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AMORPHOUS AND SPIN GLASSES.

Random magnetic anisotropy in amorphous alloys containing rare earth atoms: some recent developments

R. Ferrer, R. Harris, S. H. Sung and M. J. Zuckermann

Rutherford Physics Building, McGill University, Montreal, Canada

Abstract. — The HPZ model for random magnetic anisotropy in amorphous alloys containing non-5-state rare earth ions is analysed in detail. Magnetisation calculations using this model in conjunction with the molecular field approximation (MFA) and the Oguchi pair approximation (OPA) are presented and discussed for both ferro- and antiferromagnetic exchange coupling. The analysis of Callen et al. for hysteresis effects in amorphous alloys using the HPZ model is related to the results of Monte Carlo calculations for both ferro- and antiferromagnetic exchange coupling.

Résumé. — Le modèle HPZ relatif à l'anisotropie magnétique aléatoire dans les alliages amorphes est analysé en détail. Quelques calculs d'aimantation sont présentés et discutés en utilisant le modèle HPZ dans l'approximation du champ moléculaire et l'approximation des paires corréllées d'Oguchi, pour des interactions d'échange ferro- et antimagnétiques. L'analyse de Callen et al., qui traite des effets d'hystérésis dans les alliages amorphes, sera comparée aux résultats des calculs du type Monte Carlo pour les deux interactions.

The structure of amorphous rare-earth-transition metal/noble metal alloys is reasonably described by dense random packing of hard spheres (DRPHS) of two sizes [1, 2]. The present article examines the effect of such structures on the magnetic properties of those alloys whose rare earth component is a non-S-state (J ≠ S) magnetic ion. In this case the distribution of point charges of different values on each component atom gives rise to a set of randomly oriented easy axes of magnetisation at each rare earth site [1]. The distribution of these axes has been shown to be random for the DRPHS cluster of Cochran et al. [1]. This type of magnetic anisotropy (RMA) will be called random magnetic anisotropy in contrast to magneto-crystalline anisotropy for which there is a small number of easy directions. Cochran et al. [3] used the same cluster in conjunction with the Wigner-Eckart theorem to show that the quantum mechanical Hamiltonian describing RMA could be written as:

$$\mathcal{H}_{\text{an}} = - \sum_i A_i J_{zi}^2,$$  

where \(z_i = (x_i, y_i, z_i)\) and describes a local set of coordinate axes at the rare earth site and \(J_{zi}\) is the \(z_i\)th component of the total angular momentum vector \(J\) describing the rare-earth moment. The coefficients \(A_i\) give rise to a broad distribution of total splittings of the 4f-multiplet of \((2J + 1)\) states. Fert and Campbell [4] showed that for rare earth ions with large \(J\) (i.e. for heavy rare earths), random uniaxial anisotropy gives an excellent approximation to the Hamiltonian of (1)

$$\mathcal{H}_{\text{an}} = - D \sum_i J_{zi}^2.$$  

This is the form of the model Hamiltonian for RMA first proposed by Harris, Plischke and Zuckermann [5] and will be referred to as the HPZ model.

The magnetic interaction between the rare earth moments is taken to be a Heisenberg interaction. The total Hamiltonian for the HPZ model can then be written as:

$$\mathcal{H} = - D \sum_i J_{zi}^2 = \tilde{\Theta} \sum_{\{i,j\}} J_i J_j - g\mu_B H \sum_i J_{zi}.$$  

Here \(\tilde{\Theta}\) is the coupling constant of the exchange interaction. \(H\) is the external magnetic field taken to be in an arbitrary but fixed direction labelled the \(z\)-direction.

The HPZ Hamiltonian (3) will be analyzed using three approximations: the molecular field approximation (MFA) in both the quantum and classical limits, the Oguchi pair approximation (OPA) in the quantum mechanical case and the Monte Carlo method of calculation (MC) in the classical limit. The results of numerical calculation are presented for each type of approximation for both ferro- and anti-ferromagnetic exchange coupling and comparison with experiment is made where possible.

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1. Molecular Field Approximation (MFA). — In the MFA the HPZ Hamiltonian (3) can be written for ferromagnetic coupling $\gamma > 0$ as:

$$\mathcal{H}^{MFA} = -\mathbf{D} \sum_i J_{iz}^2 - g\mu_0 \sum_i H^{mol} J_{iz},$$

where

$$H^{mol} = 2 v \bar{J}_z/g\mu_0 + H,$$

$v$ is the average number of nearest neighbour rare-earth ions and $\langle \cdots \rangle$ implies both a thermal average and an average over the random angles $\theta_i$ between the local easy axes $z_i$ and the $z$-axis. The averaging process is described in detail in a review article by Cochrane, Harris and Zuckermann [6] and the reader is referred to this article for further information.

Comprehensive studies of amorphous alloys with the rare-earth atom as the only magnetic component were first performed by Boucher [7] who obtained low temperature magnetisation data for REAg (RE = Tb, Dy and Ho) amorphous alloys. In order to compare the HPZ theory with experiment the Hamiltonian of (4) is diagonalized for ferromagnetic exchange coupling $\gamma > 0$ and for a given value of $J$ ($J = 6, 15/2$ and $8$ for Tb$^{3+}$, Dy$^{3+}$ and Ho$^{3+}$ respectively), yielding a self consistent calculation for the magnetisation. Solving this equation at a fixed temperature and averaging over $\theta_i$ gives the reduced magnetisation as a function of applied field. The results and the comparison with Boucher’s pulsed field data [8] are shown in figure 1 and computed values for $D$, $J$ and the Curie temperature are given in ref. [8].

![Graph showing reduced magnetisation as a function of applied field](image1)

Fig. 1. — Reduced magnetisation as a function of applied field at 4.2 K calculated from the random-anisotropy model for the values of $D$ and $\gamma$ of ref. [8] (solid curves), and the experimental results of Boucher (crosses). A) HoAg; B) TbAg; C) DyAg.

The molecular fields $H^A_{mol}$, $H^B_{mol}$ are written as follows:

$$H^A = -v \bar{J}_z \mathbb{J}_z + H$$

$$H^B = -v \bar{J}_z \mathbb{J}_z + H$$

where $v$ is the average number of rare earth neighbours.

Use of equations (6) and (7) enable us to calculate the magnetisation $M(H)$ as a function of $H$ and the susceptibility $\chi$ as a function of temperature in the amorphous antiferromagnetic state [9]. These are shown in figures 2 and 3. Figure 2 indicates the existence of a spin flip transition between the amorphous antiferromagnetic state and an amorphous ferromagnetic state at a critical field $H_{cr}(T)$ which decreases with $\alpha$, where $\alpha = D/v |\bar{J}_z|$ measures the anisotropy strength for fixed exchange. The curve

![Graph showing zero temperature magnetisation as a function of external magnetic field](image2)

Fig. 2. — The zero temperature magnetisation as a function of external magnetic field of the amorphous antiferromagnetic state for several values of $\alpha$. Here $J = 15/2$, $T = 2$ K and $\bar{J}_z = -0.45$ K for all curves.

![Graph showing magnetic susceptibility as a function of temperature](image3)

Fig. 3. — The magnetic susceptibility as a function of temperature for antiferromagnetic coupling for: A) the amorphous antiferromagnetic state; B) the equivalent crystalline antiferromagnetic state. The parameters used were: $J = 15/2$, $D = 3$ K, $\bar{J}_z = -0.45$ K.
of $X_R$ versus $T$ in figure 3 for the amorphous antiferromagnetic state is very similar in shape to curves of the magnetic susceptibility found for various equilibrium spin glass models.

2. Oguchi Pair Approximation (OPA). — The Oguchi pair approximation is described in detail in Smart’s book [10] and the reader is referred to references [11] and [12] for its application to the HPZ model. Figures 4 and 5 show the results of numerical calculation (see [11]) for the spontaneous magnetisation in the HPZ model using the OPA for ferromagnetic coupling. Application of the OPA to antiferromagnetic coupling is due to Bhattacharjee and Coqblin [12] who were the first to analyse this case. Their results are qualitatively the same as those of reference [11].

3. Monte Carlo calculations. — In this section some of the results using the Monte Carlo (MC) in conjunction with the HPZ Hamiltonian [3] are reported and compared with other work. The calculations were performed at $T = 0$ using an assembly of $512 (8 \times 8 \times 8)$ classical spins on a simple cubic lattice with periodic boundary conditions.

This choice was made because the essential feature of the Hamiltonian is the RMA and therefore the real space amorphous structure is unimportant for a first approximation. The reader is referred to reference [13] for details of the calculation and for relevant references.

The results of the MC calculations are shown in figures 6, 7 and 8. The curves labelled « SG » in figures 6 and 8 refer to spin glass like states and the curve labelled « AF » in figure 8 is obtained by taking the demagnetised state to be antiferromagnetic. It should be noticed that, for high enough $D$, the MC results are close to the results of Callen et al. [14] which were obtained by using the classical MFA version of the HPZ model.

We conclude with several comments:

(a) One important result of the MC calculation is that the demagnetised state in the alloys under consideration is described by spin glass like states rather than a domain structure [13, 15]. Such spin
glass-like states are metastable states which are responsible for the initial magnetisation curves marked by «SG» in figures 6 and 8. Figure 8 also indicates that the spin flip transitions described by the curve marked «AF» in figure 8 cannot give a description of the initial magnetisation since the «AF» curve partially lies outside the hysteresis loop.

(b) The spin flip critical field \(H_{SF}\) as calculated using both the MC technique [15] and the classical MFA of Callen et al. [14] increases with \(D/|J|\), whereas we have shown above that \(H_{SF}\) calculated in the quantum MFA decreases with \(D/|J|\). This appears to be due to the fact that the quantum MFA is strictly concerned with the equilibrium ground state of the HPZ model, whereas the classical calculations include metastable states which give rise to hysteresis effects [14]. This point will be discussed in detail in a future publication.

(c) The resemblance between the hysteresis loop of figure 8 and the experimental data for TbAg of [7] should be construed as a qualitative indication that perhaps both antiferro- and ferro-magnetic exchange are present in these alloys. However the nature of the real space structure of amorphous metallic alloys would most likely tend to frustrate the formation of an antiferromagnetic ground state and hence a cluster calculation is necessary to examine the effects of anti-ferromagnetic exchange in detail. This problem is at present under consideration.

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