Asymmetric reversal of the hysteresis loop in exchange-biased nanodots

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The magnetic response of a ferromagnetic cylindrical dot in contact with an antiferromagnetic substrate and its reversal modes during the cycling of an external magnetic field H are investigated by means of Monte Carlo simulations. We found that there is a nonuniform distribution of the magnetization in the ferromagnet along the direction perpendicular to the interface. This effect gives rise to different magnetization reversals in the two branches of the hysteresis cycle.

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In recent years, a great deal of attention has been focused on the study of regular arrays of magnetic particles lithographically produced. These particles, with dimensions in the nanometer range, have potential applications in nonvolatile magnetic memory devices or high-resolution magnetic field sensors.[1] Arrays of discrete patterned magnetic elements, such as magnetic pillars, pyramids, and dots, have been proposed as a new generation of ultrahigh-density patterned magnetic storage media.[2] Within those elements or particles, different magnetic arrangements may be observed, such as leaf or flower states, in which the magnetization is quasiuniform and reaches high values close to saturation and flux closed states or vortex configurations, with low values of magnetization. In the case of cylindrically shaped particles, and for certain dot sizes, when the magnetic field is reduced from saturation, a vortex core nucleates at one edge of the dot, moves across it, and annihilates on other side.[3] In these systems, when the distance L between the particles is large enough, i.e., $L>D$, with D the diameter of the particle, the interaction between them can be safely neglected.[4,5] Then, the magnetic structure within each cylinder is basically determined by internal interactions, namely, the direct exchange between nearest-neighbors atoms, the classical dipolar coupling, a crystalline anisotropy term, and the Zeeman energy, if the system is under an external magnetic field.

In the case of systems consisting of a ferromagnet (FM) in contact with an antiferromagnet (AF) a shift of the hysteresis loop along the magnetic-field axis can occur, which is called exchange bias (EB). Often, this shift is observed after cooling the entire system in an external magnetic field below the Néel temperature T_N of the AF.[6] A remarkable EB feature is the existence of different reversal modes of the magnetization along the ascending and descending branches of the hysteresis loop. This behavior was first observed in Fe/FeF_2 and Fe/MnF_2 bilayers[7] by using neutron diffraction and later also investigated in Co/CoO samples.[8] For Fe/FeF_2 and Fe/MnF_2 systems coherent rotation of the magnetization is proposed as the reversal mechanism for the upper branch and domain wall nucleation and propagation is observed for the lower one, while the opposite occurs in Co/CoO.[8]

Most of the experimental and theoretical results are referred to the EB in a macroscopic sample where the magnetostatic interaction in the FM layer is expected to play an insignificant role. Also most of the models assume that, because of the magnitude of the exchange inside the FM, there are no magnetic domains perpendicular to the interface, i.e, the magnetic ordering inside the FM does not change from one layer to the other. However, there is experimental evidence of the importance of domain breaking inside the FM for the hysteresis loop of exchange-bias systems.[9]

As the lateral size of the FM is shrunk down to a few nanometers, the magnetostatic interaction is increasingly important in determining the reversal behavior of the ferromagnetic layer. Recently, several groups started to investigate the influence of a lateral confinement on the EB effect,[10–13] considering nanometric dots on top of an AF. In these cases it is expected that the interaction with the AF will strongly influence the reversal mechanism of the magnetization, modifying nucleation and annihilation of the vortex.

In this paper we deal with the magnetic response of a FM cylindrical dot in contact with an AF substrate and with its reversal modes during the cycling of an external magnetic field H. The exchange coupling between the FM dot and the AF is modeled, assuming an effective unidirectional anisotropy κ which acts only on the FM interface layer.[14] This model does not consider possible domain formation at the AF; however, we can study the effect of the unidirectional anisotropy inside the FM.

For particles in the range of sizes currently produced, the theoretical determination of their magnetic configurations based on a microscopic approach and with present standard computational facilities, is out of reach. This is because of the large number of magnetic moments within such structures. This can be avoided by means of a scaling technique presented recently by d'Albuquerque *et al.*,[15] which was applied to the calculation of the phase diagram of cylindrical particles of height H and diameter D. They show that such a diagram can be obtained from the one for another equivalent particle in which the exchange interaction has been scaled down by a factor $x<\mathbf{1}$, i.e., $J'=xJ$, and its diameter and height are given by $D'=Dx^{\eta}$ and $H'=Hx^{\eta}$, respectively, with $\eta\approx 0.55$. In this paper, after testing an extension of these results, we use the same approach for the calculation of the magnetic state of a dot. This technique allows the presence of a nonuniform magnetization inside the FM.

The internal energy E_{tot} of a single cylinder with N magnetic moments can be written as

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

where E_{ij} is the dipolar energy given by

$$E_{ij} = \frac{\vec{\mu}_i \cdot \vec{\mu}_j - 3(\vec{\mu}_i \cdot \hat{n}_{ij})(\vec{\mu}_j \cdot \hat{n}_{ij})}{r_{ij}^3}, \quad (2)$$

with $\hat{\mu}_i$ a unitary vector along the direction of the magnetic moment $\vec{\mu}_i$, r_{ij} the distance between $\vec{\mu}_i$ and $\vec{\mu}_j$, and $\hat{n}_{ij}$ the unit vector along the direction that connects the two magnetic moments. J_{ij} is the exchange coupling, which is different from zero only for nearest neighbors. E_K is a cubic crystalline anisotropy term which can be written as $E_K = K\Sigma_i[\alpha_i^2\beta_i^2 + \beta_i^2\gamma_i^2 + \gamma_i^2\alpha_i^2]$, with $(\alpha_i, \beta_i, \gamma_i)$ the direction cosines of $\vec{\mu}_i$ referred to the cube axis;[16] however, this term has an almost negligible effect on our results. $E_H = -\Sigma_i \vec{\mu}_i \cdot \vec{H}$ is the Zeeman energy and E_I represents the energy due to unidirectional anisotropy introduced by the exchange coupling of the FM dot with the AF substrate. This last contribution can be defined by $E_I = J\Sigma_i \kappa_i \cos\theta_i$, where θ_i represents the angle between spins and the unidirectional axis. κ_i, equal to κ for spins belonging to the FM interface and 0 otherwise, should be a function of the AF constants (AF exchange coupling J_{AF} and AF anisotropy constant K_{AF}) of the interface exchange coupling $J_{F/AF}$ and of the cooling field H_{cf}. In the case of the FM domain wall model proposed for Kiwi *et al.*,[14,17] this parameter is given by

$$\kappa = \frac{|J_{F/AF}|}{J}\left[\frac{2|J_{F/AF}| - g_{AF}\mu_B H_{cf}}{10|J_{AF}| + 2\,K_{AF}}\right], \quad (3)$$

with J the FM exchange coupling.

Since there is a bulk of experimental results on granular Fe systems, we have considered $|\vec{\mu}_i| = \mu = 2.2\mu_B$, $K = 9.6 \times 10^{-3}$ meV per spin, the lattice parameter $a_0 = 2.8$ Å (Ref. 16), and $J = 42$ meV, which lead us to obtain the experimental value of the Curie temperature for Fe bulk, 1043 K.

At this point it is important to recall the restrictions imposed upon our approach by the number of magnetic moments involved in the calculations. In fact, when one deals with cylinders with dimensions comparable to those experimentally investigated, N may be larger than 10^9, which would require a computational effort way beyond present-day standard computational facilities.[15] (Recall that the computation time increases with N^2.)

In order to circumvent this difficulty, we scale the exchange interaction by a factor of $x = 2.4 \times 10^{-3}$, so as to reduce its strength. That is to say, we replace J by $J' = 0.1$ meV in the expression for the total energy and describe our dot by means of a smaller one, according to the scaling technique explained above with $\eta = 0.57$.[15,18] We have tested our results using different values of the scaling parameter x, and we observed that, as expected, the results are independent of the choice of its value. The value for the scaling parameter x was chosen according to computational facilities available that allow us to obtain our results in a reasonable computational time and give us enough information about the behavior of the system.

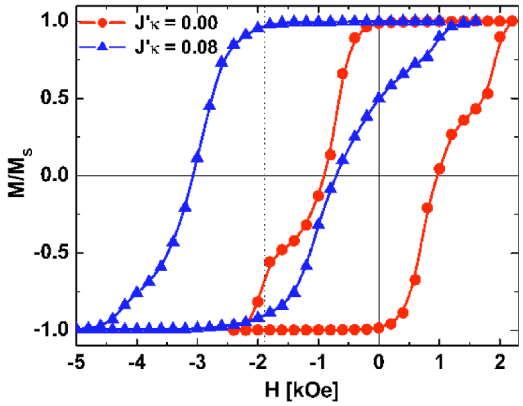

FIG. 1. (Color online) Hysteresis loops for an interacting and a noninteracting dot. Lines are guides to the eye.

In what follows we will show some hysteresis curves obtained using the scaling technique and analyze the reversion modes along both branches of the cycle. Using Eq. (1) for the energy, we simulated hysteresis curves as a function of κ, keeping all the other parameters constant. Monte Carlo simulations were carried out using the Metropolis algorithm with local dynamics and single-spin flip methods.[19] The new orientation of the magnetic moment was chosen arbitrarily 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, k_B is the Boltzmann constant, and T is the temperature. At this point it is important to discuss the temperature used in our simulations. Because of the size scaling we need also to scale down the temperature. From mean-field theories we know that the Curie temperature of a system is proportional to J. Then, in our calculations we used $T' = 0.021$ which, assuming a linear scaling, represents a "real" temperature $T = T'/x = 10$ K. The magnetic loop is started at $H = 4$ kOe with an initial configuration in which all the magnetic moments point along the external magnetic-field direction, parallel to the interface ([110] crystallographic direction), which we call the X axis from now on. $dH = 0.2$ kOe was used to decrease the external magnetic field at every calculation. We perform typically 2.8×10^5 Monte Carlo steps per spin for a complete hysteresis loop and at least five different seeds for the random number generator.

Figure 1 illustrates the hysteresis cycles for two different values of $\kappa J'$ of an Fe dot defined by $D' = 19.5$ Å and $H' = 6.0$ Å, which represents a particle of $D = 65$ nm and $H = 20$ nm. We have to remember that the "real" value of the coupling is given by $\kappa J = \kappa J'/x$, and then illustrated results correspond to $\kappa J = 0$ and 3.33 meV. This figure shows an expected bias of the hysteresis loop for $\kappa J \neq 0$, because of the coupling of the FM dot with the AF substrate. Also from Fig. 1 we can observe that the shifted hysteresis loop has different widths along the cycle, being wider for bigger M/M_S. This indicates that there are different magnetization behaviors along the two branches of the cycle. This result is independent of the number of Monte Carlo steps, an important point illustrated in Fig. 2, where the dependence of the EB field on the number of Monte Carlo steps (MCS), for $J'\kappa = 0.003$ is shown. To obtain the results depicted in this

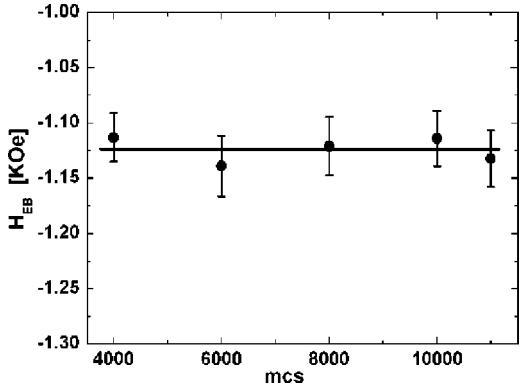

FIG. 2. EB field as a function of the number of Monte Carlo steps for equilibrating a system with $J'\kappa=0.003$ meV. Error bars are depicted with thin lines. The thick solid line is a guide to the eyes.

figure we have simulated the hysteresis cycle of our dot considering different MCS. We used MCS steps for equilibrating the system at every field, and MCS/5 steps for averaging the magnetization along the cycle. As occurs in every Monte Carlo simulation, coercivity and saturation field depend on the number of Monte Carlo steps because this number represents, on a certain scale, the time between one measure and the next one along the hysteresis curve. However, as depicted in Fig. 2 the exchange bias field, H_{EB}, is independent of this number.

In order to investigate the magnitude of the EB field as a function of the effective unidirectional anisotropy, i.e., the coupling between the FM dot and the AF substrate, we calculate the hysteresis cycle for different values of the coupling. Our results are illustrated in Fig. 3, where an increasing bias field appears for stronger coupling with the AF, as expected. In addition an almost linear behavior of the EB field is observed for $J'\kappa>0.005$.

Now we fix $\kappa J'=0.015$ meV and we obtain hysteresis cycles. We compute separately the contributions of every layer of the dot, and we depict in Fig. 4 the hysteresis of the interface and free monolayer. As we can see, both curves are different. Decreasing the external magnetic field, the change of the magnetization nucleates first at the free layer. However, in the other branch of the hysteresis the field nucleation begins at the interface. This figure clearly demonstrates that there is a nonuniform magnetization perpendicular to the interface, inside the FM dot.

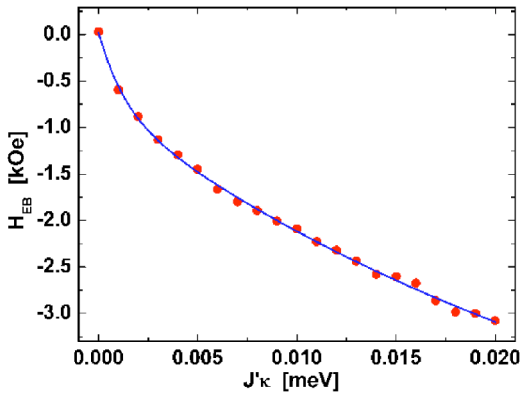

FIG. 3. (Color online) The exchange bias field as a function of the scaled effective unidirectional anisotropy. The line is a guide to the eye.

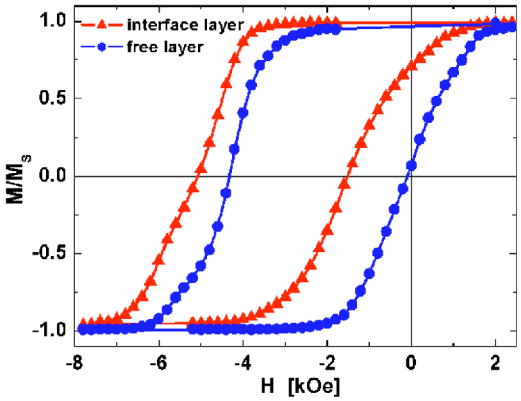

FIG. 4. (Color online) Hysteresis loops for the interface and free layer of a FM dot with scaled unidirectional anisotropy given by $\kappa J'=0.015$ meV. Lines are guides to the eyes.

It is important to clarify that the hysteresis cycles shown in Fig. 4 correspond to the average of twenty different seeds and then our results are independent of the initial conditions of our simulations. We can notice that at $H=-1$ kOe the magnetization of the free layer makes an angle of approximately 115° with respect to the magnetization of the interface layer. This rotation of the magnetization occurs slowly along 20 nm of the dot. This is equivalent to a rotation of 1.1° from one layer to a neighboring one.

To clearly understand the reversal mechanisms of the magnetization, we observe snapshots of the magnetization along the hysteresis cycle in every layer of the system. In these figures we observe that by decreasing the field from saturation, the magnetic moments of the free layer form, at the edge of the dot, what is called a *C* state. By decreasing further the field this magnetic structure moves to the center of the layer, giving rise to a vortexlike structure. The FM interface layer needs lower fields to start the formation of the *C* state. Instead, and due to the exchange interaction at the interface, the reversal of the magnetization at the right branch of the hysteresis cycle occurs through coherent rotation and nucleates first at the FM interface layer. Figure 5 illustrates snapshots of the magnetization reversal of the FM interface and free layers for two different values of the external field and $J'\kappa=0.015$ meV. At $H=-4.6$ kOe the magnetization forms what is called a *C* configuration at the FM interface layer, which precedes the appearance of the vortex, and a noncentered vortex is clearly observed at the free layer. In the other branch of the hysteresis cycle, at $H=-1$ kOe the reversal occurs by a coherent rotation, which begins at the FM interface, as occurs for the Fe/FeF_2 and Fe/MnF_2 (Ref. 7) bilayers. These snapshots, together with results depicted in Fig. 4, clearly demonstrate the existence of a nonuniform magnetization of the FM along the direction perpendicular to the interface.

It is important to clarify that the hysteresis cycles shown in Fig. 4 correspond to the average of twenty different seeds, and that our results are independent of the initial conditions

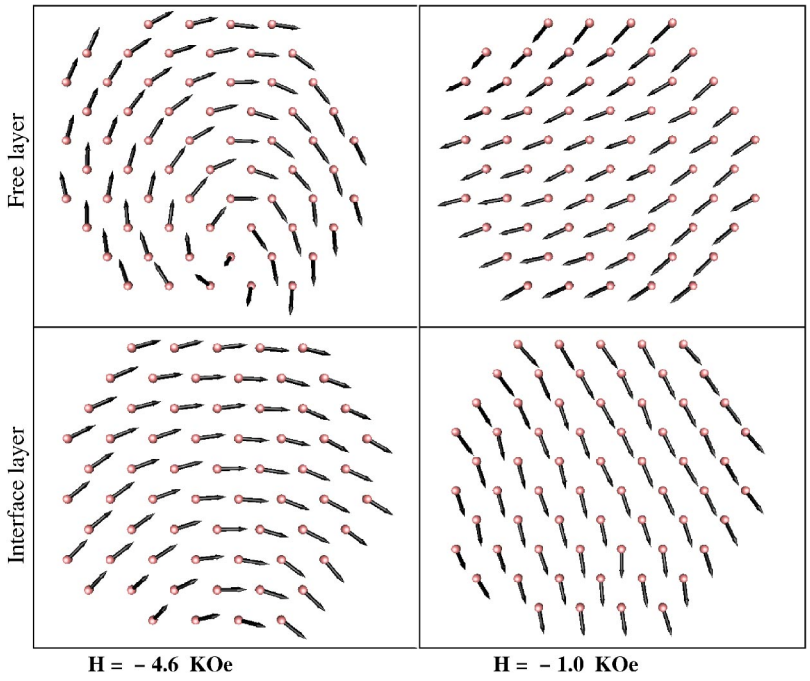

FIG. 5. (Color online) Snapshots for two different values of H of the magnetization reversal of a FM dot with scaled unidirectional anisotropy given by $\kappa J' = 0.015$meV. $H = -4.6$ kOe is referred to the left branch of the hysteresis loop while $H = -1.0$ kOe corresponds to the right branch. The points depict the position of the magnetic atoms, while the arrows illustrate the direction of the magnetic moments.

of our simulations. We can notice that at $H = -1$ kOe the magnetization of the free layer makes an angle of approximately 115° with respect to the magnetization of the interface layer. This rotation of the magnetization occurs slowly along 20 nm of the dot. This is equivalent to a rotation of 1.1° from one layer to a neighboring one.

In conclusion, by means of a scaling technique and using the ferromagnetic domain wall model we observe the reversal modes of the magnetization of a FM dot on an AF substrate. The hysteresis loop exhibits an asymmetric profile because of the different mechanisms responsible for the rotation on every branch of the cycle and the existence of a nonuniform magnetization inside the FM dot. The unidirectional anisotropy pins the FM interface layer, retarding the appearance of a vortex in it and favoring the magnetization reversal by means of a coherent rotation.

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