Microscopic model for exchange anisotropy

J. R. L. de Almeida* and S. M. Rezende†
Departamento de Física, Universidade Federal de Pernambuco 50670-901, Recife-PE, Brazil
(Received 10 August 2001; published 19 February 2002)

A simple microscopic model is used to study the effect played by interface roughness on the intriguing thermal-history-dependent properties observed in exchange-coupled antiferromagnetic (AF)/ferromagnetic (FM) bilayers. The model assumes two monolayers, one with AF-coupled compensated spins and the other with FM-coupled spins, with a fraction of them randomly substituted by spins from the AF layer to represent the interface roughness. The equations for the local magnetizations are set up in a mean-field approximation with Ising interactions and solved numerically for arbitrary temperature. Following the experimental procedure, upon cooling the system in an applied field, the model exhibits an intrinsic unidirectional anisotropy and coercitivity which are dependent on the field-temperature history. The dependence of the exchange bias field (H_e) and coercitive field (H_c) on the cooling field, initial and final temperatures, and interlayer exchange interaction are qualitatively similar to experimental observations. The results represent a definitive indication that the random field arising from interface roughness is responsible for the irreversibility and metastability properties of AF/FM bilayers.

DOI: 10.1103/PhysRevB.65.092412 PACS number(s): 75.70.Cn, 75.30.Gw, 75.50.Lk

Under appropriate preparation conditions, a ferromagnetic (FM) film in contact with an antiferromagnetic (AF) material displays a hysteresis loop shifted in field, an effect called exchange bias. Discovered more than 40 years ago,[1] this effect has attracted considerable attention lately due to its technological importance in novel magnetic memory devices (see the reviews in Refs. 2 and 3). Despite recent intensive investigations in the field, the microscopic origin of the exchange bias remains unclear. It was early recognized that the exchange coupling across the FM/AF interface was responsible for the field shift, but the values inferred from the atomic exchange interaction were too large compared to the experimentally measured ones. Later Malozemoff[4] showed that interface roughness could explain the reduction of the exchange coupling. Using a random-field treatment for the local fluctuations in the magnetic interaction he obtained an interface coupling on the same order of magnitude of the measured field shifts. However, other theoretical models assuming atomically flat interfaces also gave reduced field shifts,[5,6] challenging the need to invoke mechanisms based on roughness. With the recent increased activity in the field, several new intriguing properties have been observed in AF/FM bilayers, such as enhanced coercitivity, metastability, and thermal history dependence. Thus, the basic mechanism of the exchange bias has to account for more than just the correct order of magnitude of the field shift and the understanding of its theoretical aspects is only in its beginning.[4–11]

This paper shows that interface roughness does play an essential role in elucidating several effects observed in exchange coupled AF/FM bilayers. Of course roughness on the atomic scale exists in any real interface and in an AF material it creates a random-field system which is known to display a rich physics. In systems with randomness and frustration a very large number of parameters are involved; by nature the effect is typically one created by a complex phase space where the measured quantities depend strongly on the initial conditions. They are difficult to study and their consequences have not been fully explored in AF/FM bilayers. We have chosen to represent an AF/FM bilayer with rough interface by a simple microscopic model so that its thermodynamics could be easily formulated. As we show next, the model exhibits all essential features of the exchange anisotropy effect and allows a study of its dependence on various quantities of interest. The model also allows a study of local quantities and may be easily extended for more realistic physical cases. Consider two atomic monolayers with magnetic moments over congruent square lattices, one layer with two perfectly compensated antiferromagnetic sublattices and the other with ferromagnetically coupled moments. The moments from different layers are coupled by an interlayer exchange interaction, which can be FM or AF. The interface roughness is accounted for by randomly substituting a fraction of the atoms in the FM layer by atoms from the AF layer. The system Hamiltonian is taken as

$$H = H_{AF} + H_{FM} + H_c , \tag{1}$$

where H_{AF}, H_{FM}, and H_c are, respectively, the interaction energies in the antiferromagnetic layer (AFML), in the ferromagnetic layer (FML), and the coupling between the FML and AFML atoms, all assumed to be Ising like to simplify the calculations. Thus we have

$$H_{AF} = -\sum_{(ij)} J_{ij}^{(1)} \sigma_i^{(1)} \sigma_j^{(1)} - D_1 \sum_i \sigma_i^{(1)^2} - h \sum_i \sigma_i^{(1)} , \tag{2}$$

where $\sigma_i^{(1)}$ represents the spins on the AFML at site i interacting with the nearest neighbors (NN) through an exchange interaction $J_{ij}^{(1)} = J_1 < 0$, (ij) meaning the sum over all distinct NN pairs, D_1 is a local uniaxial anisotropy in the AFML, and h is the external field. Let the local randomly distributed variables $\eta_i = 1,0$ specify the presence $(=1)$ or absence $(=0)$ of a FML atom at site i which, in the latter case, is assumed substituted by an AFML atom. Hence, for the FM layer,

$$H_{FM} = -\sum_{(ij)} I_{ij} - \sum_{i} [D_2 \eta_i S_i^2 + D_1(1-\eta_i)(\sigma_i^{(2)})^2] - h\sum_{i} [\eta_i S_i + (1-\eta_i)\sigma_i^{(2)}], \quad (3)$$

where S_i represents the spins on the FML at site i interacting with the NN spins through the interaction I_{ij}, D_2 is a local uniaxial anisotropy in the FML, and $\sigma_i^{(2)}$ denotes the moment of an AFML atom in FM layer. Due to the random substitution of FML atoms by AFML ones, I_{ij} assumes the form

$$I_{ij} = J_2 \eta_i \eta_j S_i S_j + J_1(1-\eta_i)(1-\eta_j)\sigma_i^{(2)}\sigma_j^{(2)} + J_c[(1-\eta_i)\eta_j \sigma_i^{(2)} S_j + \eta_i(1-\eta_j) S_i \sigma_j^{(2)}], \quad (4)$$

where J_2 is the NN interaction between FML spins and J_c represents the coupling between FML and AFML atoms. The interlayer exchange interaction is

$$H_c = -\sum_{i} [J_c \eta_i S_i \sigma_i^{(1)} + J_1(1-\eta_i)\sigma_i^{(1)}\sigma_i^{(2)}], \quad (5)$$

where the sum is over all sites at the interface. All energies shall be measured in units of the absolute value of J_1. The many-body problem posed by the model expressed by Eqs. (1)–(5) is far from trivial. As in random field magnets and spin glasses, the presence of randomness results in a complex phase space exhibiting strong irreversibility and metastability effects.[12] The last terms in Eqs. (3) and (4) act like an effective random field at the interface that explicitly breaks time-reversal symmetry in the ferromagnetic subsystem, giving origin to the unidirectional anisotropy as argued in Ref. 4. In order to study the thermodynamics of the model given by Eqs. (1)–(5) we resort to the approach of Soukoulis *et al.*[13] which was successfully used to investigate spin glasses and random-field systems. The method consists of setting up mean-field equations involving the average local spin variables and solving them iteratively. The equations obtained from the free energy functional may have many minima corresponding to metastable states which play an important role in intermediate time-scale experiments. As shown by Soukoulis *et al.*,[13] as the field h or temperature T varies, the system evolves by following a given minimum on the free energy surface. Hence, the numerical calculation of a history-dependent magnetization can be done iteratively by changing h or T and looking for the new configuration close to the one in the previous cycle. The local thermally averaged magnetization $M_i^{(\mu)}$ can be calculated using a mean-field approach,[13] since the temperatures of interest are far from the critical phenomenon range. In order to obtain an analytical expression for $M_i^{(\mu)}$ it is necessary to consider a given value for the spin. Assuming for simplicity that both FML and AFML have spin 1, the thermodynamic average over the spin components $\sigma_i^{(\mu)}, S_i = 0, \pm 1$ yields

$$M_i^{(\mu)} = \sinh(\beta\phi_i^{(\mu)}) / [\cosh(\beta\phi_i^{(\mu)}) + 0.5\exp(-\beta D_\mu)], \quad (6)$$

where

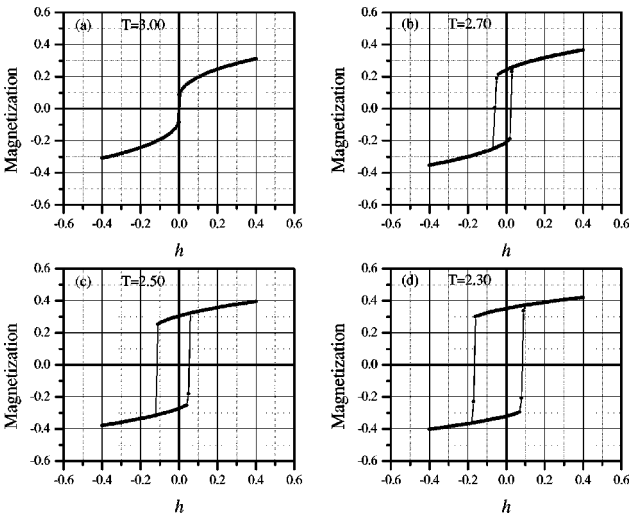

FIG. 1. Total magnetization hysteresis curves, m vs h, at several temperatures T, for a bilayer with parameters $J_1 = -1.00$, $J_2 = 1.20$, $D_1 = 1.00$, $D_2 = 0.00$, $p = 0.10$, and $J_c = +0.5$ (FM).

$$\phi_i^{(\mu)} = \sum_{\mu} \sum_{(ij)} (J_{ij} M_j^{(\mu)} + h) \quad (7)$$

is the local field in the mean-field approximation, $\mu = 1,2$ specify, respectively, FML or AFML atoms, the sum (ij) is over NN, J_{ij} is the pertinent interaction, and $\beta = 1/T$ is in units of Boltzmann constant. Following Ref. 13, Eqs. (6) and (7) are solved numerically by an iterative procedure, yielding local and macroscopic magnetizations. As we show below by some representative results, all essential features of exchange-biased bilayers are reproduced by the model.

All results presented here were obtained for two square-lattice monolayers of size $2 \times 100 \times 100$ with free boundary conditions. The moments of the FML are on sites congruent with the AFML sites, formed by two perfectly compensated AF square sublattices. The numerical calculations were done on a 500-MHz personal computer. Convergence to an accu-

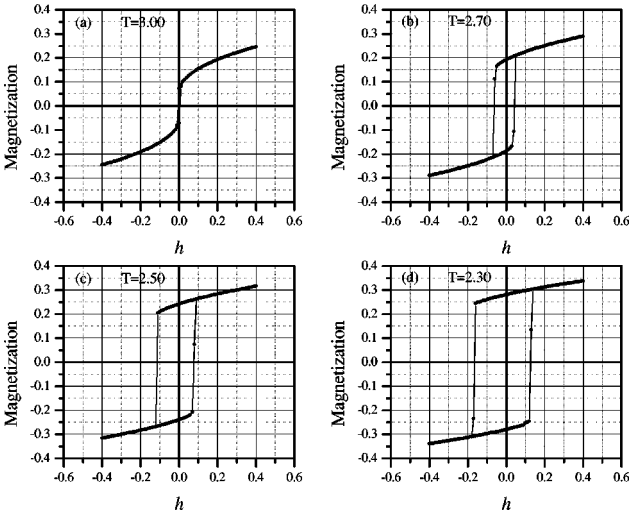

FIG. 2. Same as in Fig. 1, with AF interlayer coupling $J_c = -0.5$.

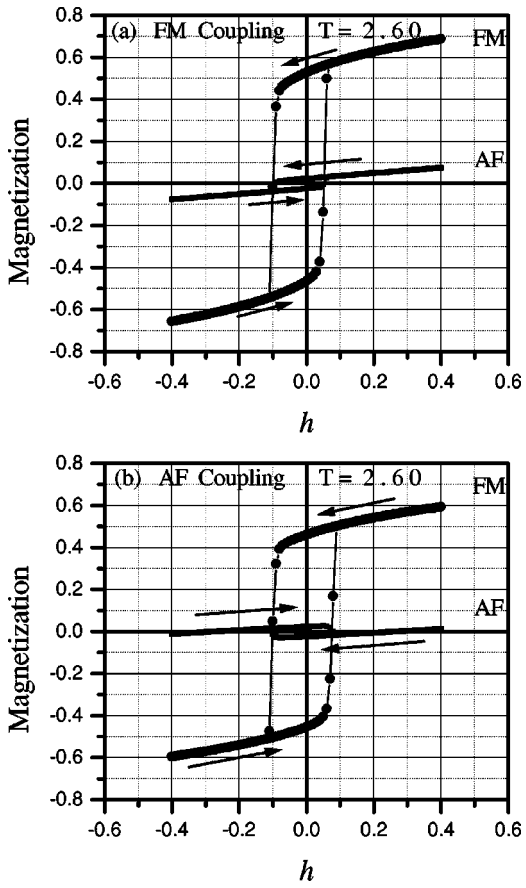

FIG. 3. Hysteresis curves for the magnetizations of the individual FM and AF layers of the same systems as in Figs. 1 and 2: (a) FM coupling $J_c=+0.5$ and (b) AF coupling $J_c=-0.5$.

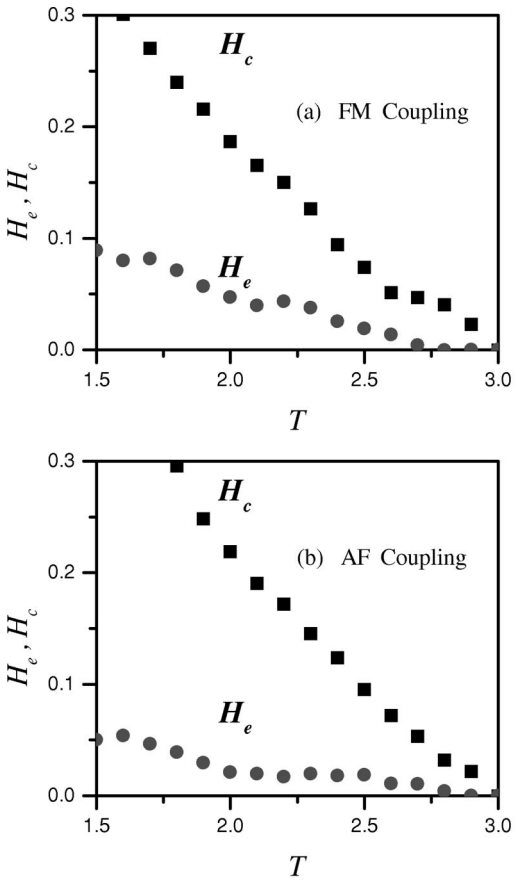

FIG. 4. Magnitude of the exchange bias field H_e and coercitivity H_c as a function of T for AF/FM bilayers with the same parameters as in Figs. 1 and 2: (a) FM coupling $J_c=+0.5$ and (b) AF coupling $J_c=-0.5$.

racy of 10^{-8} (change with respect to previous iteration) typically required 50–100 iterations for fields away from the bistability region. Near bistability the convergence is much slower and 500–1000 iterations were necessary. Without coupling between the layers and in the absence of randomness it is trivial to obtain iteratively the Curie (T_C) and Néel (T_N) temperatures of the FM and AF layers for a given set of parameters. We have chosen J_1, J_2, D_1, and D_2, such that $T_N<T_C$, as in most experimentally studied systems. In the presence of interlayer coupling and roughness, the calculations begin with a given cooling field h_{fc} at an initial temperature T_i in the range $T_N<T_i<T_C$. After convergence is achieved, the calculation is repeated at temperatures decreasing in steps ΔT, to a measuring final temperature T. Then the field is varied in steps, with T kept constant, for obtaining the hysteresis loop. The results depend sensitively on the values attributed to the parameters of the model. We show next only a few representative data. Consider initially an AF/FM bilayer with parameters $J_1=-1.00$, $J_2=1.20$, $J_c=\pm 0.50$, $D_1=1.00$, $D_2=0.00$, and roughness parameter $p=0.10$ $[=1-\text{mean}(\eta_i)]$. For these parameter values, $T_C=3.21$ and $T_N=2.93$ in the absence of interlayer coupling and disorder in the FM and AF systems. The hysteresis loops of the total system magnetization obtained with an initial $T_i=3.10$, with cooling field $h_{fc}=0.40$, at several final temperatures $T=3.00$, 2.70, 2.50, and 2.30 ($\Delta T=0.10$), are shown in Figs. 1 and 2, for $J_c=+0.5$ (FM) and $J_c=-0.5$ (AF), respectively. In both figures one observes the appearance of a field shift in the hysteresis loop and enhanced coercitivity at temperatures below T_N, characteristic of the exchange bias phenomenon. The physical origin of the shift resides in the fact that the AF spin arrangement breaks up into domains, having a net moment along the direction of the cooling field. These domains have walls similar to those found in diluted antiferromagnets under an uniform field.[14] This result lends support to the semiquantitative model of Malozemoff[4] for the origin of the exchange anisotropy. Note that the magnitude of the field shift is a small fraction of the interlayer exchange coupling, as observed experimentally. In energy units the coercitive field is much larger than observed because the anisotropy inherent to the Ising model is comparable to the exchange interaction. In real soft FM materials the anisotropy is small and the interactions are better represented by the Heisenberg model, but the calculation in this case is much more complicated. Notice in Figs. 1 and 2 that in both cases of FM and AF interlayer coupling the field shift is negative, so that from these curves alone it is not possible to determine the sign of the interlayer coupling. However, the evolution of the magnetization in the AF layer displays distinct behavior for FM and AF couplings, as shown in Fig. 3. For FM (positive) coupling the path of the AF hysteresis

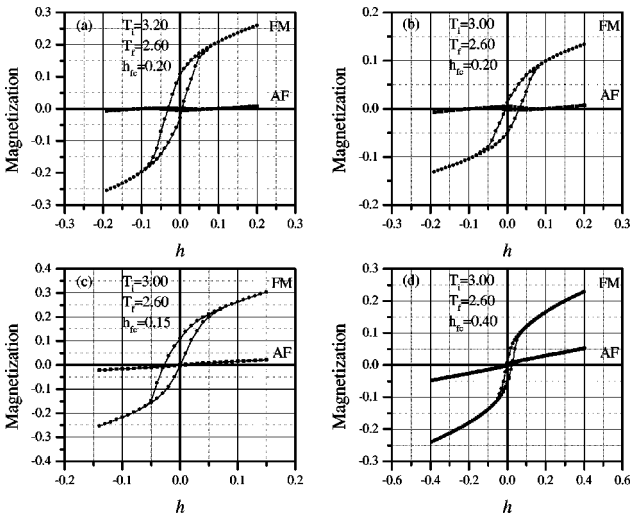

FIG. 5. Demonstration of the change in the sign of the exchange bias field with variation in the cooling conditions. The intralayer parameters are the same as in Figs. 1 and 2, except for $p=0.30$. In (a) and (b) the interlayer coupling is AF, $J_c=-0.5$, and the initial temperatures are different. In (c) and (d) the interlayer coupling is FM, $J_c=+0.3$, and the cooling field is (c) $h_{fc}=0.15$ and (d) $h_{fc}=0.40$.

cycle follows that of the FM layer, whereas for AF (negative) coupling the sense is reversed. This property may provide a way of experimentally determining the sign of the interlayer coupling.

The model can be further exploited to investigate several properties of exchange biased bilayers. Fig. 4 shows the variation of the coercitive field H_c and the magnitude of the exchange bias field H_e as a function of temperature for the same AF/FM bilayers of Figs. 1 and 2. Both bilayers, regardless of the sign of the coupling, exhibit behavior in qualitative agreement with experimental data; namely, below a temperature close to T_N, H_c increases with decreasing T, while H_e also increases with decreasing T but eventually saturates.[15,16] Calculations for other values of p show that H_c and H_e may vary in different proportions, allowing one to tailor the exchange bias and coercitivity by varying the interface roughness. Another experimental result that deserves attention is the recent observation[15,16] that in some systems, the exchange bias field changes sign as the cooling field or initial temperature vary. Our model displays this effect in bilayers with the same intralayer parameters as in Fig. 1, but with a larger roughness parameter $p=0.30$. Figures. 5(a) and 5(b) show the hysteresis loops obtained with an AF interlayer coupling, $J_c=-0.5$, with the same cooling field $h_{fc}=0.20$, but with different initial temperatures. Clearly the exchange bias field changes from negative to positive as the initial temperature is lowered, as observed experimentally.[15,16] However, the claim[15,16] that the change in sign of H_e with the variation of the cooling parameters is a characteristic feature of the AF interlayer coupling does have theoretical support. As shown in Figs. 5(c) and 5(d), the same system of two layers, coupled by a FM interaction $J_c=+0.3$, exhibits a change in the sign of the bias field as the cooling field varies.

In conclusion, we have presented a simple microscopic model for an AF/FM bilayer that allows an adequate treatment of the irreversible thermodynamics of the random-field system arising from interface roughness. Although the calculations were done for only two monolayers, they show inequivocally that roughness is responsible for several intriguing thermal history effects observed in exchange-biased systems.

This research is supported by the Brazilian agencies CNPq, CAPES, FACEPE, and FINEP.

*Electronic address: almeida@df.ufpe.br
†Electronic address: smr@df.ufpe.br

[1] W.H. Meiklejohn and C.P. Bean, Phys. Rev. **102**, 1413 (1956).
[2] J. Nogues and I.K. Schuller, J. Magn. Magn. Mater. **192**, 203 (1999).
[3] A.E. Berkowitz and K. Takano, J. Magn. Magn. Mater. **200**, 552 (1999).
[4] A.P. Malozemoff, Phys. Rev. B **35**, 3679 (1987).
[5] D. Mauri, H.C. Siegmann, P.S. Bagus, and E. Kay, J. Appl. Phys. **62**, 3047 (1987).
[6] N.C. Koon, Phys. Rev. Lett. **78**, 4865 (1997).
[7] X.W. Wu and C.L. Chien, Phys. Rev. Lett. **81**, 2795 (1998).
[8] T.C. Schulthess and W.H. Butler, Phys. Rev. Lett. **81**, 4516 (1998).
[9] M.D. Stiles and R.D. McMichael, Phys. Rev. B **59**, 3722 (1999).
[10] Z. Li and S. Zhang, Phys. Rev. B **61**, R14 897 (2000).
[11] P. Miltenyi, M. Gierlings, J. Keller, B. Beschoten, G. Guentherodt, U. Nowak, and K.D. Usadel, Phys. Rev. Lett. **84**, 4224 (2000).
[12] J. Mydosh, *Spin Glasses: An experimental introduction* (Taylor & Francis, London, 1993).
[13] C.M. Soukoulis, K. Levin, and G.S. Grest, Phys. Rev. Lett. **48**, 1756 (1982); Phys. Rev. B **28**, 1495 (1983).
[14] C. Ro, G.S. Grest, M. Soukoulis, and K. Levin, Phys. Rev. B **31**, 1682 (1985).
[15] C. Leighton, J. Nogues, B.J. Jonsonn-Akerman, and I.K. Schuller, Phys. Rev. Lett. **84**, 3466 (2000).
[16] J. Nogues, D. Lederman, T.J. Moran, and I.K. Schuller, Phys. Rev. Lett. **76**, 4624 (1996).