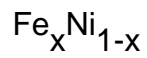


The concentration dependence of the magnetisation of the disordered ferromagnetic alloy



This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1989 J. Phys.: Condens. Matter 1 1867

(<http://iopscience.iop.org/0953-8984/1/10/008>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.90

The article was downloaded on 10/05/2010 at 17:57

Please note that [terms and conditions apply](#).

The concentration dependence of the magnetisation of the disordered ferromagnetic alloy $\text{Fe}_x\text{Ni}_{1-x}$

Qiang Hong^{†‡} and Tsung-han Lin^{†§}

[†] Department of Physics, Peking University, Beijing, People's Republic of China

[§] Centre of Theoretical Physics, CCAST (World Laboratory), Beijing, People's Republic of China

Received 18 July 1988

Abstract. The magnetisation of the disordered ferromagnetic $\text{Fe}_x\text{Ni}_{1-x}$ alloy is calculated using a single-band Hubbard Hamiltonian within the Hartree–Fock approximation. The occupation number of electrons per site is obtained in a self-consistent way. The calculated magnetisation is compared with experimental results.

1. Introduction

The magnetic properties of transition metals and their alloys have long been a challenging problem in solid state physics since Stoner's historical work [1, 2], and great progress has been made since then [3–5]. It is now generally considered that the transition metals (Fe, Co and Ni) are itinerant electron ferromagnets, i.e. the spin polarisations of the itinerant d electrons are responsible for their magnetisation. Experimental results showed that the bulk magnetisation reduces from $2.3 \mu_B$ per atom in Fe to $1.7 \mu_B$ in Co and $0.6 \mu_B$ in Ni via an increase in the number of d electrons. Because the d electrons are itinerant and sensitive to local structure, the presence of dissimilar neighbours as found in alloys must affect the magnetic properties [6].

Transition-metal alloys constitute a large group of magnetically ordered substances. Studies of the dependence of the magnetic properties on the composition and crystal structures of such alloys can give us important information about the fundamental concepts which govern the behaviour of these materials. Also, in practice, studies of these alloys are undoubtedly important, since almost all technical ferromagnetic materials are either alloys or compounds.

Among the transition-metal alloys, the alloy $\text{Fe}_x\text{Ni}_{1-x}$ is of particular interest because of not only its technological importance but also its anomalous properties. It is known that the structure of $\text{Fe}_x\text{Ni}_{1-x}$ can be classified into three types.

(i) In the Ni-rich part of the alloy, the system has a FCC structure and is ferromagnetic up to approximately 60 at. % Fe [7].

[‡] Permanent address: Department of Physics, Yantai University, Yantai, Shandong Province, People's Republic of China.

(ii) For Fe concentrations between about 60 and 80 at. %, the alloy average magnetic moment decreases drastically, and in this region there is a structure phase transition from FCC to BCC.

(iii) For Fe concentrations above roughly 80 at. %, the system is also ferromagnetic and has a BCC structure [8].

The rigid-band model [9] was first employed to study the magnetisation of Ni-based alloys. Although some features can be interpreted using this model, it is too simple to account completely for the complicated phenomena of transition-metal alloys. Disordered $\text{Fe}_x\text{Ni}_{1-x}$ has been studied within the CPA [10]. Many properties, such as the magnetic moment and the electronic specific heat coefficient, can be explained using this theory, but this method is based on an assumed electronic density of states and on ignoring the non-diagonal disorder.

In this work, we use the Bethe lattice approximation to study the magnetic moment of disordered $\text{Fe}_x\text{Ni}_{1-x}$. The Bethe lattice has the same short-range order and coordination number as the alloy but has the geometry of a Cayley tree [11]. It has been shown in previous work that this method can be successfully used for itinerant systems [12–14]. Here we use a one-band Hubbard Hamiltonian to describe the d electrons. The disordered system is represented by a Bethe lattice. In § 2, we outline the theory. Application to the $\text{Fe}_x\text{Ni}_{1-x}$ alloy is presented in § 3.

2. Theory

For a given alloy A_xB_{1-x} , we start with the Hubbard Hamiltonian [4]

$$H = \sum_{i,\sigma} \varepsilon_i C_{i\sigma}^+ C_{i\sigma} + \sum_{i \neq j} t_{ij} C_{i\sigma}^+ C_{j\sigma} + \sum_i U_i n_{i\sigma} n_{i\bar{\sigma}}. \quad (1)$$

Here $C_{i\sigma}^+$ and $C_{i\sigma}$ are the creation and annihilation operators for electrons with a spin σ in a Wannier state at site i , U_i is the intra-atomic electron–electron repulsive energy where the values U_A and U_B depend on the kind of atom at the i th site. ε_i is the single-site energy (assumed to be fivefold degenerate) which is ε_A if site i is occupied by an A atom, and ε_B if it is occupied by a B atom. The transfer integral t_{ij} is non-zero only if i and j are nearest-neighbour sites and it can have the values t_{AA} , t_{AB} and t_{BB} depending on the types of atoms on site i and j ; $\bar{\sigma}$ is the spin index opposite to σ . We assume that the energy parameters are independent of the concentration for a given alloy.

In the Hartree–Fock approximation, the above Hamiltonian can be written in the form [10]

$$H = \sum_{i,\sigma} E_{i\sigma} C_{i\sigma}^+ C_{i\sigma} + \sum_{i \neq j} t_{ij} C_{i\sigma}^+ C_{j\sigma} \quad (2)$$

where $E_{i\sigma} = \varepsilon_i + U_i \langle n_{i\bar{\sigma}} \rangle$ ($\langle n_{i\bar{\sigma}} \rangle$ denotes the total number of electrons of spin $\bar{\sigma}$ at site i).

In order to obtain the local density of electrons at an arbitrary site i , we use a Bethe lattice model to describe the disordered system. As discussed in [11], one has to define four transfer functions γ_1^σ , γ_2^σ , γ_3^σ and γ_4^σ for any given spin σ of a binary alloy. These transfer matrices satisfy the following equations:

$$\begin{aligned} \gamma_1^\sigma &= t_{AA} \{E - E_{A\sigma} - (z-1)[xt_{AA}\gamma_1^\sigma + (1-x)t_{AB}\gamma_3^\sigma]\}^{-1} \\ \gamma_2^\sigma &= t_{AB} \{E - E_{A\sigma} - (z-1)[xt_{AA}\gamma_1^\sigma + (1-x)t_{AB}\gamma_3^\sigma]\}^{-1} \\ \gamma_3^\sigma &= t_{AB} \{E - E_{B\sigma} - (z-1)[xt_{AB}\gamma_2^\sigma + (1-x)t_{BB}\gamma_4^\sigma]\}^{-1} \end{aligned} \quad (3)$$

$$\gamma_4^\sigma = t_{BB}\{E - E_{B\sigma} - (z-1)[xt_{AB}\gamma_2^\sigma + (1-x)t_{BB}\gamma_4^\sigma]\}^{-1}$$

which can be solved iteratively.

The one-particle Green functions can be expressed as

$$\begin{aligned} G_{00}^{\hat{A}\sigma}(E) &= \{E - E_{A\sigma} - z[xt_{AA}\gamma_1^\sigma + (1-x)t_{AB}\gamma_3^\sigma]\}^{-1} \\ G_{00}^{\hat{B}\sigma}(E) &= \{E - E_{B\sigma} - z[xt_{AB}\gamma_2^\sigma + (1-x)t_{BB}\gamma_4^\sigma]\}^{-1}. \end{aligned} \quad (4)$$

The local densities of states (LDOS) at a site occupied by an A atom and by a B atom with spin σ are

$$\begin{aligned} \rho_A^\sigma(E) &= -(1/\pi) \text{Im}[G_{00}^{\hat{A}\sigma}(E)] \\ \rho_B^\sigma(E) &= -(1/\pi) \text{Im}[G_{00}^{\hat{B}\sigma}(E)] \end{aligned} \quad (5)$$

respectively. The average LDOS of spin σ in the alloy is given by

$$\rho^\sigma(E) = x\rho_A^\sigma(E) + (1-x)\rho_B^\sigma(E) \quad (6)$$

and the total average LDOS is

$$\rho(E) = \sum_{\sigma} \rho^\sigma(E). \quad (7)$$

The condition that the total system is electrically neutral requires that the average number n of electrons per atom in the bulk should be related to x by

$$n = xn_A + (1-x)n_B. \quad (8)$$

Here n_A and n_B are the average numbers of electrons in pure bulk A or pure bulk B metals, respectively.

The Fermi energy E_F is determined by the number of electrons per atom through the following relation:

$$n = \int_{-\infty}^{E_F} \rho(E) dE. \quad (9)$$

Once E_F is obtained, we can determine the average numbers of electrons at a site occupied by an A or B atom with spin σ by

$$\langle n_A^\sigma \rangle = \int_{-\infty}^{E_F} \rho_A^\sigma(E) dE \quad (10)$$

and

$$\langle n_B^\sigma \rangle = \int_{-\infty}^{E_F} \rho_B^\sigma(E) dE \quad (11)$$

where $\langle n_A^\sigma \rangle$ and $\langle n_B^\sigma \rangle$ are determined self-consistently. The magnetic moment of an A or B atom in units of μ_B is obtained from

$$m_i = 5(n_{i\uparrow} - n_{i\downarrow}) \quad (i \equiv A \text{ or } B). \quad (12)$$

Here the factor 5 arises from the fivefold degeneracies of our simplified d bands.

The average magnetic moment of the alloy is given by

$$m = xm_A + (1-x)m_B. \quad (13)$$

Table 1. The energy parameters used for the calculation of magnetisation of disordered $\text{Fe}_x\text{Ni}_{1-x}$. W_I is the bandwidth, t_{II} is the transfer integral corresponding to W_I , and U_I is the on-site Coulomb interaction of pure Fe or Ni ($I \equiv \text{Fe or Ni}$).

Element	W_I (eV)	t_{II} (BCC) (eV)	t_{II} (FCC) (eV)	U_I (eV)
Fe	5.30	0.50	0.40	0.99
Ni	4.10	0.39	0.31	1.02

3. Results

Following the procedures outlined in § 2, we can calculate the magnetisation of the disordered $\text{Fe}_x\text{Ni}_{1-x}$ alloy. We assume that, in pure Fe, the number of d electrons per atom and the magnetisation are 7.2 and $2.3\mu_B$, respectively. In pure Ni the number of d electrons is 9.4 and the magnetisation is $0.6\mu_B$. For an arbitrary alloy, seven energy parameters (ε_A , ε_B , t_{AA} , t_{AB} , t_{BB} , U_A and U_B) must be given in order to calculate its electronic density of states. The energy parameters used for $\text{Fe}_x\text{Ni}_{1-x}$ are shown in table 1 in which the bandwidths of pure Fe and Ni are taken from [15] and the transfer integral t_{AA} (or t_{BB}) is chosen in such a way that the same bandwidths will be obtained by the Bethe lattice procedure, i.e. $t_{AA} = W_A/4\sqrt{z-1}$ where z is the coordination number. The transfer integral between two different atoms t_{AB} is taken to be $t_{AB} = \sqrt{t_{AA}t_{BB}}$ [16, 17]. The intra-atomic energies U_A and U_B are chosen so that in pure Fe and pure Ni the magnetisations are $2.3\mu_B$ and $0.6\mu_B$, respectively.

As pointed out in § 1, for $\text{Fe}_x\text{Ni}_{1-x}$ the system has different crystal structures in the Fe-rich part (BCC) and in the Ni-rich part (FCC) of the system. Consequently, it is difficult to choose energy parameters in these two cases. Here we assume that the bandwidths of pure Fe and Ni do not change with crystal structure and adjust the site energy difference $\varepsilon_{\text{Fe}} - \varepsilon_{\text{Ni}}$ so that when $x \rightarrow 0$ the magnetisation of the Ni atom in the alloy is $0.6\mu_B$ while, when $x \rightarrow 1$, the magnetisation of the Fe atom is $2.3\mu_B$.

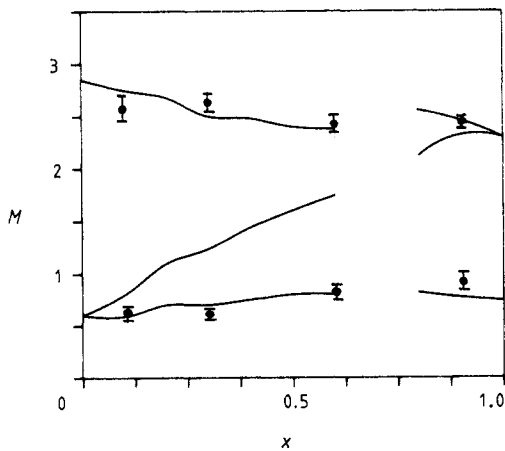


Figure 1. Plots of magnetisation of disordered $\text{Fe}_x\text{Ni}_{1-x}$ alloy against Fe concentration. The upper curve represents the magnetisation of the Fe atom in the alloy, the lower curve represents the Ni atom, and the middle curve shows the average magnetisation of an atom in the alloy. The experimental results [18] (●) are also shown.

Figure 1 shows the calculated magnetisation of disordered Fe_xNi_{1-x} . The upper curve represents the magnetisation of the Fe atom in the alloy, the lower curve represents the Ni atom in the alloy, and the middle curve shows the average magnetisation in the alloy. It can be seen that the results agree well with experiment [18]. When $0.6 < x < 0.8$ the system has a complicated magnetic order; the simple model described in § 2 does not apply to this situation.

The method discussed in this paper can be improved by considering the separation of the d bands, including the s–d hybridisation effect and the short-range order effects [16], which will be discussed elsewhere.

Acknowledgments

The authors would like to thank Dr M Robbins for kindly sending us his thesis. This work was supported by the National Science Foundation of China.

References

- [1] Stoner E C 1936 *Proc. R. Soc. A* **154** 656
- [2] Stoner E C 1938 *Proc. R. Soc. A* **165** 372
- [3] Herring C and Kittel C 1951 *Phys. Rev.* **81** 869
- [4] Hubbard J 1963 *Proc. R. Soc. A* **276** 238
- [5] Moriya T and Takahashi 1978 *J. Phys. Soc. Japan* **45** 397
- [6] Kanamori J, Akai H, Hamada N and Miwa H 1977 *Physica B+C* **91** 153
- [7] Rogge V, Neddermeyer H and Paul Th 1987 *J. Phys. F: Met. Phys.* **17** 1391
- [8] Hasegawa H and Kanamori J 1972 *J. Phys. Soc. Japan* **33** 1599
- [9] Mott N F 1964 *Adv. Phys.* **13** 357
- [10] Hasegawa H and Kanamori J 1971 *J. Phys. Soc. Japan* **31** 382
- [11] Kittler R C and Falicov L M 1976 *J. Phys. C: Solid State Phys.* **9** 4259
- [12] Moran-Lopez J L *et al* 1981 *Phys. Rev. B* **23** 5978
- [13] Dorantes-Davila J and Moran-Lopez J L 1982 *Appl. Surf. Sci.* **11–12** 689
- [14] News D M 1969 *Phys. Rev.* **178** 1123
- [15] Nguyen Manh D, Mayou D, Pastureland A and Cyrot-Lackmann F 1985 *J. Phys. F: Met. Phys.* **15** 1911
- [16] Robbins M O and Falicov L M 1982 *Phys. Rev. B* **25** 2343
- [17] Robbins M O 1983 *PhD Thesis* Berkeley
- [18] Collins M F and Forsyth J B 1963 *Phil. Mag.* **8** 401