Spin reversal in bilayer ultrathin magnetic films

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We discuss the micromagnetics of two coupled layers of ultrathin films. The spins change from a closure domain arrangement to mostly aligned as the interlayer spacing is decreased. There are remanent domains at the edges which serve as nucleation centers and control the switching behavior in a field. The domain patterns are often changed after a hysteresis cycle, consistent with recent measurement of the giant magnetoresistance in multilayer structures. Different vorticity of the edge domains can lead to very different zero-field remanent domain structures. [S0163-1829(97)03006-3]

I. INTRODUCTION

Stimulated by the success in the growth of magnetic films, there has been much interest recently in incorporating the semiconductor microelectronics technology with magnetic elements.[1,2] One of the potentially important applications of these thin magnetic films occurs in multilayer, tunnel or spin valve structures where the giant magnetoresistance is observed. In this application, the magnetizations on adjacent layers are coupled antiparallel to each other. As an external field is applied, the magnetizations are switched to a parallel configuration and the resistance of the structure is changed. To understand the spin reversal from the antiparallel to the parallel configuration we have studied the physics of two coupled layers with fourfold in plane anisotropy in a sample of rectangular geometry. The highlights of our results are:

(1) When the magnetization is obtained from cooling from high temperatures in zero field, two types of magnetization are observed as a function of the separation of the planes. When they are far apart, closure domains are formed. [An example of a closure domain is shown in Fig. 1(d).] When the planes are close, most of the spins are lined up [Figs. 1(a), 2(a) and 3(a)]. However, *there are still regions close to the edges where domains are formed. The magnetization of these edge domains can be mostly parallel or antiparallel to each other. These domains serve as nucleation centers and control the coercive field of the system*. The energies of these configurations as a function of the interplane separation is shown in Fig. 4.

(2) The switching field is usually different from that determined by considering instability against uniform rotation of the spins, but is determined by the growth of the domains at the edges. Typical hysteresis curves are shown in Fig. 5 for different values of the interlayer exchange coupling. The magnitude of the interplane exchange coupling is deduced experimentally from the switching fields assuming uniform rotation. Our results raise a flag of caution about the precise meaning of these values.

(3) When the system is cycled from a zero-field cooled state to high field and then back to zero field, the domain pattern of the system is often changed. When the edge magnetizations are parallel, the final magnetization of each plane is rotated by 90° [Figs. 2(d) and 3(d)]. When the edge magnetizations are anti-parallel, a metastable closure domain can be formed [Fig. 1(d)]. This may be related to the change of the magnetoresistance after a cycling of the magnetic field.[3] We now describe our results in detail.

II. SIMULATION

In this paper, we reported results from *finite temperature* Monte Carlo (MC) simulations, which is different from the conventional micromagnetics calculation of solving the Landau-Gilbert equation at zero temperature. One of the reasons for introducing finite temperatures is the following. The system can be in different metastable states with different domain shape and distributions. The nature of the domains depends on the past history of the system. In the present study, the system is first annealed at a high temperature ($T=1$) at zero field. The temperature is then brought down (to $T=0.1$) and equilibrated. After this the field is increased gradually to a high value and then brought down and is reversed to a negative large value.

The MC simulation corresponds to solving the master equation for the probability distribution $P(s,t)$:

$$dP/dt=\sum_{s'}\left[-w(s\rightarrow s')P(s,t)+w(s'\rightarrow s)P(s',t)\right].$$

Here the transition probabilities w are picked so that the condition of detailed balance is satisfied; i.e., $w(s\rightarrow s')/w(s'\rightarrow s)=\exp(-\Delta E/kT)$. This relaxational dynamics explores all paths from the initial to the final configuration with rates determined by the free-energy barrier. We thus expect this dynamics to produce the correct free energy of nucleation and the correct switching field but a prefactor in the nucleation rate that may be different from that of a stochastic Landau-Gilbert equation. On the other hand, nonrelaxational oscillation such as those corresponding to spin waves is not expected to be reproduced. Fortunately these oscillations are not questions of interest here.

The simulation reported here follows our earlier work on the equilibrium finite-temperature studies of ultrathin magnetic films[4,5] and on the coercive behavior in thin films[6,7] and nanostructures.[8] It is carried out for a triangular lattice of up to $60\times60\times2$ spins (our previous systematic size studies[7] suggest that this size is big enough) at a finite temperature T under free boundary condition in a rectangular region. The

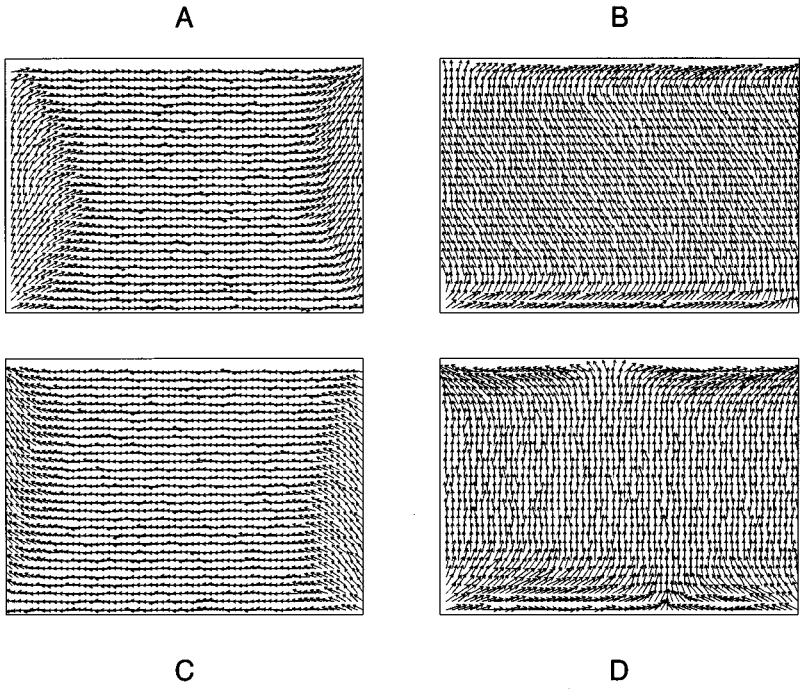

FIG. 1. Spin configurations along a hystersis line at field strengths of 0 (a), upper left, 0.6; (b), upper right, 2.5; (c), lower left and 0; (d), lower right, for an interplanar exchange of 1. A triangular lattice can be viewed as a superposition of two rectangular lattices shifted by a unit translation vector with respect to each other. To save space, only half of the spins on one of the rectangular lattices were shown.

total energy of the system is assumed to be $E_T=E_0+H\Sigma_R S_x(R)$ where the ''internal'' interaction energy between the spins is $E_0=0.5\Sigma_{ij=xyz,RR'}V(R-R')$, where $V=V_d+V_e+V_a$ is the sum of the dipolar energy $V_d(R)=g(\delta_{ij}/R^3-3R_iR_j/R^5)S_i(R)S_j(R')$; the exchange energy $V_e=-J(R-R')\delta(R=R'+d)\delta_{ij}S_i(R)S_j(R')$; and the fourfold anisotropy energy $V_a=-0.5K_1\Sigma_i(S_{ix}^2-S_{iy}^2)^2$. Here d denotes the nearest neighbors. For spins on opposite planes, the interlayer exchange coupling J_i is different from the intralayer exchange coupling J. For transition metals, the bare exchange interaction per spin is much larger than the bare dipolar coupling and the bare crystalline anisotropy interaction. We thus assume all spins in the direction perpendicular to the film to be parallel to each other and approximate it by an effective block spin. These block spins will then interact with each other with renormalized interactions. For a film of n layers and block spins with l^2 columns in the xy directions at low temperatures, the renormalized dipolar interaction g, the anisotropy K, the interlayer exchange J_i and the intralayer exchange J are increased *approximately* by factors of n^2l, nl^2, nl^2, and n respectively.[5,9]

The sum of the dipolar interaction of the atomic constituents of the block spins will also induce *short range* higher multipolar interaction between the block spins. If the size of

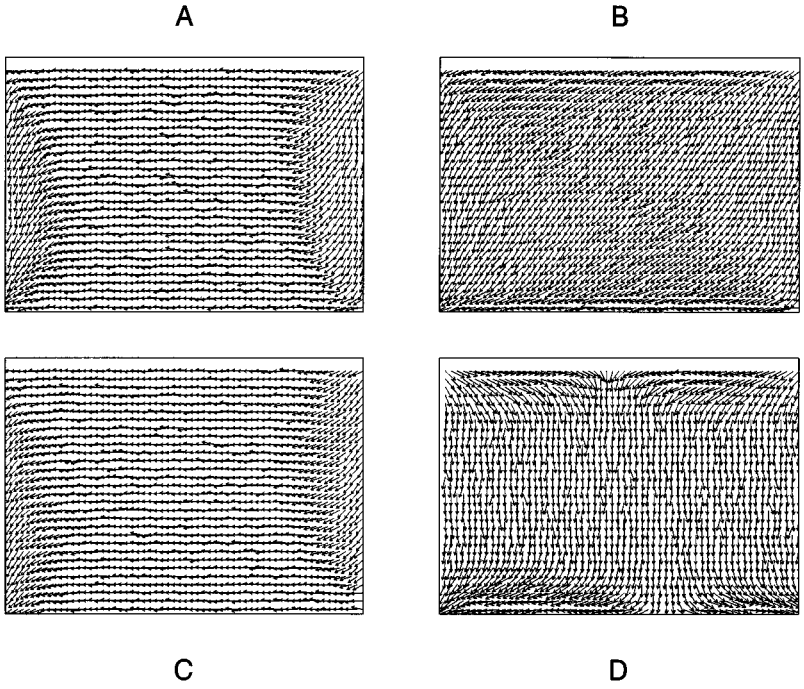

FIG. 2. Spin configurations for the top layer along a hystersis line at field strengths of 0 (a), upper left, 0.6; (b), upper right, 1.2; (c), lower left and 0; (d), lower right, for an interplanar exchange of 0.4. A triangular lattice can be viewed as a superposition of two rectangular lattices shifted by a unit translation vector with respect to each other. To save space, only half of the spins on one of the rectangular lattices were shown.

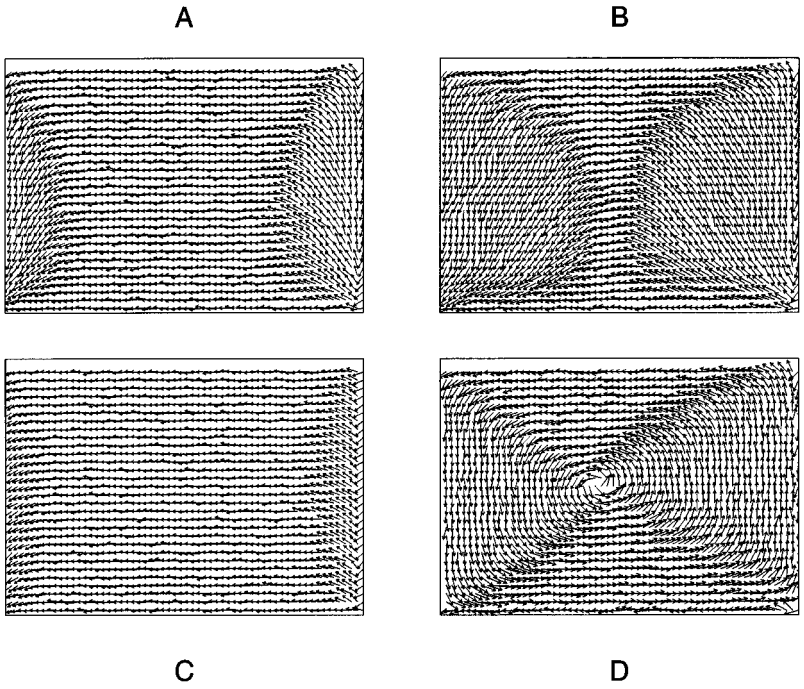

FIG. 3. Spin configurations for the bottom layer along a hystersis line at field strengths of 0 (a), upper left, 0.6; (b) upper right, 1.2; (c), lower left and 0 (d), lower right, for an interplanar exchange of 0.4. A triangular lattice can be viewed as a superposition of two rectangular lattices shifted by a unit translation vector with respect to each other. To save space, only half of the spins on one of the rectangular lattices were shown.

the block spin is big enough so that these higher multipolar interactions become comparable to the exchange, the residual multipole interactions need to be included in a realistic calculation. *In two dimensions* it is easy to estimate the magnitude of the multipoles Q_{lm}. Q_{lm} is obtained by integrating the magnetic charges that correspond to a uniform dipole moment times $r^l Y_{lm}$ over the size of the block spin. The dipole contribution corresponds to $l_0=1$, $m=\pm 1$. From parity considerations, only odd l's are allowed. Thus the first contribution that we have not included corresponds to $l_1=3$. The corresponding moment is smaller than the dipole contribution by a ratio r equal to the block spin size r_B divided by the nearest-neighbor distance a to the power l_1-l_0, $r=(r_b/a)^2\approx 0.25$. We have used a renormalized g that is half as big as J (see below), the residual multipolar interaction is thus smaller than J by approximately one order of magnitude and hence is neglected in the present case. We expect that only the *long-range* dipolar interaction is responsible for the formation of domains and thus the residual multipolar interaction not to change the physics in any case. The effect of different block spin size on the switching behavior has been studied previously.[8] This provides us with confidence that the block spin size we have chosen is adequate.

To illustrate the basic physics, we first focus on results with $J=2$, $g=1$, $K=0.2$, and $J_i=0.2$, 0.4, 1 ($T=0.1$). These parameters correspond approximately to a thickness of $n=27$ Fe layers and block spins of xy dimension $l=36$ ($J_0=270$ K). The unit of energy is $J_0 n/J=3645$ K. The bare interplane exchange is equal to $J_{i0}=J_i J_0/(Jl^2)=0.02$, 0.04,

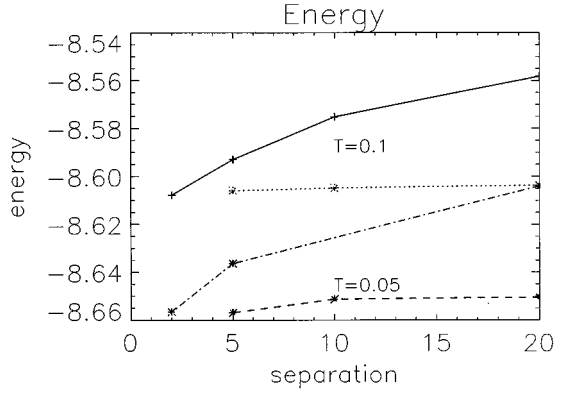

FIG. 4. The energies as a function of the separation between planes for the ''aligned'' (solid and dotted-dashed lines) and the ''closure-domain'' (dotted and dashed lines) configurations at temperatures $T=0.1$ and $T=0.05$. The distance is in units of block spin thickness $n=27$ atomic layers. The energy is for block spins in units $J_0 n/J=3645$ K.

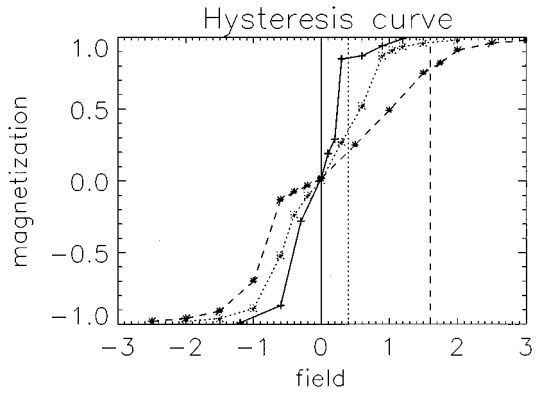

FIG. 5. Half of a hystersis loop starting from a high field decreasing to negative values for three different interplanar couplings of 0.2 (solid) 0.4 (dotted) and 1 (dashed). The bare interplane exchange is equal to $J_{i0}=J_i J_0/(Jl^2)=0.02$, 0.04, and 0.1 K, respectively. A field strength of 0.1 in our units corresponds approximately to a field of 100 Oe. The vertical lines correspond to switching fields from the high-field parallel region according to uniform rotation. The other half of the hystersis curve is obtained by plotting in addition $-M$ vs H.

and 0.1 K, respectively. A small J_i may be more appropriate for tunnel junctions whereas for metallic multilayers J_i is larger. A field strength of 0.1 in our units corresponds approximately to a field of 100 Oe. A typical run takes 4000 MC steps/spin and approximately 4 h of CPU time on a Cray J90.

We first carried out simulations for different values of the interplanar coupling at zero magnetic field. After annealing from high temperatures we found that a closure domain is obtained at large separation whereas at small separation, spins are *mostly* aligned in each plane [Figs. 1(a), 2(a), and 3(a)]. In Fig. 4 we show the energy of systems without the annealing but with the ''aligned'' (solid and dotted-dashed lines) and the ''closure-domain'' (dotted and dashed lines) initial configurations as a function of the separation between planes at $T=0.1$ and 0.05. These results suggest a crossover at a separation of around three block spin lattice spacings. Calculations with $40\times40\times2$ systems provide for a crossover distance of the same separation to within 10%.

The interplane dipolar coupling is small for the closure domain case, since there are few edge ''magnetic free poles.'' We thus expect the hysteresis behavior for that case to be similar to that of a single plane.[7] For the rest of this paper we focus on situations where the planes are close to each other (separation $dz=2$) and the spins are mostly aligned at the beginning.

In Fig. 2 we show the spin configurations of the top layer starting at zero field after the annealing (a) and then with the field increasing to 0.6 (b); to the high field parallel configuration (c) and then recycle back to zero field (d). The corresponding configurations for the bottom layer are shown in Fig. 3. Even though most of the spins are aligned at zero field there are still regions close to the edges where domains are formed. One-dimensional edge domain walls have been discussed previously by Slonczewski, Petek, and Argyle for thick coupled layers.[11] As the external field is increased, these edge domains grow and eventually merge, as we see in Fig. 2(b). After this, the external field is *perpendicular* to most of the spins. As the external field is further increased, the spins are rotated continuously until they are mostly parallel at high fields (c). Again, there are small domains left at the edges. As the field is reduced, these domains grow so that at zero field, the magnetization becomes *perpendicular* to the field and the initial magnetization.

In the previous example, the magnetization of the edge domains are parallel to each other. Because of the statistical nature of the problem, the edge magnetizations can also be antiparallel to each other. Because of a difference in the total topological vorticity of the system, the coercive behavior is changed in that case. This is illustrated in Fig. 1 where we show the spin configurations of the top layer for a run with interplane exchange coupling $J_i=1$ (a). As the edge domains grow, they cannot merge with each other (b). Eventually the vortex core moved out of the sample and the spins become mostly aligned at high fields (c). In this high-field state, the edge magnetizations remain opposite. Thus as the field is lowered to zero, the edge domain grows and a metastable closure domain results. The difference between the initial and final zero field configurations may be related to the difference in resistance of multilayers after the field was cycled.[3]

The magnetization as a function of the magnetic field from the high field configuration is shown in Fig. 5 for three values of the interplane exchange coupling. By considering the instability against uniform rotation of the spins from the parallel magnetization configuration at high field, we determine a switching field $H_{2r}=2J_i-2K+2gd'_{xx}$. Here $d'_{ij}=\Sigma_R[\delta_{ij}/R^3-3R_iR_j/R^5]$, where R measures the separation between spins on adjacent planes. d' dies off exponentially as the interlayer separation dz is increased with a length scale of the order of the lattice constant. For the triangular lattice, using the Ewald sum technique, we found that $d'_{xx}=5$, 0.11, 3×10^{-3}, 8×10^{-5} for $dz=0.5$, 1, 1.5, and 2 respectively. The uniform rotation limits are indicated by the vertical lines in Fig. 5. The switching field from the simulation is different from H_{2r}. After all, the switching is determined by the growth of the domains at the edges and not by uniform rotation. The magnitude of the interplane exchange coupling is deduced experimentally from the switching field from the parallel alignment assuming uniform rotation. The simulation suggests that instead the switching field is determined by the depinning of the edge domain walls. The length of these walls will increase when they are depinned. If the energy lost can be overcome by the energy gained from the external magnetic field, the switching will occur. We have also investigated the switching field from the antiparallel configuration. The simulation result is also different from the coherent rotation limit given by $H_{1r}=2\sqrt{K(K+\delta'+J_i)}$.

III. DISCUSSION

The possibility of a tilt in the z direction of the spins in the domain wall when the films are thick enough and in the absence of interplane exchange was emphasized previously by Sloncewski.[10] (This is called ''escape into the third dimension'' in the jargon of later work in statistical mechanics.) This usually happens for films thicker than the ''exchange length'' which is about 100 Å whereas our present interest is in ultra-thin films less than 100-Å thick.

The present result also illustrates the importance of the vorticity of the edge domains. This kind of initial state occurs because of the statistical nature of the problem. It occurs naturally in a finite-temperature simulation. However, it does not occur in a zero-temperature solution of the Landau-Gilbert equation unless the initial vorticity is introduced by hand. This illustrates the importance of doing a finite temperature calculation.

Sloncewski, Petek, and Argyle have discussed edge domain walls in the context of laminated Permalloy films.[11] It is difficult to compare their results to the present calculation quantitatively for the following reasons: (1) Their calculation assumes a one-dimensional wall whereas the walls observed here change in both x and y. This is particularly significant for small structures with small transverse dimensions. (2) Their calculation is focused on the thick film limit where the thickness of the film is larger than the exchange length which is proportional to square root of (the exchange interaction)/(magnetization squared) whereas the present paper is focused on the opposite limit of ultrathin films. In their limit the dipolar interaction is more important than the exchange. This is not true in the present case. (3) They assumed a uniaxial anisotropy in their calculation whereas the present calcula-

tion assumes a fourfold anisotropy.

To summarize, we have investigated the switching behavior of two planes of spins coupled antiparallel to each other. Our results suggest the importance of edge domains. As the interlayer spacing decreases, the width of the edge domain will decrease. When the interlayer separation becomes comparable to the bare atomic spacing, the repulsion between aligned spins at the edge will be balanced by that from the next plane, the edge domain width approaches zero. To get meaningful simulation results it is necessary to use block spins whose size is less than the width of the edge domains, whose width can become less than a normal domain wall width. For systems with more than two layers, the situation may be more complex. We hope to investigate this in future work.

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