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3D and 1D micromagnetic calculation for hard/soft bilayers with in-plane easy axes

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ABSTRACT

Macroscopic hysteresis loops and microscopic magnetic moment distributions have been determined by three-dimensional (3D) as well as one-dimensional (1D) micromagnetic models for exchange-coupled $Nd_2Fe_{14}B/\alpha$–Fe bilayers and carefully compared with each other. It is found that the results obtained from the two methods are consistent with each other, where the nucleation and coercive fields decrease monotonically as the soft layer thickness L^s increases whilst the largest maximum energy products (roughly 600 kJ/m^3) occur at $L^s=5$ nm. Moreover, the calculated angular distributions in the thickness direction for the magnetic moments are similar. Nevertheless, the calculated critical fields and energy products by 3D OOMMF are systematically smaller than those given by the 1D model, mainly due to the local demagnetization fields, which are taken into account in the 3D calculation and ignored in the 1D calculation. It is demonstrated by the 3D calculation that the large demagnetization fields in the corners of the soft layers reduce the nucleation fields and thus facilitate the magnetic reversal. Such an effect enhances as L^s increases. When $L^s=20$ nm, the differences between the coercivity is as large as 30%, while the nucleation fields obtained by the two methods have opposite signs.

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1. Introduction

Exchange spring materials, with the hard and soft phases exchange-coupled in the nanoscale, is proposed by Kneller in 1991 [1]. Such a material has drawn much attention in the past two decades [2–21] due to its expected giant energy product, with the large coercivity provided by the hard phase and the large remanence coming from the soft phase. Nevertheless, the giant energy product as large as 1 MJ/m^3 predicted by Skomski and Coey [2] has never been achieved. Experimental energy products are much smaller [3–5,7–10], even smaller than the corresponding single phased hard material, which is called energy product paradox in some literatures [13]. A close review shows that the experimental remanence is close to the predicted one however, the measured coercivity is much smaller [3–5,7–10]. Therefore, such an energy product paradox is intrinsically linked with Brown's coercivity paradox [23], where the measured coercivity is much smaller than those predicted by the available theory. Thus a reexamination of the present theories regarding hysteresis loops and energy products in the exchange spring materials, may not only provide a clue on how to increase the energy products of these materials, but also give insight on the solution of Brown's paradox.

Skomski and Coey made their prediction on the basis of a one dimensional (1D) micromagnetic model [2], which was first utilized by Goto et al. [24]. Similar model has been intensively used in the past two decades, by Leineweber and Kronmüller from Germany [6], by Fullerton and Jiang from USA [7,8], by Asti and Pellicelli et al. from Italy [11,14,19] and by Zhao et al. from China [12,13,16,18,21]. Such a simple model can reveal some important underlying physics with the derived analytical formula. However, it is not enough to take account of the magnetic distributions in the film plane as well as the sophisticated microstructures existing in nature.

In this paper, hysteresis loops and magnetic reversal process of $Nd_2Fe_{14}B/\alpha$–Fe bilayer systems have been calculated using both a 3D software (OOMMF) [22] as well as the above mentioned 1D method. The calculated results are carefully compared with each other to demonstrate the similarities as well as the differences between the two methods.

2. Micromagnetic model

The model used in this paper is an exchange–spring bilayers composed of a hard layer and a soft one. An o-xyz coordinate

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system is constructed with the origin located at the center of the interface. The magnetocrystalline axis of both the layers and the applied field are assumed to be in the y direction for simplification, as shown in Fig. 1. The superscripts s and h stand for the soft and hard layers respectively, as a result, L^s and L^h denote the thicknesses of the soft and hard layers respectively.

The three dimensional (3D) micromagnetic calculation of the software OOMMF is based on a Landau–Lifshitz–Gilbert dynamic equations [22]:

$$\frac{d\boldsymbol{M}}{dt} = -|\bar{\gamma}|\boldsymbol{M}\times\boldsymbol{H}_{eff} - \frac{|\bar{\gamma}|\alpha}{M_s}\boldsymbol{M}\times(\boldsymbol{M}\times\boldsymbol{H}_{eff}), \tag{1}$$

where $\boldsymbol{M}$ is the magnetization, $\boldsymbol{H}_{eff}$ is the effective field, $\bar{\gamma}$ is the Landau–Lifshitz gyromagnetic ratio, and α is a dimensionless damping constant. The effective field is defined as follows:

$$\boldsymbol{H}_{eff} = -\mu_0^{-1}\frac{\partial E}{\partial \boldsymbol{M}}. \tag{2}$$

Eq. (2) is valid in the limit of $\alpha \ll 1$ for dynamic studies. However, for a calculation as performed in the present work to search the equilibrium state where $\boldsymbol{H}_{eff}$ approaches 0, this restriction could be somewhat relaxed and a default value of 0.5 for α has been adopted here to allow a fast converge. The average energy density E in Eq. (2) is a function of M specified by Brown's equations [2,23]

$$E = A(r)\left[\frac{\nabla M}{M_S}\right]^2 - K(r)\frac{(\boldsymbol{M}\cdot\boldsymbol{n})^2}{M_s^2} - \mu_0\boldsymbol{M}\cdot\boldsymbol{H} - \frac{1}{2}\mu_0\boldsymbol{H}_d(r)\cdot\mathrm{M}\,, \tag{3}$$

where A and K are the exchange and anisotropy energy constants, respectively, $\boldsymbol{H}$ and $\boldsymbol{H}_d(r)$ are the applied and magnetostatic self-interaction fields while $M_S = M(r)$ is the spontaneous magnetization. These equations hold for both the hard and soft phases. The four terms at the right side of Eq. (3) correspond to the exchange energy, the anisotropy energy, the applied field (Zeemam) energy and the magnetostatic (demagnetization) energy.

The above 3D energy could be simplified to a one dimensional (1D) expression if we ignore the magnetostatic interactions, which are small for an infinitely large thin film. In one dimension, the energy density per area in the film plane is [11,18]

$$v = \int_0^{L^h}\left[A^h\left(\frac{d\theta}{dz}\right)^2 + K^h\sin^2\theta - \mu_0 H M_s^h\cos\theta\right]dz + \int_{-L^s}^{0}\left[A^s\left(\frac{d\theta}{dz}\right)^2 + K^s\sin^2\theta - \mu_0 H M_s^s\cos\theta\right]dz - \frac{2A^{hs}}{a}(\vec{m}^s\vec{m}^h - 1), \tag{4}$$

where a is the distance between the adjacent atomic planes near the interface, θ is the angle between the magnetization and the applied field and $\vec{m}$ is the magnetization unit vector at the interface. The three terms inside the bracket of the above formula are exchange energy, the anisotropy energy and the Zeeman energy, while the last term is the interface exchange coupling energy. A variational method [13] is used to minimize the energy expressed in Eq. (4), which yields the equations for the angular distribution (θ as a function of z) as follows:

For $0 < z < L^h$,

$$\frac{L^h - z}{\Delta^h} = \int_{\theta^h}^{\theta}\frac{d\theta}{\sqrt{(\sin^2\theta - \sin^2\theta^h) - 2h^h(\cos\theta - \cos\theta^h)}}. \tag{5}$$

For $-L^S < z < 0$,

$$\frac{L^s + z}{\Delta^s} = \int_{\theta}^{\theta^s}\frac{d\theta}{\sqrt{(\sin^2\theta - \sin^2\theta^s) - 2h^s(\cos\theta - \cos\theta^s)}} \tag{6}$$

where $h = H/H_k$ represents the reduced applied field with $H_k = 2K/(\mu_0 M_s)$ as the anisotropy field. $\Delta = \sqrt{A/K}$ is the Bloch wall width. θ^h and θ^s are the directions of the magnetization at the outer surfaces of the hard and soft phases, respectively. From these equations the hysteresis loops and energy products can be calculated. The 1D calculation is basically an analytical one.

In the 3D simulation carried out by OOMMF, the length and width of both the soft and hard layers are set as 300 nm. The material is divided into different cells according to different thicknesses of the soft layer. The length and width of each cell is 3 nm, which is close to the Bloch wall width of most hard materials. The height of each cell is set as 1 nm except when the thickness is 2.5 nm where the height of cell is 0.5 nm. The applied field varies from 6 T to −6 T in the simulation, starting from a positive saturation state, where magnetic moments in each cell are uniformly distributed with the initial magnetization parallel to the applied field.

In this work, $Nd_2Fe_{14}B$ is chosen as the hard layer while α-Fe is the soft one, with the following parameters [6,13]: $M_s^s = 1.71\times10^6$ A/m, $M_s^h = 1.28\times10^6$ A/m, $K^s = 4.6\times10^4$ J/m^3, $K^h = 4.3\times10^6$ J/m^3, $A^s = 2.5\times10^{-11}$ J/m, and $A^h = 7.7\times10^{-12}$ J/m. The thickness of the hard layer keeps a constant value of 10 nm while that of the soft layer varies between 1 nm and 20 nm. Analyses show that the giant energy product occurs at this thickness region [13,16], where the critical fields are not sensitive to the hard layer thickness. Only the exchange interaction between the neighboring region pair is taken into account and the free boundary conditions are chosen, The exchange energy constant between the soft and hard layers is set as $A^{hs} = 10^{-11}$ J/m in our calculation. The maximum and minimum time steps are specified as 10^{-10} s and 0 s, respectively. The actual time step depends on the thickness of the films, number of cells and other factors. According to the OOMMF outputs, the time step is around 10^{-14} s for the calculations presented in the manuscript.

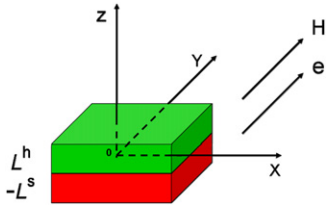

Fig. 1. The basic scheme for a double-layer calculated in this work.

3. Macroscopic hysteresis

Fig. 2 shows the major hysteresis loops of $Nd_2Fe_{14}B/\alpha$–Fe bilayer with various soft layer thicknesses, where L^h keeps a constant value of 10 nm. One can find that the hysteresis loops calculated by OOMMF and by the 1D analytical method are quite similar, especially for small L^s, justifying the reliability of our calculation. For thin soft layers, the loops are nearly rectangular with almost the same coercivities, which decrease as L^s increases. When $L^s \geq 5$ nm, the hysteresis loops calculated by the two different methods display some noticeable dissimilarities. The nucleation based on OOMMF occurs much earlier, which leads to smaller coercivities as well as the remanences compared with those by the 1D method. Such dissimilarities enlarge as L^s increases. When $L^s \geq 10$ nm, the nucleation occurs at the first quadrant of the hysteresis loops with the coercivity difference larger than 30%. These dissimilarities arise from the larger demagnetization field at the corner of the film, which is ignored in the 1D analytical calculation.

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