-1) is merged to the peak locating below the Fermi level in DOS of Co(S). The change of *d*-electron numbers for Co(S) is also seen in Table 1.

4. Summary

We have investigated the electronic structure and magnetic properties of CoTi/FeTi/CoTi(110) film by using a first-principles calculation with the all-electron full potential linearlized augmented plane wave (FLAPW) method. The magnetic moments of the surface and interface layer are 0.15, 0.65, and –0.34 μ_B for Fe(I), Co(I), and Co(S), respectively. The Co atom at the surface is antiferromagnetically coupled to that of Co(S-1).

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