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Unified nonequilibrium dynamical theory for exchange bias and training effects*

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We have investigated the exchange bias and training effect in the ferromagnetic/antiferromagnetic (FM/AF) heterostructures using a unified Monte Carlo dynamical approach. The magnetization of the uncompensated AF layer is still open after the first field cycling is finished. Our simulated results show obvious shift of hysteresis loops (exchange bias) and cycling dependence of exchange bias (training effect) when the temperature is below 45 K. The exchange bias field decreases with decreasing cooling rate or increasing temperature and the number of the field cycling. Essentially, these two effects can be explained on the basis of the microscopical coexistence of both reversible and irreversible moment reversals of the AF domains. Our simulations are useful to understand the real magnetization dynamics of such magnetic heterostructures.

Keywords: ferromagnetic/antiferromagnetic bilayers, hysteresis, exchange bias, training
PACC: 7115Q, 7550R, 7560E, 7570A

1. Introduction

Usually, when the heterostructure consisting of coupled ferromagnetic (FM) and antiferromagnetic (AF) layers is cooled in a field below the Neel temperature of its AF component, it shows the asymmetric magnetization,[1−6] which is referred to as the exchange bias effect. Furthermore, the exchange bias field, defined as the average of the two coercive fields, is observed to decrease with the increasing number of the consecutive field cycling, which is referred to as the training effect.[7] The exchange bias and training effects are very interesting and could be used in future spintronics[8−10] and data storage. Usually, the FM layer is taken as a whole and the AF layer consists of many grains.[11] The AF grain is small enough to constitute of a single domain, and some uncompensated domains (or grains) may be formed by defects or impurities[12−14] and couple with each other and with the FM domains. As the heterostructure is cooled to low temperatures, the uncompensated spins in the grains and domains become locked-in and prefer to take a unidirection in the interface, and thus contribute to the magnetization shift. Moreover, under the reversal of FM domains, the uncompensated grains or domains will be irreversibly reorganized[15−19] and thus cause the training effect. Although different models are adopted by some simulations[20,21] and theoretical investigation,[22−26] actual nonequilibrium dynamical properties of the magnetization are still waiting to be elucidated. It is highly desirable and needed to systematically investigate the two effects in a unified theory.

In this article we use a unified Monte Carlo dynamical approach[27] to study the FM/AF heterostructure in order to investigate the exchange bias and training effects. Our simulation shows the obvious shift of hysteresis loops and the cycling dependence of exchange bias. The magnetization of the uncompensated AF layer is still open after the first field cycling is finished. The exchange bias field decreases with decreasing cooling rate or increasing temperature and the number of the field cycling. With the simulations, we show the exchange bias is determined by the cooling rate, the distributive width of the anisotropy energy, or the magnetic coupling constants. Essentially, these two effects can be explained on the basis of the microscopically irreversible reversal of the AF domains. More detailed results will be presented in the following.

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The remaining part of this paper is organized as follows. In the next section we shall define our model and discuss our simulation method. In Section 3 we shall present our simulated results and analysis. In Section 4 we shall discuss the microscopic mechanism for the phenomena in a unified way. Finally, we shall give our conclusion in Section 5.

2. Model and method

According to experimental observations,[28] for both compensated and uncompensated AF layers the easy axis tends to form along the external cooling field direction rather than the later rotating field direction. In our model the AF layer consists of many AF domains, and the FM layer consists of one single domain. Assuming the cooling field is applied parallel to the AF/FM interface, then all the easy axes of AF and FM domains lie in the plane of the interface. The coupled bilayers of AF and FM domains are shown in the inset of Fig.1(a). The rectangles of the white pattern represent the AF domains and the larger rectangle is the single FM domain. The AF domains couple to each other antiferromagnetically and the single FM domain couples to all the AF domains ferromagnetically. We define the z-axis along the common easy axis which lies in the interface plane and the external field is applied to saturate the magnetization of the FM layer along the z-axis.

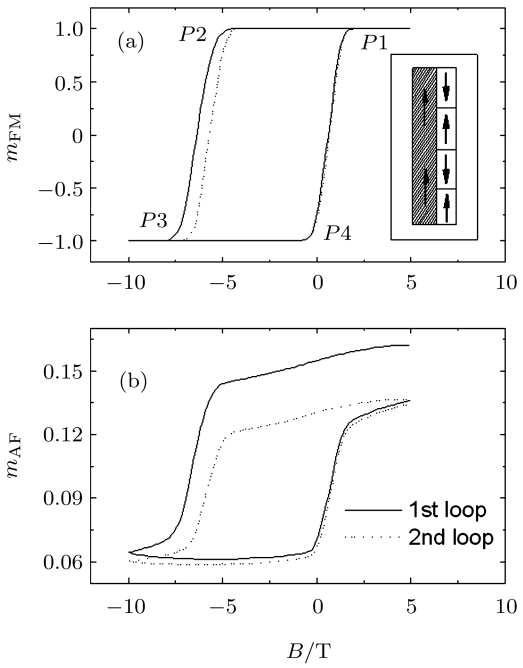


Fig.1. The first two hysteresis loops of the FM (a) and AF (b) layers at 10 K. The inset in (a) shows the AF/FM bilayers. The hysteresis loop is obtained by changing the field in the order of P1–P2–P3–P4–P1.

For simplicity, all the uncompensated spins in the AF domains are set to the same direction. We use $S's_i$ to denote the spin vector of the i-th AF domain and Ss to denote that of the single FM domain, where S' and S are the uncompensated spin values and FM spin respectively. Then the Hamiltonian of the bilayers in an external field can be written as

$$H = -K_{\rm u}(s^z)^2 - \sum_i k_{\rm ui}(s_i^z)^2 - B\cdot(\gamma'\sum_i s_i + \gamma s) + J_1\sum_{i,j} s_i\cdot s_j - J_2\sum_i s_i\cdot s, \quad (1)$$

where $\gamma' = g\mu_0\mu_{\rm B}S'$ and $\gamma = g\mu_0\mu_{\rm B}S$. The first and second terms represent the anisotropy of the FM and the AF domains, respectively and $K_{\rm u}$ and $k_{\rm ui}$ are the corresponding anisotropy constants. The third term represents the Zeeman energy of the moments due to the applied external field. The fourth term represents the antiferromagnetic couplings among the AF domains, and the last term represents the ferromagnetic couplings between the FM and AF domains.

Using θ_i and β to describe respectively the angles of the i-th AF moment and the FM moment deviating from the common easy axis, we can express the energies of the FM domain and the i-th AF domain as

$$H^{\rm FM} = -\left(J_2\sum_i s_i s + K_{\rm u}\cos\beta + \gamma B s\right)\cos\beta, \quad (2)$$

and

$$H_i^{\rm AF} = \left(J_1 s_i\sum_j s_j - J_2 s_i s - k_{\rm ui}\cos\theta_i - \gamma' B s_i\right)\cos\theta_i, \quad (3)$$

where both s_i and s are the scalars taking values of either 1 or -1. Thus for the i-th AF domain the energy increment is $\Delta E_i = k_{\rm ui}\sin^2\theta_i - h_i(\cos\theta_i - 1)$, where $h_i = (-J_1\sum_j s_j + J_2 s + \gamma' B)s_i$, and for the FM domain the energy increment is $\Delta E = K_{\rm u}\sin^2\beta - h_{\rm F}(\cos\beta - 1)$, where $h_{\rm F} = (J_2\sum_i s_i + \gamma B)\,s$. We can express ΔE and ΔE_i as

$$\Delta E = K_{\rm u}\left[\left(1+\frac{h_{\rm F}}{2K_{\rm u}}\right)^2 - \left(\cos\beta + \frac{h_{\rm F}}{2K_{\rm u}}\right)^2\right], \quad (4)$$

and

$$\Delta E_i = k_{\rm ui}\left[\left(1+\frac{h_i}{2k_{\rm ui}}\right)^2 - \left(\cos\theta_i + \frac{h_{\rm F}}{2k_{\rm ui}}\right)^2\right]. \quad (5)$$

As a result, to reverse its moment, the FM layer must overcomes a barrier $E_{\rm b}^{\rm F} = K_{\rm u}(1 + h_{\rm F}/2K_{\rm u})^2$ if $|h_{\rm F}| \leq 2K_{\rm u}$, or $2h_{\rm F}$ if $h_{\rm F} > 2K_{\rm u}$; and for the i-th AF grain a barrier $E_{\rm b}^{\rm i} = k_{\rm ui}(1 + h_i/2k_{\rm ui})^2$ if $|h_i| \leq 2k_{\rm ui}$, or $2h_i$ if $h_i > 2k_{\rm ui}$. If the condition $h_{\rm F} < -2K_{\rm u}$ or $h_i < -2k_{\rm ui}$ is satisfied, there will be no barrier for the reversal.

Actually, for the distribution of the AF anisotropy energy we use a Gauss function, $f(k_{\rm ui}) = \exp[-(k_{\rm ui} - k_{\rm u})^2/\sigma^2]$, in which σ and $k_{\rm u}$ are set to 30.0 meV and 50.0 meV respectively, unless stated otherwise. The anisotropy energy of the FM domain is set at 200.0 meV without losing physical generality. Thus, the reversal rate for a spin to reverse is $R = R_0 {\rm e}^{-E_{\rm b}/k_{\rm B}T}$, where $E_{\rm b}$ is the energy barrier and R_0 is the characteristic frequency. In our simulations, R_0 is set to 1.0×10^9/s. We adopt a square lattice for the AF domains and use 20×20 as its size. Since we are only interested in the exchange bias and training effects at a nanoscale, using the AF lattice is enough to express the main physics. Furthermore, we assume the AF domains have a uniform moment 4.0 $\mu_{\rm B}$ and the FM domain 2000 $\mu_{\rm B}$. The coupling constant J_1 is set to 4.0 meV, and J_2 8.0 meV. In our simulations the system is quenched from a high-enough temperature, such as 610 K, at which the AF layer is paramagnetic, to a low-enough temperature such as 10 K. The magnetization and exchange bias fields are calculated at the low temperature 10 K unless the temperature is explicitly stated otherwise. The basic rate of changing of temperature is $\nu_0 = 50$ K/s. The field sweeping rate is set to 0.5 T/s with the basic increment 0.1 T for each simulation step.

3. Simulated results and analysis

First, we let the AF/FM bilayers relax under a magnetic field of 5.0 T at a high temperature 610 K. This temperature is enough to make both the FM layer and the AF layer remain paramagnetic. When the temperature decreases, the average magnetization values of the two layers increase. The external field makes the average magnetization of the FM layer have a large increase below 600 K, and nearly reach the saturated value at 500 K. When the temperature becomes lower than 60 K, the average magnetization of the AF layer looks like that of an antiferromagnet under an applied field and is dependent on the cooling rate ν. Then, we further cool the bilayers under the same field. After the temperature has reached down to 10 K, we start to change the field while keeping the temperature unchanged. The field decreases from 5.0 T to -10.0 T and then increases back to 5.0 T for the first hysteresis. Repeating the field cycling, we make the second hysteresis loop. The simulated results are shown in Fig.1.

As shown in Fig.1(a), the origin of the first hysteresis is clearly shifted in the negative field direction and it shows the exchange bias. The exchange bias field is defined as $H_{\rm E} = (H_{\rm cl} + H_{\rm cr})/2$, where $H_{\rm cl}$ and $H_{\rm cr}$ are the coercivity of the left and right branches, respectively. The left branch of the second hysteresis moves towards the positive direction, but the right branches of the first two loops almost coincide with each other. Actually, any further loop almost has no difference in the right branch from the second hysteresis. The shift of the second loop clearly demonstrates that the bilayers magnetization depends on the cycling history, which is known as the training effect. Figure 1(b) shows the magnetization of the AF layer, which drops sharply and opens widely due to the irreversible reversal of the AF domains after the first field cycling has been finished. The subsequent magnetization is more smooth but still not closed, indicating the continuing cycling dependence of exchange bias. This is consistent with other Monte Carlo simulations.[20]

We also study the effect of the temperature T on the exchange bias field, $H_{\rm E}$, for different loops. Our simulated exchange bias fields as functions of T for the first two loops are shown in Fig.2. For the two curves, the data can be fitted by the simple function

$$-\mu_0 H_{\rm E} = a_1 {\rm e}^{-(T/T_1)^{b_1}}, \tag{6}$$

where a_1, T_1, and b_1 are fitting parameters. For the fitting in Fig.2, the parameters a_1, T_1, and b_1 takes 4.26 T, 17.95 K, and 1.58 for the first loop, and 3.94 T, 16.66 K, and 1.59 for the second. Our results are consistent with experimental observations that the exchange bias field decreases with increasing temperature.[13,29,30]

The exchange bias field is found to be dependent on the field cycling number n. Our simulated result from $n = 1$ to $n = 9$ is shown in Fig.3. Here, the temperature is kept at 10 K, and σ is set to 20.0 and 30.0 meV. For both of the curves in Fig.3, the data points except for $n = 1$ are well fitted by the simple

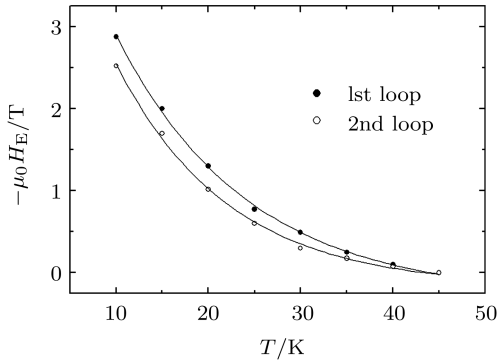


Fig.2. Temperature dependence of the exchange bias fields for the first two loops. The exchange bias field is calculated at a given temperature after the system is cooled from 610 K to that temperature. The lines are the fitting curves in terms of the simple function given in Eq.(6).

function $-\mu_0 H_E(n) = a_2\rho^n + b_2$, where a_2, b_2, and ρ are the fitting parameters, taking respectively 0.23 T, 2.26 T, and 0.76 for $\sigma = 30.0$ meV, and 0.22 T, 1.51 T, and 0.74 for $\sigma = 20.0$ meV. Usually the value of $-\mu_0 H_E(1)$ is substantially above the extrapolation of the other $-\mu_0 H_E(n)$ $(n > 1)$. These simulated results are in good agreement with experimental observation.[7]

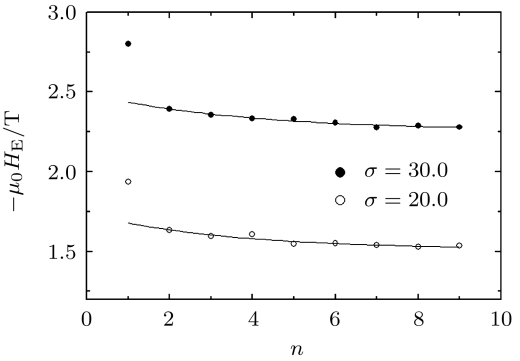


Fig.3. The loop-number dependence of the exchange bias fields for the Gaussian width $\sigma = 30.0$ and 20.0 meV, measured at $T = 10$ K. All the data except for $n = 1$ can be well fitted by a simple function $-\mu_0 H_E(n) = a_2\rho^n + b_2$.

Since the training effect reflects the nonequilibrium dynamical magnetization caused by the irreversible reversal of meta-stable domains formed during quenching, the quenching rate must affect the exchange bias field. By changing the cooling rate ν, we have studied the exchange bias field as a function of quenching rate ν, as shown in Fig.4. For both of the loops, the data can be well fitted by

$$-\mu_0 H_E = a_3 \ln\left(b_3 \frac{\nu}{\nu_0} + 1\right), \qquad (7)$$

where a_3 and b_3 are respectively 0.292 T and 20847 for the first loop, and 0.262 T and 16248 for the second loop. The exchange bias field at 10 K increases logarithmically with increasing quenching rate.

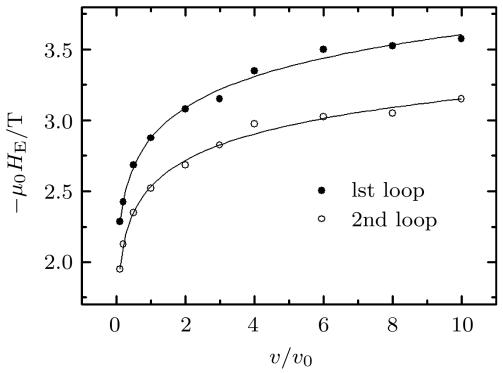


Fig.4. The cooling-rate dependence of the exchange bias fields for the first two loops. The lines are the fitting curves in terms of Eq.(7).

It is interesting to investigate the dependence of the exchange bias field on the coupling constants J_1 and J_2. The simulated results are shown in Fig.5. As shown in Fig.5(a), the exchange bias field decreases with increasing J_1. The training effect is nearly unchanged when J_1 changes from 0 to 2 meV, but diminishes to zero quickly with increasing J_1 beyond 2.0 meV. When J_1 is larger than 6.0 meV, the exchange bias field already becomes very small and the training effect is actually zero. In contrast, the J_2 data points in Fig.5(b) can be well fitted by the simple

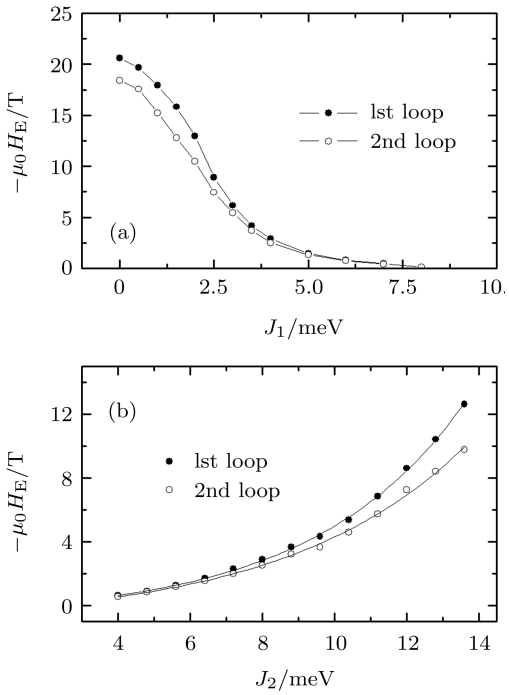


Fig.5. The exchange bias fields as functions of the coupling-constants J_1 (a) and J_2 (b) for the first two loops.

function $-\mu_0 H_{\rm E} = a_4(\exp(J_2/b_4)-1)$, where a_4 and b_4 are the fitting parameters, taking respectively 0.44 T and 4.01 meV for the first loop, and 0.51 T and 4.49 meV for the second loop. It is clearly shown that the exchange bias field increases exponentially as J_2 increases. Both of the the exchange bias field and the training effect can be enhanced by decreasing J_1 and increasing J_2, or by increasing J_2/J_1. This is consistent with the trend shown by experimental results.[31]

Fig.6 shows how the distributive width σ of the AF anisotropy affects the exchange bias fields. Clearly the exchange bias field increases with σ, and so does the training effect. Experimentally, the width can be increased by doping with nonmagnetic impurities and enhancing the roughness of the AF crystalline phases. This implies that the rougher the AF crystalline phases, the larger the exchange bias and training effects. Our result reveals that the exchange bias field is determined by both the coupling constants and the distributive width of the AF domain anisotropy. These are useful to completely understand the phenomenon.[31,32]

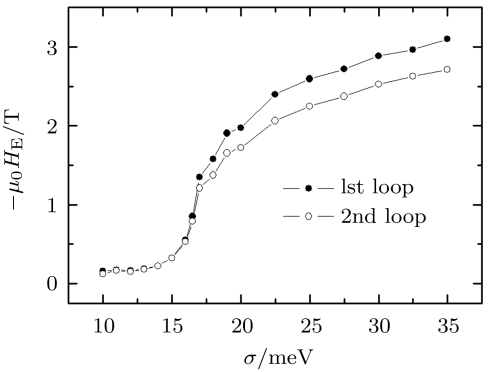


Fig.6. The exchange bias field as a function of the Gaussian width σ for the first two loops.

4. Trends and microscopic mechanism

After being cooled down to low temperatures, the AF layer has a non-zero net magnetization $M_{\rm A}$ due to the driving of both the field and the FM layer. The exchange bias field is determined by the effective moment $M_{\rm A}$, while the difference of $M_{\rm A}$ between the first two loops determines the training effect. Naturally, both the exchange bias field and the training effect increase with increasing J_2 and with decreasing J_1, as shown in Fig.5. Actually, small J_1 does not affect the effects, but a larger $J_1 > 2$ meV is harmful to the effects at 10 K. In addition, it is easily understood that $M_{\rm A}$ decreases with increasing temperature T. As a result, both the exchange bias field and the training effect decrease with increasing T, as shown in Fig.2. The exponential description in Eq.(6) reflects the fact that moment reversals are thermally activated. It is reasonable that both the exchange bias field and the training effect increase with increasing cooling rate ν, as shown in Fig.4. This is mainly because the average magnetization of the AF layer increases with ν when the temperature is below 50 K. When the cooling rate approaches zero, both the exchange bias field and the training effect should be zero. In other words, our results should approach those of corresponding equilibrium systems when the cooling rate ν approaches zero.

As shown in Fig.6, both the exchange bias field and the training effect are nearly zero when the distributive width σ of the AF anisotropy energy is smaller than 15 meV, but they increase substantially with increasing σ for $\sigma > 15$ meV. This means that the effects are dependent on a wide distribution of the anisotropy energy. This can be understood in terms of the changing of the energy barriers with the external field. From $P1$ to $P2$ in Fig.1(a), the effective barrier of the FM layer decreases but is still high enough to prevent the reversal, however, more and more spins of the AF domains are reversed due to their lower energy barriers. At the point $P2$, the FM moment is reversed with the help of the field and the reversing of the AF domains. Anyway, some AF domains with high energy barriers have their moments unchanged, even after the FM layer has been reversed, and thus there is a net average moment of the AF domains parallel to the moment of the FM layer. This net average moment increases with the distributive width σ. This explains the increase of the exchange bias field and training effect with increasing σ. As the field cycling number increases, more and more metastable AF domains reverse back and lead to the reduction of magnetization in AF layer. As a result, the exchange bias field decreases with increasing number of the field cycling. The turning point of the time scale causes the largest drop happens between the first two loops.

5. Summary

In summary, we used a unified Monte Carlo dynamical approach[27] to study the FM/AF heterostructure in order to investigate the exchange bias

and training effect. The magnetization of the uncompensated AF layer is still open after the first field cycling was finished. Our simulated result shows the obvious shift of hysteresis loops (exchange bias) and the cycling dependence of exchange bias (training effect). The exchange bias field decreases with decreasing cooling rate or increasing temperature and the number of the field cycling. With the simulations, we show that the exchange bias is determined by the cooling rate, the distributive width of the anisotropy energy, or the magnetic coupling constants. Essentially, these two effects can be explained on the basis of the microscopic coexistence of both reversible and irreversible moment reversals of the AF domains. Our simulated results are useful to have a real understanding of the magnetization dynamics of such magnetic heterostructures, which is important for spintronic devices and magnetic recording media.[31−33] This unified nonequilibrium dynamical method should be applicable to other exchange bias systems.

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