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Monte Carlo simulation of exchange bias and training effects in ferromagnetic/antiferromagnetic bilayers with different Néel temperatures

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ABSTRACT

A modified Monte Carlo Metropolis algorithm is employed to simulate the field-cooling and training dependencies of low-temperature exchange bias (H_E) and coercivity (H_C) in the ferromagnetic/antiferromagnetic bilayers with various antiferromagnetic Néel temperatures (T_N), which are modulated by altering the antiferromagnetic exchange coupling constant (J_{AF}). It is found that the smaller the J_{AF} value, the more pronounced is the H_E. However, strong cooling fields (H_{FC}) may also induce a saturated low-temperature H_E value. Interestingly, the low-temperature H_C behaviors with J_{AF} and H_{FC} both exhibit a minimum value corresponding to the steepest change in H_E. The evolutions of microscopic domain walls and domain sizes in the ferromagnetic layer are used to reflect the change in the antiferromagnetic configurations and, thus, to interpret the novel phenomena. On the other hand, H_E in the bilayers with T_N lower than the Curie temperature (T_C) indicates a training effect due to the fact that the antiferromagnetic configurations near the interface which are created partially by their adjacent ferromagnetic layer via interfacial exchange coupling during field cooling are able to be rearranged at low temperature by repeating magnetizing. In other words, the completely frozen antiferromagnetic spins in the bilayers with $T_N > T_C$ at low temperature lack the dynamics to cause the absence of training effect.

1. Introduction

Exchange bias (EB) was first discovered by Meiklejohn and Bean 50 years ago [1] and refers to a shift of hysteresis loop along the magnetic field axis when ferromagnetic (FM)/antiferromagnetic (AFM) systems are deposited in a magnetic field or field-cooled through the AFM Néel temperature (T_N) [2]. Considerable studies on EB have been carried out during the past decades mainly due to its charming and potential applications in magnetic recording media, magnetic resonance settings, spin valves, and magnetic tunnel junctions [3–6]. Yet some questions remain in the darkness as a direct consequence of experimental difficulties to produce defect-free FM/AFM interface or to determine local spin configurations in buried interface. Accordingly, computer simulations coupled with Monte Carlo (MC) techniques have been proved as powerful and useful tools to gain insights into the microscopic origin of EB [7–10]. These methods allow one to see the consequence of the change of microscopic parameters such as exchange coupling and anisotropy constants specific to real materials at hand and to take into account the specific arrangement of magnetic atoms in a lattice. As an output, macroscopically measurable quantities, such as magnetization, can be computed without losing valuable information about the microscopic magnetic configurations.

Generally, EB is observed in the composite systems where the FM Curie temperature (T_C) is much higher than T_N. Recently, some EB results on the FM/AFM systems with $T_C < T_N$ are also reported, involving multilayers [11–17], nanoclusters [18], nanocomposite films [19,20], and nanoparticles [21–23]. In these systems, a peak behavior in the EB field (H_E) versus temperature curve may be observed and was discussed in terms of evolution of interfacial exchange coupling [14,15], reduction of FM saturated magnetization [16], or competing positive and negative interfacial exchange couplings [19]. Other temperature-related phenomena, such as monotonically decreased [13], increased [20], or even oscillatory H_E [12] with temperature were observed and interpreted based on the existence of incommensurate spin-density wave in the AFM layer as well as non-collinear interfacial coupling between FM and AFM layers. Moreover, Si et al. [21,22] reported a large coercivity (H_C = 873kA/m) and a large H_E (=400kA/m) in oxide-coated manganese nanoparticles and suggested a phenomenological model to explain the phenomena. Guo et al. [20] studied the influence of cooling field (H_{FC}) on EB in $CoCr_2O_4$ (T_C = 100 K)/Cr_2O_3 (T_N = 307 K) nanocomposite films and found that below irreversibility temperature, H_E appeared and was eventually saturated to a constant value under a strong value of H_{FC} due to the frozen AFM domain states with

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sufficiently irreversible magnetization that was created after field cooling.

In a three-dimensional Heisenberg ferromagnet, a linear relation between exchange coupling and T_C has been achieved using MC simulations [24,25], implying that such critical temperature value may be strongly dependent on the intrinsic exchange coupling constant. On the other hand, a gradual degradation of H_E during consecutive hysteresis loops, known as training effect, was found in 1966 [26]. Since then a plethora of experimental investigations were reported [27–31] and a number of models were put forward to describe them [32–36]. It has been accepted that the origin of training effect is related to the change in the AFM spin states compared to the original state after field cooling [37]. Therefore, the understanding of training effect requires the exact mechanism of EB, and the study on training effect can in turn help us to understand EB further.

Conventional MC simulations based on Metropolis algorithm have an advantage of not requiring a priori knowledge of a possible state set but are computationally inefficient to deal with the quasi-equilibrium state such as hysteresis loop [38]. On the contrary, Stoner and Wohlfarth [39] used a collection of noninteracting magnetic particles to well describe the hysteresis loop half a century ago. However, their theory is only valid when magnetization is locked into the equilibrium direction, that is, when the thermal fluctuation is negligible. More recently, Xu et al. [40] and Jalil [41] presented a two-state model and its improved version, respectively, combining the MC simulations with the Stoner–Wohlfarth model. However, they both cannot extend the fluctuation state to a continuous area as it should be at low temperature. In this paper, therefore, we completely consider the reversal path of spin and exactly calculate the energy barrier during each spin reversal and present a modified MC Metropolis algorithm to study the effects of H_{FC} and training on EB in the FM/AFM bilayers with various T_N. The behaviors obtained in the bilayers with $T_N < T_C$ and $T_N > T_C$ are distinct and explained according to the AFM magnetization behaviors near the interface. The remainder of article is organized as follows. Section 2 is devoted to the descriptions of our model and method. Numerical results are shown and discussed in Section 3. Finally, Section 4 gives a summary.

2. Model and Monte Carlo simulation

At the atomic level, a model of bilayers with one FM monolayer and four AFM monolayers, consisting of 8000 spins lying at the nodes of a simple cubic lattice, is exploited. Moreover, periodic boundary conditions in the lateral directions and open boundary conditions in the out-of-plane directions are used. In the simulation, several lattice sizes have been examined and the magnetization becomes insensitive to the spin number above a certain value.

Under an external magnetic field, the Hamiltonian can be formulated as

$$\begin{aligned} H = & -J_{FM}\sum_{<i,j\in FM>} S_i\cdot S_j - \sum_{i\in FM} K_{FM}S_{ix}^2 \\ & -J_{AF}\sum_{<i,j\in AFM>} S_i\cdot S_j - \sum_{i\in AFM} K_{AF}S_{ix}^2 \\ & -J_{IF}\sum_{<i\in FM,j\in AFM>} S_i\cdot S_j - H\cdot\sum_i S_i. \end{aligned} \quad (1)$$

The Heisenberg spin S_i is a unit vector with Cartesian components of S_{ix}, S_{iy}, and S_{iz}, where i denotes a site index and angular brackets imply that the summations are restricted to the nearest neighbors only. The first two lines are the FM and AFM exchange and anisotropy energies, respectively. The last line includes the FM/AFM interfacial exchange and Zeeman energies. In this paper, the units of parameters are reduced and normalized by the FM exchange coupling constant J_{FM}, and thus the magnetic field H, H_{FC}, H_E, and H_C are given in units of $J_{FM}/g\mu_B$, the temperature T in units of J_{FM}/k_B, and the AFM and interfacial exchange coupling constants (J_{AF} and J_{IF}) and the FM and AFM anisotropy constants (K_{FM} and K_{AF}) in units of J_{FM}, respectively. J_{FM} and J_{IF} are above zero for favoring the parallel alignment of spins, and their magnitudes are 1.0, while J_{AF} is below zero and its magnitude varied from -1.00 to -0.01 in steps of $\Delta J_{AF} = 0.01$ to determine T_N. Next, $K_{FM} = 0.1$, just in order to obtain a well-defined hysteresis loop, and K_{AF} is equal to 10.0, as required to pin the AFM spins during hysteresis loops so that EB is able to be observed. Finally, the collinear FM and AFM anisotropy axes are postulated along the x axis.

During the simulation, we calculate the energy of each spin with respect to its polar and azimuthal angles in order to judge whether the energy barriers between new and initial states exist and thus to determine the "flipping" probability (p). More detailed description on the computational process has been published elsewhere [37,42–44]. If the energies of new and initial states of spin i are both lower than the minimal energy barrier and the rotation of spin i from initial to new state needs to stride over the minimal energy barrier, the energy term of new state in p will be replaced by the minimal energy barrier term,

$$p = \exp\left[-\left(E_i^{sad} - E_i^{ini}\right)/k_BT\right], \quad (2)$$

where E_i^{sad} and E_i^{ini} are the energies of saddle point and initial states, respectively. Aside from the aforementioned situation, the standard Metropolis algorithm remains,

$$p = \exp\left[-\left(E_i^{new} - E_i^{ini}\right)/k_BT\right] \quad (3)$$

for the energy of new state (E_i^{new}) > E_i^{ini}, and $p = 1$ for $E_i^{new} \le E_i^{ini}$. Our modified MC method allows one to climb to the maximum value or to drop to the minimum value by taking less MC steps. In other words, the rotational paths are considered as well as the ways to go from the absolute minimum value to the metastable one at arbitrary finite temperatures become possible, which are physically correct and consistent with both the dynamic simulation and the MC time quantification [45].

Our protocol to simulate EB mimics the experimental one: we cool a disordered system down from a high temperature $T = 4.0$ to a desired low temperature $T = 0.01$ in steps of $\Delta T = -0.01$ under an H_{FC} applied along the x axis. Once $T = 0.01$ is reached, a hysteresis loop is recorded also along the x axis and in steps of $|\Delta H| = 0.01$ from $H = 2.0$ down to $H = -2.0$ and afterwards raised again back to the initial value. The maximal applied field must guarantee the FM layer to be saturated in order to avoid the appearance of minor loops [46,47]. For a cooling magnetization and a hysteresis loop, totally 4.8×10^5 and 4.812×10^5 MC steps per spin are performed, respectively; at each temperature or field value, 200 MC steps per spin are used for thermalization followed by 1000 MC steps per spin for obtaining the thermal average of the relevant quantities. The sweep rate is slow enough to guarantee the quasi-equilibrium state, and we average over ten different realizations of the disorder to reduce the statistical errors.

3. Results and discussion

In order to obtain T_N of the antiferromagnets with different J_{AF}, a pure AFM model with a larger size of $N = 40 \times 40 \times 40$ and 3D periodic boundary conditions, which is used to simulate a bulk material, is zero-field-cooled from $T = 10.0$ to 0.01, and the zero-field susceptibility behaviors with temperature are calculated. Fig. 1(a) depicts the AFM susceptibilities as a function of temperature in the bilayers with some representative values of J_{AF}, and Fig. 1(b) indicates the evolution of T_N with J_{AF} and the T_C value of ferromagnet is also marked. Remarkably, the T_N values obtained from the antiferromagnets with $J_{AF} = -0.38$ to -0.01 are lower than T_C, while obtained from the antiferromagnets with $J_{AF} = -1.00$ to -0.38, $T_N > T_C$. Based on