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 14. ABSTRACT We present a theoretical investigation of the thermal hysteresis of iron dots exchange-coupled to an antiferromagnetic substrate. We consider a temperature interval bounded by the Néel temperature of the substrate, and we calculate the heating and cooling curves in the presence of an external field oriented opposite to the interface exchange field. The thermal hysteresis is due to the temperature variation of the interface field and the influence of the geometrical shapes and sizes of the dots on the magnetic states and switching mechanisms. We 15. SUBJECT TERMS 				
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Thermal hysteresis of interface biased ferromagnetic dots

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We present a theoretical investigation of the thermal hysteresis of iron dots exchange-coupled to an antiferromagnetic substrate. We consider a temperature interval bounded by the Néel temperature of the substrate, and we calculate the heating and cooling curves in the presence of an external field oriented opposite to the interface exchange field. The thermal hysteresis is due to the temperature variation of the interface field and the influence of the geometrical shapes and sizes of the dots on the magnetic states and switching mechanisms. We show that Fe dots on an uncompensated NiO substrate exhibit large thermal hysteresis at room temperature, and external fields of a few kOe. The width of the hysteresis loops depends on the dimensions of the ferromagnetic dot, and can be significant for dots elongated in the direction of the interface field. © 2007 American Institute of Physics. [DOI: 10.1063/1.2827478]

I. INTRODUCTION

Nanostructured materials have been extensively studied recently.¹ The motivation is largely due to their application for the development of miniaturized magneto-electronic devices and for high-density magnetic storage media.

A great deal of research effort has been dedicated to exploring the impact of the dimensions of nanoelements on their magnetic states and switching mechanisms. In this context, a key issue is the fact that a nanomagnet may become superparamagnetic at a temperature smaller than the bulk ordering temperature.¹ A possible way to combat the superparamagnetic limit is to take advantage of the magnetic coupling between the nanoparticle and a thermally stable magnetic system. This has been investigated by growing arrays of ferromagnetic (FM) nanoparticles on an antiferromagnetic (AFM) substrate.^{2–4}

Arrays of single-domain fine ferromagnetic particles are currently under investigation for the development of highdensity magnetic storage media. Thermally assisted magnetic recording allows the use of large anisotropy materials, as required in order to assure the thermal stability of small particles, and write field strengths within the available limits of ring-shaped write heads.⁵ The process is based on heating prior to writing on high anisotropy media with a magnetic field.

Thermal cycles open a discussion of another fundamental problem, namely thermal hysteresis. There have been a number of studies of thermal hysteresis in nanostructured magnetic systems. The thermal hysteresis can be quite large (200 K) and can be tuned with magnetic fields of small strengths. Recent results include studies of rare-earth and/or transition-metal multilayers,^{6,7} experimental work on ferromagnetic-antiferromagnetic exchange bias structures,⁸ and experimental and theoretical work on alloys and compounds.^{9–11}

Recently, we performed a theoretical study of thermal hysteresis in thin Dy films in the 80-179 K temperature interval.¹² The thermal hysteresis originates in the combined effect of the strong temperature dependence of the magnetization, the hexagonal anisotropy of Dy, and the modifications of the helical phase imposed by surface effects. The temperature width of the thermal hysteresis may cover the whole temperature interval between the Curie and the Néel temperatures, and may be tuned by external fields of small strength. We have also investigated trilayers composed of a thin Dy film sandwiched between two films of Fe or Gd.¹³ The point of creating these trilayer structures is that by adding ferromagnetic films on the outside, one can further modify the effects of an external field on a Dy film. The Fe film is antiferromagnetically coupled to Dy at the interfaces, while Gd is ferromagnetically coupled to the Dy at the interfaces. This difference again allows substantial changes in how the external field interacts with the structure as a whole.

In this article, we report a theoretical investigation of room-temperature thermal hysteresis of FM dots exchangecoupled to an uncompensated antiferromagnetic substrate. Within a temperature interval bounded from above by the Néel temperature of the AFM substrate, we calculate the heating and cooling curves in the presence of an external field oriented opposite to the interface exchange field. The thermal decay of the average value of AFM spins imposes a reduction in the interface field, and leads to thermal hysteresis.

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FIG. 1. (Color online) Thermal hysteresis of the dot Fe(30 nm \times 15 nm \times 15 nm)/NiO. The thermal cycle with external field opposite to the interface field. Heating takes place along path (a) and cooling along path (b).

II. MODEL

We assume that the AFM interface plane consists of a uniform sheet of spins held in a fixed direction. The magnetic structure of the dot is described by *N* cubic cells with an edge of d=3 nm (smaller than the iron exchange length^{14,15}). The energy density is given by

$$E = \frac{A}{d^2} \sum_j \sum_k (1 - \hat{m}_j \cdot \hat{m}_k) - M_s \vec{H}_{int} \cdot \sum_i \hat{m}_i$$
$$-M_s \vec{H} \cdot \sum_j \hat{m}_j - K \sum_j (m_j^x)^2$$
$$+ \frac{M_s^2}{2} \sum_j \sum_k \left(\frac{\hat{m}_j \cdot \hat{m}_k}{n_{jk}^3} - \frac{3(\hat{m}_j \cdot \hat{n}_{jk})(\hat{m}_k \cdot \hat{n}_{jk})}{n_{jk}^5} \right).$$
(1)

The energy includes the exchange energy between nearest-neighbor cells; the interface exchange energy, restricted to the interface layer cells; the Zeeman energy; the anisotropy energy, and the magnetostatic energy. \hat{m}_i is the direction of the magnetic moment of the *i*th cell and n_{ij} is the *i*-*j* cell distance in units of *d*.

We consider Fe dots on a NiO (111) substrate. For Fe, we use $A=2.5\times10^{-11}$ J/m, $K=4.7\times104$ J/m³, and M_S =1.7×10⁶ A/m.¹⁶ NiO has a Néel temperature $T_N=525$ K,¹⁷ and is frequently used for biasing purposes. Even at high temperatures, the thermal relaxation effects require a few hours to produce appreciable changes in the effective exchange bias.¹⁸

 $H_{\text{int}}=J_{\text{int}}\langle S_{\text{AFM}}\rangle = (g\mu_B n_{\perp})$ is the magnitude of the interface field, which is opposite to the AFM interface spins. $\langle S_{\text{AFM}}\rangle$ is the thermal average value of the AFM interface spins, n_{\perp} is the number of ferromagnetic atomic layers within a simulation cell, and J_{int} is the interface exchange energy. For low temperature, we chose $H_{\text{int}}=16.3$ kOe, equal to the intrinsic iron exchange field coupling neighboring



FIG. 2. (Color online) Spin maps, at room temperature, of the surface and interface layers, corresponding to the points (a) and (b) indicated in Fig. 1. The colors indicate the angle between the spins and the z axis.

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cells. $\langle S_{AFM} \rangle$ has been calculated using an S=1 Brillouin function and full coordination of bulk-like NiO spins in both sublattices. The coupling of AFM interface spins to FM spins leads to larger values of $\langle S_{AFM} \rangle$ for $T > T_N$. For a NiO (111) substrate, this amounts to having a temperature-independent contribution of 50% of the interface bonds. We have found that this extra interface stability produces negligible changes in the thermal hysteresis around room temperature, and small upshifts in the loops at high temperatures.

We use a self-consistent local field algorithm,^{19–21} and, at each temperature, the equilibrium state $[(\hat{m}_i), i = 1, 2, ..., N]$ is found by seeking a magnetic configuration in which the torque is zero in all the cells $(\vec{m}_i \times \vec{H}_{eff}^i = 0$ for i=1,2,...,N), where the effective field is $\vec{H}_{eff}^i = -(1/M_S)(\partial E/\partial \hat{m}_i)$. For each temperature, we select an initialization of the spin variables close to those corresponding to the equilibrium state at the previous value of the temperature.

III. RESULTS AND DISCUSSIONS

In Fig. 1, we show the magnetization curves along the thermal loops of a 30 nm \times 15 nm \times 15 nm Fe dot. The 30 nm length is along the x axis, parallel to the applied field. For H=4 kOe, as shown in Fig. 2(a), at low temperatures there is a twisted state, with partial alignment of the dot spins with the external field. The top surface layer spins are parallel to the external field, while the interface layer spins are kept at small angle to the interface field. As the temperature increases, the interface layer spins turn gradually into the direction of the external field because of the weakening of the interface field. Eventually the dot switches to full alignment along the external field at T=380 K. When the temperature is reduced from its highest value, the interface layer spins arrange in a buckle state, as shown in Fig. 2(b), with most spins in the middle of the bar along the external field and the spins near the yz faces of the dot perpendicular to the external field direction. This phase minimizes the surface charge of the yz face and is separated from the twisted phase, found in the heating process, by the shape anisotropy energy bar-



FIG. 3. (Color online) Thermal hysteresis for H=3 kOe of Fe dots with dimensions 30 nm×L(nm)×L(nm). The numbers in the figure indicate the values of L.

rier. The thermal loop closes at T=239 K, when the interface field is strong enough to overcome the shape anisotropy barrier. The thermal loops for external field values of 2.5 and 6 kOe have similar behavior. It is noticeable that the switching temperatures decrease as the external field is made stronger.

In Fig. 3, we show the thermal loops of Fe dots with a length of 30 nm along the uniaxial anisotropy direction and three values of the yz face area (12 nm×12 nm, 15 nm × 15 nm, and 18 nm×18 nm). As the area increases, the shape anisotropy for the structure is reduced and this allows the dot to switch more easily. It is noticeable that the temperature width of the thermal hysteresis is significantly reduced as the area is increased.

We comment that the cross-sectional area of the dot also influences the magnetic hysteresis. The width of the magnetic hysteresis of a 30 nm \times 12 nm \times 12 nm dot (not shown for brevity) is approximately 9 kOe, while that of 30 nm \times 18 nm \times 18 nm is around 4 kOe. This corresponds



FIG. 4. (Color online) In-plane and perpendicular magnetizations and spin maps for a 120 nm×60 nm×12 nm Fe/NiO dot in an external field of 4 kOe.

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to a larger shape anisotropy barrier for the dot with a smaller face and a corresponding wider magnetic hysteresis.

Most interestingly, the thermal loops of larger dots may also exhibit hysteresis in the perpendicular components of the magnetization. In Fig. 4, we show the thermal hysteresis and spin maps corresponding to a 120 nm×60 nm ×12 nm Fe dot and an external field of 4 kOe. The perpendicular components display a wide hysteresis, corresponding to the formation of vortices of opposite polarities in the two branches of the loop. The spin maps show the magnetic states in the (a) heating and (b) cooling branches at T=329 K.

We have shown that owing to the temperature change of the interface field, interface biased dots may exhibit roomtemperature thermal hysteresis, which is tunable by the external field strength, as well as the dot dimensions. This is a new kind of thermal hysteresis that might occur well below the critical temperature of the dot, and may impact the thermal stability. Controlling the thermal hysteresis might be a relevant issue for device applications.

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