Effects of surface anisotropy on hysteresis in fine magnetic particles

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We solve numerically the dissipative Landau-Lifshitz-Gilbert equations to consider hysteresis in fine magnetic particles. Finite-size effects are studied for two models with uniaxial anisotropy — bulk random axis and surface anisotropy only. It is demonstrated that the latter model introduces considerable effects for small enough particles when the coupling to the anisotropy is equal or greater than the coupling to the isotropic Heisenberg exchange. We show that some features of magnetization reversal are associated with spins at the surface of fine particles.

I. INTRODUCTION: FINE PARTICLE MAGNETISM

There is now ample experimental evidence[1] about deviations from bulk behavior in finite systems such as small magnetic particles. In addition to the purely geometric constraint of finite volume, these deviations are caused by the surfaces or interfaces due to the different environment of atoms there compared to those in the bulk. That is, there is likely to be an anisotropy as a result of the lower coordination number there. These effects can lead to interesting spatially varying magnetization on atomic length scales within the particle, especially during magnetization reversal. At the same time, thermal fluctuations may be either amplified or diminished at the surfaces, and this may influence the process of magnetization reversal. An understanding of these kinds of finite-size effects for magnetic materials will be useful for controlling coercivity, susceptibility, and other magnetic properties, as well as improving our understanding of basic magnetic interactions.

Studies of models for semi-infinite systems have been made[2–5] to understand how such an extended surface can influence phase transitions and critical properties. Benyoussef *et al.*[6] studied a spin-1 Ising model with exchange and single-ion anisotropy strengths that are different at the surface compared to the bulk. We use this idea of spatially varying anisotropy strength, but in a finite particle rather than a semi-infinite system. The emphasis in this paper is to consider how the surfaces can influence the hysteresis in the magnetization versus applied field of a small magnetic particle.

We consider the effect on a small particle due to two different types of uniaxial anisotropy, and how these anisotropy interactions compete with exchange and applied field. In the first case, magnetic ions on a lattice with randomly directed *bulk* uniaxial anisotropy are considered, this being one of the simplest models that produces hysteresis. This model has been suggested by Harris *et al.*[7–9] to describe the magnetic properties of rare earth alloys. Since then the models for disordered magnets have been studied extensively. For random field ferromagnets Imry and Ma[10] showed that the ordered state is unstable against an arbitrary weak coupling to the random field for spatial dimension $d \leq 4$, continuous order parameter with dimension $n \geq 2$ and a large enough system. In the case of random uniaxial anisotropy two regimes have been considered[11]—weak and strong anisotropy. For weak anisotropy, at $d = 3$ and $n = 3$ the correlation length is large but again there is no ferromagnetic state at $H = 0$. In the case of infinitely strong random anisotropy a nonmagnetic ground state is predicted from Monte Carlo simulations.[12] Although coercivity and remanence properties have been treated already,[13] Saslow and Koon[14] published new results recently, some of which are compared with our results on this model in the last section of this paper.

The second type of anisotropy to be considered is one that acts *only* on the atoms near the surface, assumed to be caused by the different surface environment there compared to the bulk. In addition to the finite-size effects caused by the restricted system volume, the anisotropy interactions are assumed to be *different* for the atoms near the surface compared to those in the bulk. This model also produces hysteresis, even without a bulk anisotropy. We would like to see what effects these kinds of interactions can have on the magnetic hysteresis and susceptibility.

A goal is to understand whether it is possible to distinguish purely finite-size effects from effects due to the different environment of atoms at the surface compared to those in the bulk, how the finite system size can influence the hysteresis behavior, and how the smaller coordination number of the surface sites modifies their magnetization compared to the bulk magnetization, even in the *absence* of any different interactions associated with the surface.

A very small single magnetic particle [up to 45×45 atomic spins in two dimensions (2D) and $10 \times 10 \times 10$ spins in (3D)] is considered, such that magnetic dipole-dipole interactions are negligible. Such systems are important to study since the modern state-of-the-art technology already allows production of particles with a diameter as small as 20 Å.[15] The Landau-Lifshitz-Gilbert equations with damping are used to obtain zero-temperature metastable states. The calculations are similar to micromagnetics calculations,[16] however, each element of

the system represents a single magnetic ion, rather than a finite crystal volume. Features in the magnetization curves are found to be related to reversals of groups of spins. Several different geometries are considered, including square, rectangular, and circular particles in 2D, and cubic and spherical particles in 3D. Since we have not carried out a systematic study of the 3D particles due to computational time restrictions, most of the results presented here are for the two-dimensional (2D) models. These simulations were all performed for spins on square or cubic lattices.

II. MODEL FOR MAGNETIC PARTICLES

Classical spins $\hat{\mathbf{S}}_\mathbf{n}$ of unit length, after normalization, are considered to be interacting with Heisenberg exchange constant J, in an applied field $\mathbf{H}$, where $\mathbf{n}$ labels sites on a lattice. Each site has a single-ion uniaxial anisotropy of strength $K_\mathbf{n}$, whose axis $\hat{\mathbf{k}}_\mathbf{n}$ is taken along some particular direction, depending on the type of anisotropy. Generally, the total energy is written

$$E = -J\sum_{\mathbf{n},\mathbf{a}} \hat{\mathbf{S}}_\mathbf{n}\cdot\hat{\mathbf{S}}_{\mathbf{n}+\mathbf{a}} - \sum_\mathbf{n}\left[g\mu_B S\hat{\mathbf{S}}_\mathbf{n}\cdot\mathbf{H} + K_\mathbf{n}(\hat{\mathbf{k}}_\mathbf{n}\cdot\hat{\mathbf{S}}_\mathbf{n})^2\right], \quad (1)$$

where the real magnitude of the spin S is included in the term of the external field only while $\hbar^2S^2$ is absorbed in J and K's. The factor $g\mu_B$ is the Lande' g factor times the Bohr magneton. The exchange sum is only over nearest neighbor pairs, and the set of vectors $\{\mathbf{a}\}$ are the lattice displacements to the nearest neighbors of a given site. The unit vectors $\hat{\mathbf{k}}_\mathbf{n}$ are the anisotropy axes associated with the sites.

In the first case studied, we assume that all the anisotropy axes are pointing in random directions. This random bulk anisotropy model provides a test of the simulation method by comparing with known results for random uniaxial anisotropy magnets (i.e., Stoner and Wohlfarth[17]). The finite-size effects due to a small number of random axes and the lower coordination number of the surface sites are seen to lead to features in the hysteresis curves, especially to differences in the bulk and surface magnetization curves. Values of the coupling constants obtained from experiments and mean field calculations for amorphous rare earth alloys are reported by O'Shea and Lee.[18]

In the second model studied, we assume that the physical effects due to the surfaces appear primarily as an anisotropy at the surface only and no anisotropy associated with the bulk sites. In the simplest surface anisotropy model, the uniaxial anisotropy $K_\mathbf{n}$ is included only for surface sites, with the anisotropy axes pointing outward, normal to the surface. This phenomenological assumption is based on the symmetry of the sites at the surface.[19,20] A different kind of surface anisotropy has been suggested by Aharoni[21] to account for the magnetization reversal of acicular γ-Fe_2O_3 particles, surface treated with Co, modeled as infinite circular cylinders. He has assumed that a cylindrical particle has a uniaxial anisotropy, parallel to the surface, only in a cylindrical shell on the surface.

III. METHOD OF CALCULATION: GENERATION OF HYSTERESIS LOOPS

We use the Landau-Lifshitz equations with damping to obtain the hysteresis loops. It is convenient for the purpose of the numerical simulation to rewrite the quantities in these equations in dimensionless form. In the simulations we hold the average strength of the anisotropy K to be fixed, which sets an energy scale, and then vary the exchange and applied field strengths. Scaling the Landau-Lifshitz equation by this energy scale, leads to the definitions of dimensionless time τ and dimensionless field h:

$$\tau = 2Kt/\hbar S, \quad \mathbf{h} = g\mu_B S\mathbf{H}/2K. \quad (2)$$

Then the reduced Landau-Lifshitz equations with damping are given by

$$\frac{d\hat{\mathbf{S}}_\mathbf{n}}{d\tau} = -\hat{\mathbf{S}}_\mathbf{n}\times\mathbf{h}_\mathbf{n}^{\text{eff}} - \alpha\hat{\mathbf{S}}_\mathbf{n}\times(\hat{\mathbf{S}}_\mathbf{n}\times\mathbf{h}_\mathbf{n}^{\text{eff}}), \quad (3)$$

where α is a phenomenological damping constant, and the reduced effective field acting on site $\mathbf{n}$ is

$$\mathbf{h}_\mathbf{n}^{\text{eff}} = \mathbf{h} + (J/2K)\sum_{\{\vec{a}\}}\hat{\mathbf{S}}_{\mathbf{n}+\mathbf{a}} + (K_\mathbf{n}/K)\hat{\mathbf{k}}_\mathbf{n}(\hat{\mathbf{k}}_\mathbf{n}\cdot\hat{\mathbf{S}}_\mathbf{n}). \quad (4)$$

In all cases, free boundary conditions are used, and the sites on the boundary of the system have less neighbors to which they are exchange coupled. The equations in terms of xyz spin components are integrated numerically, using a fourth-order Runge Kutta scheme, with a time step chosen according to the exchange, anisotropy strength, and applied field as follows:

$$\Delta\tau = 0.01/(1 + h + J/2K). \quad (5)$$

In this way, the time step adjusts to the higher natural frequencies of the system that result from a stronger applied field or exchange. A damping constant $\alpha = 0.5$ is used in these simulations.

Starting from some initial configuration and applied field, the integration with damping tends towards a configuration that is a local energy minimum or metastable state. As the time integration proceeds, the total energy in Eq. (1) smoothly decreases, and some criterion must be used to decide to stop the integration for the chosen applied field and proceed to the next applied field. In some situations, the energy can be changing very slowly while there are still substantial changes occurring in the spin configuration. Therefore, we proceed to the next applied field when $(1/N)\sum_\mathbf{n}|d\hat{\mathbf{S}}_\mathbf{n}/d\tau| < 0.0001$, where N is the total number of spins in the system. When this condition is met the spin configuration is very close to being stationary. After relaxing in this way at one field, the final configuration is used as the initial state

for the next field, and iteration of this process over a sequence of applied fields gives the hysteresis loop. Consistent results are obtained with a magnetic field step size of $0.0005 \leq \Delta h \leq 0.01$.

At the beginning of the simulation, the initial spin configuration is taken to be either all spins aligned with the applied large negative magnetic field, or with them pointing in random directions. We find that they relax more readily to a low energy state if there is some degree of disorder in the system, such as the random anisotropy or random initial state. For the surface anisotropy model in a square system (Sec. V), the high degree of symmetry makes it necessary either to use the random initial configuration, or, apply the magnetic field at a slight angle (about 1°) to the crystal axes. This is due to the form the anisotropy takes in the equation of motion (3), producing spin time derivatives proportional to $(\hat{\mathbf{S}}_\mathbf{n} \cdot \hat{\mathbf{k}}_\mathbf{n})(\hat{\mathbf{S}}_\mathbf{n} \times \hat{\mathbf{k}}_\mathbf{n})$, which becomes zero when $\hat{\mathbf{S}}_\mathbf{n}$ is either parallel or perpendicular to $\hat{\mathbf{k}}_\mathbf{n}$.

In the results, we present the surface magnetization, defined as the average of the moments $\hat{\mathbf{S}}_\mathbf{n}$ for those sites on the boundary of the system, projected along the applied field. We also present the average magnetization of the bulk sites, which are all other sites of the lattice. The mean magnetization is the average of all the magnetic moments at all of the sites, bulk, and surface. All calculations produce only local minimum energy states for zero temperature; there are no effects due to thermal fluctuations included.

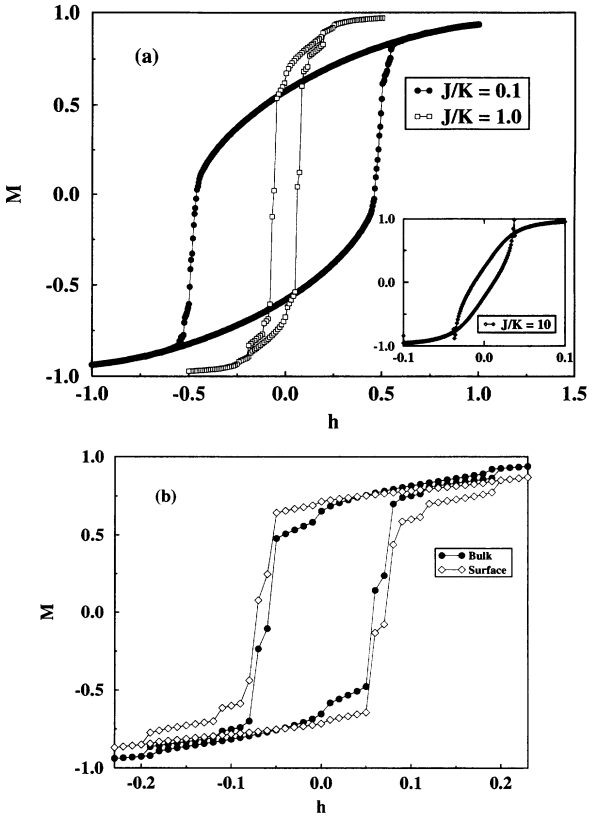

FIG. 1. Magnetization per spin for the random uniaxial anisotropy model. (a) Mean magnetization hysteresis loops for 10×10 square systems, for different values of J/K. (b) Magnetization of the bulk and surface spins, for the 10×10 square system with $J/K = 1$.

IV. RANDOM BULK ANISOTROPY

As described above, in this model, all sites, both bulk and surface, have a uniaxial anisotropy of strength K, but with randomly directed axes $\hat{\mathbf{k}}_\mathbf{n}$. In the limit $J \to 0$, this is equivalent to the Stoner-Wohlfarth model for a finite collection of random anisotropy noninteracting moments.[17] Some typical hysteresis curves for the mean magnetization of a 10×10 2D system are shown in Fig. 1(a), for three values of J/K. For $J/K = 0.1$, the exchange is weak enough relative to the anisotropy such that the spins move more or less independently, but with a *finite* collection of different anisotropy axes. The Stoner-Wohlfarth result is recovered as expected for a set of independent spins, provided the system is not too small. In the opposite limit, $J/K = 10$, the spins are strongly coupled and move approximately as one moment of effective magnitude $S_{\text{eff}} \approx NS$. In this limit the effect due to uniaxial anisotropy which varies at random from site to site is expected to diminish, leading to a decrease of the area in the hysteresis loop. As J/K gets very large, the hysteresis eventually vanishes. Finally, for $J = K$, the most interesting effects due to the anisotropy-exchange competition occur, producing noticeable jumps in magnetization due to small groups of spins reversing.

In such a small system, there are 36 surface (i.e., boundary) sites and 64 bulk sites, making it possible to have substantial finite-size effects on the surface magnetization compared to bulk magnetization. For the case $J = K$, the average surface moment is compared to the average bulk moment in Fig. 1(b). In addition to the small jumps due to having a finite set of random anisotropy axes, an effect of the lower surface coordination can be seen. The magnetization of the surface sites tends to lag behind the bulk sites, reversing more slowly than the bulk, and requiring greater in magnitude applied field to reach saturation. This can be understood to be a result of the lower surface coordination number and associated weaker effective exchange coupling for the surface sites, causing those sites to be dominated more by the local anisotropy forces.

V. UNIAXIAL SURFACE ANISOTROPY

In this model, only the sites on the boundary of the system have uniaxial anisotropy, with equal anisotropy strengths $K_\mathbf{n}$, whose axes $\hat{\mathbf{k}}_\mathbf{n}$ are taken to point normal to the surface. Some care should be taken when defining the normal to the surface on a discrete lattice. A site is considered to belong to the surface of the system if it has less nearest neighbors than the coordination number for the given lattice. For a square particle and a square underlying lattice the normal of a given site is defined along the direction perpendicular to the line connecting the nearest neighboring surface sites and the anisotropy

axes of the corner sites point outward along the [11] directions. When dealing with a circular particle and a square lattice we have always chosen the center of the particle to coincide with one of the lattice sites. Then the normal of the surface site has been defined to be along the direction from the center site to the considered surface site.

A. Square particle

Figure 2(a) shows results for a 10×10 square system, for three different values of J/K, with K fixed. The magnetic field is along the [10] direction of the lattice. For this system size, as long as J/K is fairly large compared to 1, the effect of the surface anisotropy term on the hysteresis is small. For $J = K$, the small differences in bulk and surface magnetization are shown in Fig. 2(b). The primary difference is that the magnitude of the surface magnetization is smaller than for the bulk, because a sizable fraction of the surface has its anisotropy axes at large angles to the applied field. However, for $J/K = 0.1$, the magnetization reverses through a sequence of small steps, leading to the rather interesting result shown. These nearly linear sections separated by steps in magnetization are associated primarily with the tilting of surface spins; the bulk magnetization actually reverses much sooner than the surface, as indicated in Fig. 2(c).

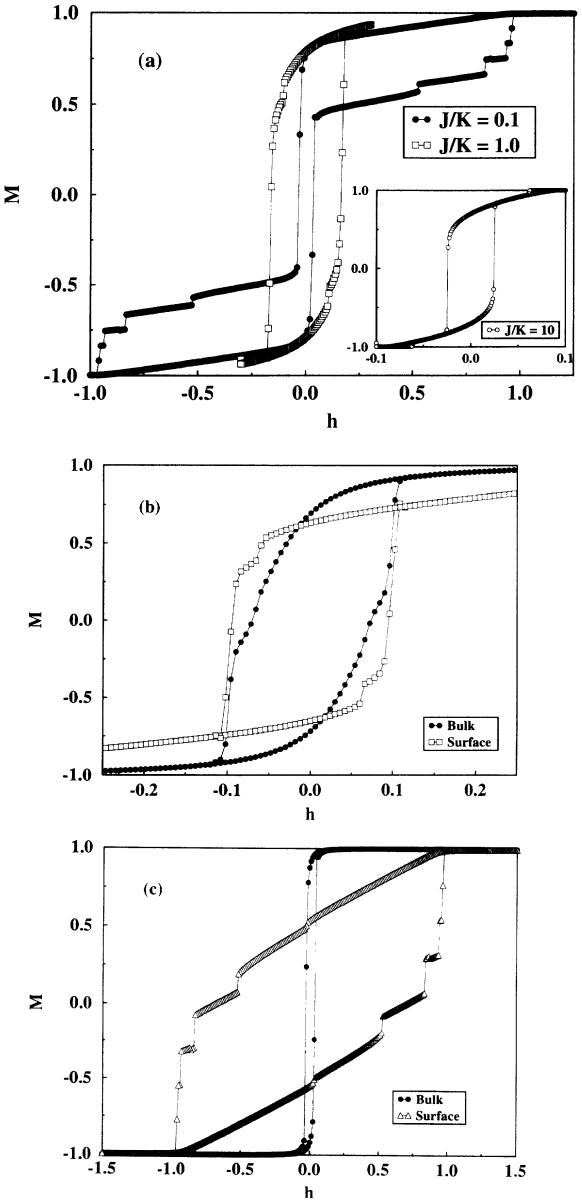

FIG. 2. Magnetization per spin for a 10×10 uniaxial surface anisotropy model. (a) Hysteresis loops for values of J/K indicated. (b) Magnetization of the bulk and surface spins, for the system with $J/K = 1$. (c) Bulk and surface magnetization for the system with $J/K = 0.1$.

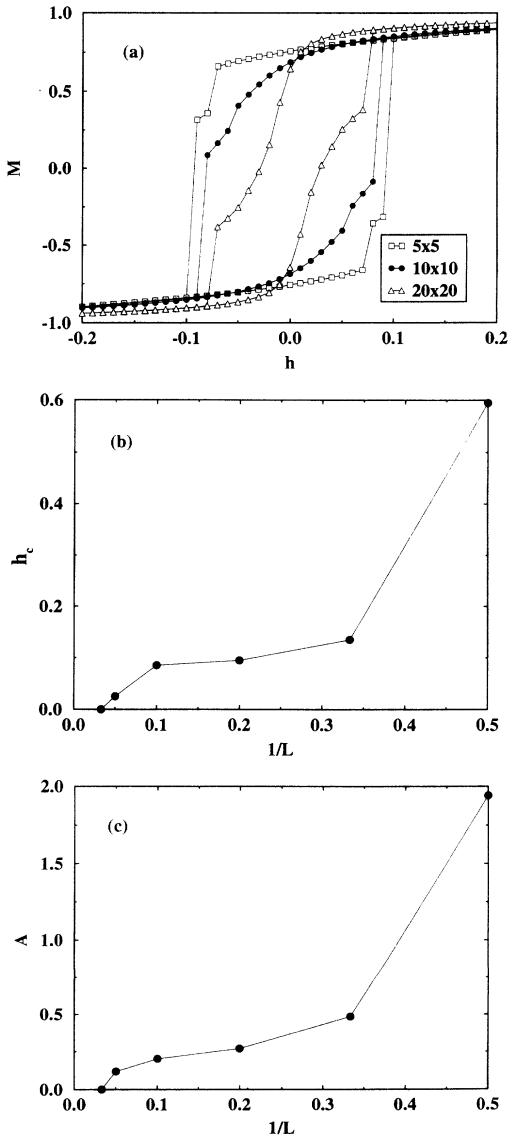

FIG. 3. (a) Size dependence of the hysteresis for the mean magnetization in the uniaxial surface anisotropy model, for square $L \times L$ systems with $J/K = 1$. (b) The coercive field h_c versus inverse system length. (c) The integrated area within the hysteresis loops versus inverse system length.

An indication of the size dependence of the results is given in Fig. 3. In Fig. 3(a), the mean magnetization is shown for systems of different sizes, with $J = K$. As the system size increases, the reduced coercive field h_c and area A within the hysteresis loop decrease. Since the ratio of the energy associated with the domain wall at the surface compared to the energy of the bulk varies as $1/L$ at sufficiently large system size, the Heisenberg term will prevail over the surface anisotropy even at very small magnitude magnetic fields, which leads to the observed decrease of h_c and the area A. These are plotted in Figs. 3(b) and 3(c) versus $1/L$.

B. Circular particle

Another set of simulations, for an approximately circular particle, is shown in Fig. 4. The radius of the particle is about 4.243 lattice constants, and contains 61 spins. This model is more realistic in that the surface spins have anisotropy axes with a wide range of directions, contrary to the situation for the square particle model. However, the J/K dependence of these results is similar to that of the square system; the magnetization reverses in a stepwise fashion when the exchange is rather weak compared to the anisotropy [Fig. 4(a)]. For $J/K = 0.2$, again the bulk magnetization reverses much sooner than the surface, as seen in Fig. 4(b). The associated spin configurations at particular points of the reversal process are shown in Fig. 4(c). Even though the exchange is relatively weak, the bulk reverses more or less as a unit, while the surface spins reverse in smaller groups, leading to the magnetization steps. The linear rises in surface magnetization between these steps are due to the tilting of the spins as the applied field competes against the uniaxial surface anisotropy.

For circular particles, the size dependence of the mean magnetization is shown in Fig. 5. Again, the coercive field and area of the hysteresis loop decreases with $1/D$, where D is the diameter of the particle.

The above results show how our choice of either a square or circular particle affects the hysteresis, especially when J/K is small. For square particles, there are more nearly linear segments in the surface magnetization [Fig. 2(c)] than for the circular particles [Fig. 4(b)]. This can be attributed to the fact that with the [10] field direction, about half of the surface sites of the square particle have their anisotropy axes parallel to the field, and about half have their anisotropy axes perpendicular to the field. The nearly linear segments in the surface magnetization are due to the slow tilting of the spins whose anisotropy axes are perpendicular to the field, as the field changes (i.e., as in the Stoner-Wohlfarth model for magnetic field perpendicular to anisotropy axis). The breaks between the linear segments correspond to some spins reversing along their anisotropy axes. On the other hand, for circular particles, there is a more uniform distribution of angles between the field and the anisotropy axes, leading to slightly curved segments in the surface magnetization, separated by jumps or breaks.

C. Three dimensions

Although we have not performed a systematic study, we can also test geometric effects in three dimensions by

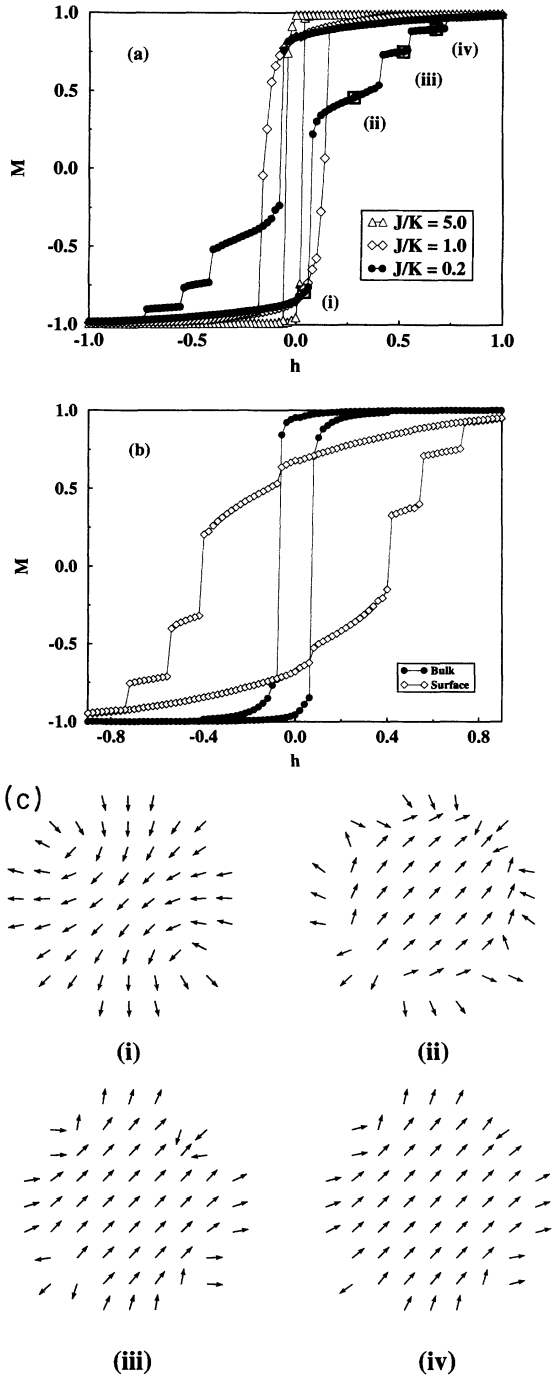

FIG. 4. Mean magnetization per spin hysteresis loops for a circular particle with uniaxial surface anisotropy. The particle radius is 4.243 lattice constants and it contains 61 spins. (a) Mean magnetization for systems with J/K values as indicated. (b) Magnetization for the bulk and surface spins, for the system with $J/K = 0.2$. (c) Spin configurations during reversal for $J/K = 0.2$, with the field near the [11] direction. Note how the bulk reverses as a single unit.

comparing results for cubic and spherical particles, with the field along the [100] direction. Magnetization results for a $10 \times 10 \times 10$ cubic particle and a spherical one with a diameter $D = 10.29$ are shown in Fig. 6. The value of J/K is 0.1. For the mean magnetization [Fig. 6(a)], the cubic particle hysteresis loop has a larger area, due to the larger energy required to reverse the spins close to the vertices and the edges of the cube, geometrical features not present in the spherical particle. For both the cubic [Fig. 6(b)] and the spherical [Fig. 6(c)] particles, the bulk magnetization reverses well before the surface. But again, the surface magnetization for the cubic particle tends to have more linear segments than for the spherical particle, probably because a large fraction of the sites have their anisotropy axes perpendicular to the field. Also, on average, the effective coupling of the surface spins to the bulk is weaker for the cubic particle than for the spherical particle, because the cubic particle's sharper edges lead to a lower average coordination number for the surface sites than in the spherical particle.

The main effect of increased dimensionality of the lattice in the transition from 2D to 3D, keeping other parameters constant, is the decreased magnitude of the coercive force h_c. This is due to the stronger exchange interaction which comes from the increased coordination number. This is even emphasized when comparing h_c of a circular particle with $J/K = 0.2$ in Fig. 4(a) and of a spherical particle with $J/K = 0.1$ in Fig. 6(a). Even

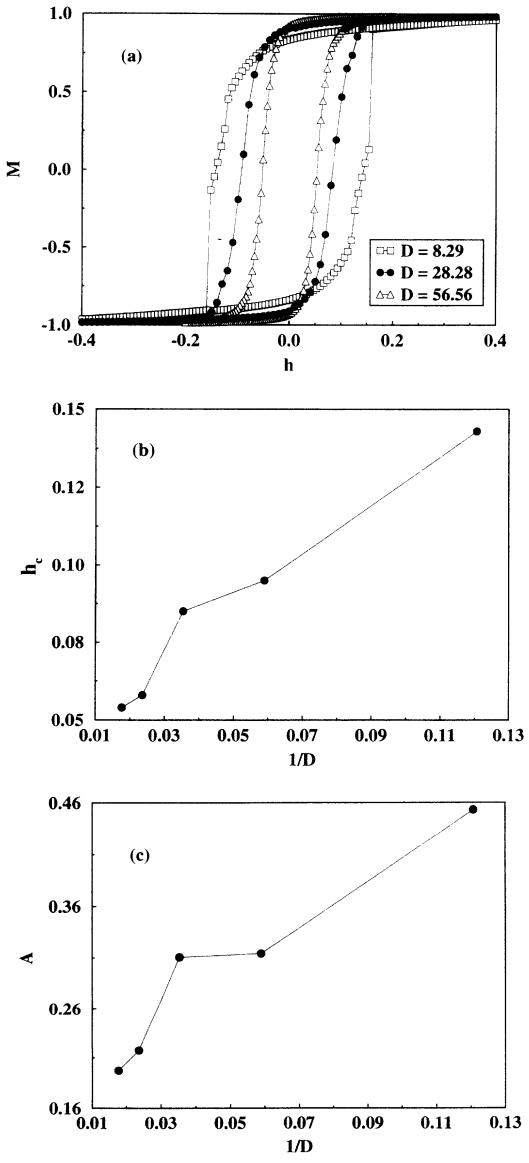

FIG. 5. (a) Size dependence of the hysteresis for the mean magnetization in the uniaxial surface anisotropy model, for circular systems with $J/K = 1$, diameters D. (b) The coercive field h_c versus inverse system size $1/D$. (c) The integrated area within the hysteresis loops versus inverse system size.

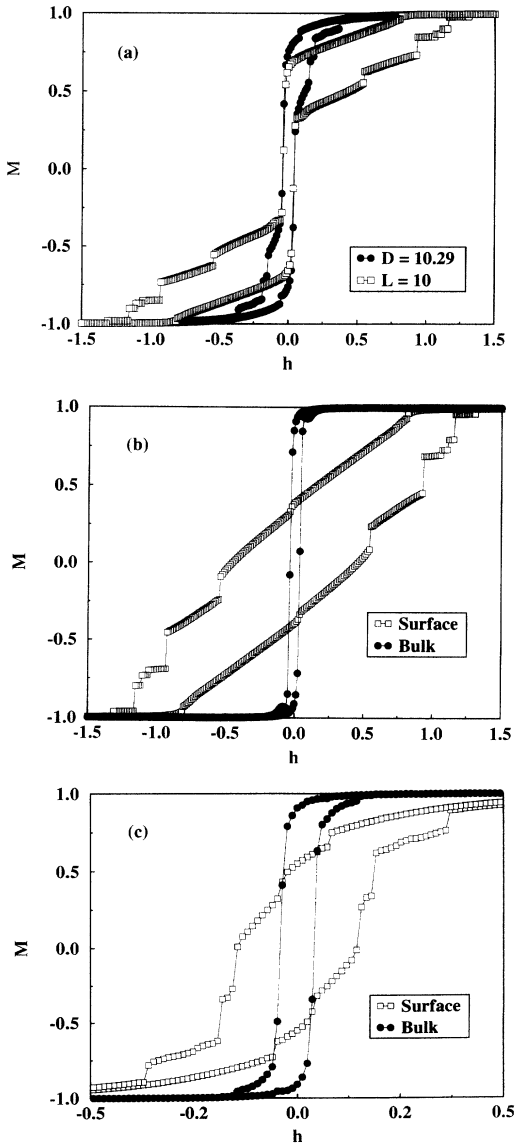

FIG. 6. (a) Magnetization per spin for 3D cubic and spherical particles with $J/K = 0.1$. The cube side and the diameter of the spherical particles are indicated in the inset in lattice constant units. Magnetization of the surface and bulk spins, for the cubic (b) and spherical (c) particles.

though the exchange to anisotropy ratio is greater for the circular particle than for the spherical one, the increased coordination number in three dimensions favors the collective motion of the spins parallel to each other and results in a smaller h_c. Another effect is the higher magnetic field required in order to saturate the surface spins for the cubic particle [Fig. 6(b)] than for the square particle [Fig. 2(c)], for similar sizes and similar values J/K. We interpret this result as due to the greater surface-to-volume ratio of the cubic particle compared to the square one and thus more energy is required to overcome the total energy barrier associated with the surface anisotropy.

VI. DISCUSSION

The results in Sec. IV for the random bulk anisotropy model indicate how the surface magnetization is different in magnitude relative to the bulk magnetization. This is because the single-ion anisotropy has a stronger effect on the surface sites than the bulk sites, since there are less nearest neighbor exchange couplings for the surface sites. When the particle undergoes magnetization reversal, the surface sites lag behind the bulk as the field changes, due to their weaker effective exchange coupling. Also, because the anisotropy axes were chosen randomly, in such a finite system there are distinct steps in the hysteresis curves due to particular sets of spins reversing before the whole. A different choice of random anisotropy axes leads to a hysteresis curve with different particular features. A weak size dependence of the hysteresis can be seen. This result is due to the moderate sized surface-to-volume ratio for the system sizes we have simulated and again to the smaller surface coordination number. Another result is the increase of coercivity when decreasing J/K. This is in agreement with Saslow and Koon's results[14] even though they have used a different algorithm, the so-called "greedy" algorithm, and periodic boundary conditions.

The results in Sec. V for the surface anisotropy models demonstrate that even though only a fraction of the total sites are affected by this anisotropy energy term, a hysteresis can result. The magnetization reversal process can take place in steps, with each step related to a particular set of spins reversing. The hysteresis eventually disappears as the particle size increases, as expected for this model with only surface anisotropy. The geometry of the particle can influence which sets of spins reverse at a particular field, as well as the shape of the hysteresis curves, especially for the surface magnetization.

In general, in three dimensions the effective coupling via Heisenberg exchange is stronger than in the 2D case due to the greater coordination number. This requires a stronger surface anisotropy constant K in the 3D case than in the 2D case in order to produce similar effects.

Apart from the obvious limitations of classical considerations and of a simulation at zero temperature our study is confined to give qualitative understanding of the dynamics of a *single* magnetic nanoparticle. In an experiment one has many such particles in a nonmagnetic matrix and statistical effects should be expected, such as disappearance of the small jumps in the magnetization associated with flipping of a small number of surface spins. We have assumed zero anisotropy for the bulk sites in the surface anisotropy model which, though not realistic, underlines the influence of the surface and gives the order of magnitude of this effect. One can improve this model by allowing bulk uniaxial anisotropy different from the surface, and comparing with the phenomenological relation for a spherical particle[22]

$$K_{\text{eff}} = K_b + \frac{6}{d} K_s, \tag{6}$$

where K_{eff} is the overall anisotropy constant per unit volume of the particle, K_b is the bulk uniaxial anisotropy constant per unit volume, K_s is the surface anisotropy constant per unit area, and d is the diameter of the particle. Another point concerning a simulation as ours is the definition of the sites that are affected by surface anisotropy. Does one consider surface anisotropy as acting only on the surface sites (those with a number of nearest neighbors less than the coordination number of the lattice), as we did, or extend the interaction into second, third layers, etc.?

In an experimental study of metallic iron nanoparticles Bødker *et al.*[22] demonstrated that the effective anisotropy energy density of a whole particle increases with decreasing particle diameter. A similar result together with some interesting temperature effects have been published also by Linderoth *et al.*[23] In a continuum material model, this result was interpreted in terms of an increased contribution from the surface anisotropy, assumed perpendicular to the surface, while the bulk anisotropy energy density remained fixed, modeled by Eq. (6) above. This would also occur in the lattice model presented here when $K > J$. However, the diameter of a nanoparticle is not more than an order of magnitude greater than the lattice constant of the material, so a continuum model may be inadequate in other respects, and particular effects due to the underlying discrete lattice may be important. Also, surface effects due to sharp edges and orientations of the surfaces faces could play roles affecting the hysteresis of fine magnetic particles, as suggested above when comparing the cubic and spherical particle results. This is an oversimplified surface anisotropy model, it is likely that other interactions should be considered, in addition to effects that might change the local surface magnetic moments compared to the bulk. However, we expect our simulation of the model with normal surface anisotropy, improved if necessary by adding nonzero bulk anisotropy, to be in qualitative agreement with the hysteresis loops measured for nanoparticles at sufficiently low temperatures.

VII. CONCLUSIONS

In an attempt to understand the surface and finite system size effects in a very small magnetic particle (consisting of about several hundred to several thousand atoms), where the discreteness of the particle has started to be seen but quantum mechanics may not be required, we

have reached the following conclusions: (i) At approximately equal exchange and anisotropy coupling constants the coercive force h_c for the random uniaxial model in 2D increases with decreasing the J/K ratio and shows a weak dependence on the size of the system for systems up to 30×30 sites. (ii) h_c of the surface anisotropy model in 2D shows strong size dependence and weaker dependence on J/K. For sufficiently big particles, keeping J/K constant, this model does not show hysteresis since the surfaces are expected to be less important for large particles. This results holds for both square and circular particles. (iii) For the surface anisotropy model, a smaller J/K ratio is needed to observe the same order of magnitude effects in 3D particles as in 2D particles.

ACKNOWLEDGMENTS

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