Disorder-induced induced mechanism for positive exchange bias fields

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(Dated: May 7, 2014)

We propose a mechanism to explain the phenomenon of positive exchange bias on magnetic bilayered systems. The mechanism is based on the formation of a domain wall at a disordered interface during field cooling (FC) which induces a symmetry breaking of the antiferromagnet, without relying on any ad hoc assumption about the coupling between the ferromagnetic (FM) and antiferromagnetic (AFM) layers. The domain wall is a result of the disorder at the interface between FM and AFM, which reduces the effective anisotropy in the region. We show that the proposed mechanism explains several known experimental facts within a single theoretical framework. This result is supported by Monte Carlo simulations on a microscopic Heisenberg model, by micromagnetic calculations at zero temperature and by mean field analysis of an effective Ising like phenomenological model.

PACS numbers: 75.70.-i, 75.60.Jk, 75.70.Cn
Keywords: Exchange Bias, Magnetic bilayers.

The exchange bias phenomenon (EB) usually appears in heterogeneous magnetic systems in the nanoscale range, such as thin-film layered systems. EB has captured the attention of many researchers due to its applications in design of spin valves. The phenomenon manifests itself when the system is cooled down in the presence of a magnetic field, provided the starting temperature is self when the system is cooled down in the presence of a cooling field (FC). An hysteresis loop performed after this procedure shows an horizontal shift called the bias field, \(H_{EB}\). Usually the bias field is opposite to the cooling field (normal exchange bias, NEB) but sometimes the displacement is in the same direction and it is called positive EB (PEB). Other important effects can appear, such as a vertical shift in the magnetization and the widening and symmetry loss of the hysteresis loops. EB disappears if the system is heated above the blocking temperature, \(T_B\), which is below but close to the Néel temperature of the antiferromagnetic (AFM).

Currently, much of the effort is focused on tuning EB and establishing the mechanisms which control the effect. The existence of uncompensated domains at the interface has been shown to be fundamental for the appearance of EB\(^{10}\). Also, at the relevant scales of the problem all the systems have some unavoidable amount of disorder which seems to play a main role. In this regard, several routes are employed in experiments to introduce and control the disorder effects\(^{11-15}\). For instance, dilution can enhance the bias field\(^{14}\). In addition, the interfacial roughness and the disorder in the anisotropy, are related to the appearance of PEB\(^{11-16}\). In any case, it is well established that a strong cooling field is necessary for the observation of PEB\(^{11-16}\). Among the bilayered systems, one of the most studied is the FM/FeF\(_2\), because the AFM FeF\(_2\) has a simple spin structure\(^{15}\). In particular, PEB was reported for the first time by Noguès et al.\(^{16}\) in this kind of systems.

Most of the theoretical works up to now has assumed that the AFM/FM interface exchange interaction is antiferromagnetic; this is a key ingredient to explain PEB\(^{11-16}\). In this paper we show that such an ad hoc assumption (hard to justify physically) is not necessary to explain PEB, as long as a large enough amount of disorder is present at the interface. To exhibit the mechanism behind such an effect we first performed Monte Carlo simulations using a microscopy model for the bilayered system. We show that PEB is related to the formation of a domain wall at the interface during field cooling (FC), hence in this case PEB is independent of the sign of the interface exchange interaction.

We considered a FM film mounted over an AFM film. The films are magnetically coupled to each other by exchange interactions and the structure of both films is \(bcc\), assuming a perfect match across the FM/AFM interface. The system is ruled by the following Hamiltonian,

\[
H = -J_F \sum_{< \vec{r}, \vec{r}' > \in FM} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - K_F \sum_{\vec{r} \in FM} (S_{\vec{r}}^z)^2 + J_A \sum_{< \vec{r}, \vec{r}' > \in AFM} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - K_A \sum_{\vec{r} \in AFM} (\vec{S}_{\vec{r}} \cdot \hat{n}_{\vec{r}})^2 - J_{EB} \sum_{< \vec{r}, \vec{r}' > \in FM/AFM} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}'} - h \sum_{\vec{r}} S_{\vec{r}}^y,
\]

(1)

where \(\vec{S}_{\vec{r}}\) is a classical Heisenberg spin (\(|\vec{S}_{\vec{r}}| = 1\)) located at the node \(\vec{r}\) of the lattice. \(< \vec{r}, \vec{r}' >\) denotes a sum over
nearest-neighbors pairs of spins. \( J_F > 0 \) is the exchange constant of the FM, \( J_A > 0 \) is the strength of the AFM exchange, and \( J_{EB} > 0 \) is the exchange coupling between the FM and the AFM at the interface. \( K_F \) and \( K_A \) are FM and AFM anisotropy constants, respectively. The disorder in the anisotropy is introduced as in the random anisotropy model, i.e. \( \hat{n}_F \) is a random direction vector for AFM spins close to the interface. Inside the AFM \( \hat{n}_F \) points in the \( y \) direction. \( h \) is an external homogeneous magnetic field oriented along the \( y \) direction. \( F \) or each point in the magnetic field, we took 10^4 Monte Carlo steps per site (MCS) to thermalize the system and the same number of MCS to calculate temporal averages. The AFM was modeled using FeF₂ fluoride parameters, setting AFM interface spin configuration uncompensated, corresponding to the (100) FeF₂ crystalline orientation.

Monte Carlo simulations were performed using Metropolis algorithm. \( L_x = L_y = L \) are the lateral dimensions of the films, and \( L_{2x} \) and \( L_{2y} \) are the number of atomic layers of the FM and AFM films, respectively. We set \( L_x = L_y = 20, 40, L_{2x} = 24 \) and \( L_{2y} = 12 \). Periodic boundary conditions were imposed in the plane of the film while open boundary conditions were used in the perpendicular direction. For each point in the magnetization curve, we took 10^4 Monte Carlo steps per site (MCS) to thermalize the system and the same number of MCS to calculate temporal averages. The AFM was modeled using FeF₂ fluoride parameters, setting AFM interface spin configuration uncompensated, corresponding to the (100) FeF₂ crystalline orientation.

In Fig.1 we show the field \( H_{EB} \) versus the number of disordered AFM layers \( k \) in the interface region. The temperature of the system is well below the Néel temperature \( (T/T_N = 0.1) \). As a general rule the bias field decreases in module as the number of planes with disorder increases, as expected according to previous results (see e.g. Ref.[20]). The bias field is normal up to \( k = 7 \), and for larger values it becomes positive. Notice that the absolute value of \( H_{EB} \) varies continuously at the transition from normal to PEB, as observed experimentally. We also observe a vertical shift in the hysteresis loops correlated with the sign of the bias field (see Fig.1), as observed in fluoride iron compounds. In Fig.2 we plot \( H_{EB} \) versus temperature for a system with a fixed number of AFM disordered layers (\( k = 12 \)) and for different cooling fields. If the cooling field is strong \( (H_{CF} > 0.24J_A) \), \( H_{EB} \) is positive in the whole range of temperatures whereas, as \( H_{CF} \) decreases, the sign of \( H_{EB} \) changes twice at intermediate temperatures. A change of sign of \( H_{EB} \) as a function of the temperature has been observed in diluted AFM and in random anisotropy AFM. As we will discuss later, while \( NEB \) is expected at low temperatures, the presence of PEB at very low temperatures appears to be a spurious finite size effect, as suggested by the strong enhancement of fluctuations in the sign of \( H_{EB} \) as the lateral size of the system is reduced (see inset of Fig.2).

An inspection of the local magnetization at each layer shows that, in the case of PEB, an antiferromagnetic domain wall (DW) forms during FC in the disordered region. In this way the system reduces the exchange energy cost due to frustration while it stores energy at the interface through the Zeeman coupling of the AFM spins. This energy is restored during the field reversal producing a positive bias in the hysteresis loop. On the contrary, in the case of NEB no DW is observed for positive field. In other words, the whole AFM slab (both the ordered and the disordered regions), exhibits a single Neel state without frustration. In this case, a DW forms for negative fields, giving rise to a negative bias of the hysteresis loop. It is noting to note that in our simulations, the DW formed in the disordered region is responsible for the shift in the magnetization.

Let’s analyze the conditions for the formation of a do-
continuous line is a fit of Eq.(5) with \( \theta_0 = 0.45 \) and \( l_w = 11 \). Inset: AFM magnetization profile, the dashed box indicates the disordered region.

main wall under an applied field in the disordered region of the AFM. The energy per unit of area of an AFM disordered region of length \( l_w \) under the applied field is given by

\[
E = \int_0^{l_w} \left[ \frac{J_F}{2} \left( \frac{d\theta}{dz} \right)^2 - \frac{H_{CF}}{2} \sin(\theta) \left( \frac{d\beta}{dz} \right) \right] dz. \tag{2}
\]

Assuming that randomness averages the effect of the anisotropy, we neglected it considering only the exchange interaction between layers (\( J_l \)) and the coupling with the field. We will test this approximation later. Note the field interacts through the gradient of the angle \( \theta \) since this region is antiferromagnetically ordered, i.e. the magnetization in the direction of the field is 

\[
m(z) = \frac{1}{2} \sin(\theta) \left( \frac{d\theta}{dz} \right).
\]

Minimizing this energy we obtain \( \theta = \frac{\pi - \theta_0}{l_w} z + \theta_0 \), where \( \theta_0 \) is a free parameter (\( 0 < \theta_0 < \pi \)). The total energy is,

\[
E = \frac{J_l}{2} \left( \frac{\pi - \theta_0}{l_w} \right)^2 l_w - \frac{H_{CF}}{2} \left( 1 + \cos(\theta_0) \right), \tag{3}
\]

and a domain wall forms if \( E < 0 \) implying \( H_{CF} > H^* \), where

\[
H^* = \frac{J_l}{2} \frac{\left( \frac{\pi - \theta_0}{l_w} \right)^2}{1 + \cos(\theta_0)} l_w. \tag{4}
\]

The magnetization profile is:

\[
m(z) = \frac{1}{2} \frac{\pi - \theta_0}{l_w} \sin \left( \frac{\pi - \theta_0}{l_w} z + \theta_0 \right). \tag{5}
\]

We checked Eq.(5) simulating (Eq.(1)) a system containing a region without anisotropy. In Fig. 3 we plot the profile of the net magnetization \( \tilde{M}(z) = [m_y(z) + m_y(z + 1)]/2 \) pointing in the direction of the applied field. The continuous line is a fit of Eq.(5) with \( \theta_0 = 0.45 \), showing a good agreement with the Monte Carlo simulation.

Moreover, when randomness is considered (\( K_A \neq 0 \)), the agreement is still good, verifying our previous assumption.

According to Eq.(4) there is a threshold for the appearance of a domain wall and therefore PEB. Using the parameters of the simulations (Fig. 5), and \( J_l = 4J_A \) we obtain \( H^* = 1.38J_A \) (\( \sim 5.5 \) T). However, in simulations of the net magnetization in the direction of the field is antiferromagnetically ordered, i.e. the magnetization profile is:

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\tilde{M}(z) = \theta \sin(\theta) \left( \frac{d\theta}{dz} \right)\]

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and a domain wall forms if \( E < 0 \) implying \( H_{CF} > H^* \), where

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\]

FIG. 3: (Color online) Net magnetization of the AFM \( \tilde{M}(z) \) obtained through Monte Carlo simulations, RAM refers to random anisotropy. The solid line corresponds to Eq.(5) with \( \theta_0 = 0.45 \) and \( l_w = 11 \). Inset: AFM magnetization profile, the dashed box indicates the disordered region.
sibilities and compared them for different values of $H$ and $T$. In Fig. 4 we show a typical example of both free energies when $H < J_{AF}$. We see that the minimum free energy solution changes from NEB to PEB as the temperature increases. Conversely, for each temperature we have a minimum field $H^*(T)$ (see lower inset of Fig. 4) such that PEB becomes the minimum energy state when $H > H^*(T)$, even for temperatures close to $T_N$. The upper inset of Fig. 4 shows the DW in the PEB case (compare with the inset of Fig. 3). A change in the sign of $H_{EB}$ as a function of the temperature has been observed in disordered fluorides\textsuperscript{11,13–15} following the same trend we observed in the MF calculations. In particular, in the Fe$_x$Ni$_{1-x}$F$_2$/Co bilayer\textsuperscript{15} a domain wall at the interface has been reported, where Fe$_x$Ni$_{1-x}$F$_2$ is a random anisotropy antiferromagnet. Since the critical field $H_c$ depends on the amount of disordered layers, inhomogeneities at the interface can give rise to a distribution of $H_c$ as is observed in FeF$_2$/FM\textsuperscript{14} bilayers. Finally, the effect of the disorder of the anisotropy at the interface is similar to that considered in the spin glass model of exchange bias\textsuperscript{21}, since disorder reduces the anisotropy at the interface, but in our case the coupling of this region with the applied field turns out to be important to produce PEB.

Summarizing, the reduction in the anisotropy for a large enough amount of interfacial disorder can induce the formation of a domain wall in the cooling field process inducing a symmetry breaking in the antiferromagnet. The energy stored in this domain wall is released during the field reversion, resulting in PEB. In this way, the PEB phenomenon can be explained as an exclusive result of interfacial disorder, without relying on ad hoc assumptions about the sign of the coupling between FM and AFM.

This work was partially supported by grants from CONICET, and SeCyT Universidad Nacional de Córdoba (Argentina).

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35 We fixed the parameters to be: $J_F = 9.56J$, $J_A = -J$, and $K_F = -0.5J$, where $J$ is an arbitrary parameter that sets the energy units. $J_EB = 0.5J$, $J$ and $K_A = 1.77J$.
36 See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.88.020405 for more details about these calculations.
37 The molecular field of FeF$_2$ is $8J_A \sim 32$ T.
38 The blocking temperatures in Fig. 2 are about 0.9 the Néel temperature.
39 See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.88.020405 for more details about the derivation of the free energy and the calculations described in what follows.
40 We used in the calculations $J_{AF} = 1$, $J = J_{AF}/2$ and $t_F = 5$. 
