Deep Potential Effect on Magnetism of Binary Including Spintronic Material

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Magnetic moments on transition elements strongly depend on their circumstances. Generally, the magnetic moments, surrounded by neighbor atoms having deep potential, seem to be enhanced. For example, the moment on Iron (Fe) is indeed enhanced in the Ni₃Fe and Ni-Fe-Ga as shown in the previous calculation.¹⁾ In both alloys, the nearest neighbors of Fe are Nickel (Ni) atoms, having deeper potential than Fe.

To examine the effect of surrounding deep potential, the electronic structures of binary alloys between 3d-transition-metal elements are calculated for the B2 and L1₂ structure. The surrounding deeper potential draw the electronic states of the subject atoms into lower energy range and bring the various moments and interesting features. In other words, the effects of surrounding potential can control energy level of *DOS* peak or the band gap. Were the structure of Cu₃V to be the L1₂, the magnetic moment on V would become unusually large (1.99 μ_B). Some alloys calculated show the high spin polarization at the *Fermi level* (E_F). The values of the spin polarization at the E_F evaluated from the *density of states* (*DOS*) for Ni₃Cr, Ni₃Co and CoFe are 0.94, -0.86 and -0.88 respectively. To control the energy level of *DOS* peak or the band gap would give us another means for finding new spintronic materials. The relations between whole magnetic moment and the valence electron concentration show the Slater-Pauling like behavior.

(Received October 29, 2004; Accepted January 13, 2005)

Keywords: electronic structure, magnetic moment, L1₂, Ni₃Co, Ni₃Cr, spintronic

1. Introduction

The enhancement of magnetic moments on Iron (Fe) in compounds and alloys has been actively discussed as in the Fe₁₆N₂. In the previous calculations, the large Fe moments were estimated in the Ni-Fe-Ga and Ni₃Fe.¹⁾ The nearest neighbor atoms of Fe are eight Nickel (Ni) atoms in the Ni-Fe-Ga with the L2₁ structure (full-Heusler) and twelve Ni atoms in the Ni₃Fe with the L1₂ structure. It was also reported that the moment on Fe surrounded by Co was also enhanced in the Co-Fe-Al with the L2₁ structure.²⁾ The results suggest that there are two factors to enhance Fe moment: the enlargement of interatomic distances caused by Gallium (Ga) and the surrounding deep potential made by Ni. We pay attention to the latter factor.

In this paper, we consider the deep potential effect on the 3d-transition-metal elements (V, Cr, Mn, Fe, Co) in the two kinds of circumstances. The circumstances are assumed in the B2 structure as a bcc-type and the L1₂ structure as an fcc-type which are shown in Fig. 1. The surrounding neighbor elements are chosen among the 3d-transition-metal elements (Fe, Co, Ni, Cu) to have the larger atomic number than the subject element. These circumstances are not meet all the real phase for the subject elements. Some alloys actually exist as ordered in such structures but some do not.

As shown in the previous work,¹⁾ the local *density of states* (*DOS*) of Fe in the Ni₃Fe with the L1₂ structure have peculiar feature. The majority-spin *DOS* scarcely exist over the E_F and very high peak of minority-spin *DOS* exist just above the E_F . If one can move this high peak to just on the E_F , the spin polarization at the E_F of the alloy becomes high: one can get a candidate of a spintronic material.

Fig. 1 The crystal structures of the B2 and L1₂ structures. The electronic structures of the subject atoms (V, Cr, Mn, Fe and Co) are calculated for these two types of the structures.

2. Crystal Structure and Method of Calculation

To clarify the effect of circumstances on the electronic structure, we choose typical distinctive two structures, the B2 (CsCl-type) and L1₂ (Cu₃Au-type) structures. Both of the structures have the same symmetry as the $pm\bar{3}m$, the 221st space group symmetry in the 'International Tables for Crystallography'.³⁾ The unit cells of both structures are shown in Fig. 1. The numbers of the nearest neighbor atoms are eight in the B2 structure and twelve in the L1₂ structure. The L1₂ structure is one of the close-packed structures.

Band calculations are carried out self consistently by the LMTO-ASA method.⁴⁾ The exchange correlation potential is treated within the framework of the local-spin-density (LSD) approximation.⁵⁾ To find the reasonable equilibrium lattice constants, the lattice constant dependence of the *total energy* is calculated and determined the theoretical lattice constant and the ratio of the atomic spheres. The radii of the atomic spheres of V (r_V), Cr (r_{Cr}), Mn (r_{Mn}), Fe (r_{Fe}), Co (r_{Co}), Ni

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Table 1 Theoretical lattice constants of the B2 and L1₂ structures.

		Lattice constant, nm				
X:	V	Cr	Mn	Fe	Co	
B2	Fe-X	0.288	0.283	0.281	0.282	
	Co-X	0.288	0.286	0.284	0.283	0.279
	Ni-X	0.291	0.286	0.289	0.283	0.277
	Cu-X	0.294	0.287	0.293	0.285	0.280
L1 ₂	Fe ₃ -X	0.356	0.352	0.354	0.346	
	Co ₃ -X	0.354	0.351	0.348	0.353	0.352
	Ni ₃ -X	0.357	0.355	0.355	0.354	0.351
	Cu ₃ -X	0.368	0.367	0.365	0.360	0.357

(r_{Ni}) and Cu (r_{Cu}) are used in the same ratio for both of the structures. In any alloys, the charge neutrality in the spheres is fulfilled. The ratio of the radii is $r_{\text{V}}:r_{\text{Cr}}:r_{\text{Mn}}:r_{\text{Fe}}:r_{\text{Co}}:r_{\text{Ni}}:r_{\text{Cu}} = 1.102:1.080:1.068:1.044:1.022:1.000:0.999$.

3. Results

3.1 Total energy

To determine the lattice constants theoretically, the *total energies* are calculated as a function of the lattice constants. The minimum value of the *total energy* gives the theoretical value of the lattice constant. The theoretical lattice constants taken in this calculation are summarized in Table 1. In our method, the theoretical lattice constant for ordered intermetallic compound sufficiently coincide with the experimental ones, especially for close-packed structures. For instance, the experimental lattice constant of Ni₃Fe is 0.3545 nm.⁶⁾ In this paper, we will discuss the electronic structures calculated at the theoretical lattice constants. However, some alloys does not have ordered phase as the B2 or L1₂ structure so that these structures for such alloys are virtual.

3.2 Magnetic moments

Among pure transition metals, Iron is a ferromagnet and Manganese is a complicated antiferromagnet in the bcc structure, while Cobalt and Nickel are ferromagnets in the fcc structure. Here, we examine the change of the magnetic properties of the 3d-transition-metal elements in the bcc and fcc circumstances, where the surrounding potential is deeper than the self potential. The surrounding potential made by neighbors becomes deeper in the order of Fe, Co, Ni and Cu.

The magnetic moments due to the spin polarization are estimated in both structures. The total magnetic moments of alloys can be understood as a function of valence electron concentration. The relation between the whole magnetic moments and the valence electron concentration is given in Fig. 2. The relations between them show the Slater-Pauling like behavior.

The values of the magnetic moments on the subject elements (V, Cr, Mn, Fe and Co) in the B2 and L1₂ structures are listed in Table 2. Paying attention to pure Iron (Fe), the magnetic moment is $2.2 \mu_{\text{B}}$ in the bcc structure and $0.15 \mu_{\text{B}}$ in the fcc structure. In the both circumstances, the Fe moment is enhanced where the surrounding potential becomes deeper. Especially, when the surrounding element changes from Fe to Co, the increase is very large in the fcc circumstances.

Fig. 2 The relation between the total magnetic moment and valence electron concentration.

Table 2 Magnetic moments on X (X = V, Cr, Mn, Fe and Co) in the B2 and L1₂ structures.

		Moment on X, μ_{B}				
X		V	Cr	Mn	Fe	Co
B2	Fe-X	-0.30	0.33	1.22	2.20	
	Co-X	0.26	1.53	2.68	2.73	1.76
	Ni-X	0.28	1.74	3.42	2.77	1.71
	Cu-X	—	0.97	3.43	2.55	1.46
L1 ₂	Fe ₃ -X	-0.58	-0.92	-2.22	0.15	
	Co ₃ -X	—	-1.12	2.04	2.53	1.63
	Ni ₃ -X	0.73	1.95	3.01	2.85	1.70
	Cu ₃ -X	1.99	3.27	3.52	2.56	1.22

Roughly speaking, the magnitude of the magnetic moment increases as the surrounding potential becomes deeper. Moreover, the marvelous result is seen in the V moments. Although Cu and V are immiscible, the magnetic moment on V in case where V is surrounded by Cu in ordered Cu₃V with the L1₂ structure would have an unusual value ($1.99 \mu_{\text{B}}$). On the other hand, not every value of the magnetic moment on the subject atoms is enhanced. The magnetic moments on X (= Cr and Mn) in the Fe₃X and Co₃X are antiparallel to that on the neighbor Fe and Co.

These features described above are reflected in the *densities of states (DOS)*. They are explained in terms of the changes of *DOS* shape caused by the difference of the crystal structures and the surrounding potential, in the next section.

3.3 Density of state

3.3.1 Magnetic property

To understand the various magnetic moments of the subject atoms, it is significant to examine the effect of neighbor atoms. The *densities of states (DOS)* help us to understand the effect of surrounding neighbors.

At first, we pay attention to the large V moments in the Cu₃V with the L1₂ structure. This phase is not likely to exist because Cu and V are immiscible, and Y. X. Shen *et al.* conclude in their calculation report that the L1₂ structure is not stable as Cu-V ordered phase.⁷⁾ Whether the Cu₃V with the L1₂ structure exist or not, the large magnetic moment in

Fig. 3 The paramagnetic local DOS of V and their neighbor atoms (above) and ferromagnetic DOS of V (below) in Co_3V , Ni_3V and Cu_3V . The vertical line shows the E_F .

this circumstances suggest significant thing. The paramagnetic local DOS of V and their neighbors (Co, Ni and Cu) in the L_{12} structure are shown in the upper part of Fig. 3. When the neighbors change from Co to Cu, the electronic states of V move to the low energy range as the result of the d-states hybridization with the neighbors. In other words, as the surrounding potential become deeper, the DOS of V move to the lower energy range. Then, the high peak of DOS of V are situated at the E_F in the Ni_3V and Cu_3V . The DOS of V in these alloys satisfies the Stoner condition for the occurrence of ferromagnetism. The lower part of Fig. 3 shows the ferromagnetic DOS of V in the Co_3V , Ni_3V and Cu_3V . The same tendency can be seen as the deep potential effect on the paramagnetic DOS of subject atoms. As the surrounding potential become deeper, the DOS of the subject atoms move to the lower energy range, and then we can guess the magnetic property of the subject atoms from the DOS near the E_F . In the virtual alloys of Cu_3V with the L_{12} structure, the effect on V cause an unusual large magnetic moment ($1.99 \mu_B$).

In Fig. 4, the paramagnetic DOS of Fe are shown for the bcc and the fcc structure. The E_F is situated at the high peak of the DOS in the bcc structure, while the value of the DOS at the E_F are not so large in the fcc structure. This is reflected in the magnetic moments on Fe in the B2 and L_{12} structures described in the previous section. When the neighbors change from Fe to Cu in the L_{12} structure, the DOS of the subject atoms move to the lower energy range and the DOS near the

Fig. 4 The paramagnetic local DOS of Fe in pure Iron with the bcc and the fcc structure, and in the CuFe with the B2 structure and in the Ni_3Fe with L_{12} structure. The vertical line shows the E_F .

E_F become higher and form a peak. The same tendency is seen in the B2 structure. The features are seen in Fig. 4. Thus, Fe surrounded by deeper potential than self-potential becomes easy to carry a large magnetic moment.

The total DOS of the Fe_3Cr are shown in Fig. 5, where the E_F is situated in the large valley. This suggests that the Fe_3Cr exhibits antiferromagnetism as pure Cr which is antiferro-

Fig. 5 The paramagnetic total DOS of the Fe_3Cr . The vertical line shows the E_F .

magnetic and the E_F is situated in the large valley of the DOS . The moment on Cr in the Fe_3Cr is really antiparallel to that on the neighbor Fe. The E_F in the Fe_3X and the Co_3X ($X = Cr$ and Mn) is also situated in the large valley of the total DOS . Therefore, we can guess that the moments on X ($= Cr$ and Mn) in the Fe_3X and Co_3X are antiparallel to those on the neighbors.

In the same way, the surrounding deep potential affects the overall subject atoms (V , Cr , Mn , Fe , Co). Namely, as the surrounding potential become deeper, the majority-spin DOS of the subject elements are drawn into the lower energy range. Then the DOS of the subject elements at the E_F change and the result cause the changes of magnetic property.

3.3.2 Spintronic material

Paying attention to the DOS at the E_F , we notice that there are some alloys with characteristic property. The high spin polarization at the E_F cause spin dependent conduction and that conduction is useful for a GMR (giant magnetoresistance), TMR (tunneling magnetoresistance) or MRAM (magnetic random access memory) application. Hereafter, we turn our eyes to the candidates for such spintronic materials. The spin polarization P at the E_F is defined as

$$P = \frac{D_{\text{major.}} - D_{\text{minor.}}}{D_{\text{major.}} + D_{\text{minor.}}}$$

where D_σ ($\sigma = \text{major.}, \text{minor.}$) is the *density of states* at the E_F with spin σ (majority, minority). The spin polarizations at the E_F of the candidates are listed in Table 3.

In our calculation, the $CoMn$ in the B2 structure shows the high spin polarization at the E_F (0.92). Even if the B2 structure of $CoMn$ is not reported experimentally, this calculated result suggests the characteristics of the DOS to be the high spin polarization in bcc circumstances. Figure 6 shows the DOS of the $CoMn$. The local DOS of Mn and Co have two peaks, which are characteristics for the bcc 3d-

Fig. 6 The local DOS of Mn and its neighbor Co in $CoMn$ (above), and the total DOS of $CoMn$ (below). The vertical line shows the E_F .

transition metals. When the E_F exists at the 'wedge-shaped' valley in the minority-spin state, the alloys show the high spin polarization at the E_F . This situation is similar to those of the bcc pure Iron (Fe) that P calculated is 0.55. If the E_F locates in the 'wedge-shaped' valley in the minority spin state, the alloys in the bcc circumstances will be the candidates as the high spin polarization alloy.

Next, we turn our attention to the Ni_3X ($X = Cr, Mn, Fe$ and Co) with the $L1_2$ structure. The probability of existence of these alloys seems to be high, so that the grand state of pure Ni is in the fcc structure. In fact, for instances, the $L1_2$ ordered phase of the Ni_3Cr and Ni_3Fe is reported.^{8,9)} The local DOS of the X atoms are shown in Fig. 7. The peak move to the lower energy range as the X changes Cr to Co , and are mostly occupied for $X = Fe$ and Co . The high peak of DOS is situated at the E_F in the majority-spin for $X = Cr$ while in the minority-spin for $X = Co$.

The local DOS of the neighbor Ni are shown in Fig. 8. The DOS shape of Ni in the Ni_3Co is similar to that of Ni with the fcc structure. Generally, the DOS of typical fcc transition metals show no large valley. However, the Ni DOS of minority-spin in the Ni_3Cr or Ni_3Mn have a valley: the band gap of d-states in minority-spin clearly exists near the E_F . As the subject atoms change from Co to Cr , the DOS of Ni move to the higher energy range. We consider this the result of the hybridization between the d-states of Ni and the subject elements. The shallow potential effect of the subject elements

Table 3 Spin polarization at the Fermi level.

Spin polarization				
$L1_2$	Ni_3Cr	Ni_3Fe	Ni_3Co	Cu_3Fe
P	0.94	-0.66	-0.86	-0.80
$B2$	$FeCr$	$CoCr$	$CoMn$	$CoFe$
P	0.79	0.56	0.92	-0.88

Fig. 7 The local DOS of X (X = Cr, Mn, Fe and Co) in Ni_3X . The vertical line shows the E_F .

Fig. 8 The local DOS of Ni in Ni_3X (X = Cr, Mn, Fe and Co). The vertical line shows the E_F .

on Ni can be seen.

The total DOS of this series are shown in Fig. 9, which reflect the characteristics of the DOS of Ni and X atoms described previously. Although Ni_3Cr is not a half-metallic alloy, the electronic structure of this alloy shows the half-metallic-type high spin-polarization at the E_F . The DOS of the Ni_3Co and Ni_3Cr show the high spin-polarization at the E_F . The Ni_3Co is categorized as a typical strong ferromagnetic-type high spin polarization alloy, in which the majority-spin states are mostly occupied. This type strong ferromagnetic-type high spin polarization alloy seen in the B2 structure is CoFe that P calculated is -0.88 .

4. Discussion

In the previous work,¹⁾ we notice the peculiar features of the local DOS for Fe in the Ni_3Fe with the L1_2 structure. The majority-spin DOS scarcely exist over the E_F and very high peak of minority-spin DOS exist just above the E_F shown in Fig. 7. To move the peak to just on the E_F , we can use the

deep potential effect. Figure 10 shows the local and total DOS of Cu_3Fe . As the effect of the deep potential of Cu, the majority-spin local DOS of Fe in the Cu_3Fe move to the lower energy range and the high peak of the minority-spin locates at the E_F . On the other hand, in the minority-spin states, the states in the lower energy range decrease and form the high peak near the E_F as the consequence of the d-d exchange interaction. This result suggests that to change the surrounding potential lead some candidates to suitable for spintronic materials.

5. Conclusion

The electronic structures of binary alloys were calculated for the B2 and the L1_2 structures to make clear the surrounding deep potential effect on magnetic property. The magnetic moments on the subject elements (V, Cr, Mn, Fe and Co) are strongly affected by the surrounding potential. As the surrounding potential becomes deeper, the DOS of the subject atoms move to the lower energy range. Roughly

Fig. 9 The total DOS of Ni_3X ($\text{X} = \text{Cr}, \text{Mn}, \text{Fe}$ and Co). The vertical line shows the E_F .

speaking, the effect brings the enhancement of the magnetic moment of the subject elements. The relation between the whole magnetic moments and valence electron concentrations show the Slater-Pauling like behavior.

Some alloys show the high spin-polarization at the E_F . The high spin polarization alloys are categorized in two types: the halfmetallic-type and the strong ferromagnetic-type. In the L1_2 structure, the Ni_3Cr shows the halfmetallic-type and the Ni_3Co shows the strong ferromagnetic-type. In the B2 structure, the high spin polarization of CoMn suggests a necessary condition for high spin-polarization in bcc circumstances. This condition is common with those of Heusler alloys. When the E_F exists in the ‘wedge-shaped’ valley in either spin state, the spin-polarization at the E_F becomes high. The strong ferromagnetic-type of the B2 structure is CoFe ($P = -0.88$).

The effects of surrounding potential can control energy level of DOS peak or the band gap. To control the energy

Fig. 10 The local DOS of Fe and Cu in Cu_3Fe (above), and the total DOS of Cu_3Fe (below). The vertical line shows the E_F .

level of DOS peak or the band gap lead us another idea for finding new spintronic materials.

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