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Effect of Interface Roughness on Exchange Bias of an Uncompensated Interface: Monte Carlo Simulation

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By means of Monte Carlo simulation, we investigate the effects of interface roughness and temperature on the exchange bias and coercivity in ferromagnetic (FM)/antiferromagnetic (AFM) bilayers. Both exchange bias and coercivity are strongly dependent on interface roughness. For a perfect uncompensated interface a domain wall is formed in the AFM system during FM reversal, which results in a very small exchange bias. However, a finite interface roughness leads to a finite value of the exchange bias due to the existence of pinned spins at the AFM surface adjacent to the mixed interface. It is observed that the exchange bias decreases with increasing temperature, consistent with the experimental results. It is also observed that a bump in coercivity occurs around the blocking temperature.

Keywords : exchange bias, interface roughness, Monte Carlo simulation

1. Introduction

Exchange bias, which is a shift of a hysteresis loop along the magnetic field axis, has received much attention over the past several decades [1-5] because of its great potential for technological applications [6-10]. The origin of the exchange bias effect in a ferromagnetic (FM) layer coupled to an antiferromagnetic (AFM) layer is the interfacial exchange coupling between the FM and AFM systems [3, 4]. As such, any insight into this interface structure is crucial for our understanding or ability to control the properties of magnetization reversal in FM/AFM bilayers. Although many works have concentrated on clarifying the underlying mechanism of exchange bias, a comprehensive understanding of this phenomenon remains elusive due to lack of experimental tools that are capable of extracting detailed information about the interface structure. Therefore, we believe an atomistic simulation, which takes into account detailed atomic level information about the microstructure of system, is a practical way to investigate the effects of interface structure on the exchange bias.

A number of theoretical models with various interface structures have been proposed for describing the exchange bias effect exhibited in FM/AFM systems [4, 5]. For instance, the earliest macroscopic model proposed by Meiklejohn and Bean [1] can be used to explain the origin of exchange bias in FM/AFM systems. However, this model predicts a much larger exchange bias field than that observed experimentally, which can be partly ascribed to their assumption of an ideal interface structure. Later, Malozemoff proposed a model for exchange anisotropy based on the assumption of interface roughness, and acquired a relatively reasonable estimate for exchange bias [11]. Recently, a domain state model was developed to investigate the exchange bias by involving a domain state caused by the structural defects in AFM material [12, 13].

In real FM/AFM materials, disorder or defects are unavoidable both at the interface and inside the bulk material. Spray and Nowak [14] reported on the substantial effect of interface roughness on exchange bias for a *compensated* interface. Hence, it is very important to analyze the interface structure in order to understand the exchange bias of FM/AFM systems from a theoretical point of view [15]. In this work, we study the effect of mixed interfaces on the exchange bias and coercivity of $Fe/FeF_2(100)$ bilayers with an *uncompensated* interface in a FeF_2 single crystal by means of a Monte Carlo method

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[16]. We also study the temperature dependence of the exchange bias and coercivity for various mixed interfaces. Our results show that the exchange bias and coercivity depend strongly on the interface structure. In our model, the exchange bias is almost zero for a perfect uncompensated interface due to the formation of a domain wall in the AFM. However, the exchange bias grows with increasing interface roughness, which is caused by the rotation of AFM surface spins as well as the rotation of interfaces spins. At a certain interface roughness, we get a positive exchange bias as a result of an antiparallel coupling between the FM spins at the interface and the pinned spins at the AFM surface adjacent to the mixed interface. In addition, the coercivity exhibits a bump around the blocking temperature, as has been reported in previous experiment [16].

2. Model and Method

The model system we use consists of a single crystal FeF_2(100) coupled to a Fe layer. The FeF_2 crystal has a body-centered tetragonal structure with the Fe^{2+} ions at the center of the unit cell ordered antiferromagnetically with those at the corners [17]. For FeF_2(100), all spins are parallel within a plane but antiparallel to those spins in adjacent planes. An uncompensated AF spin structure for a perfect interface exists along the [001] easy axis, below the Néel temperature T_N = 78.4 K, as shown in [16]. The lateral dimensions of our system are $L_x = L_y = 30$ (spins or unit cells) and the thickness is $t_{FM} = 4$ and $t_{AFM} = 10$ layers with one mixed interface monolayer. Periodic boundary conditions are applied along the in-plane direction, and free boundary conditions are assumed in the out-of-plane direction. The easy axis of the FM is parallel to that of the AFM and is aligned in the x-axis direction. For the FM layer, the dipolar interaction is approximated by including an anisotropy term (shape anisotropy) that leads in-plane magnetization. The Heisenberg model is used to describe both FM and AFM systems with the Hamiltonian.

$$\begin{aligned}\mathscr{H} = &-\sum_{i,j\in FM} J_{FM}\vec{S}_i\cdot\vec{S}_j - \sum_{i\in FM}(D_xS_{ix}^2 + D_zS_{iz}^2 + \vec{H}\cdot\vec{S}_i)\\ &-\sum_{i,j\in AFM} J_{AFM}\vec{s}_i\cdot\vec{s}_j - \sum_{i\in AFM}(d_x s_{ix}^2 + \vec{H}\cdot\vec{s}_i)\\ &-J_{INT}\sum_{\substack{i\in AFM\\ j\in FM}}\vec{s}_i\cdot\vec{S}_j\end{aligned} \qquad (1)$$

$\vec{S}_i(\vec{s}_i)$ is the unit vector of a spin in the FM (AFM). The first two terms describe the energy of the FM system and the terms in the second line contains energy contributions of the AFM system, where J_{FM} and J_{AFM} denote effective nearest exchange coupling constants for the FM and AFM spins, respectively. D_x, D_z are the uniaxial anisotropy and shape anisotropy in the FM and d_x is the uniaxial anisotropy in the AFM. $\vec{H}$ is the external magnetic field applied along the easy axis of the FM and AFM layers. The last term describes the interfacial exchange coupling with an exchange constant, J_{INT}, between the FM and AFM spins. The parameters used in this paper are taken from previous literature [18, 19]. The nearest and next-nearest exchange constants between the FM spins are $J_{FM} = 0.02$ eV and $J_{FM}^1 = 0.5J_{FM}$, respectively, and the nearest and next nearest exchange constants between the AFM spins are $J_{AFM} = -0.2J_{FM}$ and $J_{AFM}^1 = 0.1J_{FM}$, respectively. The uniaxial anisotropies are $D_x = 0.0003J_{FM}$ per FM atom and $d_x = 0.5J_{FM}$ per AFM atom, and the shape anisotropy is $D_z = -0.02J_{FM}$ per FM atom. The interfacial exchange constant is taken as $J_{INT} = -J_{AFM} = 0.2J_{FM}$. Here the spins are normalized to unity, so that the magnetic field H has the units of energy.

Our simulations are carried out using a Monte Carlo method with the Metropolis algorithm [20]. During the simulation process, the trial step of each spin update, one Monte Carlo step (MCS), involves a small variation around the initial spin. With the FM system magnetized fully along the +x-axis, we first perform a field cooling process with an external field $H = 0.25J_{FM}$ applied also along the +x direction from $T = 150$ K to 10 K, which starts above and ends below the ordering temperature of the AFM. After field cooling, the simulation of each hysteresis loop starts with an initial field $H = 0.4J_{FM}$ and ends with a field $H = -0.4J_{FM}$ decreasing in steps of $0.004J_{FM}$, then the field rises again to its initial value (increasing branch) [21]. We perform 4×10^5 MCS per spin for a complete hysteresis loop, 2×10^5 of these MCS

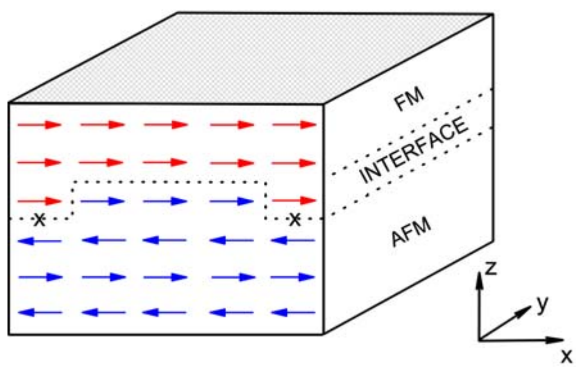

Fig. 1. (Color online) The schematic illustration of the FM (red spins) and AFM (blue spins) layers with one mixed interface layer after the application of a field cooling. The dashed line marks the boundary between the FM and AFM. The cross indicates frustrated interactions of FM spins.

are used for thermalization and the other 2×10^5 MCS are used for computing average values. Fig. 1 sketches the spin microstructure of the system after field cooling, which shows the FM, AFM and one mixed interface layer. A parameter R is introduced to describe the mixed interface. We define R as the proportion of FM spins to total spins at the interface. $R = 0$ or 1 corresponds to a perfect interface fully covered with AFM or FM spins and $R = 0.5$ corresponds to the maximally imperfect interface.

3. Result and Discussions

Fig. 2 displays the effect of R on the exchange bias field (H_{EB}) and coercivity (H_C) at various temperatures. We can see that the mixed interface has a strong influence on the exchange bias (Fig. 2(a)). At temperature below T_N (= 78.4 K), e.g., at T = 20 K or 60 K, a very small exchange bias field is found in the cases of a relatively perfect interfaces ($R \leq 0.2$ or $R \geq 0.8$). At R = 0.6, the exchange bias field is the largest. We also observe a positive exchange bias field at R = 0.3. Above T_N, e.g., at T = 90 K, no exchange bias exists in any case due to the fact that spins in the AFM system are orientated randomly. The coercivity strongly depends on the composition of the interface as well (Fig. 2(b)). The coercivity is large for a perfect interface (i.e. R = 0 or 1), but tends to decrease as R approaches 0.5.

The almost zero exchange bias while $R \leq 0.2$ or $R \geq 0.8$ is caused by the domain wall formation at the top surface plane of the AFM during FM reversal. In Fig. 3, we illustrate the hysteresis loop of the FM system and the spin configuration of the four FM and AFM layers near

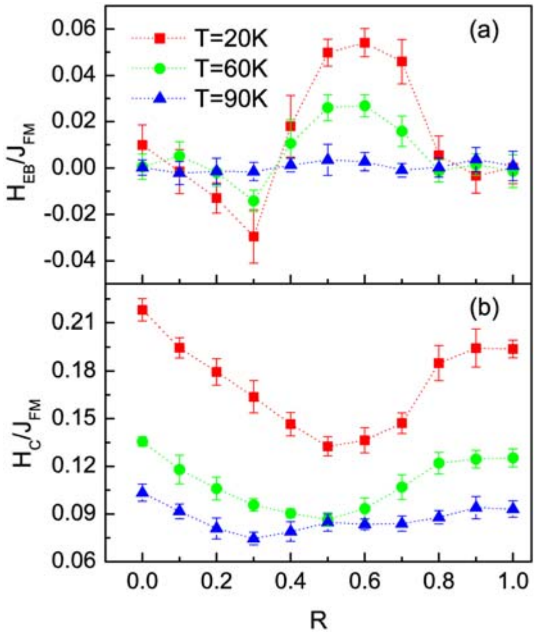

Fig. 2. (Color online) The variation of exchange bias field (H_{EB}/J_{FM}) (a) and coercivity (H_C/J_{FM}) (b) with the mixed interfaces R at three different temperatures T = 20, 60, and 90 K.

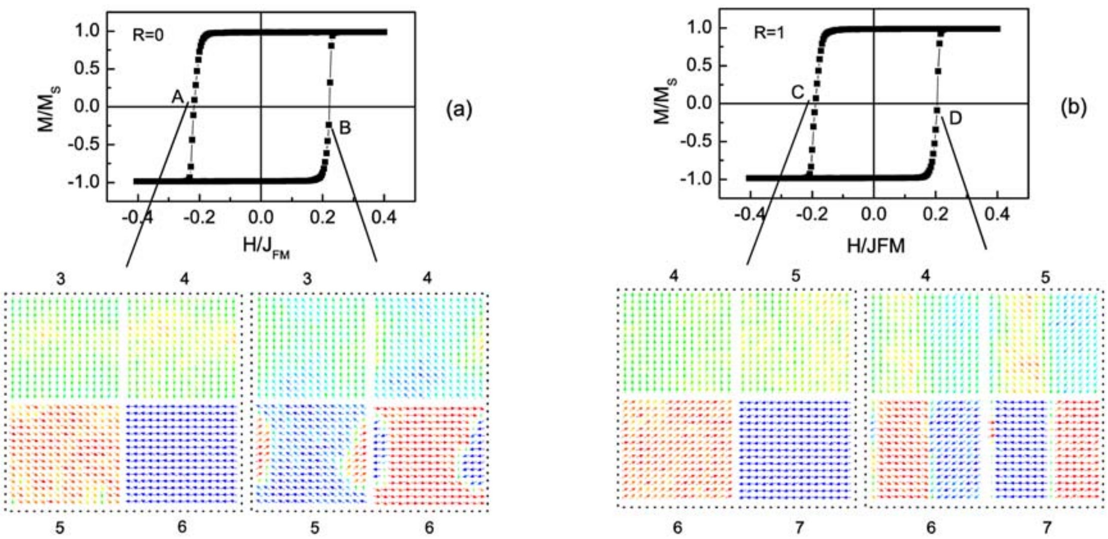

Fig. 3. (Color online) The hysteresis loop for the FM system and the spin configurations of layers around the interface at 20 K. (a) at R = 0, the hysteresis loop and spin configurations of layers 3-6 labeled 3, 4, 5, 6 for the points marked A and B in the figure. Layers 3, 4 are FM layers and layers 5, 6 are AFM layers, and (b) at R = 1, the hysteresis loop and the spin configurations of layers 4-7 labeled 4, 5, 6, 7 for the points marked C and D in the figure. Layers 4, 5 are FM layers and layers 6, 7 are AFM layers. The colors indicate the spin orientation. The four in-plane directions are represented by red (right), blue (left), and green (up and down).

the interface. Fig. 3(a) shows the spin configuration for layers 3-6 with R = 0, whereas Fig. 3(b) shows the spin configuration for layer 4-7 with R = 1. This is due to the fact when R is 0 (or 1), the fifth layer can be treated as a part of the AFM (or FM) system. It is clear that at one branch of the hysteresis loop (H > 0), a domain wall is formed in the top surface of the AFM. In this branch, the other AFM layers remain unchanged when the FM reverses. However, we did not observe any domain wall formation in the other branch (H < 0). In other words, the AFM spins have a small rotation in one field direction, but rotate strongly and form a domain wall in the opposite field direction. This asymmetry results in a reduction of the exchange bias. Our results are in good qualitative agreement with experimental ones [22-26], where an exchange bias was not found in the Fe/FeF_2(100) system even though the FeF_2(100) orientation possesses uncompensated spins at the interface. Therefore, domain wall formation in AFM systems is a good candidate to explain the zero exchange bias in experiments.

After field cooling, we observe that at $R \leq 0.3$, an antiparallel alignment between the FM spins at the interface and the AFM spins at the surface layer is preferential in terms of energy. This assists the rotation of the FM spins on the decreasing branch of the loop (H < 0) but disturbs their rotation on the increasing branch (H > 0), which results in the positive exchange bias field. When R is larger than 0.3, field cooling leads to a parallel exchange coupling between the FM spins and AFM spins at the interface. Therefore, there is a transition of exchange bias field from a negative to a positive value. The exchange bias field reaches a maximum at R = 0.6. This large negative exchange bias field is often caused by the direction and magnitude of the cooling field. Cooling fields with different magnitudes can lead to different alignments between the FM and AFM spins resulting in an exchange bias field with a different sign. For instance, Hauet *et al.* [27] observed experimentally that the $Gd_{40}Fe_{60}/Tb_{12}Fe_{88}$ system shows a transition from a positive to negative exchange bias field as the cooling field is increased from a small value to a large positive value.

The above results indicate that a mixed interface results in frustrated interfacial exchange interactions. The temperature can cause a change in interfacial configuration, so we can say temperature causes different behavior of the exchange bias and coercive field. In Fig. 4, we show the temperature dependence of the exchange bias and coercivity at two mixed interfaces: R = 0.5 and 0.7. The exchange bias decreases as the temperature increases in both cases. The blocking temperatures when R = 0.5 and 0.7 are about 80 K and 70 K, respectively. This is evidence that blocking temperature is partly related to interface roughness. Interestingly, a peak of coercivity occurs at the so-called blocking temperature when the exchange bias field becomes zero, qualitatively consistent with experimental results [22-26].

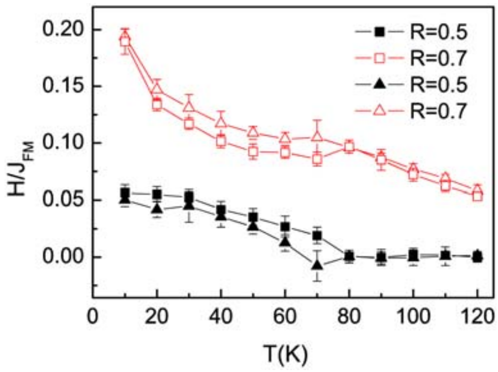

Fig. 4. (Color online) The temperature dependence of H_{EB} and H_C for mixed interfaces R = 0.5 and 0.7. The open symbols denote H_C and the solid symbols denote H_{EB}.

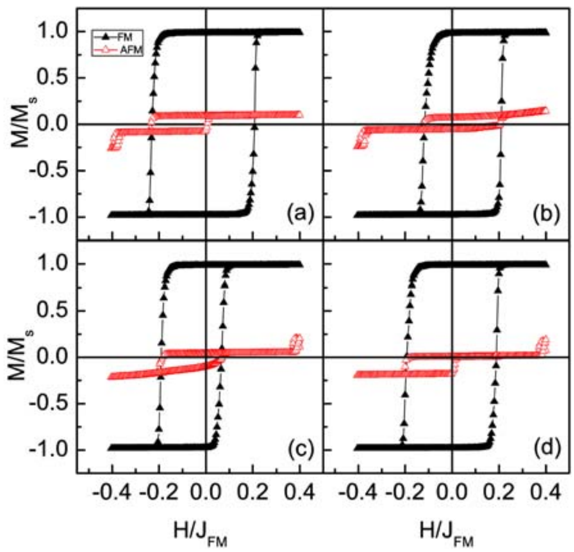

Fig. 5. (Color online) The hysteresis loops of the FM and AFM systems at T = 20 K with different mixed interfaces (a) R = 0, (b) R = 0.3, (c) R = 0.6 and (d) R = 1. The solid triangles are for the FM system and the open triangles are for the AFM system.

Fig. 5 shows the hysteresis loops of the FM and AFM at T = 20 K for four types of interfaces. Note that the full variation of the M/Ms in the AFM is much smaller than in the FM, indicating that only a small portion of AFM spins rotate as a function of the field. For a perfect interface, i.e., R = 0 or 1 (Fig. 5(a) and 5(d)), the magnetization reversal in the AFM coincides with that in the FM on the decreasing branch (H < 0). However, on the other branch, the magnetization reversal in the AFM occurs at H = 0 and is independent of the reversal in the FM, caused by the domain wall formation, as shown in Fig. 3 (The domain wall width in the AFM is about one atom layer in the plane and about 2 atom layers in the out-of-plane direction, which is smaller than the thickness of an AFM layer.). For the cases where R = 0.3 and 0.6 (Fig. 5(b) and 5(c)), the switching fields of the AFM coincide with those of the FM. This illustrates that a more imperfect roughness results in a stronger coupling between the FM and AFM spins. As a result, the AFM spins at the interface can rotate by following the magnetization of the FM and the other AFM spins are not affected by the reversal of the FM.

4. Summary

By using a Monte Carlo method, we studied the dependence of exchange bias and coercivity on mixed interfaces and temperature in Fe/FeF_2 bilayers with an uncompensated interface. The results reveal that interface roughness has an important role in determining the exchange bias and coercivity. We found four consequences of the effect of interface roughness (R) on exchange bias field and coercivity; (i) at R = 0 or 1, even at a perfect uncompensated interface, an almost zero exchange bias is found due to the domain wall formation at the top surface of the AFM layers, (ii) at R = 0.3, there is a positive exchange bias due to antiparallel alignment of FM and AFM spins after field cooling, (iii) at around R = 0.5, the negative exchange bias is maximized whereas coercivity is minimized, and (iv) there is a bump in coercivity at the blocking temperature. The results listed above have been also observed in experiments. Therefore, our model, which includes interface roughness, seems reasonable and is able to explain previous experimental results well when the appropriate exchange constants are chosen. From this study we can conclude that the exchange bias and coercivity in FM/AFM bilayer systems can be controlled by the tuning of interface roughness, which could prove useful in designing the characteristics of magnetic devices.

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