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## Electronic structure calculations for amorphous Co and Ni

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**Abstract.** Self-consistent electronic structure calculations were performed for amorphous Co and Ni metals using the most localized linear muffin-tin orbital method together with the recursion method. The calculated results for the paramagnetic states suggest that these metals exhibit ferromagnetism according to the Stoner criterion. Spin-polarized calculations were also performed. The resultant magnetic moments were  $1.63\mu_B$  for amorphous Co, and  $0.61\mu_B$  for amorphous Ni. These values agree well with the experimental values obtained by extrapolation to the pure amorphous limit in several Co- or Ni-based amorphous alloys. The stability of ferromagnetism is discussed for both the amorphous metals on the basis of the electronic structures obtained.

### 1. Introduction

In order to investigate the magnetism of amorphous transition metals and alloys, it is important to clarify the electronic structures of pure amorphous transition metals. Fujiwara [1] first developed the method to calculate the electronic structure self-consistently in an amorphous phase and applied it to pure amorphous Fe metal. He suggested that amorphous Fe did not exhibit uniform ferromagnetism according to the Stoner criterion. It was found that, in the case of Fe–Zr amorphous alloys, the ferromagnetism disappeared beyond an Fe content of 90 at.%, in association with the appearance of spin-glass state [2, 3]. Similar phase transitions were also observed in several Fe-based amorphous alloys [4, 5].

There have also been many experimental reports on the magnetism of other amorphous transition-metal alloys in the vicinity of pure amorphous metal. For example, Fukamichi *et al* [6] found that the Curie temperatures of Y–Co amorphous alloys were higher than those of their crystalline counterparts. The magnetism of Ni-based alloys has been investigated for Ni–Y [7], Ni–Ce, Ni–La [8] and Ni–Hf [9] amorphous alloys. These exhibit a weak ferromagnetism for a Ni content beyond 80 at.%. In contrast, there have been few reports on the electronic structure of pure amorphous Co and Ni metals, which might contribute to a basic understanding of the magnetism in these amorphous metals and alloys. Although Ching *et al* [10] calculated the electronic structure of pure amorphous Ni using a method consisting of orthogonalized linear combination of atomic orbitals, it was not a self-consistent calculation. These facts prompted us to report the results of our band calculations for amorphous Co and Ni metals. The magnetism of these metals is discussed on the basis of the calculated electronic structures.

## 2. Methods

The local atomic structures of amorphous Fe, Co and Ni are quite similar to each other [11, 12]. For example, figure 1 shows a comparison of the pair distribution functions (PDFs)  $g(r)$  for amorphous Fe and Ni obtained by Ichikawa [12], employing the x-ray diffraction method. The distances are normalized by the first peak positions  $r_1$  for each PDF in the figure. Yamamoto and Doyama [13] constructed an atomic structure model for amorphous Fe using a model with relaxed dense random packing of hard spheres. The PDF obtained from the atomic structure model agreed well with the experimental value (see figure 1(b) in [13]). We therefore employed this model for the atomic structure models of amorphous Co and Ni, after scaling it by their first peak position in the PDF. The model structure consists of 1450 atoms. The number densities obtained from the model structure are  $0.0851 \text{ \AA}^{-3}$  for amorphous Co, and  $0.0882 \text{ \AA}^{-3}$  for amorphous Ni.

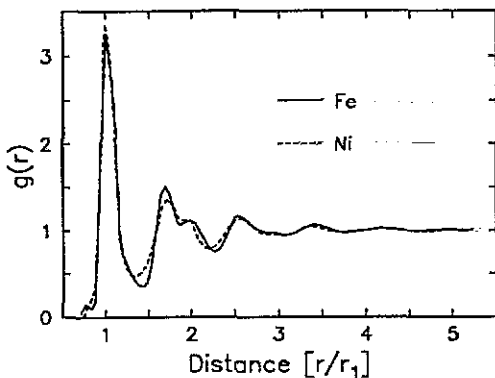


Figure 1. Comparison of the PDFs  $g(r)$  for amorphous Fe (—) and amorphous Ni (---) [12]. The distances are normalized by the first peak position  $r_1$  for each curve.

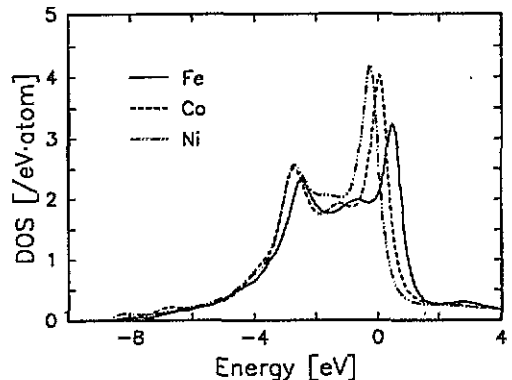


Figure 2. Comparison of the total DOS for amorphous Fe [1] and the total DOSs obtained in the present calculation for amorphous Co and Ni. The zero energy level denotes the Fermi level.

On the basis of the atomic structure model, we calculated the electronic structures using the most localized linear muffin-tin orbital method together with the recursion method [1]. We employed a local-spin-density-functional approximation in the form suggested by von Barth and Hedin [14]. Self-consistency was achieved within the averaged muffin-tin potential for each atom. This approximation is sufficiently valid to use in a discussion of the average density of states (DOS) [15]. In the recursion process, we restricted electrons to hopping within a cluster consisting of the 883 innermost atoms of the above atomic structure model to avoid the influence from the surface of the structure model. This cluster size was determined so that the screened structure constants for the atoms within the cluster were negligible at the surface of the structure model. The averaged DOS was obtained by averaging local DOSs for the 203 innermost atoms. There was little change in the resulting average DOS when we increased the number of atoms to more than 203 in the averaging process. We used a square-root terminator [16] with the asymptotic recursion coefficients evaluated by the method of Beer and Pettifor [17].

### 3. Results

#### 3.1. Paramagnetic states

In figure 2, the present calculated total DOS for amorphous Co and Ni are compared with that calculated by Fujiwara [1] for amorphous Fe. On the whole, the general shapes of the total DOS for these three amorphous metals are quite similar, because they are determined mainly by the local atomic structure. The band width of the total DOS decreases systematically as the d electron number increases, in the order Fe, Co and Ni. This systematic decrease in the band widths, which is also observed in the DOS of crystalline FCC Fe [18], Co and Ni [19] can be explained by the Friedel [20] model.

The figure also shows that the highest peak position in the DOS shifts towards low energies with increasing d electron number because of band filling of the d states. The Fermi level of amorphous Fe lies on the low-energy side and away from the peak position, whereas in the case of crystalline BCC Fe it lies near the highest peak position of the total DOS. Fujiwara [1] suggested that amorphous Fe metal was expected not to exhibit a uniform ferromagnetism because the DOS at the Fermi level does not satisfy the Stoner criterion. The DOS at the Fermi level, the Stoner exchange parameters calculated by Janak [21], and their products are summarized in table 1 for the present amorphous Co and Ni, together with the values calculated by Fujiwara [1] for amorphous Fe. Both amorphous Co and amorphous Ni satisfy the Stoner criterion and are expected to exhibit ferromagnetism. In particular, the Fermi level in amorphous Co lies almost on the peak position of the DOS as shown in figure 2, and therefore the DOS at the Fermi level is higher than for crystalline HCP Co. This leads to a gain in the exchange energy, resulting in the enhancement of ferromagnetism in the amorphous Co over that in the crystalline HCP phase. Recently, Kakehashi [22] showed that this enhancement in ferromagnetism remained even at a finite temperature by employing a functional integral method and a distribution function method. The enhancement of the Curie temperature observed for Y-Co amorphous alloys at high Co contents [6] can be attributed to the enhancement of the DOS at the Fermi level. On the other hand, the Fermi level of amorphous Ni lies on the high-energy side and away from the peak position of the DOS, as shown in figure 2, and therefore the DOS at the Fermi level is lower than for crystalline FCC Ni. The ferromagnetism in amorphous Ni is expected to be weaker than that in the crystalline FCC phase.

**Table 1.** DOS  $n(E_F)$  at the Fermi level, the Stoner exchange parameters  $I$  obtained by Janak [18], and their products for amorphous Fe [1], Co and Ni. The Stoner criterion is satisfied for amorphous Co and Ni.

System	$n(E_F)$ (Ryd <sup>-1</sup> /atom)	$I$ (Ryd)	$n(E_F)I/2$
a-Fe	28.24	0.068	0.96
a-Co	53.77	0.072	1.94
a-Ni	37.57	0.074	1.39

### 3.2. Spin-polarized state

We also calculated the spin-polarized electronic structures of amorphous Co and Ni metals. The calculated total and projected DOSs are shown in figure 3 for amorphous Co, and in figure 4 for amorphous Ni. The DOSs for these two metals are also quite similar except that the exchange splitting of d states is larger for amorphous Co than for amorphous Ni. Their shapes are well explained by the simple rigid band splitting of the paramagnetic DOS that is shown in figure 2.

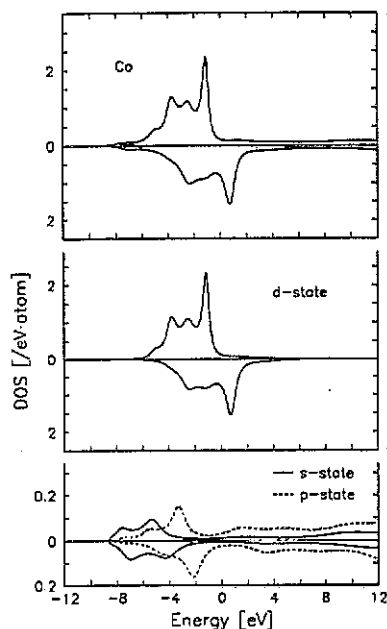


Figure 3. The total and projected DOSs for amorphous Co in the spin-polarized state. The zero energy level denotes the Fermi level.

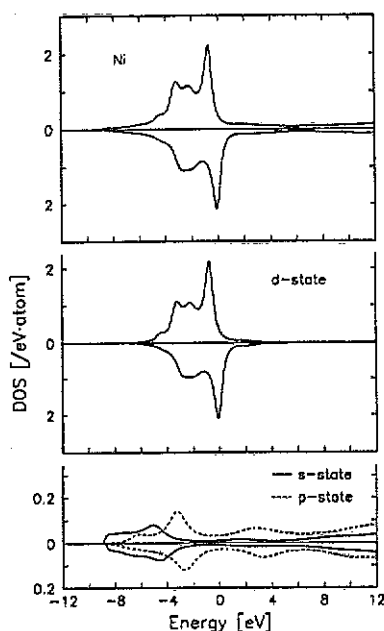


Figure 4. The total and projected DOSs for amorphous Ni in the spin-polarized state. The zero energy level denotes the Fermi level.

Figure 5 shows a comparison of the total DOS of the amorphous Co and Ni. Note that the Fermi level (vertical lines in the figure) lies near a local minimum of the total DOS in amorphous Co metal. This indicates that the strong ferromagnetism is stable. On the other hand, the Fermi level of amorphous Ni lies near a local maximum of the total DOS, although it lies near a local minimum of the total DOS for crystalline FCC Ni. It is therefore expected that the ferromagnetism in amorphous Ni is not so stable as in the crystalline FCC phase. In fact, weak ferromagnetism has been observed in the vicinity of pure amorphous Ni in Y-Ni, Ce-Ni [7, 8], La-Ni and Hf-Ni [9] amorphous alloys.

The electron occupation numbers for each state and the magnetic moments of amorphous Co and Ni are listed in table 2. The calculated magnetic moment of amorphous Co is  $1.63\mu_B$ , which agrees closely with the experimental values obtained from the extrapolation to the pure amorphous Co limit in Y-Co, La-Co, Zr-Co [23], Gd-Co [24] and Co-B [25] amorphous alloys. On the other hand, the calculated magnetic moment of amorphous Ni is  $0.61\mu_B$ , which also agrees well with the values

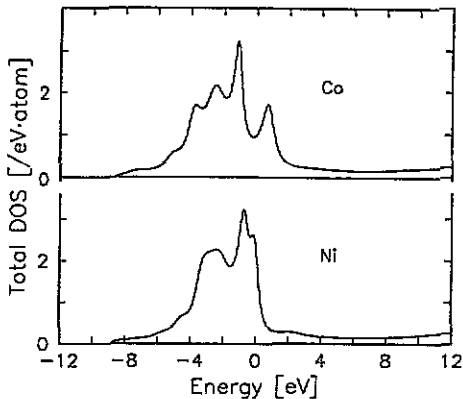


Figure 5. Comparison of the total DOSs for amorphous Co and Ni. The zero energy level denotes the Fermi level.

Table 2. Electron occupation numbers of each state and resultant magnetic moments for amorphous Co and Ni.

System	Spin	Occupation number			$M$ ( $\mu_B$ )
		s	p	d	
a-Co	Up	0.31	0.39	4.62	1.63
a-Co	Down	0.36	0.45	2.88	
a-Ni	Up	0.32	0.42	4.56	0.61
a-Ni	Down	0.32	0.40	3.97	

extrapolated to the pure amorphous Ni limit in Y-Ni, Ce-Ni [7, 8], Hf-Ni and Ta-Ni [9] amorphous alloys.

The changes in the magnetic moments were investigated with respect to changes in the Wigner-Seitz radius or, in other words, changes in the volume density for both amorphous Co and amorphous Ni. Varying the Wigner-Seitz radius by 1% changed the magnetic moment by about  $0.03\mu_B$  (about 2%) for amorphous Co, and by about  $0.10\mu_B$  (about 16%) for amorphous Ni. This means that the magnetic moment of amorphous Ni is more sensitive to the volume density than is the magnetic moment of amorphous Co. Therefore, it is expected that local magnetic moments in amorphous Ni fluctuate more widely than in amorphous Co, because of fluctuation of the local volume densities. These facts indicate that amorphous Ni is less ferromagnetic than amorphous Co.

#### 4. Conclusion

We calculated the self-consistent electronic structures of amorphous Co and Ni metals. The calculated results in the paramagnetic state suggest that both amorphous metals exhibit ferromagnetism according to the Stoner criterion. Spin-polarized calculations were also performed. It is expected that the ferromagnetism in amorphous Co metal is stable, because the Fermi level lies on a local minimum of the total DOS. On the other hand, the ferromagnetism in amorphous Ni metal seems to be unstable, because the Fermi level lies near a local maximum of the total DOS. The resultant magnetic moments are  $1.63\mu_B$  for amorphous Co, and  $0.61\mu_B$  for amorphous Ni.

These values agree well with the experimental values obtained from extrapolation to the pure amorphous limit in several Co- and Ni-based amorphous alloys.

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