Exchange bias in ferromagnetic/compensated antiferromagnetic bilayers

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By means of micromagnetic spin dynamics calculations, a quantitative calculation is carried out to explore the mechanism of exchange bias (EB) in ferromagnetic (FM)/compensated antiferromagnetic (AFM) bilayers. The antiferromagnets with low and high Néel temperatures have been both considered, and the crossover from negative to positive EB is found in the case with low Néel temperature. We propose that the mechanism of EB in FM/compensated AFM bilayers is due to the symmetry breaking of AFM that yields some net ferromagnetic components during cooling process.

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Exchange anisotropy was first discovered in 1956 by Meiklejohn and Bean,[1] who found that the hysteresis loop of Co/CoO after cooling in a magnetic field was no longer centered at zero field ($\mathbf{H}=0$) but was shifted along the field axis. The shifted direction was found to be opposite to the applied magnetic field (negative exchange bias $H_B<0$) and the magnitude of this shift is known as exchange bias (EB). It was subsequently established that this might be a general phenomenon for any ferromagnet (FM)/antiferromagnet (AFM) system cooling in an applied magnetic field (cooling field) from above the Néel temperature (T_N) of the AFM, with the FM Curie temperature (T_C) greater than T_N. In recent years, since the phenomenon of exchange bias has become the basis for an important application in information storage technology,[2] tremendous efforts have been made at exploring the mechanism.[3,4]

Meiklejohn and Bean originally suggested that exchange bias was a consequence of the presence of interfacial uncompensated AFM spins. In view of this argument, a natural question to ask is whether the exchange bias also exists in a FM/compensated AFM system. Surprisingly, in a compensated Fe/FeF_2 bilayer system, Nogués *et al.* observed not only the usual negative exchange bias but also an unexpected positive exchange bias ($H_B>0$) under large cooling fields.[5]

Several important theories have existed to study the exchange bias in compensated AFM. Koon[6] presented a microscopic explanation of EB due to an irreversible AFM domain wall and found a perpendicular orientation between the FM/AFM axis directions: namely, a spin-flop state. Schulthess and Butler[7] obtained that spin-flop coupling gave rise to a uniaxial anisotropy rather than leading to EB with consideration of magnetostatic interactions for a perfectly flat interface and attributed EB to the interfacial defects similar to Malozemoff's random field.[8] Hong[9] argued that interface spin configuration persisted after cooling below T_N, and negative or positive bias, respectively, corresponded to parallel or perpendicular easy axes of FM and AFM. Kiwi *et al.*[10] suggested a canted AFM spin configuration frozen into a metastable state and proposed the incomplete FM domain wall model to explain positive exchange bias. However, the former two theories were carried out with micromagnetic calculations without consideration of the cooling field; the latter two theories pointed out the cooling field without micromagnetic calculations and lacked much more detailed and sufficient microscopic information. Up to now, the exchange bias mechanism is still controversial.

In this paper, based on the assumptions that an antiferromagnetic interface coupling between FM/AFM is responsible for exchange bias in FM/compensated AFM,[5,11–13] and that the biased hysteresis loop is basically determined by the spin configurations in the underlying antiferromagnetic layer after cooling,[14–16] we carry out micromagnetic calculations using spin dynamics to explain the mechanism of EB in the FM/compensated AFM systems. *Physically the key point different from previous micromagnetic calculations,*[6,7] *is addressing the cooling field during cooling process*. We succeed to reproduce both the negative and positive EB effects. Qualitatively speaking, it is a competition among (i) the cooling magnetic field, (ii) the interface coupling of FM/AFM, and (iii) the spin-spin interaction and anisotropy of AFM that eventually determines the spin configurations in AFM during the cooling process.

For an AFM with weak spin-spin interaction (low T_N), the spin configuration of AFM at low cooling magnetic field is dominated by an AF-type interface coupling of FM/AFM. Therefore, the initially compensated AFM layers, especially the interface AFM layer, become weakly uncompensated, resulting in a net ferromagnetic component opposite to the cooling field (or the magnetization in FM). The hysteresis loop is then measured at low temperature after removing the cooling field, while the spin configuration in AFM is frozen. Similar to the arguments given by Meiklejohn and Bean, it can easily be deduced that the broken symmetry of AFM in this case favors the negative exchange bias. However, on the other hand, if the cooling field H_{CF} is large and comes to dominate, then a net ferromagnetic component along the cooling field is expected. Because of the AFM-type interface coupling of FM/AFM, it turns out that the broken symmetry of AFM in this case favors a positive exchange bias. On the other hand, for AFM with a strong spin-spin interaction (high

T_N) only negative EB can be found in a reasonably high H_{CF}. The quantitative results are given in the following to reveal in detail how these different terms affect the broken symmetry of AFM layers and its correlation with the exchange bias.

Our model Hamiltonian is

$$H = H_{A\text{-}A} + H_{F\text{-}F} + H_{A\text{-}F}, \tag{1}$$

where $H_{A\text{-}A}$ is the part of AFM layers, $H_{F\text{-}F}$ and $H_{A\text{-}F}$ the FM and the interface coupling between AFM and FM layers. They are

$$H_{A\text{-}A} = \sum_{\langle i,j \rangle} J_{A\text{-}A} \mathbf{S}_i \cdot \mathbf{S}_j - D_A \sum_i (S_i^x)^2 - H_{CF} \sum_i (g_A u_B) S_i^x, \tag{2}$$

$$H_{F\text{-}F} = -\sum_{\langle i,j \rangle} J_{F\text{-}F} \mathbf{S}_i \cdot \mathbf{S}_j - H_{CF} \sum_i (g_F u_B) S_i^x, \tag{3}$$

$$H_{A\text{-}F} = \sum_{\langle a,f \rangle} J_{A\text{-}F} \mathbf{S}_a \cdot \mathbf{S}_f, \tag{4}$$

where g_A, g_F, u_B, D_A, and H_{CF} denote AFM Landé factor, FM Lande factor, Bohr magneton, antiferromagnetic anisotropy, and cooling field in parallel with AFM anisotropy, respectively. The exchange coupling among spins is considered for nearest-neighbor sites only. The subscripts a and f are associated with AFM and FM, respectively. It is noticed that the anisotropy of the FM layer is neglected based on the fact that most experiments used soft ferromagnets. The dipole-dipole interactions in the system are not considered here, since they affect only quantitatively rather than qualitatively the symmetry breaking of AFM. As the previous models, we also assume that $J_{A\text{-}F} \sim J_{A\text{-}A}$.[6,7] The Néel temperature increases monotonically with $J_{A\text{-}A}$; thus the interface coupling is stronger in the FM/AFM systems with higher T_N and vice versa.

Now we calculate the EB by the following spin dynamics approach;[7] i.e., the local effective field is determined from the gradient of the energy, $\mathbf{H}_i^{\text{eff}} = -\partial H / g u_B \partial \mathbf{S}_i$, and $\{\mathbf{S}_i\}$ is required to satisfy the Laudau-Lifshitz equation of motion with the Gilbert-Kelley form for the damping term:

$$\frac{\partial}{\partial t} \mathbf{S}_i = g u_B \mathbf{S}_i \times \left(\mathbf{H}_i^{\text{eff}} - \eta \frac{\partial}{\partial t} \mathbf{S}_i \right),$$

where η denotes the damping parameter. This damping term is phenomenological and is included to remove the energy from the system and to ensure that the magnetic system is in a stable or metastable equilibrium after sufficient iterating calculating steps. A lattice with $50 \times 50 \times 2$(FM) and 10 layers of AFM is used in our calculation. In the beginning, the temperature T of the system is set at $T_c > T > T_N$. Therefore, the initial spin configuration in our spin dynamics calculation is such that the spins are randomly arranged for AFM but are ferromagnetically arranged for FM. A cooling field is then applied along the x direction that is also the easy axis of AFM. Meanwhile, it is known that the spins of FM will be easily aligned according to the cooling field. After taking a long step of spin dynamics calculation, a stable state of FM/AFM under the cooling field is finally approached. Then the system is cooled down to low temperature, and we switch off the cooling field and start to do a simulation of hysteresis loop of FM layers while the spin configuration of AFM is fixed.

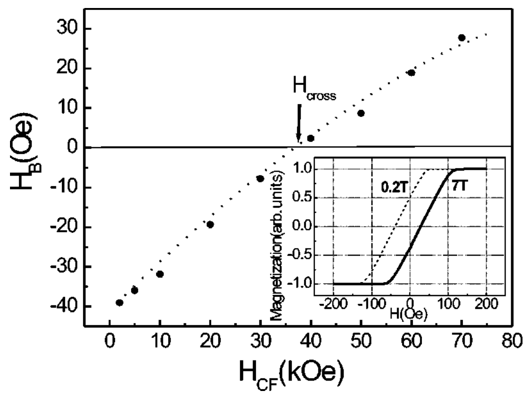

FIG. 1. Exchange bias H_B as a function of cooling magnetic field H_{CF} for FM/AFM with lower T_N (FeF_2). Dashed and solid lines in the inset show the negative and positive magnetic loops at 2 kOe and 7 T cooling field, respectively.

Figure 1 shows EB as a function of cooling field for a AFM/FM system with low T_N such as FeF_2 ($T_N \sim 78.4$ K) or MnF_2 ($T_N \sim 67.3$ K). In doing this we set the parameters in Hamiltonian as $g_A = g_F = 2.0$, $J_{F\text{-}F} = 10$ meV, $J_{A\text{-}A} = 0.8$ meV, $J_{A\text{-}F} = J_{A\text{-}A}/2 = 0.4$ meV, and $D_A = 0.4$ meV per site.[3,6,7] As a natural output from the calculation, it is indeed observed in this figure that the exchange bias H_B changes sign from negative to positive as the cooling field increases, and a crossover field H_{cross} is found at about 3.7 T. Dashed and solid lines in the inset show the negative and positive loops at 2 kOe and 7 T, respectively.

For systems with low T_N, i.e., weak spin-spin interaction $J_{A\text{-}A}$ in AFM, the spin configuration of AFM at low cooling magnetic field is dominated by AFM-type interface coupling of FM/AFM. In this case, symmetry breaking of compensated AFM layers appears. Some net ferromagnetic component along the $-x$ axis is expected, which means that the broken symmetry of AFM in this case favors the negative exchange bias. However, for higher cooling magnetic field H_{CF}, the cooling field comes to dominate the broken symmetry so that a net ferromagnetic component along the positive x direction is expected; i.e., the broken symmetry of AFM in this case favors a positive exchange bias.

For a quantitative description of the FM components in AFM, we define the ferromagnetic component in the nth AFM layer:

$$S^x(n) = \sum_i S_{na}^x(i) / N_n, \tag{5}$$

where $S_{na}^x(i)$ is the AFM spin at site i of the nth layer and N_n is the number of lattices in the nth AFM layer, while the first layer is defined as the interface layer of AFM. This quantity

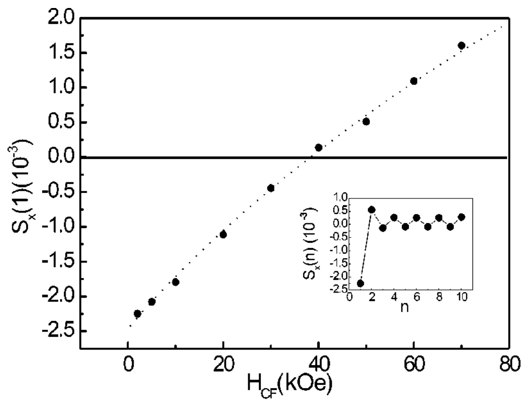

FIG. 2. The ferromagnetic component along the x axis as a function of cooling field for the interface AFM layer. The inset shows the layer dependent ferromagnetic components of AFM layers at 2 kOe.

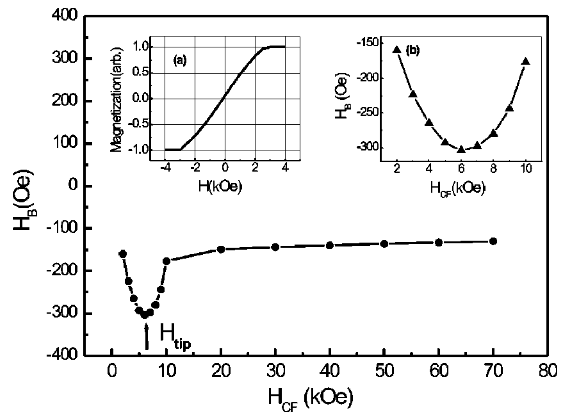

FIG. 3. The relationship between exchange bias H_B and cooling field H_{CF} for FM/AFM with higher T_N (FeMn). Inset (a) presents a magnetic loop at 3 T cooling field. Inset (b) shows clearly the EB around cooling field H_{tip} indicated by the arrow in the figure.

$S^x(n)$ describes the degree of symmetry broken in each layer of AFM. It is found from our calculation that the ferromagnetic components are layer dependent. As expected, it will be larger when the layer is near the interface and become smaller when the layer is far from the interface. In Fig. 2 the ferromagnetic component of the interface AFM layer, $S^x(1)$, is shown as a function of H_{CF}, using the same parameters as obtaining Fig. 1. Similar results as Fig. 1 are found: that $S^x(1)$ is negative at the beginning when the cooling field is small, then reaches zero at a critical field (~ 37 kOe), and finally becomes positive as the field further increases. Since the first AFM layer should be the most important one in the interface coupling, it is reasonable to see that the ferromagnetic component of the interface AFM layer should be responsible for the EB effect. The inset of Fig. 2 gives the layer-dependent ferromagnetic components when the cooling field is fixed at 2 kOe. The oscillation is caused by the antiferromagnetic exchange interaction between the layers of AFM.

Figure 3 shows the same relationship but for a AFM/FM system with higher T_N such as FeMn (~ 500 K). The parameters used here are $J_{F\text{-}F}=10$ meV, $J_{A\text{-}A}=5$ meV, $J_{A\text{-}F}=J_{A\text{-}A}=5$ meV, and $D_A=3$ meV per site.[3] In this case, it is found that H_B is always negative and changes little when H_{CF} ranges from 2 to 7 T. This result also agrees qualitatively with experiment.[3] Inset (a) of Fig. 3 shows the magnetization loop at 3 T cooling field. In fact, $J_{A\text{-}A}$ is large when the AFM layer of the system has high T_N; thus, the interface coupling $J_{A\text{-}F}$ also becomes large ($J_{A\text{-}F}\sim J_{A\text{-}A}$), and then the AFM-type interface coupling controls the symmetry broken of AFM. In this case, if H_{CF} is reasonably high (2–7 T) but not too high, H_B is found to be always negative. This can explain why a positive EB was reported in the FM/AFM thin films with low T_N.[5,11–13]

One distinguished feature of Fig. 3 is that a tip EB is found at cooling field H_{tip} indicated by the arrow, and this tip also is clearly shown in inset (b). As previously mentioned, the preceding discussions are subject to both cooling field and applied magnetic field parallel to the AFM easy axis. In fact, an orthogonal FM/AFM spin configuration similar to Koon's conclusion can also be recovered with zero or smaller cooling field for a stable spin configuration. With increasing cooling field from zero to H_{tip}, the FM spins will gradually rotate direction from perpendicular to parallel to the AFM easy axis during the cooling process, and the interface coupling contribution to the negative bias will enlarge and nearly saturate at H_{tip}. On the other hand, with increasing cooling field above H_{tip}, the cooling field contribution to the potentially positive bias will raise; in other words, the contribution to the negative bias will lessen. Thus for a cooling field parallel to the AFM easy axis situation, there exists a tip EB associated with a cooling field H_{tip}.

In summery, micromagnetic spin dynamics calculations are carried out to explain the mechanism of EB in the FM/compensated AFM system. Different from previous micromagnetic calculations, we address the key role of the cooling field. Some important experimental results, such as the cooling-field-dependent transition from negative to positive EB in AFM/FM layers with low T_N, can be reproduced. It is proposed that the symmetry breaking of AFM during the cooling process plays a key role in explaining the exchange bias.

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