Phase transitions in ferro-antiferromagnetic bilayers with a stepped interface

D.P. Landau a,*, Shan-Ho Tsai a,c, Thomas C. Schulthess b

a Center for Simulational Physics, University of Georgia, Athens, GA 30602
b Center for Computational Sciences and Computer Science & Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831
c Enterprise IT Services, University of Georgia, Athens, GA 30602

Abstract

We have studied magnetic ordering in ferro/antiferromagnetic (F/AF) bilayers using Monte Carlo simulations of classical Heisenberg spins. For both flat and stepped interfaces we observed order in the AF above the Néel temperature, with the AF spins aligning collinearly with the F moments. In the case of the stepped interface there is a transition from collinear to perpendicular alignment of the F and AF spins at a lower temperature.

Key words: Ferromagnetic-antiferromagnetic bilayer, classical spin, anisotropy, Monte Carlo simulation

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Magnetic properties of ferro/antiferromagnetic (F/AF) bilayers can be very different from those of free F and AF films. These coupled systems exhibit a shift in the hysteresis loop (exchange bias) and larger coercivity than the free F film [1]. Other effects of the F/AF coupling include the order in the AF observed above the Néel temperature[2] and the perpendicular orientation of the F with the AF moments[3,4]. Understanding these effects and the nature of the F/AF interfaces remains a challenge.

In this paper we use Monte Carlo simulations to study the effect of the interfacial exchange and roughness on the magnetic ordering in F/AF bilayers. The work is motivated by recent experiments for Fe3O4/CoO multilayers[2]. We consider a ferromagnetic (F) film coupled to an antiferromagnetic (AF) film where the lattice is coherent across the F/AF interface. Each film is a bcc lattice, with linear sizes \(L_x = L_y = L \leq 96\) and 12 staggered (because of the bcc structure) layers of classical spins \(|S_r| = 1\), which interact via the Hamiltonian

\[
\mathcal{H} = -J_F \sum_{\langle r, r' \rangle \in F} \mathbf{S}_r \cdot \mathbf{S}_{r'} - K_F \sum_{r \in F} (S^z_r)^2 - J_A \sum_{\langle r, r' \rangle \in AF} \mathbf{S}_r \cdot \mathbf{S}_{r'} - K_A \sum_{r \in AF} (S^y_r)^2 - J_I \sum_{\langle r, r' \rangle \in F/AF} \mathbf{S}_r \cdot \mathbf{S}_{r'}
\]

where \(\langle r, r' \rangle\) denotes nearest-neighbor pairs of spins coupled with exchange interactions \(J_F = 5J > 0\) in the F film, \(J_A = -J < 0\) in the AF film, and \(J_I = -J\) at the F/AF interface. Spins in the AF film have a uniaxial single-site anisotropy \(K_A = J\), whose easy axis is along the y axis. The demagnetizing field on the F film is modeled with a hard-axis \((K_F = -0.5J)\) along the z direction, which is perpendicular to the F/AF interfacial plane. No external magnetic field is applied. We use periodic boundary conditions along the z and y directions and free boundary conditions along the z direction. We model flat interfaces that are fully uncompensated as well as uniformly stepped ones that are compensated on average.
The stepped interface has 6, L, and one spin per terrace in the x, y, and z directions, respectively.

The F and AF order parameters are the uniform (m) and staggered (m_s) magnetization per spin, respectively[6]. m_x and m_y denote the two components of m in the interfacial plane. We perform Monte Carlo simulations with Metropolis algorithm at fixed temperature T. Typically we discard 3 × 10^5 Monte Carlo Steps/site (MCS) for thermalization and then use about 2 × 10^5 MCS for averages. Whenever not shown, error bars in the figures are smaller than the symbol sizes.

The T-dependence of m shown in Figs.1(a) and 1(b) plus finite-size analysis (not shown) indicate an F ordering transition at T_c ≈ 9.3J/k_B. A free 12-atomic-layer AF film undergoes a phase transition at the Néel temperature[5] T_N ≈ 2.2J/k_B. For both flat and stepped interfaces, the spins on the F film orient predominantly in a direction collinear with the easy axis of the AF at high T (see Fig.1), even above T_N. This is an indication that there is still order in the AF above T_N due to the coupling to the ferromagnet. As T is lowered in the case of the stepped interface the F spins switch to orient in a direction that is perpendicular to the AF spins. Our results suggest that the onset of this perpendicular orientation is very sharp and it occurs at a temperature below T_N. The z-components of m and m_s are very small for all T. In the absence of the AF film, spins on the F film have global rotation symmetry in the x-y plane, which is their easy plane. The preferential orientations of the F spins observed either below or above T_N result from the exchange coupling to the AF film.

Fig.2 shows m_s versus T for different L for stepped and flat interfaces. In the former case the decay to zero of m_s at T ≈ 2.2J/k_B becomes sharper for larger L (see the inset), suggesting an AF phase transition at T_N. In contrast, with a flat ( uncompensated) interface there is no finite-size dependency of m_s near T_N, suggesting the absence of an AF phase transition there.

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Fig. 2. Staggered magnetization as a function of temperature for stepped and flat interfaces.

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