Monte Carlo simulations of ordering in ferromagnetic-antiferromagnetic bilayers

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Monte Carlo simulations have been used to study phase transitions on coupled anisotropic ferromagnetic-antiferromagnetic (FM/AFM) films of classical Heisenberg spins. We consider films of different thicknesses, with fully compensated exchange across the FM/AFM interface. We find indications of a phase transition on each film, occurring at different temperatures. It appears that both transition temperatures depend on the film thickness.

INTRODUCTION

Most of the attention given to ferromagnetic-antiferromagnetic (FM/AFM) bilayers is normally directed to the changes of the magnetic properties of the FM when it is in contact with the AFM. The commonly observed effects are a unidirectional shift (exchange bias) and a significant increase of the coercivity. The blocking temperature, $T_B$, below which these effects are observed, is comparable to the bulk Neel temperature when the AFM film is thick, but can be considerably lower when the AFM film is thin. It is generally believed that this reduction of the blocking temperature is due to finite size effects in the AFM, i.e. the ordering temperature of the AFM is decreased due to its finite thickness. In a recent neutron experiment on CoO/Fe$_3$O$_4$, however, van der Zaag et al. have found that the AFM shows signs of ordering above $T_B$. This indicates that the proximity of the FM influences the phase transition in the AFM in a way that cannot be predicted from studying free AFM films.

In this paper we use Monte Carlo simulations to analyze the effect of the FM on the transition between disordered and ordered states in the AFM for various film thicknesses and compensated exchange across the FM/AFM interface.

MODEL AND METHODS

The system studied here consists of a multi-layered ferromagnetic (FM) film coupled to an underlying multi-layered antiferromagnetic (AFM) film with no lattice mismatch at the FM/AFM interface. The Hamiltonian of the model is given by

$$
\mathcal{H} = -J_F \sum_{(\mathbf{r}, \mathbf{r}') \in \text{FM}} \mathbf{S}_r \cdot \mathbf{S}_{r'} - K_F \sum_{\mathbf{r} \in \text{FM}} (S^z_r)^2
$$

$$
- J_A \sum_{(\mathbf{r}, \mathbf{r}') \in \text{AFM}} \mathbf{S}_r \cdot \mathbf{S}_{r'} - K_A \sum_{\mathbf{r} \in \text{AFM}} (S^z_r)^2
$$

where $\mathbf{S}_r = (S^x_r, S^y_r, S^z_r)$ is a three-dimensional classical Heisenberg spin of unit length, $(\mathbf{r}, \mathbf{r}')$ denotes nearest-neighbor pairs of spins coupled with exchange interactions $J_F > 0$ on the FM film, $J_A < 0$ on the AFM film, and $J_{AF}$ at the FM/AFM interface, which is on a (001) plane. Spins on the AFM film have a uniaxial single-site anisotropy $K_A > 0$, whose easy axis is along the $y$ axis. In contrast, the single-site anisotropy for spins on the FM film has a hard-axis ($K_F < 0$) along the $z$ direction, which is perpendicular to the FM/AFM interfacial plane. No external magnetic field is applied on the films. The structure of the films is a body-centered cubic lattice, with linear sizes $L_x$, $L_y$, and $L^A_z + L^F_z$, measured in terms of two-spin unit cells. $L^A_z$ and $L^F_z$ denote the number of unit-cell layers on the AFM and FM films, respectively. Hence, the total number of spins in the lattice is $N = 2L_x L_y (L^A_z + L^F_z)$. We use periodic boundary conditions along the $x$ and $y$ directions and free boundary conditions along the $z$ direction.

The effect of the film thickness on the FM and AFM transition temperatures is studied for fixed interaction parameters. We consider $J_F = J > 0$, $J_A = -J$, $K_A = J$, $K_F = -0.5J$, and a compensated interface with $J_{AF} = r J$, where $r$ is a random number uniformly sampled in the interval $[-1, 1]$. Values of the film thickness used are $L^A_z = L^F_z = 3, 6, 12$, with several cross sections ($L_x = L_y = 12, 20, 40, 60$) to analyze finite-size effects.

The order parameter for the ferromagnetic transition is the uniform magnetization per spin $m = |\sum_{\mathbf{r}} \mathbf{S}_r|/N$, whereas to characterize the antiferromagnetic transition it is necessary to divide the BCC lattice into two simple cubic sublattices, denoted I and II, and consider the staggered magnetization per spin defined as $m_s = |\sum_{\mathbf{r} \in I} \mathbf{S}_r - \sum_{\mathbf{r} \in II} \mathbf{S}_r|/N$.

Our simulations were carried out using importance sampling Monte Carlo methods, with Metropolis algorithm, at fixed temperature $T$. Typically $3 \times 10^5$ Monte
Carlo Steps/site (MCS) were used for computing averages after about $1 \times 10^5$ MCS were discarded for thermalization. Whenever not shown, error bars in the figures are smaller than the symbol sizes.

RESULTS

Figs. (1a) and (1b) show the uniform and staggered magnetizations per spin for films of different thicknesses and fixed cross section. At low temperature, both $m$ and $m_s$ tend to 0.5, indicating ordered FM and AFM films (note that both quantities are computed for the entire lattice and thus go to 0.5 instead of 1.0 when the films are ordered). As the temperature increases, both $m$ and $m_s$ decay to zero, indicating disordered spin configurations on both films at higher temperatures. In simulations of finite lattices, occurrence of phase transitions cannot be ascertained with the use of only one lattice size. Therefore, we have considered different cross sections for each film thickness. Illustrations of finite-size effects on the uniform and the staggered magnetizations near the phase transitions are presented in Figs. (2a) and (2b), respectively. These figures show that as the cross section increases, the decay of the magnetizations $m$ and $m_s$ to zero becomes sharper. Such dependence of order parameters on finite lattice sizes is characteristic of real phase transitions. Similar finite-size effects were observed for the uniform and the staggered magnetizations of films of other thicknesses. The behavior of the uniform and staggered magnetizations shown in Figs. (1a) and (1b), with finite-size effects described above, suggests that for a given film thickness there are two distinct phase transitions, one occurring on the AFM film and one on the FM film. The AFM transition temperature seems to be slightly higher than the FM one, presumably due to the higher anisotropy on the AFM film. In addition, it appears that the transition temperatures on both the FM and the AFM films increase with film thickness. We use

![Graph](image1)

**FIG. 1**: (a) Uniform and (b) staggered magnetizations as a function of temperature for several film thicknesses, with $L_x = L_y = 20$ and $L_z^a = L_z^f = L_z$.

![Graph](image2)

**FIG. 2**: (a) Uniform and (b) staggered magnetizations as a function of temperature, for $L_x^a = L_y^a = 6$ and several cross sections.
crossings of reduced fourth-order cumulants of order parameters defined as \( U_{4r} = 1 - \langle m^4 \rangle / (3 \langle m^2 \rangle^2) \) and \( U_{4s} = 1 - \langle m^4 \rangle / (3 \langle m^2 \rangle^2) \), to locate the phase transition temperatures on the FM and AFM films, respectively. Preliminary analyses of cumulant crossings indicate that the AFM transition for \( L_A^z = L_F^z = 6 \) occurs at \( T_c = (2.235 \pm 0.005)J/k_B \), and it is consistent with the two-dimensional Ising universality class. For the same film thickness, the FM transition appears to be at \( T_c = (1.95 \pm 0.01)J/k_B \); however, the nature of this transition has not been determined yet.

Figs. (3a) and (3b) show the x, y, and z components of the uniform magnetization per site as a function of film layer, for \( L_A^z = L_F^z = 6, L_x = L_y = 20 \) and (a) \( T = 0.6J/k_B \) and (b) \( T = 2.0J/k_B \). The solid lines are guides to the eyes.

CONCLUSIONS

We have used extensive Monte Carlo simulations to study a system of coupled FM/AFM films, with compensated exchange across the interface. For the values of anisotropies and interaction parameters considered, it appears that the FM and the AFM phase transitions occur at different temperatures. The latter transition is consistent with the two-dimensional Ising universality class. Our preliminary simulations suggest that both phase transition temperatures increase with the film thickness.

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