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## Effect of misaligned unidirectional and uniaxial anisotropies on angular dependence of exchange bias



Yong Hu\*, Xiaoling Wang, Ning Jia, Yan Liu, An Du

College of Sciences, Northeastern University, Shenyang 110819, China

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## ABSTRACT

We report a numerical study of the angular dependences of low-temperature exchange bias field (ADEB) and coercivity in the ferromagnetic/antiferromagnetic bilayers with misaligned unidirectional and uniaxial anisotropies. Through choosing a proper antiferromagnet the conventional symmetry in the ADEB may be broken, while the novel behaviors are also dependent on the angle between induced unidirectional and intrinsic uniaxial anisotropies. Finally, we draw conclusions that the two anisotropies with a small misalignment together determine the asymmetric ADEB properties around the easy axis. In contrast, after the magnetically hysteretic measurement rotating through the hard axis, a large misalignment between the anisotropies may change the magnetization reversal mode at the decreasing branch of loop, besides weakening the positive loop shift. Thus the strength of exchange bias field is suppressed while the coercivity is enhanced.

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## 1. Introduction

When ferromagnetic (FM)/antiferromagnetic (AFM) materials' combinations are field cooled through the AFM Néel temperature ( $T_N$ ) a shift of magnetic hysteresis loop in the FM material toward a given field direction, referred to as exchange bias (EB), is often observed [1]. Since its discovery in 1950s [2,3], EB is heavily used to stabilize the magnetization of FM reference layer along one preferred direction in spintronic devices [4–7] or to measure the FM/AFM interfacial coupling for determining the AFM surface order parameter that is difficult to probe experimentally [8,9]. Despite extensive research, unfortunately, there are still ongoing controversies about the fundamental mechanisms governing it.

It is well established that the studies on angular dependence of EB (ADEB) are used to explore the properties of unidirectional anisotropy or to reveal the origin of EB to a great extent [10–15]. For example, our previous work [16,17] studied the angular dependences of EB, coercivity ( $H_C$ ), and magnetization reversal process systematically in the FM/AFM bilayers not subjected to a field-cooling treatment in order to highlight the role of intrinsic anisotropies. It was found that strong AFM anisotropies elevated the energy barriers to trap the AFM spins in metastable states and caused an asymmetric and magnetic-history-related ADEB behavior, forming a noncollinearity between unidirectional and

uniaxial anisotropies. Nevertheless, Jiménez et al. [18] proposed that there was commonly another significant factor, which was also dependent on the anisotropy magnitudes, that spontaneously induced a noncollinear anisotropy due to the existence of magnetic frustration at the FM/AFM interface. In addition the unidirectional anisotropy, which serves to establish the direction of EB, can be promoted extrinsically via special field-cooling procedures. In other words, the cooling field direction with respect to the easy axis has a significant impact on the ADEB properties. Interestingly, through systematic investigations, some groups [19,20] not only illustrated a rich phase diagram originating from the noncollinearity of the involved anisotropies, but also pointed out that the unidirectional anisotropy was not necessarily along the cooling field direction.

To demonstrate the role of cooling field direction in establishing the unidirectional anisotropy and to further unveil the effect of misaligned anisotropies on ADEB, in this paper, we focus on the evolution of ADEB at low temperature after cooling under a rotatable strong field by employing a modified Monte Carlo simulation, and interpret the numerical findings by means of the angular dependences of coercive fields and magnetization reversal modes.

## 2. Model and Monte Carlo simulation

In the following, we consider one FM monolayer exchange coupled to an AFM film consisting of four monolayers. A lateral size  $40 \times 40$  is chosen, and in this plane (the  $xy$  plane) periodic

\* Corresponding author. Tel.: +86 24 83687658; fax: +86 24 83678686.

E-mail address: [huyong@mail.neu.edu.cn](mailto:huyong@mail.neu.edu.cn) (Y. Hu).

boundary conditions are used while open boundary conditions are used along the  $z$  axis. To avoid the finite-size effect we have checked several models with different lateral sizes, and for larger systems only a negligible vertical shift exists in the ADEB curve. The Hamiltonian under an external magnetic field can be written simply as

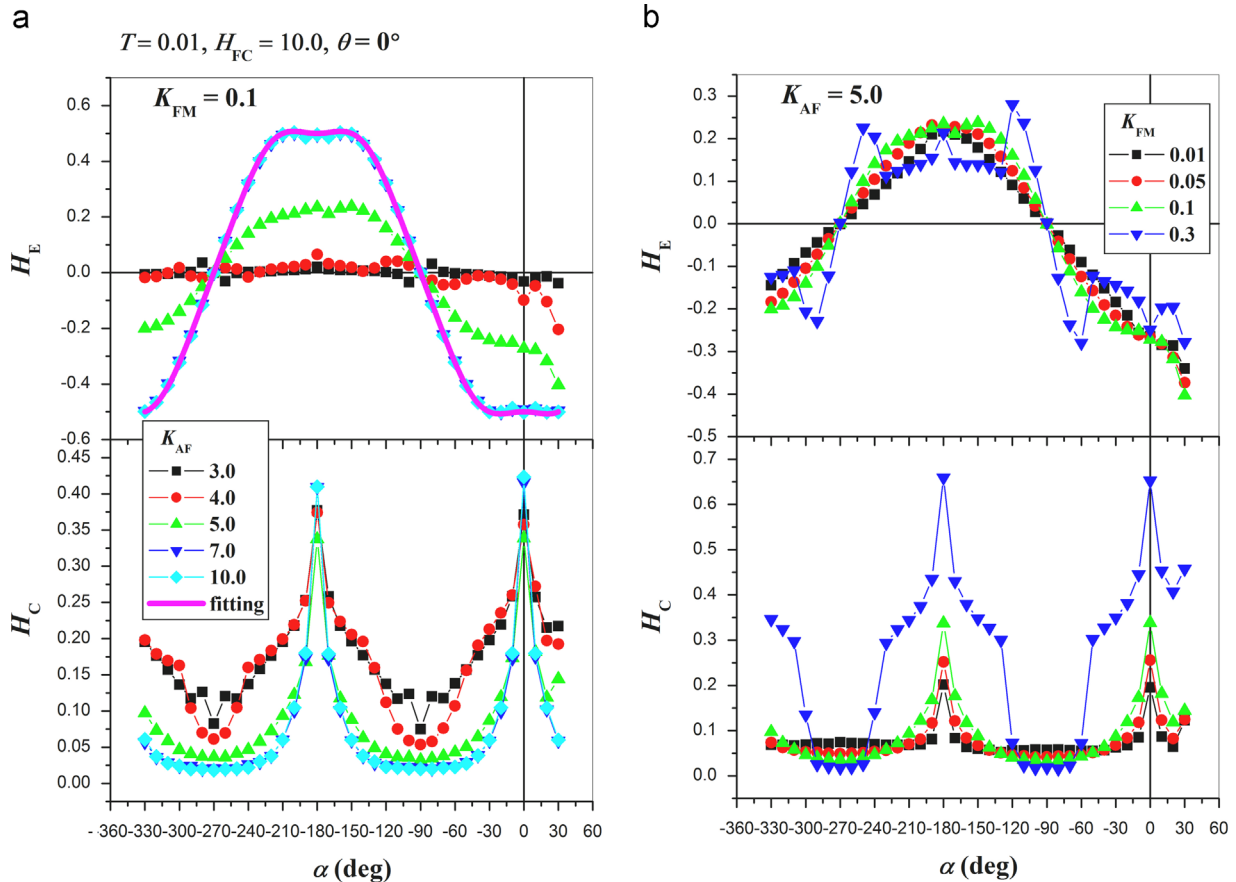
$$\begin{aligned}
 H = & -J_{\text{FM}} \sum_{\langle ij \in \text{FM} \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i \in \text{FM}} K_{\text{FM}} (S_i^x)^2 \\
 & -J_{\text{AF}} \sum_{\langle ij \in \text{AFM} \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i \in \text{AFM}} K_{\text{AF}} (S_i^x)^2 \\
 & -J_{\text{IF}} \sum_{\langle i \in \text{FM}, j \in \text{AFM} \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{H} \cdot \mathbf{S}_i,
 \end{aligned} \tag{1}$$

where  $\mathbf{S}_i$  is a Heisenberg spin variable at lattice site  $i$  and the angular brackets denote a summation over the nearest neighbors only. That is exchange interactions between the nearest neighboring spins in the FM and AFM layers, and across their interfaces, are considered. Meanwhile, to obtain results that are general and easily translated into any other kind of bilayers characterized as above, the FM exchange constant  $J_{\text{FM}}$  serves as a normalized energy unit. Correspondingly the AFM exchange constant  $J_{\text{AF}}$  is below 0 and  $|J_{\text{AF}}|=J_{\text{FM}}$ , while the interfacial one  $J_{\text{IF}}=J_{\text{FM}}/2$ . Next uniaxial magnetocrystalline anisotropies of FM ( $K_{\text{FM}}$ ) and AFM spins ( $K_{\text{AF}}$ ) are also included, and their easy axes are both along the  $x$ -axis. In the next section, the FM and AFM anisotropy strengths are discussed briefly. Finally, an external magnetic field  $H$  with a unit of  $J_{\text{FM}}/g\mu_B$  is applied in the film plane and coupled to spins, where  $g$  is the Lande factor and  $\mu_B$  is the Bohr magneton.

In the simulation, the protocol is divided into two stages: a field-cooling procedure followed by an isothermally magnetizing process.

In the first stage, the system with a disordered configuration is field cooled from a high temperature  $T=4.0$  with a unit of  $J_{\text{FM}}/k_B$  down to a desired  $T=0.01$  in constant steps of  $\Delta T=-0.01$ . The strength of  $H_{\text{FC}}$  keeps a constant value of 10.0 while its orientation is varied to create the unidirectional anisotropy with different directions. We define  $\theta$  as the angle between the positive  $x$ -axis and  $H_{\text{FC}}$ ; when  $H_{\text{FC}}$  is applied pointing to the positive  $x$ -axis  $\theta=0^\circ$ , and  $\theta > 0^\circ$  indicates that  $H_{\text{FC}}$  rotates by  $\theta$  clockwise from the positive  $x$ -axis. Four values of  $\theta$  (i.e.,  $60^\circ$ ,  $30^\circ$ ,  $0^\circ$ , and  $-60^\circ$ ) are selected. Then, at  $T=0.01$ , the second stage starts. We introduce  $\alpha$  to represent the angle between the positive  $x$ -axis and the positive field of magnetic hysteresis loop; the criterion for the sign of  $\alpha$  is the same as that of  $\theta$  and the range of  $\alpha$  is chosen from  $30^\circ$  to  $-150^\circ$  in steps of  $-10^\circ$  unless otherwise specified. It is noteworthy that the  $0^\circ$  definitions of  $\theta$  and  $\alpha$  are independent of each other, agreeable with the theoretical hypothesis of Beckmann et al. [15] while different from the experimental conception proposed by Jiménez et al. [11,12] using the cooling field direction as  $0^\circ$  of  $\alpha$ . For each  $\alpha$ , the magnetic hysteresis loop is recorded by cycling  $H$  between 1.0 and  $-1.0$  in constant steps of  $|\Delta H|=0.01$ . At low temperature after the field-cooling procedure along a given  $\theta$ , a complete ADEB curve is plotted by executing alternately the magnetically hysteretic measurement and the demagnetizing rotation without any interval.

Furthermore, to obtain a realistically magnetic hysteresis loop, we modify the “flipping” probability used in the Metropolis algorithm of Monte Carlo simulation, considering the energy barriers during a spin reversal by calculating the energy of the spin with respect to its polar and azimuthal angles. The method reported is based on the same methodology used previously in our recent work [16,17] to which the reader is referred for details.



**Fig. 1.** Exchange bias field and coercivity as functions of angle between easy axis and magnetically hysteretic measurement at low temperature after cooling under a strong field applied along the easy axis in the ferromagnetic/antiferromagnetic bilayers with different anisotropies, where the symbol-line curves denote the simulation results while the solid line in (a) is the fitting result of empirical law.

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