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Coercive mechanisms in ferromagnetic-antiferromagnetic bilayers

Zhanjie Li and Shufeng Zhang

Department of Physics and Astronomy, University of Missouri–Columbia, Columbia, Missouri 65211

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The magnetization reversal of polycrystalline ferromagnetic-antiferromagnetic bilayers is investigated by employing the Landau-Lifshitz-Gilbert equation. The magnetic interaction at the interface is modeled by a random field. It is found that the random field breaks the ferromagnetic layer into domains during magnetization reversal. The domain size is usually much smaller than that without the underlying antiferromagnetic layers. We quantitatively determine the enhanced coercivity as a function of the thickness of the ferromagnetic layer, the grain size, and the interface random field.

An exchange interaction at the interface of a ferromagnetic (F) and an antiferromagnetic (AF) layer results in several unique macroscopic magnetic properties. Among many distinct experimental observations, the most interesting properties are the shifted hysteresis loop and enhanced coercivity of the ferromagnetic layer.[1] To understand the shifted loop theoretically, a convenient scheme is to saturate the ferromagnetic layer and then to rotate the magnetization in the plane[2] so that one can avoid complicated reversal mechanisms. Indeed, most of the theoretical models assume a single domain state of the ferromagnetic layer and focus on the domain structure of the AF layer for different types of interfaces. Mauri *et al.*[3] considered the AF domain wall formation of a perfect uncompensated interface during the coherent rotation of the F layer. Koon,[4] as well as Schulthess and Butler[5] find some interesting spin-flop states for a perfect compensated interface, which will effectively contribute a uniaxial anisotropy to the ferromagnetic layer. Other theories[2,6–10] of the exchange bias also assume a uniform magnetization of the F layer.

While the assumption of a uniform magnetization of the F layer greatly simplifies the problem and might be sufficient to understand the hysteresis loop shift, it masks important details during the magnetization reversal of F/AF bilayers. In particular, the enhanced coercivity observed in almost all F/AF bilayers can not be quantitatively derived from the model of coherent rotation of the magnetization. In fact, it has been pointed out that the single-domain character of a magnet is largely irrelevant to the problem of coercivity in general.[11] Recently, several experiments have begun to study detailed domain structures in a F/AF bilayer.[12] For example, the ferromagnetic domain size during magnetization reversal has been observed to be much smaller in an exchange biased bilayer than in a single F layer without the exchange bias.[13] The domains can be as small as the grain size when the F layer thickness is small.[14] These observations indicate that the formation of small domains is crucial to understand the magnetization reversal or the hysteresis of the F/AF bilayer. In this paper, we investigate the magnetic reversal of the exchange coupled bilayer without assuming a uniform magnetization of the F layer. Instead, we compute these domains from various competing interactions in the bilayer. With our model, the enhanced coercivity can be explicitly related to the *experimentally controllable parameters* such as the thickness of the F layer and the grain size of the AF layer. In addition, we have obtained some useful scaling relations.

We start with a Hamiltonian of a bilayer

$$H = E_F^e + E_F^a + E_{AF}^e + E_{AF}^a + E_d + E_Z + E_{int}, \tag{1}$$

where the first two terms represent the exchange and anisotropy energy of the F layer, and the third and fourth terms are those for the AF layer. E_d is the magnetostatic energy, E_Z is the Zeeman energy due to the external magnetic field, and the final term is the interaction between AF and F spins at the interface. The magnetic hysteresis of the above Hamiltonian is obtained via solving the standard Landau-Lifshitz equation with the following procedures. The sample was laterally divided into $N\times N$ blocks. Each block represents a grain which consists of $n\times n$ atomic spins in each plane parallel to the the interface so that the grain size is $D = na_0$, where a_0 is the lattice constant. We have found that as long as N is large enough, the calculated results will be independent of N. In our case, $N=20$ is sufficient. Within each grain, the ferromagnetic layer is assumed to be a single domain state. The exchange energy between the nearest-neighbor ferromagnetic blocks scales as $E_F^e = -J_F(t_F/a_0)S^2\mathbf{S}_i^F\cdot\mathbf{S}_j^F/n^2$, where t_F is the thickness of F layer, J_F is the microscopic exchange constant, S is the atomic spin, $\mathbf{S}_i^F$ represents a unit vector along the direction of the magnetization of the i^{th} block, and we have assumed a linear variation of the moments from one block to the next. The anisotropy energy E_F^a is assumed uniaxial $E_F^a = K_F t_F \sin^2\theta_i$, where θ_i is the angle between the direction of the magnetization and the easy axis. In the AF layer, we define two unit vectors $\mathbf{S}_{i1}^{AF}(k)$ and $\mathbf{S}_{i2}^{AF}(k)$ to represent the directions of the magnetization of the two sublattices, where k labels k^{th} atomic plane in the AF layer. The exchange interaction in the AF is the sum of the contributions within a grain and between the grains, $E_{AF}^e = \Sigma J_{AF}\mathbf{S}_{i1}^{AF}\cdot\mathbf{S}_{i2}^{AF} + \Sigma J'_{AF}[\mathbf{S}_{i1}^{AF}\cdot\mathbf{S}_{j2}^{AF} + \mathbf{S}_{j1}^{AF}\cdot\mathbf{S}_{i2}^{AF}]$, where we only consider the nearest AF exchange coupling between two sublattices. The summation is over all the sublattice sites including the interlayer exchange coupling of each AF grain, and J'_{AF} is the intergrain AF coupling (we will take $J'_{AF} = J_{AF}/n$). The anisotropy energy of the AF layer is $E_{AF}^a = K_{AF}\sin^2[\theta(k)-\theta_i]$, where θ_i is the anisotropy axis of ith grain and $\theta(k)$ is the magnetization direction for either of two AF sublattices. We will take an isotropically random anisotropy axis within the plane of the layer to model a polycrystalline film. The demagnetization energy takes a simple form $E_d = 4\pi(t_F/a_0)M_s^2(S_i^{Fz})^2$ where the z axis is normal to the planes. Since we have used a model of a linear variation of the magnetization between the neighboring F blocks, the magnetostatic interaction at the grain boundary is negligible. The Zeeman term is written as $E_Z = -\mu_B \Sigma_{ik}[\mathbf{S}_{i1}^{AF}(k) + \mathbf{S}_{i2}^{AF}(k)] \cdot \mathbf{H} - \mu_B S(t_F/a_0)\Sigma_i \mathbf{S}_i^F \cdot \mathbf{H}$, where H is the external magnetic field and μ_B is the Bohr magneton.

The interaction between the F and AF layer, E_{int}, is least known. The present model is based on the general idea of random fields in the presence of impurities.[15] The application of this random-field picture to the exchange interaction of F/AF interfaces was first proposed by Malozemoff[7] who has shown in a great detail that the random interaction is a valid model to describe the exchange interaction in the presence of the interfacial roughness. We adopt this random field to model the interface interaction throughout this paper. Introducing two random numbers r_1 and r_2 which are bounded between -1 to 1, we write the interface energy as

$$E_{int} = -J_s \sum_i r_1 \mathbf{S}_i^F \cdot [(1 + r_2/n)\mathbf{S}_{i1}^{AF}(1) + (1 - r_2/n)\mathbf{S}_{i2}^{AF}(1)], \tag{2}$$

where J_s characterizes the average microscopic exchange constant between the first atomic plane of the AF layer ($k = 1$) and that of the F layer. The first random number r_1 represents the random exchange interaction between the nearest-neighbor sites of F and AF layers at the interface. We will show below that it is this random interaction which controls the enhanced coercivity of F/AF bilayers. The second random number in Eq. (2), r_2, characterizes the finite-size effect of the grains, i.e., the numbers of the two sublattices for a given grain are statistically fluctuated. Their difference (normalized by the total number of spins) scales as $1/\sqrt{n \times n} = 1/n$. In fact, we will illustrate that the finite grain size is the main parameter to control the exchange shift.

We first comment on the general features of the calculated magnetic reversal by taking the intrinsic parameters such as J_F, J_{AF}, K_{AF} from commonly quoted values of bulk NiFe and CoO.[5] Due to the large AF anisotropy constant, the magnetic moments of the AF sublattices only changes slightly and the spin-flop transition does not occur during the hysteresis cycle. The competition of the interlayer coupling in AF layers and the interface random exchange energy leads to small angle variation between different AF monolayers (typically only a few degrees). We also find that the weak intergrain coupling (J_F') does not significantly change the calculated magnetic properties given below. The ferromagnetic layer reversal is mainly controlled by two energy terms, the ferromagnetic exchange interaction between neighboring ferromagnetic blocks and the random field acting on a ferromagnetic block due to interfacial interactions. If the former is much stronger than the latter, ferromagnetic blocks are aligned together and the ferromagnetic domains are much larger than the grain size. Then the net coercive force (random fields from the AF gains) acting on the ferromagnetic layers is averaged out and one would have a smaller enhanced coercivity on the F layer. If the interface interaction is stronger than the ferromagnetic coupling, the domain size of the ferromagnetic layer during magnetic reversal will not be much larger than the grain size. In this case, each ferromagnetic domain receives different random fields from the AF layer, and, due to fluctuation of the random field from each grain, the reversal will take place at different external fields for different ferromagnetic domains. Therefore the breakup of the ferromagnetic layer into small domains is essential for the increased coercivity. This general picture is quantitatively supported by the following detailed variation of the coercivity with respect to the thickness of the ferromagnetic layer, the grain size, and the interface interaction.

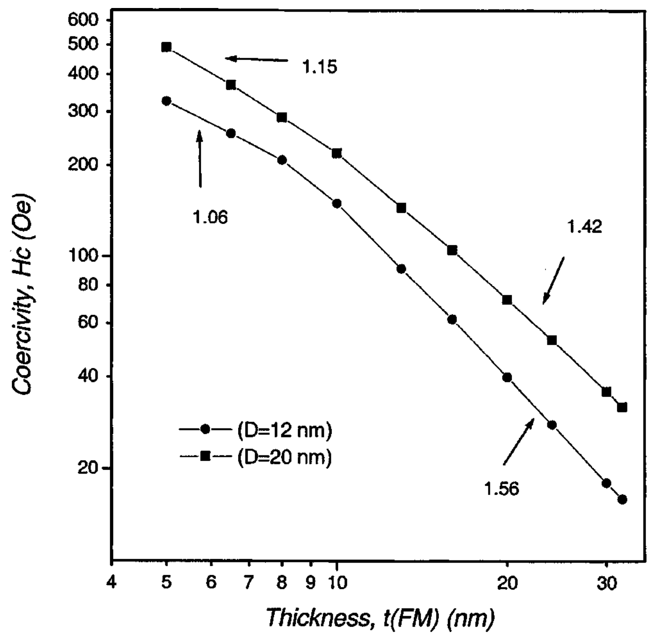

FIG. 1. Coercivity as a function of the thickness of a ferromagnetic layer for two grain sizes $D = 12$ nm and $D = 20$ nm. The slopes of the curves are indicated by the arrows. The parameters are the same as those used in Ref. 5: $J_F = 16$ mev, $J_s = 2$ mev, $J_{AF} = 2$ mev, and $K_{AF} = 3$ mev. The demagnetization field of NiFe is $4\pi M_s = 8300$ Oe.

The ferromagnetic domain size L can be estimated roughly by equating the ferromagnetic exchange energy and the random field energy. The exchange energy per unit area scales as $\frac{1}{2}(t_F/a_0)J_F/L^2$. The random field energy is the statistically averaged energy of $N = L^2/a_0^2$ spins within a domain, which scales as $(J_s/a_0^2)/\sqrt{N} = J_s/a_0 L$. By minimizing these two energies, we find the domain size is about $L = t_F J_F/J_s$. This size is comparable to the grain size when the thickness of the F layer is of the order of 100 Å. We note that the same reasoning was applied by Malozemoff to estimate the AF domain size.[7]

In Fig. 1, we show the coercivity of the ferromagnetic layer for a fixed interfacial random field. We have used the CoO anisotropy energy $K_{AF} = 3$ mev per site.[5] For such a large anisotropy constant, the domain wall width in the AF layer will be small. The calculated coercivity will be independent of the AF layer thickness as long as it exceeds five monolayers. For smaller K_{AF}, one would need a thicker AF layer to simulate the coercivity. The calculated coercivity depends slightly on the anisotropy constant of the AF layer.

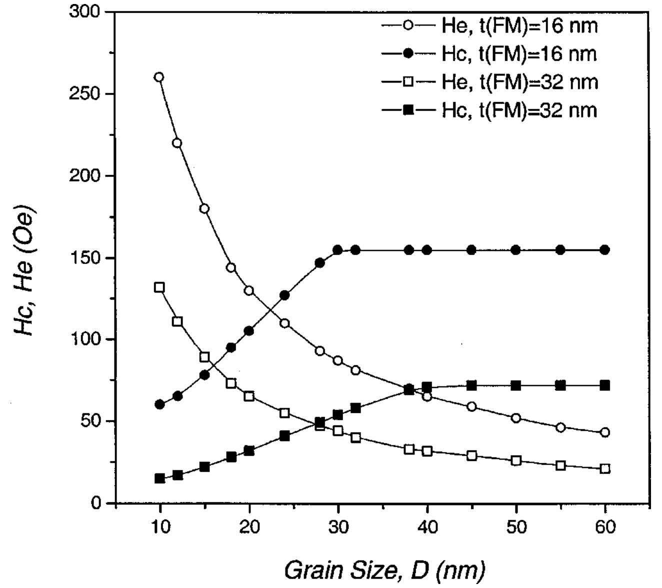

FIG. 2. Coercivity H_c and loop shift H_e as a function of the grain size for two different F layer thicknesses. The parameters are the same as in Fig. 1.

The dependence of the coercivity on the F layer thickness is rather strong, and it approximately satisfies a power law. We can understand the result in terms of the picture described in the last paragraph. Since the ferromagnetic coupling between two neighboring blocks is proportional to the thickness of the F, larger thicknesses produce larger domain sizes in the F layer. For larger domains, the average of the random field (per site) is small. Thus the coercivity decreases. For a small thickness, e.g., below 8 nm, the ferromagnetic layer breaks into domains whose size is not too much larger than the grain size. This is the situation when the coercive energy from the random field ceases to increase even if the thickness is further reduced, because the minimum size of the domain is limited by the grain site. It is thus reasonable that the coercivity scales with the F layer thickness as $H_c \propto t_F^{-\alpha}$ with α nearly one (note that the random field is only acting on the interface—thus $\alpha=1$). When one increases the thickness beyond 8 nm in the figure, the domain size of the F layer begins to grow and the coercive energy decreases faster than $1/t_F$. In this case, α is approximately 3/2. This scaling relation has been suggested earlier from a general argument and it has been experimentally verified.[16]

In Fig. 2, we show both the hysteresis shift and coercivity as a function of the grain size. It is expected that the loop shift is inversely proportional to the grain size. This is because the average of the random field per unit area within a grain is inversely proportional to the grain size, as it was first pointed out by Takano *et al.*[17] The coercivity shows quite interesting behavior. Upon increasing the grain size, the effective interaction between the ferromagnetic blocks decreases as $E_J \propto 1/D^2$. Thus the domain size of the F layer is much larger than the grain size when the grain size is small, and it becomes comparable when the grain size reaches 40 nm. When the grain size is more than 40 nm, the coercivity stays at its maximum value. We point out that the magnetic structure within a grain could be quite complicated when the size of the grains is equal to or larger than the domain wall width. To model the spin structure within a grain, one should in principle choose ferromagnetic meshes whose size is sufficiently small. In our model we have neglected these complicated spin structure within grains, i.e., we have assumed that the spin structure is linearly varied from one grain to the next. However, the general trend shown in Fig. 2 on the variation of the coercivity as a function of the grain size remains qualitatively correct.

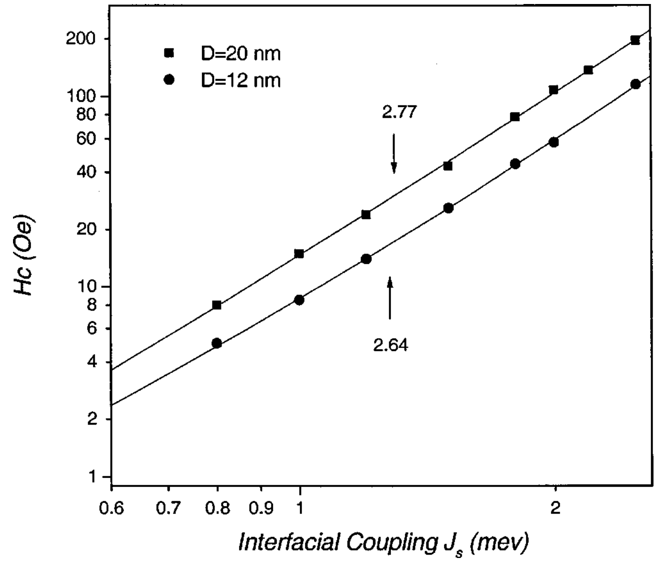

FIG. 3. Coercivity as a function of interface coupling strength J_s for two different grain sizes. The arrows indicate the slopes of the curves. The parameters are the same as in Fig. 1.

In Fig. 3, we show the coercivity as a function of the interface random fields. From the above argument, a stronger interface interaction will lead to a smaller F domain size and thereby a larger enhancement of the coercivity. Experimentally, the variation of the interface coupling can be controlled by inserting a wedged Cu or Ag layer at the F/AF interface so that one can quantitatively compare this prediction with experimental data.[18]

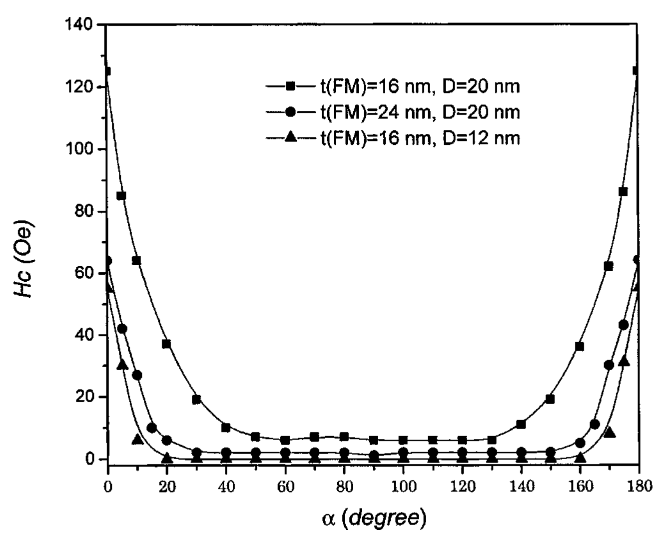

FIG. 4. Angular dependence of the coercivity for two F layer thicknesses and two domain sizes. The parameters are the same as in Fig. 1.

Finally we address the angular dependence of the coercivity. We first apply a large external magnetic field in the x direction to simulate the cooling direction. Then the magnetic field is reduced to zero. This remanent state is our initial state to perform the calculation of the angular dependence of the hysteresis when an external field is applied in a direction which makes an angle α with respect to the x axis. The calculated magnetization always refers to the direction of the applied field. When we change to a different angle of the applied field, we repeat back to the the initial remanent state. Figure 4 shows the calculated results for two F layer thicknesses. The angular dependence of the coercivity clearly indicates that the coercivity only appears in a very narrow range of angles of the cooling field. This is a quite different from the unbiased ferromagnetic film in which the Stoner Wohlfarth model gives a much larger range of angle. Figure 4 is in qualitative agreement with experimental observations.[19] Note that we have set the F layer anisotropy constant equal to zero so that we do not have a background coercivity. Experimentally, there is always a small coercivity even for $\alpha=90°$; the origin of the finite background value may come from the finite F layer anisotropy and the dipolar interaction between ferromagnetic domains.

In summary, we have incorporated a random field at a F/AF interface into Landau-Lifshitz equation. The presence of the random field results in the formation of domains in the ferromagnetic layer. There is a new length scale for the ferromagnetic domains associated with two competing interactions: the ferromagnetic exchange and the interface random field. As a result, the ferromagnetic domains are much smaller in exchange biased bilayers. We have shown that the random field model can account for the observed enhancement of the coercivity in F/AF bilayers as a consequence of the formation of lateral domains. We have derived various relations between the coercivity and experimentally controllable parameters.

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