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Exchange bias of patterned systems: Model and numerical simulation

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ABSTRACT

The magnitude of the exchange bias field of patterned systems exhibits a notable increase in relation to the usual bilayer systems, where a continuous ferromagnetic film is deposited on an antiferromagnet insulator. Here we develop a model, and implement a Monte Carlo calculation, to interpret the experimental observations which is consistent with experimental results, on the basis of assuming a small fraction of spins pinned ferromagnetically in the antiferromagnetic interface layer.

A complete theoretical understanding of the exchange bias (EB) phenomenon has posed a formidable challenge to condensed matter theorists for over five decades. The challenge has several sources: the intrinsic interest of EB, the many supplementary physical phenomena that are involved and the important technological applications it has generated. EB was discovered more than 60 years ago, by Meiklejohn and Bean [1,2], and its characteristic signature is the shift of the center of magnetic hysteresis loop from its normal position at $H=0$ to $H_{EB}\neq 0$. It occurs in a large variety of systems [3] which are composed by an antiferromagnet (AF) that is in atomic contact with a ferromagnet (FM) when the sample is grown, or after the system is cooled, below the respective Néel and Curie temperatures T_N and T_C, in an external field H_{cf}. Examples of the type of systems where EB has been observed are clusters or small particles, FM films deposited on single crystal or polycrystalline antiferromagnets, F/AF thin films bilayers, and spin glasses. A comprehensive review, which emphasizes experimental results and provides an up-to-date list of relevant publications, was published by Nogués and Schuller [3], while the theory was reviewed by Berkowitz and Takano [4], Kiwi [5] and Stamps [6]. A comprehensive review of exchange bias in polycrystalline films, containing small grains, was published short time ago by O'Grady et al. [7] stressing the importance of the antiferromagnetic bulk structure and the interplay of bulk and interfacial effects.

In particular, the relevance of the magnetic structure of the antiferromagnet (AF) for the proper description and understanding of the EB phenomenon has emerged from several recent experiments. Morales et al. [8] focused on the three dimensional AF bulk structure, Dutson et al. [9] and Vallejo-Outon et al. [10] emphasized the importance of interface effects and AF bulk dynamics, while Roy et al. [11] investigated in detail the depth profile of uncompensated spins in the AF. In a recent contribution Vallejo-Outon et al. [12] presented a numerical simulation of patterned exchange bias systems consisting in an array of squares containing metallic polycrystalline AF layers. They obtained values for the EB field as a function of square size and AF thickness. The difference with continuous thin film values was obtained quantitatively, on the basis of assuming that each individual grain supports a single magnetic domain. This way the relevance of the AF grain size distribution becomes a key ingredient, an issue already pointed out previously [13].

In this context experiments on patterned systems [14] may provide an important clue to improve the theoretical understanding that has been developed so far. These experiments proved that replacing a continuous 30 nm thick FM nickel film by a patterned one, built up by dots 110 nm in diameter, reduced the cooling field necessary to generate similar EB values by a full order of magnitude [14]. The AF substrate used in these experiments was 30 nm thick FeF_2. The results of Li et al. [14] were interpreted by the authors on the basis of a rather long range "domain" structure (of the order of 500 nm) unfolding in the AF. Here we develop a simple model, that provides an alternative interpretation of the experiments to the one put forward in the paper by Li et al. [14].

Our purpose is to describe, on the basis of a model based on the FM pinning of a small fraction of spins on the AF interface layer which, in combination with a Monte Carlo calculation, provides a proper description of the observed results. The physical idea for the FM pinning of a fraction of the spins rests on the work by Gaunt [15], which in the EB context was already explored by

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O'Grady et al. [9,10,16]. Gaunt's basic idea is that the ferromagnetic magnetization $M(t)$ varies in time as

$$M(t) = M(t_0) \pm S \ln(t/t_0), \tag{1}$$

where S is a constant [15]. The function $\ln(t)$ reflects a broad distribution of energy barriers for pinned spins which, in agreement with the grain size distribution mentioned above [7,12,13], we assume also exists in the AF [17], particularly in the interface layer. The picture we put forward is that a significant fraction of the pinned spins has such a long decay time that for all practical purposes they can be assumed to be static. The rest of them is able to follow the cooling field, at least to a certain degree. This picture is consistent with the EB bias model for continuous overlayers that we developed some time ago [5,18–20]. However, if one FM dot of the overlayer "sits" on just a single region of pinned spins pointing in a particular direction, with a very large energy barrier (i.e. with basically no dynamics), then the effect does not average out, as it does for a continuous film, but on the contrary spreads across the whole dot. In terms of the cartoon of Fig. 1, if the dot covers a single region of pinned spins with a net FM moment then its dynamics, and consequently the magnitude both of the exchange bias field H_{EB} and the coercivity H_c, are quite different from the configuration with several differently oriented FM pinned regions lying under the dot. In our picture a FM dot that extends over several pinned regions behaves almost as a continuous film, as far as the EB phenomenon is concerned.

Here we focus our attention on the effect of these FM pinned spins, in the AF interface layer, on the EB phenomenon of patterned systems. While these spins are subject to the external cooling field $\vec{H}_{cf}$ the details of the consequences of varying the magnitude of $\vec{H}_{cf}$ are left open for the time being. Analytically the model is formulated as follows:

$$\mathcal{H} = \mathcal{H}_{AF} + \mathcal{H}_{F/AF} + \mathcal{H}_F, \tag{2}$$

where

$$\mathcal{H}_{AF} = -J_{AF} \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - K_{AF} \sum_j (\vec{S}_j \cdot \hat{e}_{AF})^2 - \mu_B g_{AF} \sum_j \vec{S}_j \cdot \vec{H}, \tag{3}$$

$$\mathcal{H}_{F/AF} = -J_{F/AF} \sum_{\langle j,k \rangle} \vec{S}_j \cdot \vec{S}_k, \tag{4}$$

$$\mathcal{H}_F = -2J_F \sum_{\langle k,\ell \rangle} \vec{S}_k \cdot \vec{S}_\ell - \mu_B g_{FM} \sum_k \vec{S}_k \cdot \vec{H}. \tag{5}$$

Above $\mathcal{H}_{AF}$,$\mathcal{H}_{F/AF}$ and $\mathcal{H}_F$ describe the AF, the interface and the FM, respectively. The symbol $\langle m,n \rangle$ implies that the summation is restricted to nearest neighbors only; the set of labels $\{i,j\}$ and $\{k,\ell\}$ label the AF and the FM, respectively, while μ_B denotes the Bohr magneton and g the gyromagnetic ratio. $\vec{H}$ is the external applied magnetic field and J_{AF}, $J_{F/AF}$ and J_F are the AF, interface and FM Heisenberg exchange parameters, respectively. K_{AF} is the AF anisotropy constant. Eq. (3) contains the uniaxial anisotropy direction $\hat{e}_{AF}$, which points parallel to the interface. Moreover, we limit the dynamics of the AF spins to planes parallel to the interface. Since the FM is polycrystalline, and in addition the anisotropy of the FM is much smaller than K_{AF}, we simply consider that the FM does not have magnetic anisotropy.

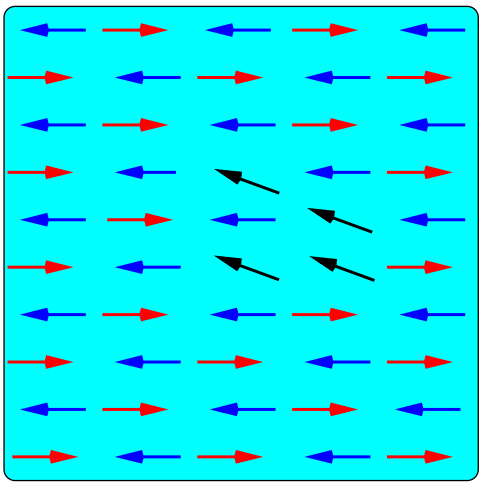

Fig. 1. Cartoon of the AF interface layer with a fraction of the spins pinned and pointing in an arbitrary fixed direction.

To extract quantitative information from our model we implemented a Monte Carlo calculation for the system defined by the Hamiltonian of Eq. (2). In particular, we modeled a system that consists in FM Ni dots deposited on an AF FeF_2 substrate, which corresponds to the measurements reported by Li et al. [14]. The parameters we adopt are $J_{AF} = -0.1$, $J_{F/AF} = -0.5$, $K_{AF} = 0.08$, all in units of $J_F = 1$. For the gyromagnetic ratios we used $g_{AF} = 3.5$ and $g_{FM} = 1.5$, which correspond to Ni and FeF_2 (i.e. for these parameter values, and using Monte Carlo, we obtain the experimentally observed Curie and Néel temperatures).

Monte Carlo simulations were carried out using the Metropolis algorithm with local dynamics and single-spin flip dynamics [21]. The new orientation of the magnetic moment was chosen arbitrarily, in such a way that the spin components vary within an interval of 0.2 around the initial ones, with a probability $p = \min[1, \exp(-\Delta E/k_B T)]$, where ΔE is the energy change due to the reorientation of the spin, k_B the Boltzmann constant and T the temperature. We set $T = 10\,\mathrm{K}$, which corresponds to the usual hysteresis loops measurements. In the simulation, the magnetization curve starts at $H = 10\,\mathrm{T}$ applied along the [1 0 0] crystallographic direction, labeled as the x-axis, and initially all of the FM magnetic moments point along this direction. We define the coercivity field as $H_c = (H_2 - H_1)/2$ and the EB field $H_{EB} = (H_2 + H_1)/2$, where H_1 and H_2 are the values of the external field that yield zero magnetization. Field steps of $\Delta H = 0.01\,\mathrm{T}$ are used in all the calculations. Typically, we perform 1.2×10^6 Monte Carlo steps (MCS) for a complete hysteresis loop, which is equivalent to 600 MCS per field value. Five different seeds for the random number generator were used to improve the statistics. These five simulations are averaged and used to generate the results we present.

A basic issue is to make sure that the number of MCS is sufficient to generate reliable results. To simulate the presence of pinned spins in the AF we allowed a fraction of them to remain fixed, parallel to each other and pointing in an arbitrary direction in the AF interface layer, as illustrated in Fig. 1. In Fig. 2 we illustrate the results for the exchange bias field H_{EB} and coercivity H_c as a function of the number of steps per spin, half of which are allowed for thermalization and the rest for averaging. On the basis of these results we adopted 600 MCS per spin to determine the magnitude of H_{EB} and H_c. As expected, the results we obtain for the coercivity H_c only converge to a constant value asymptotically with time.

The results we obtained for the EB field H_{EB} and the coercivity H_c as a function of dot size, with 36 (6×6) spins pinned in the same spatial direction, are displayed in Fig. 3. Obviously, the magnitude of H_{EB} decreases as the fraction of FM pinned spins diminishes, but it is quite remarkable that with less than 5% of the interface layer pinned, which corresponds to $\sim 0.1\%$ of the total number of spins in the system, the value of H_{EB} still turns out to be around 200 Oe. The results for H_{EB} scale approximately as $L^{-1.8}$. The coercivity H_c shows a monotonic increase as a function of the lateral size of the system, which approaches its maximum value as $L \to \infty$.