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Role of antiferromagnetic bulk exchange coupling on exchange-bias propagation

Xiaodan Chi [a], Fenghua Ma [a], An Luo [a], An Du [a], Jinren Wang [b], Yong Hu [a,c,*]

[a] College of Sciences, Northeastern University, Shenyang 110819, China
[b] Sifang College, Shijiazhuang Tiedao University, Shijiazhuang 050043, China
[c] MOE Key Laboratory for Anisotropy and Texture of Materials, Northeastern University, Shenyang 110819, China

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ABSTRACT

We report a numerical study on the propagation behaviors of exchange-bias (EB) field (H_E) and coercivity (H_C) influenced by the magnitude of antiferromagnetic (AFM) bulk exchange coupling (J_{AF}) in ferromagnetic (FM)/AFM/FM trilayers. The H_E propagation for the AFM thin spacer with different J_{AF} may encourage or discourage EB. On the contrary, the H_C propagation only increases H_C, however, this increment shrinks for large J_{AF}. This theoretical work deepens our understanding of the EB effect in magnetic multilayers and provides a picture to optimize the EB properties through choosing a proper AFM material.

1. Introduction

Ferromagnetic (FM)/antiferromagnetic (AFM)/FM trilayers have attracted much attention not only due to the technological point of view as a spin-valve unit exhibiting giant magnetoresistance [1–3] but also the scientific point of view to probe the internal AFM spin distribution using exchange bias (EB) [4–7]. EB has been a significant phenomenon for the applications in areas such as nonvolatile storages and sensors [8], while it is still as an unresolved fundamental issue in condensed matter physics. EB commonly characterized by a shift of magnetization hysteresis (M–H) loop along the field axis in an amount (defined as EB field, H_E) originates from magnetically heterostructural (AFM/FM) interface when the interface is grown or cooled in the presence of an external magnetic field (called as field depositing or field cooling) [9]. In the magnetic trilayers, double EB are generated at the top AFM/FM and bottom FM/AFM interfaces simultaneously, which may induce diverse phenomena due to the fact that the variation of multiple EB is not independent. Normally, EB is strongly dependent on some intrinsic (e.g., AFM [1,10–12] or FM thicknesses [1,10,13] and interface roughness [14,15]) and extrinsic (e.g., temperature [16–20] or cooling field [21–24]) factors. It is accepted that the layer thicknesses mainly determine the loop shape (single or double shift), while the interface roughness changes the interfacial coupling and the temperature or the cooling field affects the spin structure directly.

However, conventional experimental techniques encountered some difficulties when they dealt with these magnetic trilayer systems. At first, EB in the FM/AFM/FM trilayers may exhibit distinct trends using different material species and/or undergoing different magnetic/heat treatments [16,22]. Secondly, it is difficult to systematically adjust one microstructural parameter without inadvertently changing another [7]. Thirdly, structure imperfections such as interface roughness, interdiffusion, chemical nonstoichiometry, grain boundary and reduced coordination number at the interface inevitably exist in the process of the thin-film preparation [11]. These structure imperfections further frustrate the exchange-coupled AFM/FM spins in a very complicated fashion. Additionally, direct characterizations of the AFM interfacial and bulk spin configurations in the thin-film structure are difficult due to the negligible magnetization in the AFM materials, and most of the studies have to resort to the FM magnetization indirect measurements [5]. Therefore, a fundamental understanding on the EB properties in trilayers is still lacking.

On the other hand, recent studies indicated that in the FM/AFM/FM trilayers, an EB propagation phenomenon was observed between multiple interfaces across an AFM thin spacer [22]. These findings provide a feasible avenue to realize to control EB only by a simple structure modification from the bilayers to the trilayers [25]. By virtue of the EB propagation, Hu et al. [26] have ele-

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[*] Corresponding author at: College of Sciences, Northeastern University, Shenyang 110819, China.
E-mail address: huyong@mail.neu.edu.cn (Y. Hu).

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vated the EB blocking temperature, above which EB disappeared, even by a factor of 2 as compared to that obtained from the bilayers with the same materials. It indicates that the EB propagation is potential to extend the EB working temperature, meantime, enhance the EB thermal stability. In this letter, we perform a modified Monte-Carlo (MC) simulation and focus on the dependence of EB propagation on AFM bulk exchange coupling in the FM/AFM/FM trilayers. We also establish AFM/FM bilayers to quantify the EB propagation, and ultimately, all the findings are interpreted microscopically.

2. Model and Monte-Carlo method

In the experiment, two critical thicknesses of the AFM layer are found normally when one studies EB in the FM/AFM/FM trilayers. One is the minimum thickness ($t_{\mathrm{AF}}^{\mathrm{min}}$) below which EB cannot emerge and the other is the maximum thickness ($t_{\mathrm{AF}}^{\mathrm{max}}$) above which the EB propagation disappears. Both of them are different for different material combinations. For example, in NiFe/FeMn/NiFe trilayers, $t_{\mathrm{AF}}^{\mathrm{min}}$ may be 2.5 nm [1] or 2 nm [5], while up to 5 nm in Co/FeMn/Co [7], NiFe/FeMn/CoFe [11] and FeCoV/NiO/FeCoV trilayers [27]. On the other hand, $t_{\mathrm{AF}}^{\mathrm{max}}$ may be 20 nm [1] or 15–16 nm in NiFe/FeMn/NiFe trilayers [5], 10 nm in Co/FeMn/Co trilayers [7] and 40 nm in FeCoV/NiO/FeCoV trilayers [27]. Remarkably, for the studies on the EB propagation in the FM/AFM/FM trilayers, the AFM layer thickness (t_{AF}) should be chosen in the range between $t_{\mathrm{AF}}^{\mathrm{min}}$ and $t_{\mathrm{AF}}^{\mathrm{max}}$. Although their sizes have reduced to nanoscale, thin films may still have over 10^9 magnetic moments, far beyond present-day standard computational facilities. As a consequence, the determination of the low-temperature magnetic configuration of thin films using Monte Carlo technique becomes prohibitively time-consuming. Therefore, a fast and reliable scaling approach [28,29] is used in order to deal with these systems theoretically.

We only consider short-range exchange interactions in the FM and AFM layers and their interfaces and single-ion anisotropies of the FM and AFM spins to calculate the low-temperature magnetic configuration. Under an external magnetic field, the Hamiltonian is written as follows.

$$\begin{aligned}\mathcal{H} = &-J_{\mathrm{FM}} \sum_{\langle i,j \in \mathrm{FM}\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i \in \mathrm{FM}} K_{\mathrm{FM}} (\mathbf{S}_i \cdot \mathbf{e})^2 \\ &+ J_{\mathrm{AF}} \sum_{\langle i,j \in \mathrm{AFM}\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i \in \mathrm{AFM}} K_{\mathrm{AF}} (\mathbf{S}_i \cdot \mathbf{e})^2 \\ &- J_{\mathrm{IF}}^{t} \sum_{\langle i \in t\mathrm{FM}, j \in \mathrm{AFM}\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J_{\mathrm{IF}}^{b} \sum_{\langle i \in b\mathrm{FM}, j \in \mathrm{AFM}\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\ &- \mathbf{H} \sum_i \mathbf{S}_i, \end{aligned} \tag{1}$$

where $\mathbf{S}_i$ denotes the unit vector of magnetic moment with the module of $|\mathbf{S}_i| = 1$ and the parameters J and K are set to be positive. For simplicity, a series of realistic parameters are set while do not correspond to any specific materials. Therefore, we set $J_{\mathrm{FM}} = 10$ meV in the range between 0.2 meV and 20 meV for most of the transition metals, a small K_{FM} (= 0.008 meV) for well-defined M–H loops, $J_{\mathrm{AF}} = 0.25 \sim 6$ meV based on a common principle that the Curie temperature (T_{C}) is higher than the Néel one (T_{N}) in FM/AFM typed EB systems, and a large K_{AF} (= 0.16 meV) for EB. Generally, the interfacial exchange interaction (J_{IF}^{t} and J_{IF}^{b}) is unknown and should be different from the bulk values, hence we set $J_{\mathrm{IF}}^{t} = 5$ meV and $J_{\mathrm{IF}}^{b} = 10$ or 0 meV directly. The influence of the different values of J_{IF}^{t} and J_{IF}^{b} will be addressed later. According to Refs. [28] and [29], we need to scale J by a factor x, so as to reduce its strength, while K does not change. Correspondingly, the film dimension (e.g., the layer thickness) is scaled by a factor $x^{0.55}$. We set the lattice parameter $a_0 = 3.5$ Å and use 60×60 spin array to stand for 300×300 nm^2 in the film plane, so $x^{0.55} = \frac{0.35 \times 60}{300} = 0.07$ and thus $x \approx 0.008$. Using the parameters set above, we obtain $t_{\mathrm{AF}}^{\mathrm{min}} \approx 2.5$ nm and $t_{\mathrm{AF}}^{\mathrm{max}} \approx 15$ nm, which are close to the values obtained in NiFe/FeMn/NiFe trilayers [1,5] and we set $t_{\mathrm{AF}} = t_{\mathrm{FM}} = 5$ nm as a study case. All the parameters used in the simulation are generalized in Table 1. Moreover, periodic boundary conditions are used in the film (xy) plane to eliminate finite-size effect [see Fig. 1(a)] and this has been checked using a larger size of the lateral extension (200×200 spin array).

Table 1
Values of magnetic parameters and thicknesses in the trilayers and bilayers adopted in the simulation.

J_{FM} (meV)	K_{FM} (meV)	J_{AF} (meV)	K_{AF} (meV)	J_{IF}^{t} (meV)	J_{IF}^{b} (meV)	t_{FM} (nm)	t_{AF} (nm)
10	0.008	0.25–6	0.16	5	10 or 0	5	5

$J_{\mathrm{IF}}^{b} = 10$ meV in the trilayers while $J_{\mathrm{IF}}^{b} = 0$ in the bilayers.
t_{FM} and t_{AF} denote the ferromagnetic and antiferromagnetic layer thicknesses.

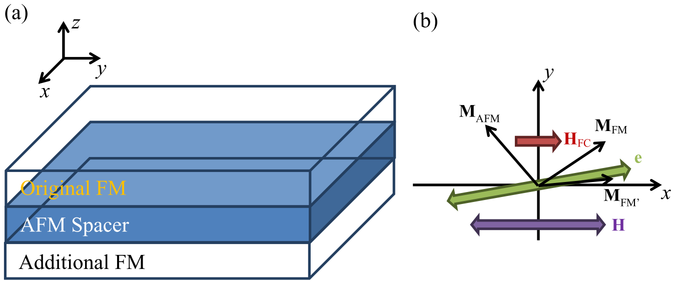

Fig. 1. Schematic illustrations of trilayers (a) and orientations of magnetization, easy axis and magnetic field (b), where different symbols have been defined in the text and the subscripts FM and FM′ are used to distinguish between the original and additional ferromagnetic layers.

Field-cooling and M–H loop measuring processes are simulated. The initial spin states in the trilayers or bilayers are disordered with no net magnetization and then they are cooled through T_{N} from $T/T_{\mathrm{N}} = 1.428$ to $T/T_{\mathrm{N}} = 0.01428$ under a magnetic field (cooling field) $H_{\mathrm{FC}} = 2$ kOe. At the target temperature ($T/T_{\mathrm{N}} = 0.01428$), the M–H loop is measured by cycling the magnetic field between −7 kOe and 7 kOe. The anisotropy (easy-axis) directions of the FM and AFM layers are set to be collinear. The cooling field and the M–H loop measuring field are applied along the same axis, while the positive magnetic field deviates from the one end of the easy axis by a small angle of 10 degree, as shown in Fig. 1(b).

It is well known that many metastable states exist during the magnetization reversals in the M–H loops, and in order to better probe these states using MC techniques, a modified Metropolis algorithm proposed by Du et al. [30] is adopted to update the spin configurations. For a temperature or a magnetic field, 10^5 MC steps are performed and discarded to equilibrate the system, and then the magnetization is determined by averaging the results repeatedly calculated by another 10^5 MC steps. Finally, 200 independent initial configurations are used to calculate the M-T and M–H curves, which are averaged to minimize the statistical errors (not shown in our plots accordingly).

3. Results and discussion

Fig. 2 depicts some representative results of the M–H loops in the trilayers and bilayers with different J_{AF} and some distinct features are observed between them. Firstly, with increasing J_{AF}, the trilayer loop shrinks rapidly from a wide and symmetric shape towards the center, while the bilayer one moves rightwards gradually