Modeling the magnetic properties of $DyFe_2/YFe_2$ superlattices

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(Presented 12 November 2002)

The Stoner–Wohlfarth model has proved reasonably successful in describing the coercivities of antiferromagnetically coupled $DyFe_2/YFe_2$ hard/soft superlattices in the absence of magnetic exchange springs. In particular, the coercivity rises sharply as the net magnetic moment of the superlattice approaches zero. However the situation becomes more complicated as the thickness of the YFe_2 layers is increased. Two distinct "instability fields" can be identified: the bending field B_B, signifying the onset of a magnetic exchange spring, and the irreversible switching field B_{IS} associated with magnetic reversal. We have developed a computational model to address this problem. In particular, it is shown that the two instability fields in question are characterized by vanishing eigenvalues in the matrix formed by the double energy derivatives $\partial^2 E/\partial\theta_i\partial\theta_j$, where E is the total energy and θ_i the angle of each individual monolayer. It is shown that the model provides a very good description of the $M-B_{\rm app}$ loops of $DyFe_2/YFe_2$ multilayer films. In particular, the coercivity of a nearly magnetically compensated multilayer (75 Å $DyFe_2$/150 Å YFe_2) is much reduced below the prediction of the Stoner–Wolhfarth model, in accord with experiment. [DOI: 10.1063/1.1539072]

INTRODUCTION

The Stoner–Wohlfarth or single-domain coherent rotation model is perhaps the simplest model that can provide an explanation for magnetic hysteresis.[1–3] This model is easily generalized to describe artificially engineered multilayer films and has proved reasonably successful in describing the coercivity of molecular beam epitaxy (MBE)-grown $DyFe_2/YFe_2$ superlattices.[4] However, as the thickness of the magnetically soft YFe_2 layers is increased, additional features come into play. Magnetic exchange springs, set up in the magnetically soft YFe_2 layers,[5–7] exert torque on the spins in the hard layer, thereby changing the magnetization M, and the irreversible switching field B_{IS} of the composite film. This problem is tackled in this article.

STONER–WOHLFARTH MODEL WITH MAGNETIC EXCHANGE SPRINGS

In the generalized Stoner–Wohlfarth model, the coercivity B_C is given by

$$B_C=\frac{2(K_H t_H+K_S t_S)}{M_H t_H \pm M_S t_S}, \tag{1}$$

where K_H (K_S) is the anisotropy of the hard (soft) layer, M_H (M_S) is the magnetic moment of the hard (soft) layer, t_H (t_S) is the thickness of the hard (soft) layer, and $\pm$ refers either to ferromagnetic (antiferromagnetic) coupling between the hard and soft layers, respectively. We seek to generalize this expression to include magnetic exchange springs.

Following work reported in Refs. 8–11, the total energy of an exchange spring can be written in the form

$$E_{\rm tot}=\sum_i^N -\tfrac{1}{2}\mu(i)B_{\rm ex}\{\cos(\theta_{i+1}-\theta_i)[1-\delta_{i,N}]+\cos(\theta_i-\theta_{i-1})[1-\delta_{i,1}]\}-K_A(i)\cos^2\theta_i-\mu(i)B_{\rm app}\cos(\theta_i-\theta_H) \tag{2}$$

$B_{\rm ex}$ and $B_{\rm app}$ are the magnetic exchange and applied fields, respectively, the magnetic field is applied along θ_H, with respect to the uniaxial crystal field axis, and the delta functions indicate that the film is finite. For stability, the partial derivative of the total energy, with respect to a small variation in θ_i, must be zero:

$$\frac{\partial E_{\rm tot}}{\partial\theta_i}=-\mu(i)B_{\rm ex}\{\sin(\theta_{i+1}-\theta_i)[1-\delta_{i,N}]-\sin(\theta_i-\theta_{i-1})[1-\delta_{i,1}]\}+K_A(i)\sin 2\theta_i+\mu(i)B_{\rm app}\sin(\theta_i-\theta_H)=0. \tag{3}$$

In general, numerical methods are employed to solve Eq. (3). The reader is referred to the iterative procedure developed by Trallori *et al.*,[8–11] the Monte Carlo method of Fullerton *et al.*,[12,13] and the linearized procedure of Bowden *et al.*[14] In this article we use the last, because this method lends itself readily to a discussion of stability.

In practice, the amount of computing time required to find the shape of the exchange spring in a repetitive multilayer film could be excessive. But the time can be reduced significantly by using "cyclic boundary" conditions. In place of the delta functions in Eq. (3), we set $\theta_0=\theta_N$ and

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$\theta_{N+1}=\theta_1$. Following the procedure in Ref. 14, we assume that an initial set of angles $\{\theta_i\}_0$ close to the desired equilibrium set is already available. Thus by choosing new angles $\theta_i \rightarrow (\theta_i)_0 + \delta\theta_i$ it should be possible to move even closer to the equilibrium set $\{\theta_i\}$. On expanding Eq. (3) to first order in $\delta\theta_i$ we find

$$\frac{\partial E_{\rm tot}}{\partial \theta_i} \rightarrow \left(\frac{\partial E_{\rm tot}}{\partial \theta_i}\right)_0 + \left(\frac{\partial^2 E_{\rm tot}}{\partial\theta_{i-1}\partial\theta_i}\;\frac{\partial^2 E_{\rm tot}}{\partial\theta_i^2}\;\frac{\partial^2 E_{\rm tot}}{\partial\theta_{i+1}\partial\theta_i}\right)_0 \begin{pmatrix}\delta\theta_{i-1}\\ \delta\theta_i \\ \delta\theta_{i+1}\end{pmatrix}. \tag{4}$$

This equation is easily generalized to

$$\left(\frac{\partial E_{\rm tot}}{\underline{\partial\theta}}\right) \rightarrow \left(\frac{\partial E_{\rm tot}}{\underline{\partial\theta}}\right)_0 + \mathbf{E}_0''(\underline{\delta\theta})=0, \tag{5}$$

where the $(\partial E_{\rm tot}/\underline{\partial\theta})$ are column vectors and $\mathbf{E}''$ is an $N \times N$ matrix. Thus the revised set of corrections $(\delta\theta)$ can be found by inverting Eq. (5). In practice, this procedure rarely requires more than half a dozen iterations. However, it remains to be shown whether the final set $\{\theta_i\}$ represents a maximal or minimal energy solution.

From Taylor expansion we have

$$\begin{aligned} E_{\rm tot} &\rightarrow (E_{\rm tot})_0 + \sum_{i=1}^{N}\left(\frac{\partial E_{\rm tot}}{\partial\theta_i}\right)_0 d\theta_i \\ &+ \frac{1}{2!}\sum_{i}^{N}\sum_{j}^{N}\left(\frac{\partial^2 E_{\rm tot}}{\partial\theta_i\partial\theta_j}\right)_0 d\theta_i d\theta_j + \ldots, \\ &= (E_{\rm tot})_0 + (E_{\rm tot})' + (E_{\rm tot})'' + \ldots\ldots . \end{aligned} \tag{6}$$

For the equilibrium set $\{\theta_i\}=\{\theta_i\}_0$ the set of first derivatives $(\partial E_{\rm tot}/\partial\theta_i)_0$ must, of course, be zero [see Eq. (3)]. But in addition the second order term should be positive semidefinite. To tackle this problem we note that $(E_{\rm tot})''$ can be reexpressed in matrix form

$$(E_{\rm tot})'' = \tfrac{1}{2}(d\theta)^* \mathbf{E}_0''(d\theta), \tag{7}$$

or, alternatively, in diagonal form

$$(E_{\rm tot})'' = \tfrac{1}{2}[\lambda_1 \mathbf{d}\theta_1^2 + \lambda_2 \mathbf{d}\theta_2^2 + \lambda_1 \mathbf{d}\theta_3^2 + ,\ldots\ldots,\;\; \lambda_N \mathbf{d}\theta_N^2], \tag{8}$$

where **d**'s have been used to symbolize that a unitary transformation has been implemented. So for the second order change in the energy is to be positive, all the eigenvalues λ_K must be greater than zero. If just one of the eigenvalues, say, $\lambda_K \rightarrow 0$, then the associated second order change in energy $\lambda_k \mathbf{d}\theta_k^2 \rightarrow 0$. In practice, soft modes occur at the bending field B_B and the irreversible switching field B_{IS}. Finally, we remark that if one or more eigenvalues is negative, then the set of angles $\{\theta_i\}$ corresponds to a maximal energy solution and should be discarded.

RESULTS AND DISCUSSION

All the calculations presented below are for $T=0$ K. The parameters used were $K_A(\mathrm{DyFe_2})=10$ K, $K_A(\mathrm{YFe_2})=0$, $M_{\mathrm{DyFe_2}}=7\,\mu_B$, $M_{\mathrm{YFe_2}}=3\,\mu_B$, and $B_{\rm ex}=600$ K. From experiments on $\mathrm{DyFe_2/YFe_2}$ multilayers, $K_A(\mathrm{DyFe_2}) \sim 9(3)$ K.[4] In principle, it is possible to simulate an increase in temperature by reducing K_A, but neglecting thermal activation.

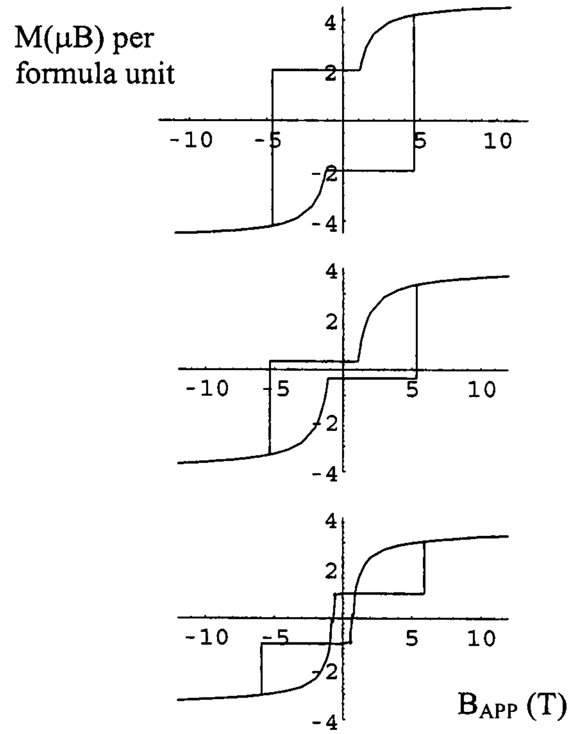

FIG. 1. Calculated magnetization curves at 0 K for multilayer films $N_{\mathrm{YFe_2}}=60/N_{\mathrm{DyFe_2}}=60$ (top), $N_{\mathrm{YFe_2}}=60/N_{\mathrm{DyFe_2}}=30$, and $N_{\mathrm{YFe_2}}=88/N_{\mathrm{DyFe_2}}=22$ (bottom).

In Fig. 1, calculated magnetization curves can be seen for the three superlattice films: a $\mathrm{DyFe_2}$ magnetically dominated, $N_{\mathrm{YFe_2}}=60/N_{\mathrm{DyFe_2}}=60$, an almost magnetically compensated, $N_{\mathrm{YFe_2}}=60/N_{\mathrm{DyFe_2}}=30$ film, and a $\mathrm{YFe_2}$ dominated film, $N_{\mathrm{YFe_2}}=88/N_{\mathrm{DyFe_2}}=22$. The number of monolayers has been chosen to correspond to the multilayer films $[150\,\text{Å}\,\mathrm{YFe_2}/150\,\text{Å}\,\mathrm{DyFe_2}]\times 10$, $[150\,\text{Å}\,\mathrm{YFe_2}/75\,\text{Å}\,\mathrm{DyFe_2}]\times 18$, and $[220\,\text{Å}\,\mathrm{YFe_2}/55\,\text{Å}\,\mathrm{DyFe_2}]\times 15$. The measured magnetization loops for the last of the three can be seen in Fig. 2. From a comparison of Figs. 1 and 2 it can be observed that there is good semiquantitative agreement between theory and experiment. Better agreement can be had by fine tuning the principle parameters $B_{\rm ex}$, K_A, and N, the multilayer number per Å. But the reader is warned that the crystal field anisotropy should be modified to include fourth- and sixth-order rare earth (RE) single-ion terms, plus the magnetoelastic strain term.[15] The calculated "instability fields" B_B and B_{IS} for the three films are listed in Table I. Note that the B_{IS} calculated for the nearly magnetically compensated film, Fig. 1(b), is 5.321 T; cf. the measured result of ~8 T. However, if we use the Stoner–Wohlfarth model of Eq. (1), we find $B_C \sim 35$ T, considerably higher than that of experiment. Finally, we note that for the $N_{\mathrm{YFe_2}}=88/N_{\mathrm{DyFe_2}}=22$ multilayer, $B_{\rm app}$ is still positive when the magnetization goes negative in the top right-hand quadrant. In a conventional sense, this corresponds to "negative coercivity."[15] However, the $\mathrm{DyFe_2}$

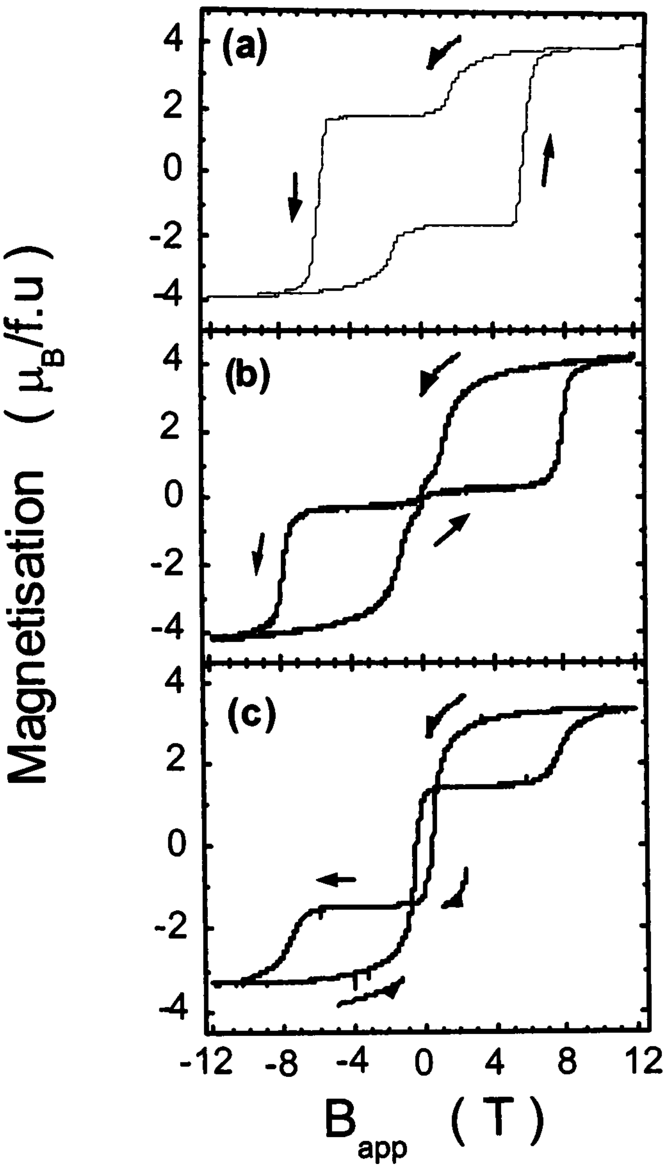

FIG. 2. Measured magnetization curves at 10 K for multilayer films [150 Å YFe_2/150 Å $DyFe_2$]×10 (a), [150 Å YFe_2/75 Å $DyFe_2$]×18 (b), and [220 Å YFe_2/55 Å $DyFe_2$]×15 (c).

layers are reversed at the much higher field of $B_{IS} = 5.927$ T.

CONCLUSIONS

In this article it was shown that the Stoner–Wohlfarth model, adapted to include magnetic exchange springs, can be used to provide a good semiquantitative interpretation of $DyFe_2/YFe_2$ multilayer films. In particular, it was noted that the incipient presence of magnetic exchange springs brings about a large reduction in the irreversible switching field B_{IS} of nearly magnetically compensated samples.

TABLE I. Calculated instability fields B_B and B_{IS}.

N_{YFe_2}/N_{DyFe_2}	B_B (T)	B_{IS} (T)
60/60	1.094	4.338
60/30	1.085	5.321
88/22	0.5486	5.927

ACKNOWLEDGMENTS

This work was supported by the Advanced Magnetics Program of the EPSRC and funded, in part, by QinetiQ Ltd. (formerly DERA Farnborough).

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