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MAGNETIC PROPERTIES OF Ni- AND Co-ALLOYS CALCULATED BY KKR-CPA-LSD METHOD

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Abstract. - Electronic structure of fcc Ni-M (M = Ti, V, Cr, Mn, Fe, Co, Cu) and fcc-M (M = Cr, Mn, Fe) are calculated with KKR-CPA, in which the lattice constant as well as the charge and spin densities are determined self-consistently. The calculation well explains the observed magnetic properties of these alloys.

Alloys among 3d transition metals show variety of magnetic properties. Although many theoretical studies on these alloys have been made, there are still few realistic calculations. Accordingly most experiments have been compared with the calculations based on the tight-binding model combined with the coherent potential approximation (CPA) and the Hartree-Fock approximation (TB-CPA-HFA) [1]. Although the basic understanding of the magnetic properties of these systems is reached with a help of such model calculations they are certainly not enough for more detailed information like, e.g. cohesive properties. The purpose of the present paper is to discuss the magnetic properties of ferromagnetic Ni and Co based fcc alloys (Ni-Ti, V, Cr, Mn, Fe, Co, Cu and Co-Cr, Mn, Fe) in the light of realistic calculation based on the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) [2, 3].

KKR-CPA is one of the best alloy versions of the usual KKR band structure calculation. Use of a fast KKR-CPA procedure [4] makes a full self-consistent, i.e. both in charge (and spin) densities and in the coherent $t$-matrix, calculation practicable with reasonable computational time.

In the following, the density functional theory in the local spin-density approximation (LSD) with exchange-correlation potential by von Barth and Hedin [5] is used to remain in line with obtained successful description of dilute alloys [6, 7]. The lattice constant is directly determined in each concentration by energy minimization. Core states are rigorously included; the Brillouin zone integration is performed with 500 independent $k$-points. The final convergence attains $10^{-8}$Ry/atom stability of the total energy, guaranteeing good accuracy for calculated quantities. See references (Refs. [4, 8]) for computational details.

Figure 1 shows the calculated magnetization of these alloys, which reproduces well the trend of the experimental data shown in figure 2. The local magnetic moments of Ti, V and Cr of Ni based alloys and those of Cr and Mn of Co based alloys couple antiparallel...
to the bulk magnetization whereas they couple parallel for other cases. For Co-Mn a state with parallel moment is also obtained.

First we focus on Ni-Fe and Ni-Mn. Both systems undergo the ferro-to-nonmagnetic transition which follows after initial increase of magnetization, with increasing Fe or Mn concentration. For Ni-Fe the calculation predicts a first-order transition in contrast to the experiments where a smoother transition is observed. In addition, the choice of the exchange-correlation potential affects the critical concentration considerably for Ni-Fe.

The mechanism underlying the magnetic instability of Ni-Fe has been discussed by many authors [9]. The discrepancy of the calculation from experiment may arise from the following possibilities: (i) LSD may not take account well of the renormalization of the ground state due to the electron-magnon scattering discussed, for instance, by Igarashi [10]; (ii) the possibility of more-than-one magnetic states of Fe atoms, e.g. one with magnetic moment parallel and another antiparallel, may require an extension of the present treatment; (iii) since the magnetic instability occurs near the boundary where the fcc phase is no more available, the experimental condition is much complicated i.e. it is not guaranteed that the calculation should suitably simulate the experimental situation.

In conclusion, more detailed comparisons with experiments are desirable to judge if the present theory is applicable to Ni-Fe or if any modification accounting for various effects not yet included is necessary.

For the Ni-Mn system, the calculated ferro-tononmagnetic transition is of second order, which seemingly explains the observed behavior satisfactorily. However, a discrepancy shows up if the calculated equilibrium lattice constants are compared with experimental ones (Fig. 3). The calculated lattice constant reaches maximum around 10 atom. % of Mn and then rapidly decreases. The experimental one, on the other hand, monotonously increases with increasing Mn.

The reason of this discrepancy lies in the fact that Mn atoms retain their magnetic moment even in the paramagnetic state. More realistic treatment is, therefore, to take account of the coexistence of more than a single magnetic states for each component atom, as is pointed out by Jo years ago [11]. He calculated such a situation by use of TB-CPA-HFA to explain the NMR data which clearly show the existence of two Mn magnetic states in Ni-Mn.

Incidentally we notice that the self-consistent determination of the lattice constant is essential in these calculations. For instance, if a fixed lattice constant suitable for pure Ni is used, the calculation predicts a smooth transition for Ni-Fe, instead of a first order one.

Finally we turn our attention to other systems. It certainly is true that CPA is less justifiable for the strongly perturbed systems like Ni-Ti, V, Cr and Co-Cr. The reasonable agreement with experiments for these alloys, however, implies that the average properties nevertheless are moderately accounted for by CPA even in such cases. For weakly perturbed systems (Ni-Co, Ni-Cu, Co-Fe) the present theory seems satisfactory as naturally is expected. Further discussion will appear in future publications.

In summary, we successfully calculated Ni and Co based ferromagnetic alloys by KKR-CPA-LSD, which confirms the applicability of the present theory to wide range of the transition metal alloys. For Ni-Fe and Ni-Mn, however, some extension of the theory may be required.


\[\text{[7]}\] see e.g. Dederichs, P. H., Akai, H., Blügel, S., Stefanou, N. and Zeller, R., Proc. of the NATO Advanced Study Institute on “Alloy Phase Stability” (Malme, Crete) 1987, in press.

\[\text{[8]}\] Akai, H., to be published.

