Effect of interfacial coupling on the magnetic ordering in ferro-antiferromagnetic bilayers

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Monte Carlo simulations have been used to study magnetic ordering in coupled anisotropic ferro/antiferromagnetic (FM/AFM) films of classical Heisenberg spins. We consider films with flat interfaces that are fully uncompensated as well as rough interfaces that are compensated on average. For both types of interfaces above the “Néel temperature” we observed order in the AFM film, with the AFM spins aligning collinearly with the FM moments. In the case of rough interfaces there is a transition from collinear to perpendicular alignment of the FM and AFM spins at a lower temperature.

Ferromagnetic/antiferromagnetic (FM/AFM) bilayers have been shown to exhibit a unidirectional shift in the hysteresis loop (exchange bias) and a significant increase of the coercivity \cite{1}. Magnetic properties of FM/AFM bilayers can also be drastically different from those of free FM and AFM films. For example, even though in most exchange bias systems the blocking temperature is lower than the Néel temperature of the antiferromagnet, order in the AFM has been observed above the Néel temperature due to the coupling to the ferromagnet \cite{2}.

Earlier theoretical work \cite{2,3,4} has shown that for compensated interfacial exchange (\textit{i.e.} zero net exchange interaction across the FM/AFM interface) the FM aligns perpendicular to the AFM easy axis. Although similar perpendicular orientation has been observed in numerous FM/AFM systems \cite{3}, understanding the nature of the interfacial coupling and roughness in FM/AFM bilayers remains a challenge.

In this paper we use Monte Carlo simulations to study the effect of interfacial exchange interaction and roughness on transitions from ordered to disordered states in FM/AFM bilayers. The work is motivated by recent experiments of Ijiri et. al. \cite{6}, which show for CoO/Fe\textsubscript{3}O\textsubscript{4} multilayers, that the transition to perpendicular ordering takes place at temperatures considerably lower than the FM and AFM ordering temperatures.

The model studied here consists of a ferromagnetic (FM) film coupled to an underlying antiferromagnetic (AFM) film where the lattice is coherent across the FM/AFM interface. The structure of the films is a body-centered cubic (BCC) lattice, with linear sizes \(L_x = L_y = L \leq 96\). Each film is composed of 12 staggered (because of the BCC structure) layers of classical unit length spins \(S_r = (S^x_r, S^y_r, S^z_r)\), which interact via the Hamiltonian

\[
\mathcal{H} = -J_F \sum_{\langle r, r' \rangle \in \text{FM}} S_r \cdot S_{r'} - K_F \sum_{r \in \text{FM}} (S^z_r)^2
\]

where \(\langle r, r' \rangle\) denotes nearest-neighbor pairs of spins coupled with exchange interactions \(J_F > 0\) in the FM film, \(J_A < 0\) in the AFM film, and \(J_I\) at the FM/AFM interface. Spins in the AFM film have a uniaxial single-site anisotropy \(K_A > 0\), whose easy axis is along the \(y\) axis. The demagnetizing field on the FM film is modeled with 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. We use periodic boundary conditions along the \(x\) and \(y\) directions and free boundary conditions along the \(z\) direction.

We consider interaction and anisotropy parameters \(J_F = 5J > 0\), \(J_A = -J\), \(J_I = -J\), \(K_A = J\), and \(K_F = -0.5J\). We model flat interfaces as well as “rough” ones which are comprised of uniformly spaced steps, with 6, 1, and one spin per terrace in the \(x\), \(y\), and \(z\) directions, respectively. The terrace sizes along the \(x\) and \(z\) directions are kept fixed for the different film cross sections used. For both types of interfaces the exchange coupling across the interface is uniform \((J_I = J)\); therefore, the flat interfaces are fully uncompensated while the rough ones are compensated on average.

The FM and AFM order parameters are the uniform and staggered magnetization per spin, respectively. These are defined as \(m_x = |\sum_r S^x_r|/N_F\) and \(m_y = |\sum_{r \in I} S^y_r - \sum_{r \in II} S^y_r|/N_A\), where I and II denote the two simple cubic sublattices of the BCC lattice and \(N_F\) and \(N_A\) denote the number of spins on the FM and on the AFM films, respectively. The summations here are performed over all sites on both types of films. The magnitude of the two components of the uniform magnetization parallel to the interfacial plane is denoted as \(m_x\) and \(m_y\). Our simulations were carried out using importance
Neel temperature. The is very sharp and it occurs at a temperature below the suggest that the onset of this perpendicular orientation axis, which is the direction of the AFM spins. Our results in a direction that is perpendicular to the AFM easy axis, the direction of the FM spins. As the temperature is lowered in the case of the rough interface the FM spins switch to orientation is constant. These data suggest the existence of staggered magnetization are very small for all $T$ in the absence of the AFM film, spins on the FM film have global rotation symmetry in the $x$-$y$ plane, which is the easy plane for spins on this film. The preferential orientations of the FM spins observed here either below or above $T_N$ result from the exchange coupling to the AFM film.

In studying thin films, it is also interesting to examine the layer magnetization since this can vary significantly depending on the proximity to the interface or to the free boundaries. Figs. and show the layer magnetization and the magnitude of its $y$-component, respectively, as a function of the film layer for a system with rough interface and $L = 96$. In our notation, layers 1 to 12 comprise the AFM film, layer 13 has uniform terraces belonging alternately to the AFM and FM films, and layers 14 to 24 form the FM film. For each temperature, the slightly lower magnetization on the surface layers is a consequence of the free boundary condition along the $z$-axis. In addition, the compensated exchange on average across the interfacial plane reduces the layer magnetiza-
tion for the layers near the interface. The perpendicular orientation of the FM spins with the AFM spins at low 
$T$ can also be seen in Fig. 3b, where e.g. for $T = 0.6J/k_B$ the magnetization on the FM layers has a very small $y$-component. At a higher $T$, e.g. $T = 1.8J/k_B < T_N$ the magnetization on the FM layers has a large $y$-component. When the interface is flat with uncompensated exchange across it, the reduction of the magnetization on the layers near the interface is not very large, at low $T$ (see Fig. 4 where layers 1 to 12 comprise the AFM film and layers 13 to 24 the FM film).

Simulations using $J_F = 5J > 0$, $J_A = -J$, $J_I = -2J$, $K_A = J$, and $K_F = -0.5J$ (i.e. with a stronger interfacial coupling) with rough interface suggest that the onset of the perpendicular orientation of the FM with the AFM easy axis occurs at a lower $T$ when the interfacial coupling increases in magnitude. We also find that for a film with a rough interface that is compensated on average, when the interaction and anisotropy parameters are such that the AFM becomes disordered at a higher temperature than the FM (e.g. with $J_F = J$,

$J_A = -J$, $J_I = -J$, $K_F = -0.5J$, and $K_A = J$), the perpendicular orientation of the FM and AFM spins is present throughout the FM phase.

Besides the usual critical slowing down near critical points, studies of phase transitions in thin films are further complicated by the fact that order in the films varies layer by layer, as illustrated above. Therefore, determining the nature of phase transitions may require a layer order parameter. However, the goal of our current work is not to study the thermodynamic limit of these bilayers, but rather to understand experimental observations of finite systems.

Monte Carlo simulations have been used to study a system of coupled FM/AFM films, with flat interfaces that are fully uncompensated as well as rough interfaces that are compensated on average. For both types of interfaces above the Néel temperature we observed order in the AFM with the AFM spins aligning collinearly with the FM moments. As the temperature is lowered in the case of the rough interface, we have seen a transition from collinear to perpendicular alignment of the FM and AFM spins.

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