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Influence of thermal energy on exchange-bias studied by finite-element simulations

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In this article we describe the thermal relaxation in anti-ferromagnetic/ferromagnetic bilayers using a hybrid method that combines a kinetic Monte Carlo technique with magnetization dynamics following the Landau Lifshitz Gilbert equation. A granular anti-ferromagnetic layer is exchange coupled to an amorphous ferromagnetic layer and discretized using a finite element method. Calculations are made to help clarify how the underlying magnetic structure is related to the measured exchange bias fields as a function of temperature for the case of amorphous $Co_{65.5}Fe_{14.5}B_{20}$/granular $Ir_{22}Mn_{78}$ bilayers. Our calculations are in excellent agreement with experimentally measured macro-magnetic properties of these bilayers. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4816664]

When a ferromagnetic (FM) and anti-ferromagnetic (AF) layers are coupled, a shift in the hysteresis loop is generated.[1,2] The shift of the hysteresis loop, known as the "exchange bias field," H_{ex}, is also accompanied in some sample configurations with a "training effect."[3,4] This is where H_{ex} reduces gradually over successive field cycles until the sample has been fully "trained" and relaxed to its lowest energy state. It has been observed that the exchange bias field and magnitude of the training effect are highly dependent on the thickness of the system, most notably the AF layer.

A thicker AF IrMn layer, up to a saturating limit, increases H_{ex} while larger training effects are observed for thinner IrMn layers. Qualitatively, thermal energy can overcome anisotropy energy (anisotropy constant-volume product, KV) and therefore influence the exchange-bias phenomenon observed in the coupled system. In this work we show that thermal relaxation over energy barriers may explain of the dependence of the training effect on temperature.

The phenomenon of exchange bias is used extensively in information storage devices using granular thin films. However, to date, the exchange bias properties have been optimized through empirical work. Therefore, there is significant motivation to develop a model with the predictive ability of the influence of material properties and structure, and in particular, include the effect of the thermal stability on the granular AF layer.

Here we use a finite element model, which incorporates the structural parameters of an amorphous $Co_{65.5}Fe_{14.5}B_{20}$/granular $Ir_{22}Mn_{78}$ bilayer. This is combined with a previously modified micromagnetic algorithm that includes the influence of thermal energy based upon a kinetic Monte Carlo approach.[5] We choose to model this specific bilayer due to its technological relevance. Hybrid Monte Carlo-Landau-Lifshitz-Gilbert (HMC-LLG) simulations are used to calculate the underlying magnetic structure and exchange bias fields within the exchange-biased bilayer as a function of temperature and intergrain exchange. This article first describes the HMC-LLG algorithm, previously used to successfully study thermal effects in recording media. This is then implemented to study directly the thermal effects in an exchange-biased system at finite temperatures. Finally we compare our computational results with experimental measurements.

At a finite temperature, T, the mean lifetime, τ, of a magnetic orientation in a magnetic single domain can be estimated by the Arrhenius-Néel equation

$$\frac{1}{\tau} = f_0 e^{\frac{-E_b}{k_B T}}, \tag{1}$$

where the energy barrier, $E_{B,}$ is the energy required to switch between two magnetically stable configurations. The pre-exponential factor f_0 is the attempt frequency at which the magnetization tries to switch orientation. This approach has been successful in estimating probability of switching in granular media when subjected to thermal energy and external fields.[6]

One method to compute the energy barrier of the individual grains is assuming each grain in single domain and applying the nudged elastic band method, which enables rapid estimates of the thermal stability of the system. In macroscopic granular assemblies, such as exchange-biased systems, a distribution of energy barriers is inherent due to a spread of the grain volume. To study a temporal evolution of the magnetization in systems with energy barrier distributions, such as a hysteresis loop, kinetic Monte Carlo methods can be applied.[7] We implement an approach as outlined by Suess[5] based on the work of Chantrell.[7] In the method by Suess *et al.*[5] grains are allowed to switch according to their switching probability. Once a grain is switched, the system is relaxed towards the next local minimum by solving the LLG equation. Switching between the Monte Carlo and LLG calculations provides a methodology of solving the magnetic

evolution of the magnetization in systems for time spans of minutes and hours while accounting for thermal energy. This method has proved to be a good approximation to the energy barriers for grains up to 20 nm thick.[5]

Here we use it to simulate the AF granular microstructures where the probability of switching, P_r, for each grain within a time step, t_m, can be calculated using

$$P_r = 1 - e\frac{-t_m}{\tau}. \quad (2)$$

The simulation proceeds as follows: In a pre-simulation step the energy barriers of the AF grains are precomputed and tabulated for a various total fields H^* and field angles acting on the grain. A local minimum energy configuration is computed by solving the LLG equation. For this configuration the exchange fields H^* that act on the AF grains are computed. H^* takes into account the exchange field with the ferromagnet and the intergrain exchange field from neighboring AF grains. Then an AF grain is chosen randomly. From the value of H^* and its angle corresponding barrier E_B is taken from the precomputed values by interpolation. The switching probability within time t_m is calculated according to Eq. (2). On average all grains are picked on time within the time step t_m. After each switching event according to Eq. (2) the system is relaxed to the next local minimum by a standard LLG solver. The Monte Carlo time step t_m is chosen sufficiency small so the simulations are independent of this time step. To calculate the effective field, we use a previously modified micromagnetic finite element code for exchange bias.[8–10]

We base our simulations upon experimental measurements where possible. A 5 nm thick layer is first meshed using tetrahedral cells to represent the amorphous $Co_{65.5}Fe_{14.5}B_{20}$ layer. To simulate the hysteretic behavior of the exchange coupled system using our hybrid finite element code we replicated a "field cool" protocol for the sample following the experimental sample preparation. An annealing field of 15 kOe is simulated over the sample alongside a temperature of 513 K. This increase in thermal energy increases the probability of the IrMn switching. This HMC-LLG can then be used to simulate the reversal of the granular layer in a 5-h period. After a simulation period of 1 h the thermal energy is then reduced to 300 K. The field is then removed in the simulation allowing the exchange-coupled system to relax to an energy minimum remnant state forming the "field cool" state. This generates an exchange bias effect parallel to the "field cooled" direction. The local coupling between the AF grain and the FM plays a major role in forming the AF state after field cooling. Hysteresis loops are also matched using HMC-LLG to represent the experimentally measured times and field ramp rates of 0.3 Oe s^{-1} (i.e., quadrant taking approximately 3150 s to complete).

Due to the field cooling process in the fabrication a uniaxial anisotropy is induced in the FM layer, as measured experimentally, of $K_{FM} = 2000\,J\,m^{-3}$.[11] The magnetic exchange stiffness and polarization were set as $A_{FM} = 1.3 \times 10^{11}\,J\,m^{-1}$ and $M_{FM} = 1.4\,T$, respectively.[11]

Experimentally measured grain size distributions[9] are used to generate the structure for the polycrystalline $Ir_{22}Mn_{78}$ layer. Thicknesses of 12.5 nm (grain size diameter of 7.7 ± 0.8 nm), 9 nm (7.0 ± 1.1 nm diameter), and 6 nm (5.0 ± 0.8 nm diameter) are used for comparison. Errors represent the standard deviation for each set. We incorporate a grain boundary phase within the IrMn granular structure, 0.5 nm thick, consistent with transmission electron microscopy observations,[9] texture to the magnetic anisotropy direction of {111} out-of-plane, and random orientation in-plane, as determined by selected area electron diffraction.[9] Interlayer and intergrain exchange values of $J_{INT} = 2.7 \times 10^{-13}\,J\,m^{-1}$ and $A_{GRAIN} = 0.1 \times 10^{-13}\,J\,m^{-1}$, respectively, are based on fitting to experimental data, described previously.[8,9] Roughness and atomic steps at the CoFeB and IrMn interface, as well as IrMn grain boundary grooving, are modeled using a random dispersion, evenly distributed (1:1), of an uncompensated interface and compensated interface spin coupling.

The IrMn anisotropy strength to be used in the micromagnetic simulations depends on the way thermal effects are incorporated. In our previous calculations that did not take into account thermal activations were based on values of $100 \times 10^3\,J\,m^{-3}$.[12,13] This value allowed us to simulate such systems at room temperature and successfully predicted the behavior of exchange bias films.[8–10] In this research, the model includes thermal activation over the energy barriers. Therefore a higher anisotropy value of $K_{AF} = 550 \times 10^3\,J\,m^{-3}$ as measured experimentally by O'Grady[14–16] is used here. O'Grady and co-workers use measurements of the medium blocking temperature of the IrMn/CoFe bilayers together with Eq. (1), in order to estimate the magnetocrystalline anisotropy of the AF grain. For their calculation the use $E_B = K_{AF}V(1 - H^*/H_k^*)$,[2] where H^* is the exchange bias field and H_k^* is the anisotropy field of the AF grain, and $f_0 = 10^9$ Hz. Similarly we assumed an attempt frequency of $f_0 = 10^9$ Hz in our simulations.

This single set of parameters allows us to pre-compute the energy barrier distribution of the IrMn grains for the three different thicknesses examined experimentally, 12 nm, 9 nm, and 6 nm. As an approximation, we consider the energy barrier E_b as the difference between the individual anisotropy energy for each AF grain ($E_a = K_{AF}V$) and the interfacial energy at the AF/FM interface of $E_{int} = 2J_{int}(A/d)$ where A is the cross sectional area of the grain and d is the lattice constant, in this case $d = 0.378$ nm.[9] Depending on the state of the FM with respect to the anisotropy direction of the antiferromagnetic grain, the interface energy increases or decreases the energy barrier. Both these energies scale with cross sectional area; however, the anisotropy energy increases with granular thickness. Switching of an AF grain is temperature driven, and the switching probability decreases for larger grains. The predicted lifetime calculated for the individual IrMn grains are shown in Fig. 1 for 12.5 nm, 9 nm, and 6 nm thicknesses. The overlaid shaded region from 10^{-10} to 10^3 s highlights grains that possess a high probability of switching as the FM layer is switched. Those with high lifetimes are likely to remain pined an unchanged as the adjacent FM layer is switched during reversal.

These calculations predict that for a 12.5 nm thick media fewer than 2% of the AF grains are expected to switch as the FM progresses through the hysteresis loop. This is in contrast to a 6 nm thick granular sample where over 66% of the grains have a high probability to switch during the hysteresis loop measurement. It should be noted that this approach is

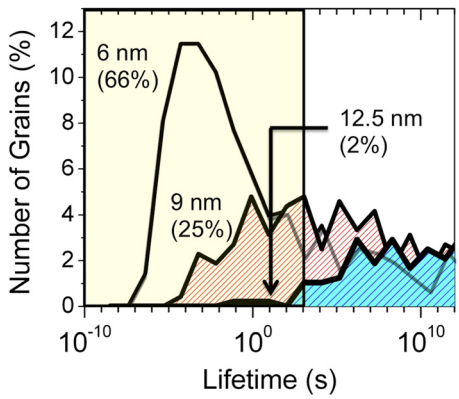

FIG. 1. A plot of the calculated lifetime (up to 10^{12} s) of each grain in the exchange biased system at 300 K for different IrMn layer thicknesses: 12.5 nm, 9 nm, and 6 nm. The rectangular shaded region (from 10^{-10} to 10^{3} s) highlights grains that possess a high probability of switching as the FM layer is switched in realistic systems. The percentage values predict the fraction of grains that will switch with each field sweep.

limited and only relevant for decoupled grains and will only affect the exchange bias field, H_{ex}, if the grains are coupled via an uncompensated interface. Here this approach is limited to decoupled grains. Experimentally we observe sharp grain boundary transitions, so to account for this the model is now extended to incorporate inter-granular exchange.

We first use the HMC-LLG method to simulate exchange bias fields and training effects found by experimental measurements at 300 K. These have previously been simulated using a micromagnetic simulation without temperature dependence and only in the nanosecond timescale. Here we simulate using HMC-LLG both temperature and the field ramp rates obtaining exchange bias fields for three different thickness of IrMn of 12.5 nm, 9 nm, and 6 nm, presented in Figures 2(a)–2(c), respectively.

With no intergrain exchange, grains are fully decoupled. In this case any grain whose inherent energy barrier is lower than the energy exerted by the interfacial energy will switch in each field-loop resulting in no further change in the exchange bias as highlighted in Figure 1. This fast training effect is shown in Figure 2 where after a maximum of two field-loops the exchange bias has reached its minimum region. For a 6 nm thick grain, the average fraction of grains switching was calculated to be 45%, 42%, 43%, 44%, and 42% for the first 5 successive loops of the external field, respectively. This is lower than the predicted value of 66% in Figure 1, which could be attributed to the mix of compensated and uncompensated interfaces used in the AF/FM model; however, it can be seen that this number remains relative constant after the first loop leading to a relatively constant exchange bias of 50 Oe after the initial loop. With the inclusion of intergrain effects the IrMn grains are weakly coupled, thus neighboring grains will also contribute to the stability of the individual grains, reducing the speed at which they switch. Over 5 loops of the external field, the average number of grains switching are found to be 44%, 39%, 36%, 35%, and 32% reaching a similar minimized state to that of the decoupled system. The number of grains switching has reduced due to the intergrain energy stabilizing the switching leading to a slower decrease in the exchange bias field and indeed it is observed experimentally.

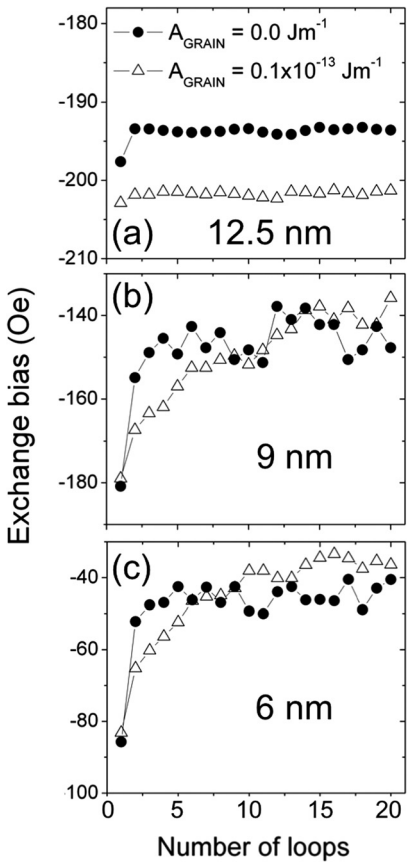

FIG. 2. Finite element simulation of the exchange bias over 20 successive loops of the external field for IrMn layer thicknesses of (a) 12.5 nm, (b) 9 nm, and (c) 6 nm.

Using the HMC-LLG method we can simulate the hysteretic behavior of exchange coupled systems at different temperatures. The simulations, based upon the experimentally measured samples, follow the protocol developed by Fernandez-Outon.[17] Here the field-cooled exchange coupled system is placed under a magnetic field of 2×10^4 Oe for 1 h at 373 K in order to reset the magnetic alignment of the grains in the AF layer. Then, with the field still applied, the sample is cooled to the measurement temperature of 100, 200, or 250 K ($\pm$0.1 K) and the magnetization of the sample measured during magnetic field cycling from +700 Oe to −1700 Oe in 20 Oe steps. This cycle was applied three consecutive times to track the training effect. Fig. 3(a) shows the experimental results at a measurement temperature of 100 K, which shows an increase in the exchange-bias field to approximately 390 Oe. In the following cycles, the magnetization curves are similar, indicating that the training effect is negligible. At a measurement temperature of 200 K (not shown), the exchange bias field decreases to 200 Oe reducing further to 70 Oe for measurements undertaken at 250 K [Fig. 3(c)]. At these higher temperatures, a training effect is now observed in the ascending branch of the magnetization curve. For the hysteresis curves measured at 250 K, H_{EX} is observed to decrease by approximately 25 Oe and 15 Oe in consecutive cycles.

These experimental measurements are compared to the results of the HMC-LLG simulations shown in Figs. 3(b) and 3(d). At 100 K the simulated loops show an exchange bias of

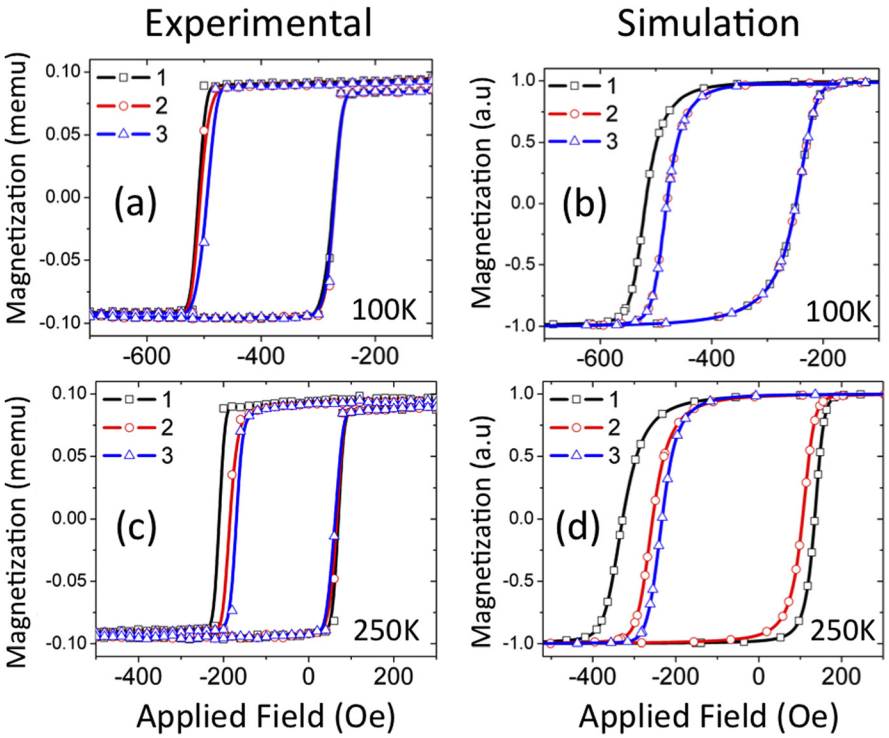

FIG. 3. The comparison between experimental and simulated hysteresis loops of a 6 nm thick IrMn layer at two different temperatures, with three successive hysteresis loops shown for each. The temperature is varied from (a), (b) 100 K and (c), (d) 250 K.

over 350 Oe reducing to 100 Oe as the temperature is increased to 250 K. This increase in thermal energy also leads to a subsequent training effect. The temperature dependency of the training effect is plotted in Figure 4 over 20 loops and can be related to the lifetime approximation of the grains as shown in Figure 5. As a guide to the eye, grains that possess a high probably of switching during the measurement of the hysteresis loop have been shaded, thus highlighting the significance of the stability of the grain and the effect on the exchange bias and training effects.

At higher temperatures the increased thermal energy reduces the stability of the grains, creating more grains that are susceptible to rotation. The predicted probability of switching thus increases, to approximately 60% of the system. This leads directly to an increase in the training effects and a reduction in the exchange bias field. As the thermal energy of the system is reduced, the probability of switching decreases to fewer than 9% of the grains, resulting in an increase of the exchange bias field to over 350 Oe and a reduced training effect.

In summary, we presented temperature dependent calculations on an exchange bias system of amorphous $Co_{65.5}Fe_{14.5}B_{20}$ and granular $Ir_{22}Mn_{78}$. A modified micromagnetic code is used along with a hybrid Monte Carlo technique to predict the influence of thermal energy on bias and training effects. We have incorporated all available experimentally measured parameters in order to build an exchange bias model. This method has also allowed us to use the experimental field ramp rates, waiting times, and field cooling protocols resulting in an agreement between simulated and experimental exchange bias fields and training effect. By incorporating the experimentally characterized microstructure of the IrMn layer, we show that the thickness of the AF layer is critical in determining the exchange bias properties, thus enabling to design and tailor bilayers for their desired

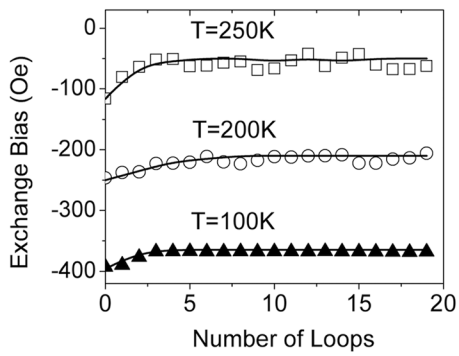

FIG. 4. The training effect, calculated by the finite element simulation algorithm presented in this work, as a function of temperature for a 6 nm thick IrMn layer. At low temperatures, a small training effect is observed where, at higher temperatures, the training effects become greater with a decrease in the exchange bias field.

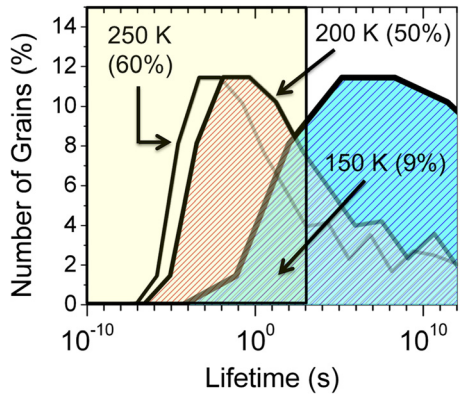

FIG. 5. The calculated lifetime (up to 10^{12} s) of each grain in the exchange biased system at 300 K for a 6 nm thick IrMn layer at 250 K, 200 K, and 100 K. The rectangular shaded region (from 10^{-10} to 10^{3} s) highlights grains that possess a high probability of switching as the FM layer is switched. The inset percentages show the predicted fraction of grains that will switch with each field sweep.

performance before fabrication and the subsequent extensive experimental measurements. Furthermore, we also show that including intergrain exchange is critical for such calculations. Without intergrain exchange, the training effect occurs only over the first loop cycle and is not consistent with experimental observations.

It is also shown that at low temperatures, the thermal stability of the grain dominates over the interlayer energy, increasing the exchange bias field to over 400 Oe when compared to a room temperature measurement of 100 Oe.

This hybrid modelling technique shows excellent agreement with experimentally measured macro-magnetic properties of these exchange-coupled systems and helps to explain the resultant exchange bias properties and training effects from the balance of the interlayer and anisotropy energies that make up such systems.

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