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# ON THE MAGNETIZATION OF RARE EARTH-TRANSITION METAL ALLOYS*

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A simple model of a disordered alloy with spins localized on the rare earth atoms and interacting with a narrow *d*-band is considered. The saturation magnetization of the alloy is calculated using the molecular field and Hartree–Fock approximations. Disorder is treated by the coherent potential approximation. Result sare in good agreement with the experimental data for GdFe and GdCo alloys.

## *1. Introduction*

The magnetic properties of rare earth metals are mainly due to the partially filled 4f shell. The magnetic 4f electrons are strongly localized and the magnetic moments of rare earth ions are coupled to their neighbours by exchange interaction with the conduction band electrons. From the energy-band calculations, it follows that the conduction bands in hcp rare earth metals are identical with those of the 3d transition metals having hcp structure. They are overlapping and strongly hybridized s-like and d-like bands [1]. On the other hand, the magnetization of pure iron-group transition metals is currently described in terms of itinerant 3d electrons. Because of the large magnetic moments of some of the rare earth metals and considerably high Curie temperature some of the iron-group metals, the rare earth-transition metal intermetalic compounds are very interesting as magnetic materials.

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Saturation magnetization of $Fe_xGd_{1-x}$ alloys in the crystalline [2] as well as in the amorphous [3] state suggests an antiparallel alignment of gadolinium and iron moments. Magnetic moment per atom of the alloy in both states (crystalline and amorphous) is qualitatively consistent with the average value $m_{\text{alloy}} = |xm_{\text{Fe}} - (1-x)m_{\text{Gd}}|$, where $m_{\text{Fe}}$ and $m_{\text{Gd}}$ are the saturation moments of the pure iron and pure gadolinium metals. This suggests that the magnitude of magnetization in at least gadolinium-iron alloys is roughly independent of structure. Assuming this to be true we can apply here the coherent potential approximation (CPA), which has been shown to be successful in studying transition metal alloys [4].

## 2. *Model Hamiltonian of the alloy*

We shall consider a simple model consisting of spins localized on sites occupied by rare earth metal atoms and the narrow band formed by the 5d and 3d states from the rare earth and transition metals respectively. The coupling between localized spins and band electrons is assumed to be a typical exchange interaction. Each site of the lattice is occupied at random by a rare earth or transition metal atom with, respectively, propabilities $c_{\text{R}}$ and $c_{\text{T}} = 1 - c_{\text{R}}$. The corresponding Hamiltonian is assumed to have the form

$$H = H_{\text{f}} + H_{\text{d}} + H_{\text{f+d}}. \tag{1}$$

Here

$$H_{\text{f}} = -g\mu_{\text{B}}\mathcal{H}\sum_i p_i S_i^z \tag{2}$$

is the Zeeman energy of spins in an external magnetic field and $p_i = 1$ or 0 depending on whether the site at $r_i$ is or is not occupied by a rare earth atom,

$$H_{\text{d}} = \sum_{i,s,s'} (\varepsilon_i - \tfrac{1}{2} g'\mu_{\text{B}}\mathcal{H}\sigma_{ss'}^z) c_{is}^+ c_{is'}$$
$$+ \tfrac{1}{2}\sum_{i,s} U_i n_{is} n_{i-s} + \sum_{i\neq j,s} T_{ij} c_{is}^+ c_{js} \tag{3}$$

is the form of the nondegenerate narrow band Hubbard Hamiltonian and

$$H_{\text{f-d}} = -\tfrac{1}{2} J \sum_{i,s,s'} p_i \boldsymbol{S}_i \boldsymbol{\sigma}_{ss'} c_{is}^+ c_{is'} \tag{4}$$

is the localized spins-band electron exchange interaction. Clearly this model ignores 5-fold d-band degeneracy, which can however be qualitatively taken into account if $U$ is thought of as an effective Coulomb repulsion and calculated quantities e. g. average number of electrons multiplied by five. Disorder in the transfer term $T_{ij}$ is also treated approximately because we assume

$$T_{ij} = \alpha_i t_{ij} \alpha_j^*, \tag{5}$$

where the parameters $\alpha_i$ depend on the type of atom occupying the $i$-th site (they characterize the band width of pure metals) and $t_{ij}$ is configuration independent.

The known methods for dealing with disordered systems can not be applied to Hamiltonian (1) directly. Therefore, we have to introduce the following approximations:
(*i*) molecular field approximation for f–d exchange interaction and (*ii*) Hartree-Fock approximation for intraatomic Coulomb repulsion, which has been widely used in transition metal alloys [4]. Making use of it, we replace Hamiltonian (1) by

$$H = \tilde{H}_{\mathrm{f}} + \tilde{H}_{\mathrm{d}}, \tag{6}$$

where

$$\tilde{H}_{\mathrm{f}} = -\sum_i p_i h_i S_i^z \tag{7}$$

with

$$h_i = g\mu_{\mathrm{B}}\mathscr{H} + \tfrac{1}{2} J(\langle n_{i+}\rangle - \langle n_{i-}\rangle) \tag{8}$$

and

$$\tilde{H}_{\mathrm{d}} = \sum_{i,s} \varepsilon_{is} n_{is} + \sum_{i \neq j,s} T_{ij} c_{is}\, c_{js}, \tag{9}$$

here

$$\varepsilon_{is} = \varepsilon_i + U_i \langle n_{i-s}\rangle - \tfrac{1}{2}(g'\mu_{\mathrm{B}}\mathscr{H} + J p_i \langle S_i^z\rangle)\sigma_{ss'}^z. \tag{10}$$

In order to find to find configuration averaged magnetic moments for both kind of atoms we will do as follows:
(*i*) We assume that the molecular field $h_i$ and $\varepsilon_{is}$ will be selfconsistently determined such that they depend only on the type of atom occupying the $i$-th site. It means that now

$$\langle n_{is}\rangle = \begin{cases} n_{\mathrm{R}s} & \text{for rare earth sites} \\ n_{\mathrm{T}s} & \text{for transition metal sites.} \end{cases}$$

(*ii*) We apply the locator formalism of the single site CPA (see e. g. Ref. [5]) to find the local densities of states on both the rare earth and transition metal atoms.

Following Shiba [5] let us introduce the bare locator

$$L_{is}(\omega) = \frac{\omega - \varepsilon_{is}}{|\alpha_i|^2},$$

where $i$ = R (or T) depending on whether site $i$ is occupied by a rare earth (or transition metal) atom and coherent locator $L_s(\omega)$. The CPA equation for $L_s(\omega)$ in this formalism takes the form

$$c_{\mathrm{R}}(L_{\mathrm{R}s}(\omega) - I_s(\omega))^{-1} + c_{\mathrm{T}}(L_{\mathrm{T}s}(\omega) - I_s(\omega))^{-1} = F_s(\omega), \tag{11}$$

where

$$I_s(\omega) = L_s(\omega) - F_s^{-1}(\omega),$$

$$F_s(\omega) = \frac{1}{N}\sum_k \frac{1}{L_s(\omega) - \varepsilon_k} = \int_{-\infty}^{\infty} \frac{\mathscr{N}(\varepsilon)d\varepsilon}{L_s(\omega) - \varepsilon} \tag{12}$$

and $\varepsilon_k$ is defined through

$$t_{ij} = \frac{1}{N} \sum_k \varepsilon_k e^{-ik(r_i - r_j)}.$$

The main quantities that we are looking for are local (or partial) densities of states at the rare earth and transition metal atoms

$$\varrho_{is}(\omega) = -\frac{1}{\pi |\alpha_i|^2} \operatorname{Im} \frac{1}{L_{is}(\omega) - I_s(\omega)}. \tag{13}$$

For ease of computation, we use the simple analytic form of the density of states

$$\mathcal{N}(\omega) = \begin{cases} \frac{2}{\pi} \sqrt{1-\omega^2} & \text{for } |\omega| \leqslant 1 \\ 0 & \text{otherwise.} \end{cases} \tag{14}$$

This assumption means that the half band width of a pure transition (or rare earth) metal is given by $|\alpha_T|^2$ (or $|\alpha_R|^2$). Then $I_s(\omega) = F_s(\omega)/4$ and the CPA equation (11) is replaced by

$$c_R(L_{Rs}(\omega) - \tfrac{1}{4} F_s(\omega))^{-1} + c_T(L_{Ts}(\omega) - \tfrac{1}{4} F_s(\omega))^{-1} = F_s(\omega) \tag{15}$$

and

$$n_{is} = \int_{-\infty}^{\infty} f(\omega) \varrho_{is}(\omega) d\omega$$

$$= -\frac{1}{\pi |\alpha_i|^2} \int_{-\infty}^{\infty} f(\omega) \operatorname{Im} \frac{1}{\omega - \varepsilon_{is} - \frac{1}{4} F_s(\omega)} d\omega, \tag{16}$$

where $f(\omega)$ is the Fermi distribution function. The average value of the localized spin at a rare earth atom is

$$\langle S^z \rangle = S B_S \left( \frac{S h_R}{k_B T} \right) \tag{17}$$

with

$$h_R = g \mu_B \mathcal{H} + \tfrac{1}{2} J (n_{R+} - n_{R-}). \tag{18}$$

The expectation values for the number of electrons of spin $s$ on a R and T sites are determined by solving the selfconsistency conditions (16) and (17) with Eqs (10), (15) and (18). In this way we get contributions to the magnetic moments of the transition metal atom

$$m_T = \tfrac{5}{2} g' \mu_B (n_{T+} - n_{T-}) \tag{19}$$

and rare earth atom

$$m_R = g\mu_B\langle S^z\rangle + \tfrac{5}{2}\, g'\mu_B(n_{R+} - n_{R-}) \tag{20}$$

coming from both band electrons (including 5-fold degeneracy of the d-band) and localized spin. The total magnetic moment per atom of an alloy is

$$m = c_T m_T + c_R m_R. \tag{21}$$

### *3. Numerical results and discussion*

We will proceed to compare magnetic moments coming from the model presented above with experimental data for GdFe and GdCo alloys. The parameters of our model that have to be chosen are the energies $\varepsilon_R$, $\varepsilon_T$, $U_R$, $U_T$, $|\alpha_R|$, $|\alpha_T|$ and the exchange constant coupling $J$. Because only the difference $\varepsilon_T - \varepsilon_R$ is important we will assume in the following that $\varepsilon = 0$ then our estimation gives (all energies with the exception of $J$ are in transition metal half band width units) $\varepsilon_{Fe} = -1.8$ and $\varepsilon_{Co} = -1.9$. For the intraatomic effective Coulomb repulsion we assume $U_{Gd} = 1.67$, $U_{Fe} = 1.75$ and $U_{Co} = 1.80$, it can be compared with about 1.0 for Fe and 1.2 for Co pure metals as calculated in Ref. [6] or 1.25

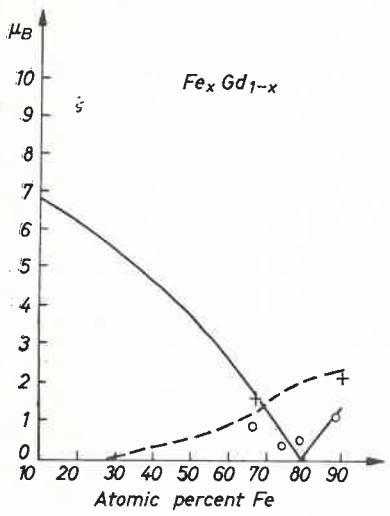


Fig. 1

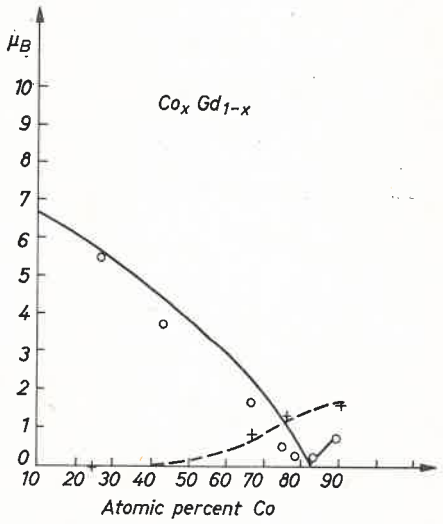


Fig. 2

Fig. 1. Concentration dependence of the saturation magnetic moments of $Fe_xGd_{1-x}$ alloy (——— — theory, ○ — experiment) and Fe ion (– – – — theory, + — experiment)

Fig. 2. Concentration dependence of the saturation magnetic moments of $Co_xGd_{1-x}$ alloy (——— — theory, ○ — experiment) and Co ion (– – – — theory, + — experiment)

for Fe and 1.4 to 1.8 for Co assumed by Hasegawa and Kanamori [4]. There are also some ambiguities about exchange coupling $J$. Burzo has estimated from his experimental data that $J_{s-f} = 0.24$ eV and $J_{d-f} = -0.05$ eV, on the other hand, Gomes and Guimaraes [8] suggested that $J_{s-f}$ is of the order 0.05 eV. In these circumstances, our assumption that

$J = 0.24$ eV for both alloys seems quite reasonable. The assumed band half-widths of a pure transition metal $|\alpha_T|^2$ and gadolinium metal $|\alpha_R|^2$ are 1 and 3.5 respectively in our energy units. We also put $S = 3.5$ and $g = g' = 2$. All our calculations are performed at $T = 0°K$.

In Figs 1 and 2 we present the results of numerical calculations of saturation magnetic moment per atom of alloy as given by Eq. (21) and magnetic moment of the transition metal ion (Eq. (19)) in comparison with experimental data taken from review papers by Taylor [2] and Burzo [7]. It is seen that in spite of the simplicity of our model and rough approximations qualitative agreement is quite satisfactory. It should be stressed that some of the parameters of the model ($\varepsilon_i$, $U_i$ and $|\alpha_i|$) were chosen to obtain the best fit of the calculations to the experimental data. They differ slightly from values used by other authors studying e. g. transition metal alloys. This is due to not the quite realistic density of states function and the neglecting of the spin-flip scattering of electrons on localized spins. We hope that if some of the deficiences of our theory are removed, better agreement will be obtained.

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