Monte Carlo simulations of a ferromagnetic-FeF_2 system

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Abstract

In this work we perform Monte Carlo simulations to study the magnetization reversal mechanism in ferromagnetic thin films on FeF_2. In particular, we emulate a bilayer AFM/FM structure, where the AFM interface corresponds to an uncompensated (100) plane. The magnetic moments are modeled by classical Heisenberg spin variables. Our analysis focus on the role of the exchange interaction J_{AF} between the FM spins and the spins belonging to the AFM interface on the reversal mechanisms of the magnetization. By simulating hysteresis loops we study the effect of temperature on the bias field.

Key words: Exchange bias, Monte Carlo simulation, Thin films.

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1 Introduction

Exchange bias (EB) is an effect arising typically at an interface between a ferromagnetic (FM) and an antiferromagnetic (AFM) material when the Curie temperature of the former is larger than the Nèel temperature of the latter. If the system is cooled under an applied field H_{cf} below the ordering temperature of the antiferromagnet, the center of the hysteresis loop usually shifts opposite to the cooling field by an amount H_{EB}, called the exchange bias field. Although this phenomenon was observed long time ago (1) there are still many controversies concerning the underlying mechanisms responsible for this effect (2; 3; 4). Beyond the theoretical interest, this phenomenon is also relevant in practical applications like for instance magnetic sensors and magnetic recording media (3). The characterization of the spin structure in the nearest planes to the interface is a main topic in the understanding of the EB phenomena. In particular, interfaces can be roughly classified as compensated and uncompensated, depending on whether they have zero or non zero net magnetization, respectively. Most of the earliest models that explain EB assume an uncompensated interfacial spin structure even when this requirement is not always fulfilled in experiments. In fact, experiments carried out by Moran *et al.* (5) and Nogués *et al.* (6) on Fe films grew over FeF_2 single crystals cut along different orientation showed that H_{EB} is larger when the interface is compensated ((110) plane) in comparison with the uncompensated interface in the (100) plane. This effect was supposed to be associated with spin rearrangement at the interface (3; 6).

In this work we analyze the hysteresis loop of a bilayer FM–FeF_2 with an uncompensated interface corresponding to the (100) plane using Metropolis

Monte Carlo simulations to analyze the existence of spin rearrangement. We are mainly concerned with the influence of the strength of the interaction between the FM and AFM layers.

2 Model

We studied one FM film mounted over other AFM film. The films are magnetically coupled each other by exchange interactions and the structure of both films is a body-centered cubic lattice with a perfect match across the FM/AFM interface. To perform the numerical simulations we used the following Hamiltonian

$$\begin{aligned} H = -J_F \sum_{<\vec{r},\vec{r}'>\in \mathrm{FM}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - K_F \sum_{\vec{r}\in \mathrm{FM}} (S^z_{\vec{r}})^2 \\ -J_A \sum_{<\vec{r},\vec{r}'>\in \mathrm{AFM}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - K_A \sum_{\vec{r}\in \mathrm{AFM}} (S^y_{\vec{r}})^2 \\ -J_{AF} \sum_{<\vec{r},\vec{r}'>\in \mathrm{FM/AFM}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - h \sum_{\vec{r}} S^y_{\vec{r}} \end{aligned} \tag{1}$$

where $\vec{S}_{\vec{r}}$ are classical Heisenberg spins vector of module one at the site $\vec{r}$, $< \vec{r}, \vec{r}' >$ denotes nearest neighbors pairs of spins coupled with exchange interactions, $J_F > 0$ is the exchange constant of the FM, $J_A < 0$ is the exchange constant of the AFM and $J_{AF} > 0$ represents the exchange coupling between the FM and the AFM layer. The anisotropy constant $K_F < 0$ introduces a planar anisotropy in the FM and the anisotropy constant $K_A > 0$ in the AFM introduces an easy axis single site anisotropy along the y axis. L_x and L_y are the lateral dimensions of the films in units of the lattice parameter and L_{za} and L_{zf} are the thicknesses of the FM and AFM films in same units, respectively. The total number of spins is then $N = 2\, L_x\, L_y\, (L_{za} + L_{zf})$. Periodic boundary conditions were imposed in the plane of the film while in the direction perpendicular to the film open boundary conditions were used. For each point in the simulated magnetization curves we took 10^4 Monte Carlo step per site to thermalize and the same number to calculate the temporal averages. We set the following dimensions for the system: $L_x = L_y = 20$ and $L_{za} = Lzf = 6$ and employ the following parameters: $J_F = 9.56J$, $J_A = -J$, J_{AF} in the interval $[J_A, J_F]$, $K_F = -0.5J$ and $K_A = -1.77J$, following the ideas introduced in (7) in order to emulate FeF_2 materials.

3 Results

In Fig. 1 we present the bias field H_{EB} as a function of J_{AF} keeping frozen the spin configuration of the AFM film at the interface. According to the model of Meiklejhon (8) the bias field is given by

$$H_{EB} = \frac{4J_{AF}}{L_{zf}} \tag{2}$$

Notice that for $J_{AF} \lesssim 1$ this relation (continuous line) holds very well, suggesting that the inversion of the magnetization takes place by a coherent rotation, i.e. the magnetization rotates in the plane of the film. For $J_{AF} > 1$ the simulated points depart from the model, and this can be explained by the formation of a domain wall in the FM film which is parallel to the interface. Fig. 2 displays the hysteresis loops of interfacial FM layer, of the top FM layer and of the complete film, confirming the formation of the domain wall. The top FM plane is the easiest to rotate whereas the layer at the interface is pinned by the AFM spins. Since the FM anisotropy is planar, the curves do not show hysteresis.

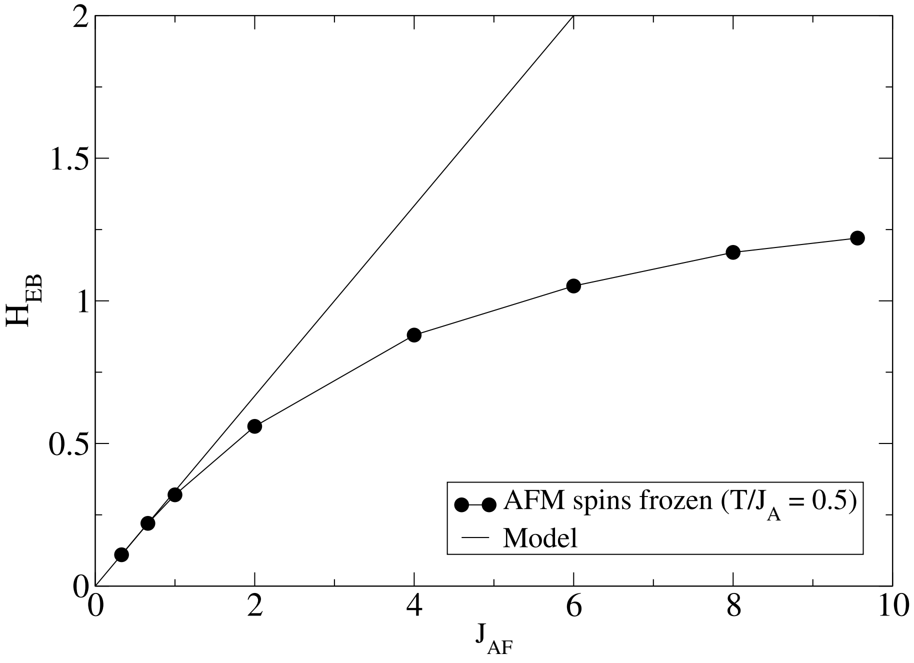

Fig. 1. Bias field for a frozen AFM spin configuration and different values of J_{AF}. The line is a plotting of eq. (2).

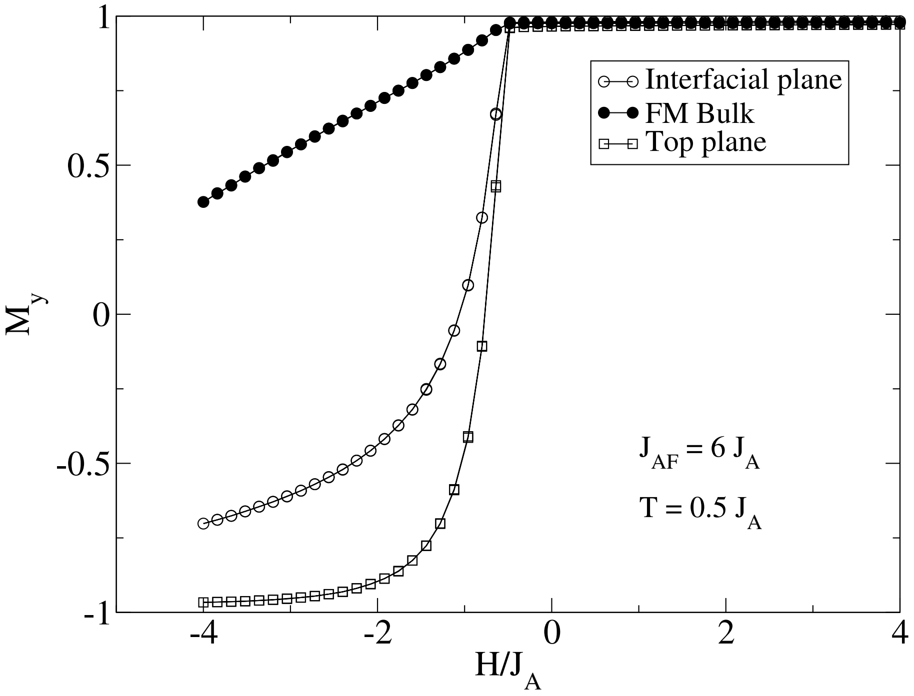

Fig. 2. Bulk, bottom layer, and top layer magnetization in the direction of the applied field for $J_{AF}/J_A = 6$ and $T/J_A = 0.5$. The curves split indicating the presence of a wall parallel to the FM film.

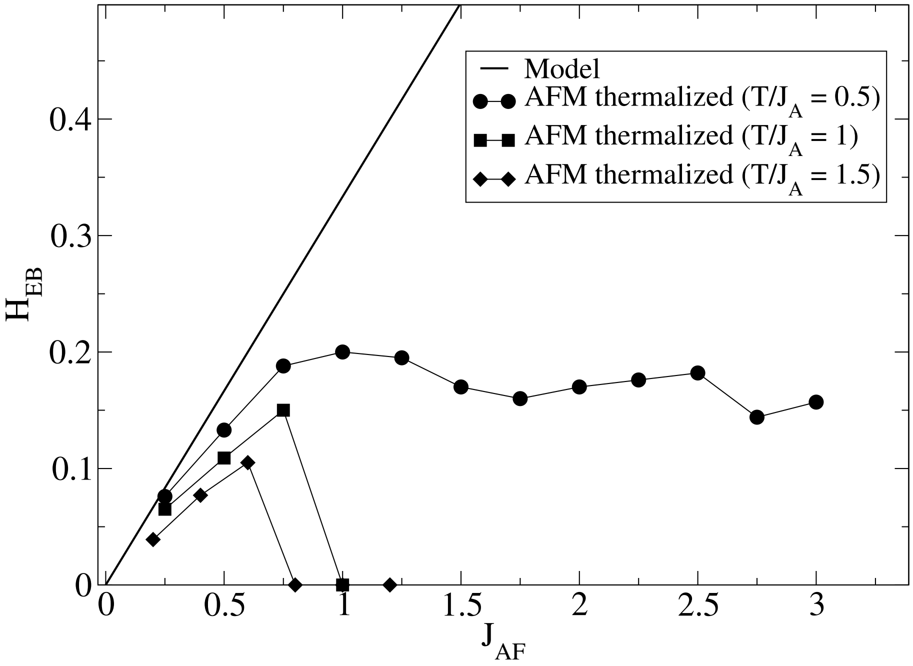

Fig. 3. Bias field as function of the exchange coupling between the layers for three different temperatures. The line is a plot of eq. (2).

In Fig. 3 we show the bias field as a function of J_{AF} for three different temperatures, when the AFM spins are allowed to thermalize. The simulated points show a bias field that is always smaller than the values predicted by Eq. (2) even in the region where a domain wall is not present in the FM (Fig. 1). As the temperature increases the bias field goes to zero at lower values of J_{AF}.

Fig. 4 shows the magnetization loop of the AFM plane nearest to the interface together with magnetization loop of the FM film at $T/J_A = 1.5$, for $J_{AF}/J_A = 0.2$ (Fig. 4a) and $J_{AF}/J_A = 1.2$ (Fig. 4b), respectively (see Fig. 3). The demagnetization curve of the AFM layer in Fig 4a remains almost constant until the applied field is close to the bias field of the FM loop, when abruptly changes to a lower value and attains again a constant value. This behavior can not be associated to coherent rotation of the AFM spins and a spin rearrangements in the interface seems to be necessary. As J_{AF}/J_A increases

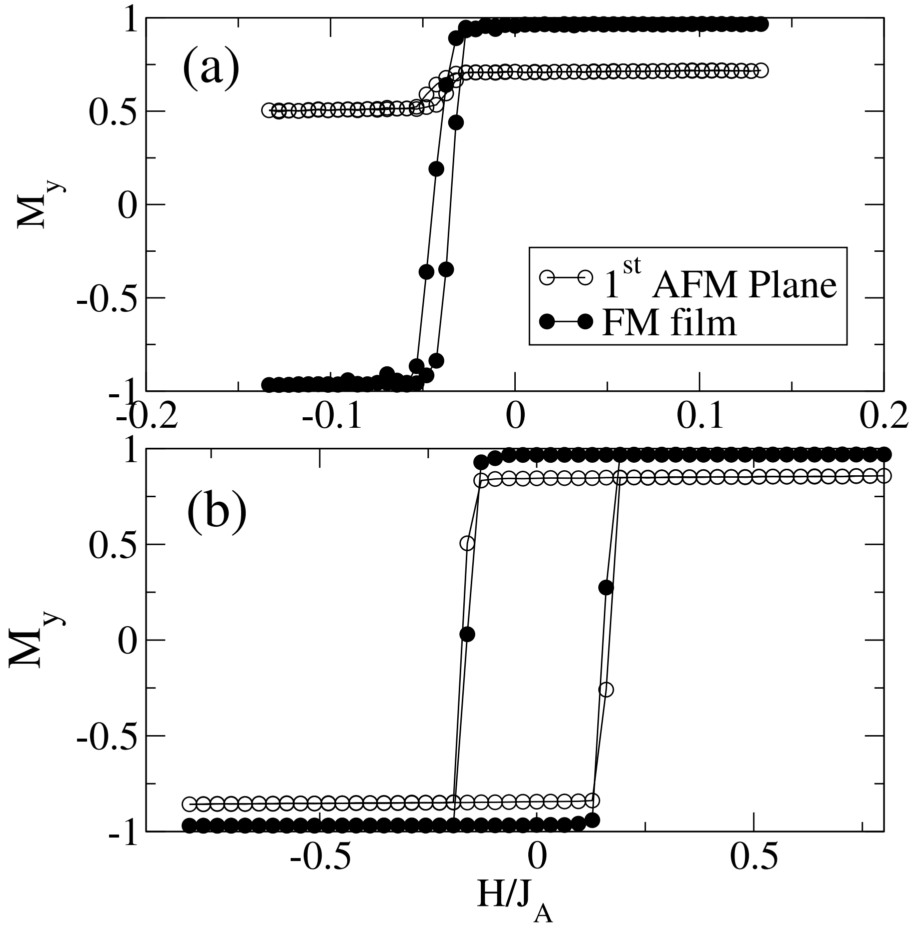

Fig. 4. Hysteresis loop corresponding to the first plane of the AFM (hollow symbols) and the FM film (fill symbols) for $T/J_A = 1.5$. Two different interface interactions are considered, $J_{AF} = 0.2$ (a) and $J_{AF} = 1.2$ (b).

(Fig. 4b) the change in the demagnetization curve of the AFM layer becomes sharper and the magnetization aligns to the inverse applied field. In this case the bias field of the FM is equal to zero and the spin rearrangements at the interface, which are irreversible, result in a non null value of the coercivity of the FM film.

Summarizing, when the AFM spins in the interface are frozen a domain wall develops if the interaction between the films is high enough. For small values of this interaction the bias is well described by Eq. (2). Allowing the AFM to thermalize results in a decrease in the bias field which is associated to spin rearrangements that begins at the interface. For large values of the FM-AFM interaction, instead of a wall formation in the FM film the spin rearrangement becomes more irreversible in detriment of the bias field, raising the coercivity of FM film.

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