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Perpendicular Magnetic Anisotropy

Monte Carlo modeling of mixed-anisotropy $[Co/Ni]_2/NiFe$ multilayers

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Abstract—The magnetic properties of a thin film consisting of an exchange-coupled $[Co/Ni]_2/NiFe$ multilayer has been studied as a function of the NiFe thickness by using Monte Carlo modeling and compared with experimental results of $[Co/Ni]_4/Co/NiFe$ multilayers. Both modeling and experiment showed that the NiFe thickness controls the effective anisotropy. The direction of the easy axis is determined by a competition between the perpendicular crystalline anisotropy of the Co/Ni and the shape anisotropy of the multilayer. As the thickness of the NiFe layer increases the reversal mechanism of the thin film changes from the nucleation of reverse domains to vortex propagation. Therefore our results revealed the magnetic configurations and the easy axis reorientation of mixed-anisotropy multilayers.

Index Terms—Perpendicular magnetic anisotropy, hysteresis, multilayers, reversal modes.

I. INTRODUCTION

Systems with mixed anisotropies which consist of hard anisotropy films coupled with soft magnetic films have been widely studied because of their potential for perpendicular magnetic recording media, spin-transfer torque switching and nanooscillator devices [Dumas 2014, Rippard (2010), Houssameddine (2007), Davies (2005), Dobin (2006), Victoria (2005), Fullerton (1999)]. Such exchange-coupled multilayers can provide precise control of the magnetic properties by adjusting the composition, the number of layers and their thickness. There have been several studies of different systems with mixed anisotropies including $Co_{0.66}Cr_{0.22}Pt_{0.12}/Ni$ multilayers [Navas (2012), Pellicelli (2008), Wang (2009), Bollero (2006), Girt (2007), Pandey (2009)]; $[Co/Pd]_5/Co/NiFe(t)$ and $[Co/Pd]_5/Co/CoFeB(t)$ [Nguyen (2011), Tacchi (2014), Nguyen (2014b), Tryputen (2015)], $[Co/Ni]_4/Co/NiFe$ [Chung (2013)] and [Co/Pd]/Fe/[Co/Pd] [Dou (2013)]. Navas *et al*. [2012] showed experimentally that the change of the direction of the effective anisotropy in $Co_{0.66}Cr_{0.22}Pt_{0.12}/Ni$ multilayers depends on the Ni thickness. Chung *et al*. [2013] showed in $[Co/Ni]_4/Co/NiFe$ that for NiFe thickness of 2.6−3.0 nm, a well-defined remanent magnetization tilt angle can be tuned from 0 to 90 degrees. We recently [Tryputen 2015] showed a change in the sign of the anisotropy with varying NiFe thickness in $[Co/Pd]_5/NiFe(t)$ multilayers. Domains with out-of-plane magnetization were present even for multilayers with a thick NiFe layer as a result of the perpendicular [Co/Pd] anisotropy. On the other hand, Heldt *et al.* [Heldt 2014] observed a mutual imprint of vortices in the NiFe and in the stripe domains in the [Co/Pd] multilayers, which could allow the control of vortex core motion.

To model these results, micromagnetic simulations based on a one-dimensional free energy model were used [Chung 2013, Anh Nguyen 2014a, Anh Nguyen 2014b], solving the Landau-Lifshitz-Gilbert equation with a hybrid finite element/boundary method [Heldt 2014] or a zero temperature, two-spin magnetic model [Morrison 2015]. Although they showed a good agreement with experimental results, the models did not include thermal nor sample shape effects. To explore these factors we used a Monte Carlo (MC) method that includes thermal effects, typically neglected in micromagnetic simulations. Due to its non-deterministic behavior, the MC approach allows observation of different possible reversal modes starting from the same initial state.
Other systems and geometries have been studied using this method, showing a very good agreement with experimental results [Mejía-López 2006]. A [Co/Ni] multilayer coupled to a NiFe film was used for this study due to the relatively weak perpendicular anisotropy of the [Co/Ni]. In this case, changes in the magnetic properties of the full multilayer structure can be observed even for a thin NiFe layer.

II. MODEL

Our system consisted of a rectangular NiFe thin film deposited on top of a $[Co/Ni]_2$ multilayer (see Fig. 1). The film had a length $L = 300$ nm and width $w = 100$ nm. Each Co and

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Ni layer was 2.5 nm thick, with a total $[Co/Ni]_2$ thickness of h = 10 nm. The NiFe film thickness was varied from t = 0 to 20 nm, and the total thickness of the sample was $h_1 = h + t$.

We carried out simulations on a square sample of 300 nm x 300 nm and found qualitatively similar results to those of a 300 nm x 100 nm sample. However, in the square sample reverse domains nucleated at the four borders, making a more complex reversal process. Results from the rectangular sample are reported here.

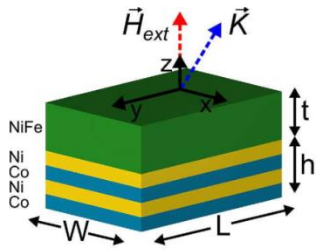

Fig. 1. Schematic of the multilayer used in the Monte Carlo model.

To simulate the magnetic properties of the film we assumed that all magnetic moments $\{\vec{\mu}_i\}$ occupied the positions $\{\vec{R}_i\}$ in a fcc lattice of constant $a_0 = 3.6$ Å. Considering exchange and dipolar interactions, anisotropy and external fields, the total magnetic energy of the system can be written as

$$E_{tot} = \frac{1}{2}\sum_{i\neq j}\left(E_{ij} - J_{ij}\hat{\mu}_i \cdot \hat{\mu}_j\right) + E_H + E_K, \qquad (1)$$

where E_{ij} is the dipolar energy given by

$$E_{ij} = \left[\vec{\mu}_i \cdot \vec{\mu}_j - 3\left(\vec{\mu}_i \cdot \hat{n}_{ij}\right)\left(\vec{\mu}_j \cdot \hat{n}_{ij}\right)\right]/r_{ij}^3 , \qquad (2)$$

with $r_{ij} = |\vec{R}_i - \vec{R}_j|$, and $\hat{n}_{ij} = (\vec{R}_i - \vec{R}_j)/r_{ij}$. The exchange interaction J_{ij} is equal to J for nearest-neighbor magnetic moments and zero otherwise. $E_H = -\sum_i \vec{\mu}_i \cdot \vec{H}$ is the Zeeman energy associated with an applied magnetic field $\vec{H}$, and the anisotropy is given by $E_K = -\sum_i (\vec{\mu}_i \cdot \hat{K})^2 K$.

In principle the magnetic configuration can be found by minimizing the total energy of the system, but this is computationally extremely expensive. For particles in the nanometer scale an atomistic simulation would be prohibitively time consuming due to the large number of magnetic moments within each particle. This problem can be overcome by combining the Monte Carlo method with a scaling technique introduced previously to obtain the phase diagram of magnetic nanoparticles [d'Albuquerque e Castro 2002]. This method has been used to study the magnetic behavior of nanoparticles, yielding results in excellent agreement with experiments [Mejía-López 2003]. It is based on scaling down the strength of the exchange interaction J, the number N of moments and the temperature T according to the relations $J' = \xi J$, $N' = \xi^{3\eta} N$, and $T' = \xi^{3\eta} T$, where ξ is a scaling parameter in the range $0 < \xi < 1$ and $\eta \approx 0.56$. A proper value of the ξ allows to reduce the size of the system so as to make Monte Carlo calculations feasible. The geometrical parameters are scaled as $L' = \xi^\eta L$, $w' = \xi^\eta w$, $h' = \xi^\eta h$ and $t' = \xi^\eta t$, with $\xi = 0.001$. The results thus obtained are rather insensitive to the precise value of the scaling parameter.

Monte Carlo simulations were carried out using the Metropolis algorithm with local dynamics and single-spin flip method [Binder 2002]. The new orientation of the magnetic moment was chosen randomly with a probability $p = min[1, exp(-\Delta E/k_B T')]$, where ΔE is the change in energy due to the reorientation of the spin and k_B is the Boltzmann constant. In this case we used $T = 300$ K corresponding to $T' = 0.003$ K. The magnetic parameters were $\mu = 1.72, 0.62$ and $1.60\ \mu_B$; $J' = 0.039, 0.045$ and 0.038 meV for Co, Ni and NiFe respectively as [Neumann 2013].

To obtain the hysteresis we started with most of the magnetic moments pointing along a 6 kOe field applied perpendicular, (**OP**), and parallel, (**IP**), to the plane of the film. In the latter case, the field was applied along the y (longer) axis. Field steps of $\Delta H = 0.01$ kOe are used in all calculations so that 2403 ΔH values are needed to complete a hysteresis loop.

The perpendicular magnetic anisotropy (PMA) of [Co/Ni] multilayers [Rouelli Sabino 2014, Wu 2013] was introduced into the MC simulations by including an anisotropy constant of 1% of the value of $J_{Co-Ni} = \sqrt{J_{Co}J_{Ni}} = 11.76$ meV [Neumann 2013], giving $J_{Co-Ni} = 0.12$ meV. The exchange constant for the Ni/NiFe interface was calculated as $J_{Ni-NiFe} = \sqrt{J_{Ni}J_{NiFe}} = 11.74$ meV. No other anisotropy terms were present in the NiFe layer aside from its shape anisotropy. In the [Co/Ni]/NiFe multilayer we therefore have two coexisting anisotropies with orthogonal directions, the out-of-plane interface anisotropy $\vec{K}_0$ and the shape anisotropy, $\vec{K}_s$, leading to an effective uniaxial anisotropy, $\vec{K}_{eff}$. Experimentally, high PMA is obtained for Co/Ni multilayers with 4 repeats consisting of 1−2 atomic layers of Co (i.e. Co thickness below 0.5 nm) and a thickness ratio [Co:Ni] of 1:2 [Daalderop 1992, Girod 2009, Gimbert 2012]. The model uses thicker layers but because the PMA is an input parameter applied throughout the film, the PMA is independent of layer thickness.

III. RESULTS AND DISCUSSION

Fig. 2 illustrates hysteresis cycles obtained by using MC simulations for different NiFe thicknesses and IP and OP external fields. From these results we observe that the IP remanence and coercivity *Hc* increased with *t*. The coercivity was 0.24 kOe for *t* = 0 and 1.30 kOe for *t* = 20 nm. When applying an IP field it was easier to saturate thicker samples.

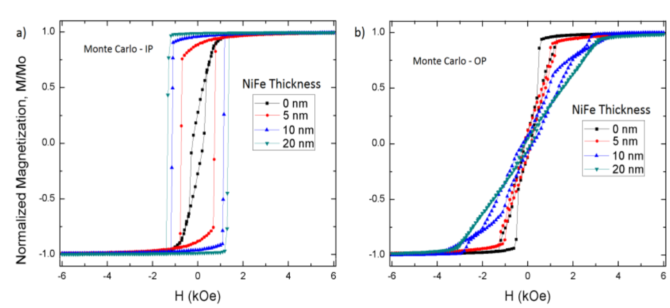

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Fig. 2. Monte Carlo calculations of hysteresis loops of a 100 nm × 300 nm $[Co/Ni]_2$/NiFe nanostructure for magnetic fields (a) parallel and (b) perpendicular to the plane, with t varying from 0 to 20 nm.

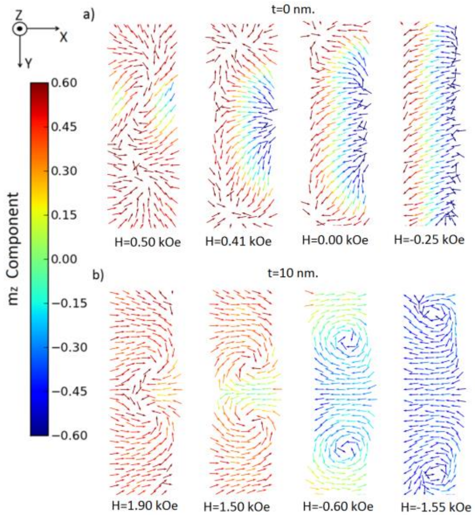

Fig. 3. Spin configuration of the first layer (surface) during the reversal of a 100 nm × 300 nm $[Co/Ni]_2$/NiFe nanostructure with a OP field and NiFe thickness of (a) t = 0 nm (results are similar to t = 5 nm) and (b) t = 10 nm (results are similar to t = 20 nm.)

In contrast, when an OP field is applied, larger fields are needed to saturate thicker samples. These results indicate an easy axis reorientation from OP towards IP while increasing the permalloy thickness. Figure 3 illustrates the spin configuration of the surface layer for different NiFe thicknesses. These snapshots are taken at specific values of the OP field during the reversal process. The system started saturated along the z axis with H = 6 kOe. The color scale represents the z component of the magnetization and the arrows depict the IP direction of the magnetization. While these figures show the magnetic structure of the surface layer, other layers exhibit a similar spin structure. When t = 0 the reversal started with the formation of reverse domains at the longer edges of the sample, delineated by Néel walls. Then, by decreasing the field, one reverse domain expands and propagates across the width of the sample, fully reversing the magnetization. The low OP remanence is a result of the reverse domain nucleation. For t = 5 nm the reversal process was almost the same. However, for t =10 nm, for fields of around 2 kOe, the sample had a large in-plane magnetization component and the reversal process was initiated by the formation of a pair of vortices near the center of the sample that propagated to the ends of the sample, reversing the magnetization. Similar results were obtained for t = 20 nm.

Fig. 4 shows the depth-dependence of the magnetization direction at remanence. Starting with the system saturated along the z direction, the system was relaxed for 10^9 Monte Carlo steps at zero field. Fig. 4(a,b) depicts a top-view of the magnetization of the saturated sample (a) and relaxed sample (b), respectively for t = 20 nm. In this Fig. it can be seen that the magnetization at the top is now IP oriented. Fig. 4(c) shows a cross-section in which the tilting of the magnetization varies from OP at the bottom of the [Co/Ni] to IP at the top of the NiFe. The gradual tilt of the magnetization is shown in Fig.4(d) for all NiFe thicknesses, which plots the average angle θ_i between the magnetization of each layer with respect to the z axis. $\theta_i = 0°$ represents a OP magnetization, and $\theta_i = 90°$ denotes a fully IP magnetization. Even for the thickest NiFe layer, the magnetization at the top surface is not fully IP, and the [Co/Ni] retains its OP magnetization.

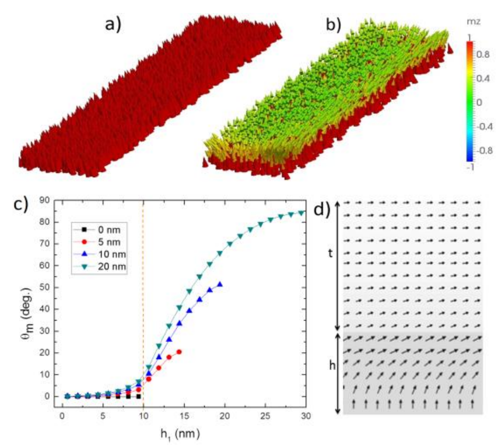

Fig. 4. (a,b) Snapshot of the magnetization for (a) out-of-plane saturation; (b) at remanence. The color represents the z component of magnetization. (c) θ vs. depth through the sample for the four samples considered in the study. The dashed line represents the interface between the CoNi and NiFe layers. (d) magnetic moment configuration in the Y Z plane for t = 20 nm at remanence. The grey scale represents the gradual change in the angle.

A comparison was made with experimentally determined hysteresis loops measured on a series of exchange-coupled unpatterned multilayers Ta(5 nm)/Cu(8 nm)/Co(0.3 nm)/$[Ni(0.9\ nm)/Co(0.3\ nm)]_4$ /NiFe(t nm)/Ta(5 nm), where t = 0 to 3 nm. The films were grown on thermally oxidized Si(100) substrates at room temperature using a confocal magnetron sputtering system in a chamber with a base pressure below 4 × 10^{-8} Pa (3 × 10^{-8} Torr) at an Ar pressure of 5 mTorr. The Ta (5 nm)/Cu(8 nm) seed layers promoted a (111) texture to ensure a perpendicular magnetic anisotropy in the Co/Ni multilayers [Chung 2013]. The hysteresis loops were measured by vibrating sample magnetometry (VSM) at room temperature.

Fig. 5(a,b) illustrates the IP and OP hysteresis loops, evidencing the magnetization reorientation from IP to OP as the NiFe thickness increased. In the absence of a NiFe layer, and for NiFe thicknesses of 1 and 2 nm, the films had a square OP loop with an in-plane hard axis. The multilayers with the NiFe layer of 3 nm thickness and above showed in-plane hysteresis loops and low coercivity. Therefore the magnetic easy axis reorients from OP to IP for the NiFe thicknesses in the range of 2−3 nm. This resembles the behavior of similar films grown with a NiFe wedge of varying thickness [Chung 2013].

The MC model describes a rectangular slab of the multilayer, so the domain structures and reversal mechanism will differ from those of an extended film. Despite this, key results of the model are in qualitative agreement with the experimental data. Both show a change in the sign of the anisotropy with increasing NiFe thickness, although the MC model predicts a reorientation at higher NiFe thickness than was observed experimentally.

A reorientation was also predicted from a one-dimensional model applied to [Co/Pd]/NiFe and [Co/Ni]/Co/NiFe stacks [Chung 2013, Anh Nguyen 2014a, Anh Nguyen 2014b] which calculates the through-thickness tilt angle of the magnetization that minimizes the free energy. This model predicted that in [Co/Ni]/Co/NiFe [Chung 2013] the magnetization in the film reoriented to IP as the NiFe thickness increased from 2.5 to 3 nm, and the magnetization tilt angle throughout the film varied by at most 7°, i.e. the magnetization in the [Co/Ni] and NiFe layers remained nearly parallel. In contrast, the one dimensional model for [Co/Pd]/Co/NiFe [Anh Nguyen 2014a, Anh Nguyen 2014b] predicted a greater NiFe thickness for reorientation and a larger variation in tilt angle, e.g. over 50° for 8 nm NiFe. The [Co/Pd] had a higher anisotropy (and lower magnetization) compared to [Co/Ni]. The MC model results are more similar to those of the one-dimensional model for [Co/Pd]/Co/NiFe, suggesting that the MC model may have been based on an overestimate of the anisotropy of the [Co/Ni] stack.

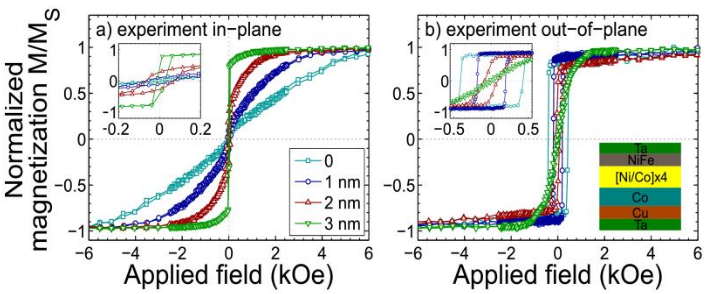

Fig. 5. Hysteresis loops for magnetic fields parallel (a) and (b) perpendicular to the plane, for an unpatterned multilayer of $[Co/Ni]_4$ /Co/NiFe, with NiFe thickness varying from 0 to 3 nm. The insets show details of the loops in a smaller field range.

IV. CONCLUSIONS

In summary, we have studied the magnetic properties of rectangular sections of exchange-coupled [Co/Ni]/NiFe multilayers as a function of the NiFe layer thickness by using Monte Carlo simulations, and compared our results with experimental magnetic hysteresis loops. Both the MC model and measurements on unpatterned multilayer films show that by increasing the NiFe thickness the magnetic easy axis changes its direction from out-of-plane to in-plane. The model demonstrated a depth-dependent tilt in the magnetization direction which results from the competition between the [Co/Ni] out-of-plane anisotropy and the in-plane shape anisotropy of the multilayer. This reorientation is accompanied by a decrease of the out-of-plane remanence and by changes in the reversal mode. Our results are in qualitative agreement with the results of a one-dimensional model applied to [Co/Ni]/Co/NiFe [Sunjae2013] and [Co/Pd]/NiFe [Anh Nguyen 2014a, Anh Nguyen 2014b], though the MC model predicted a larger difference in tilt angle between the [Co/Ni] and NiFe layers, and a greater NiFe thickness before reorientation, which are characteristic of higher PMA in the [Co/Ni] multilayer compared with the experimental samples. Furthermore, the MC model predicted that the reversal mechanism of a 100 nm x 300 nm film changed from domain formation and propagation for NiFe thickness of 0 and 5 nm to reversal via vortex formation for NiFe thickness of 10 and 20 nm. The results show the applicability of Monte Carlo modeling in a range of mixed-anisotropy multilayers to reveal the details of the magnetic configurations inside the system.

V. ACKNOWLEDGMENT

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