COERCIVITY MECHANISM OF MELT-SPUN $Sm(Fe_{11}Ti)$

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Abstract

Hysteresis loops of randomly oriented grains with uniaxial anisotropy were computed on the basis of an array of 27 Wigner Seitz cells representing crystallites which interact by exchange coupling at the grain boundaries. The computed coercivity increases linearly with increasing interatomic exchange. Using the experimental anisotropy and exchange parameters for $Sm(Fe_{11}Ti)$, we found $\mu_0 H_c$=1.2 T in good agreement with results on melt-spun ribbon. The main insight is that strong intergrain coupling is beneficial for developing coercivity in nanocrystalline alloys with uniaxial anisotropy.

1. INTRODUCTION

The aim of this study is to gain a better understanding of the mechanism responsible for the coercivity of nanocrystalline alloys with strong uniaxial anisotropy. An example of this type of material is a melt-spun ribbon of $Sm(Fe_{11}Ti)$ which is composed of randomly-oriented crystallites with average diameter ($\approx$50 nm), smaller than or comparable to the critical diameter for single-domain structure [1,2]. There is no secondary intergranular phase. The shape of the magnetization curves is similar to that predicted by the Stoner-Wohlfarth (S-W) model of non-interacting single domain particles, but magnitude of the observed coercivity B_c is an order of magnitude less than the S-W model prediction. The S-W model assumes the system adopts a metastable state, so that each monodomain grain exhibits a coercivity equal to the anisotropy field H_a. However such large coercivities are not found in practice. When only the energy minimum state is considered, there is zero coercivity for each monodomain grain, and interactions between the monodomain grains then play the decisive role in determining H_c. In other words, the coercivity is the collective property of the system of interacting grains.

We recently considered the analogy between the magnetization of a single-domain grain and a spin in an amorphous material with random axial anisotropy (HPZ model[3]). Transposing the extensive results of computer simulations on the HPZ model, we found that H_c should vary as the interatomic exchange coupling, and increase as the inverse crystallite size in the nanocrystalline case [2]. In order to further investigate the dependence of H_c on exchange and anisotropy, we have now carried out computer simulation on a realistic model of the grain configuration.

2. MODEL AND CALCULATION

2.1 Grain Generation

We used a 343,000 point face-centered cubic array as the basis of the simulation. First, 27 seed points were chosen at random, and the Wigner Seitz cells (grains) were grown around each of them using an algorithm which searches for those lattice points in ever-increasing spheres which are closest to a particular seed point. Periodic boundary conditions are applied. A histogram showing the distribution of the number of lattice points in the 27 grains is shown in Fig. 1. The number of nearest neighbour-pairs crossing the interfaces between grains was evaluated for each one of the grains. It is on average 11 % of the number of nearest neighbour pairs within the grains. Next, an anisotropy direction is randomly assigned to each grain. The arrangement is shown schematically in Fig. 2. Only the small fraction of nearest neighbour exchange bonds that cross an interface (grain boundary) are active in coupling the grains together and there is competition between these exchange interactions and the different anisotropy directions on either side of the interface.

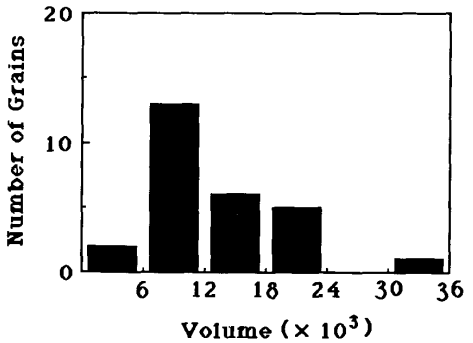

Fig. 1 Distribution of volumes (numbers of lattice points) of the array of grains used in the simulation.

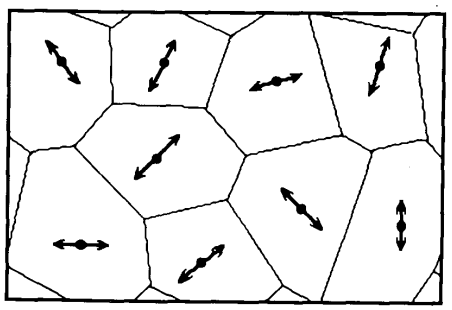

Fig. 2 Schematic representasion of the grains used in the simulation. Each grain has a randomly oriented uniaxial anisotropy axis indicated by the double arrow.

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2.2 Coercivity for Strongly Coupled Grains

In our simulation, we abandon the S-W approach entirely; the difference between the S-W model and the present model is illustrated in Fig. 3. focussing on an isolated single domain grain, the S-W model allows the grain to adopt a metastable energy state which leads to coercivity. However in our model the direction of the grain magnetization, obtained by assuming uniform rotation within the grain, always corresponds to the energy minimum, so the isolated grain has no coercivity.

When the single domain grain is surrounded by neighbours, and the exchange coupling between the grain and the surrounding grains is taken into account, the situation for the grain is changed as illustrated in Fig. 4. Again focussing on a single grain, one now distinguishes two fields which act on it, the external field $\mathbf{H}_0$ and the exchange field $\mathbf{H}_{ex}$. The direction of the effective local field $\mathbf{H}_{local}$, which determines the direction of the moment, is obtained as the sum of these two. Plotting the magnetization of the grain as a function of the external field, the magnetization curve is shifted along the field axis. On calculating the ensemble average for the grains in the system, the coercivity is obtained.

In this calculation, we assume the following free energy for each grain j

$$E^j = E^j_{ex} + E^j_a + E^j_m. \qquad (1)$$

The first term is the effective exchange energy between grains assumed to be governed by the interatomic exchange interaction of Fe atoms located at the surface of adjacent grains:

$$E^j_{ex} = -\mu_0 \mathbf{H}^j_{ex} \cdot \mu_j, \qquad (2)$$

where

$$\mathbf{H}^j_{ex} = \frac{J_{FeFe}}{12 n_j} \sum_{i(nn)} n^{ij}_p \, S_i. \qquad (3)$$

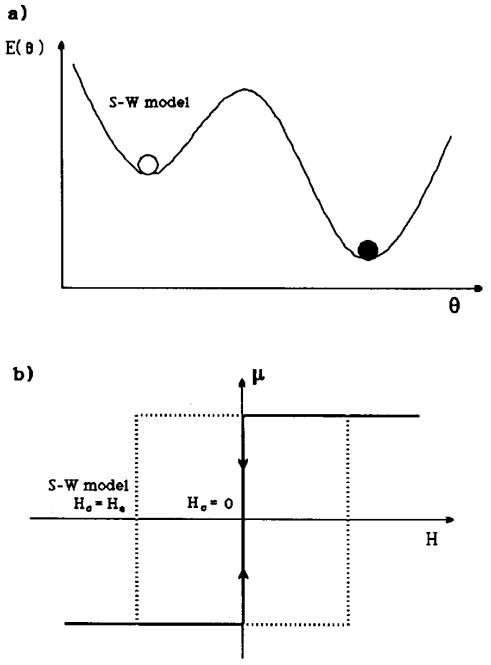

Fig. 3 (a) Free energy E of the single domain grain as a function of the angle θ between the easy axis and the moment. The open circle shows the metastable state used in the S-W model and the solid circle shows the stable state used in our model. (b) The S-W model yields the hysteresis loop with $\mu_0 H_c = \mu_0 H_a$ whereas our model shows no coercivity.

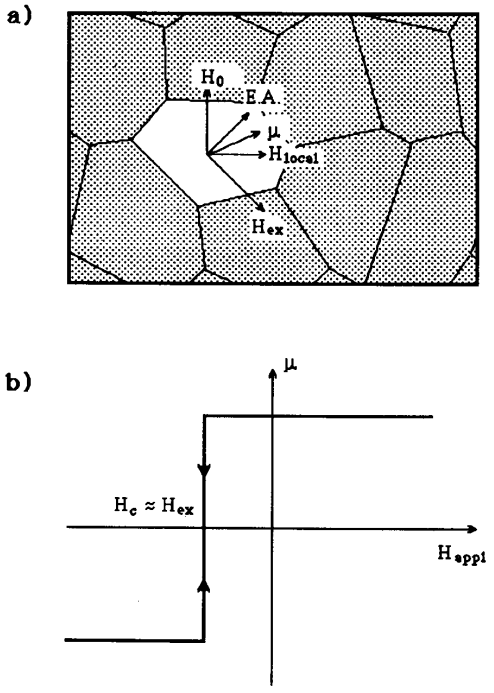

Fig. 4 Schematic illustration of the relation between the applied field $\mathbf{H}_0$, the exchange field $\mathbf{H}_{ex}$, the local field $\mathbf{H}_{local}$, the easy axis E.A. and the magnetization μ of the grain.

In Eqs. 2 and 3, $\mathbf{H}^j_{ex}$ is the exchange field, μ_j is the magnetization of the grain j expressed as $\mu_j = n_j g \mu_B \mathbf{S}_j$, where n_j is the number of the spin within the grain and $\mathbf{S}$ is the classical spin vector, J_{FeFe} is the Fe-Fe interatomic exchange coupling constant, n^{ij}_p is the number of the nearest neighbour pairs located at the interface between the grain j and its nearest neighgour grains and the factor of 12 is the average number of nearest neighbour grains.

The second term is the magnetocrystalline anisotropy energy:

$$E^j_a = n_j D \sin^2\theta_j , \qquad (4)$$

where θ_j is the angle between $\mathbf{S}_j$ and the anisotropy axis of the grain. D is the anisotropy constant. The third term is the magnetic energy in an external magnetic field $\mathbf{H}_0$:

$$E^j_m = -\mu_0 \mathbf{H}_0 . \mu_j . \qquad (5)$$

In order to calculate the interesting quantities such as coercivity and hysteresis loops, the energy E^j is first minimized as E^j_{min} and it follows that the total energy for the array of 27 grains is given by

$$E_{tot} = \sum_j \left(E^j_{min} + \frac{1}{2} \mu_0 \mathbf{H}^j_{ex} . \mu_j \right), \qquad (6)$$

where the second term is included to take account of double counting. For a given external field $\mathbf{H}_0$, the magnetic configuration of the array is determined by iteration giving a self-consistent set of {S}.

3. RESULTS AND DISCUSSION

A series of hysteresis loops calculated, using D=5 K and J_{FeFe}=1.5, 2.5, 5 and 10 K is shown in Fig. 5. There is a sharp collective reversal of most of the magnetization at a well defined field H_c, which is proportional to J_{FeFe} (Fig. 6). The most interesting point is that the coercivity is very much less than the anisotropy field (D=5 K implies $\mu_0 H_a$=10 T). So the intergranular interactions have the effect of reducing the coercivity below the S-W prediction, $H_c = H_a$. The measured value of J_{FeFe} from Curie temperature for the case of $Sm(Fe_{11}Ti)$ is 10 K, which corresponds to a coercivity of 1.5 T. The observed coercivity in nanocrystalline melt-spun $Sm(Fe_{11}Ti)$ is 0.6 T at room temperature, and 1.2 T below 50 K which is in good agreement with our (zero temperature) prediction. Our model clearly suggests that the way to improve the coercive field is to increase the effective coupling between the grains which can be achieved in a given material by reducing the grain size.

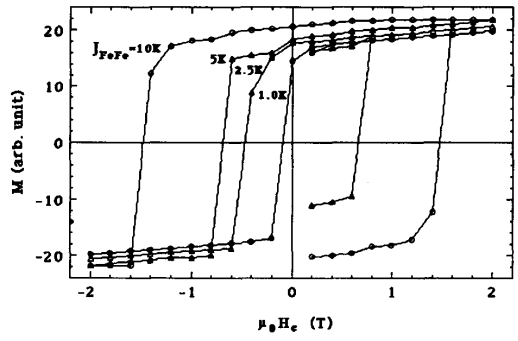

Fig. 5 Calculated hysteresis loops for different exchange constants J_{FeFe}.

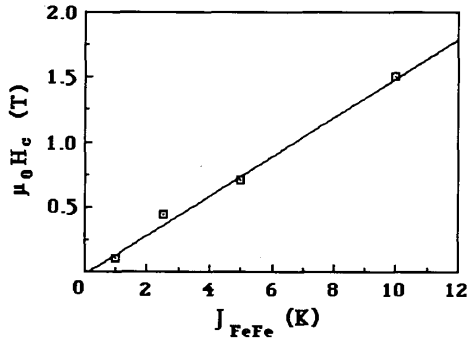

Fig. 6 The relation between the exchange constant J_{FeFe} and the computed coercivity $\mu_0 H_c$, indicating that these quantities are proportional.

Acknowledgments

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