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Magnetization switching in small ferromagnetic particles: Nucleation and coherent rotation

U. Nowak[a] and D. Hinzke
Theoretische Tieftemperaturphysik, Gerhard-Mercator-Universität-Duisburg, 47048 Duisburg, Germany

The mechanisms of thermally activated magnetization switching in small ferromagnetic particles driven by an external magnetic field are investigated. For low uniaxial anisotropy the spins rotate coherently while for sufficiently large uniaxial anisotropy they behave Ising-like, i.e., the switching then is due to nucleation. The crossover from coherent rotation to nucleation is studied for the classical three-dimensional Heisenberg model with uniaxial anisotropy by Monte Carlo simulations. From the temperature dependence of the metastable lifetime the energy barrier of a switching process can be determined. For the case of infinite anisotropy we compare numerical results from simulations of the Ising model with theoretical results for energy barriers for both, single- and multidroplet nucleation. The simulated barriers are in agreement with the theoretical predictions.

With decreasing size ferromagnetic particles become single domain which improves their quality for magnetic recording. On the other hand, when the particles are too small they become superparamagnetic and then due to thermal fluctuations no magnetic information can be stored (see e.g., Ref. 1 for a review). Hence, much effort has been devoted to an understanding of the behavior of small magnetic particles experimentally,[2–4] analytically,[5] and in computer simulations. In the latter case, mainly magnetization switching by nucleation[6–8] has been studied using Ising models of finite size, but also other reversal mechanisms in models with continuous degrees of freedom like coherent rotation, single-droplet nucleation, and multidroplet nucleation have been discussed.[8,9]

In this article we focus on different thermally activated reversal mechanisms occuring in ferromagnetic particles. We will consider a finite, spherical, three-dimensional system of magnetic moments. These magnetic moments may represent atomic spins or also block spins following from a coarse graining of the physical lattice.[10] Our system is defined by a classical Heisenberg Hamiltonian,

$$\mathcal{H}=-J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j-d\sum_i\,(S_i^z)^2-\mathbf{B}\cdot\sum_i\,\mathbf{S}_i\,, \tag{1}$$

where the $\mathbf{S}_i$ are three-dimensional vectors of unit length. The first sum which represents the exchange of the spins is over nearest neighbors with the exchange coupling constant J. The second sum represents an uniaxial anisotropy which favors the z axis as easy axis (anisotropy constant $d>0$). The last sum is the coupling of the spins to an applied magnetic field, where $\mathbf{B}$ is the strength of the field times the absolute value of the magnetic moment of the spin. We neglect the dipolar interaction. Therefore, the validity of our results is restricted to particles which are small enough to be single domain in the remanent state.[11]

In the following we will investigate the thermally activated reversal of the magnetization of a particle which is destabilized by a magnetic field pointing into the direction antiparallel to the initial magnetization which is parallel to the easy axis of the system initially. In this case, after some time the particle will reverse its magnetization.

Due to the many degrees of freedom of a spin system numerical methods have to be used for a detailed microscopic description. Since we are especially interested in the thermal properties we use Monte Carlo (MC) methods for the simulation. Although a direct mapping of the time scale of a Monte Carlo simulation on experimental time scales is not possible this method provides information on the dynamical behavior since it solves the master equation for the irreversible behavior of the system.

We consider spins on a simple cubic lattice of size $L\times L\times L$ and simulate spherical particles with radius $R=L/2$ and open boundary conditions on this lattice using the MC algorithm described in Ref. 8. We start our simulations with an initial spin configuration where all spins are pointing up $[\mathbf{S}_i=(0,0,1)]$. The magnetic field $\mathbf{B}=(0,0,-B)$ destabilizes the system and after some time the magnetization will reverse. The metastable lifetime τ is defined by the condition $M_z(\tau)=0$ where M_z is the z component of the magnetization $\mathbf{M}=(1/N)\Sigma_i\mathbf{S}_i$.

For sufficient low anisotropy the spins can be expected to rotate coherently. Such a reversal process is shown in Fig. 1 where a spin configuration of a simulated system of size $R=6$ spins during the reversal process is represented. The spins are nearly parallel except of thermal fluctuations. Following the theory of Néel[12] and Brown[13] the energy barrier which has to be overcome during the reversal is only due to the anisotropy of the system,

$$\Delta E_{\mathrm{cr}}=\frac{4\pi R^3 d}{3}-\frac{4\pi R^3 BM}{3}+\frac{\pi R^3 B^2 M^2}{3d}, \tag{2}$$

where M is the saturation magnetization of the system.

For a system with a sufficient large anisotropy it is energetically favorable to divide into parts with opposite direc-

[a]Electronic mail: uli@thp.uni-duisburg.de

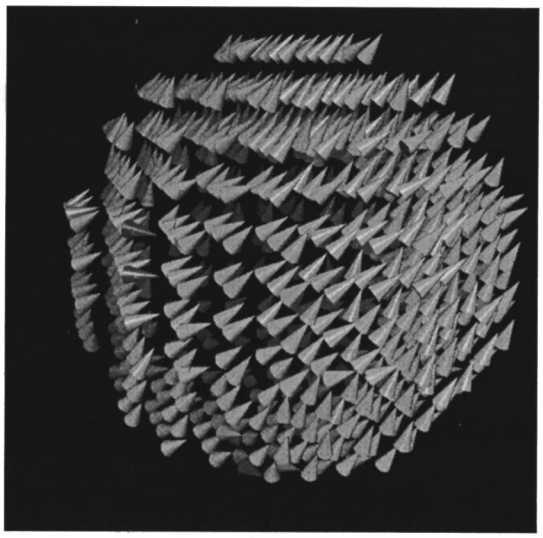

FIG. 1. Snapshot of a simulated spin system during coherent rotation. In the picture we omit the interior part of the system and show only the outer spins of the sphere. $R=6$ spins, $B=0.7$ J, $d=0.35$ J/spin, $T=0.09$ J.

tions of magnetization parallel to the easy axis in order to minimize the anisotropy energy barrier. This kind of reversal mechanism is called nucleation[14] (see Ref. 6 for a recent review). The simplest case of a reversal process driven by nucleation for a system of finite size is the growth of one single droplet starting somewhere at the boundary. Due to the growth of the droplet a domain wall will cross the system and the energy barrier which has to be overcome is caused by the domain wall energy. This is shown in Fig. 2. Here the domain wall is in the center of the system dividing the particle into two oppositely magnetized parts of equal size.

The energy barrier ΔE_n which has to be overcome during the reversal by nucleation of one single droplet in a three-dimensional system with open boundary condition has been derived in Ref. 8. It can be expanded with respect to MBR/σ resulting in

$$\Delta E_n \approx 2\pi R^2\sigma - \frac{4\pi BR^3M}{3} + \frac{3\pi B^2R^4M^2}{8\sigma} + \ldots, \tag{3}$$

where σ is the domain wall energy density. The corresponding lifetime of the metastable state for the single-droplet nucleation is then

$$\tau \sim \exp\left(\frac{\Delta E_n}{T}\right) \tag{4}$$

for temperatures $T \ll \Delta E_n$. Equation (3) has an interesting interpretation: for small fields B the energy barrier of a nucleation process is the energy of a flat domain wall in the center of the particle plus corrections which start linearly in B. In contrast to the Néel–Brown theory, here for vanishing magnetic field the energy barrier is proportional to the cross-sectional area of the particle rather than to its volume.

Hence, comparing the two energy barriers for coherent rotation [Eq. (2)] and nucleation [Eq. (3)] one can evaluate the critical particle size R_c where the crossover from coherent rotation to nucleation sets in. For vanishing magnetic field this critical particle size is given by

$$R_c = \frac{3\sigma}{2d}. \tag{5}$$

For particles larger than R_c reversal by nucleation has the lower energy barrier while the opposite is true for particles smaller than R_c.

Another possibility of a reversal process driven by nucleation is the growth of several droplets at the same time (multidroplet nucleation). This reversal process occurs when the probability for the growth of large droplets is high enough and when the critical droplet size is smaller than the system size so that many droplets may occur in the system at the same time. This is the case for higher fields or larger temperatures.[15,16] The lifetime for the multidroplet nucleation in D dimensions is[14]

$$\tau \sim \exp\left(\frac{\Delta E_n}{(D+1)T}\right). \tag{6}$$

Hence, the exponent of the exponential function changes by a factor of $1/(D+1)$ which is 1/4 in our case. In order to quantify the crossover from single droplet to multidroplet nucleation we consider the case of infinite anisotropy in which case we can directly simulate an Ising system. We performed a standard MC simulation of the Ising Hamiltonian

$$\mathcal{H} = -J\sum_{\langle ij\rangle} S_iS_j - B\sum_i S_i \tag{7}$$

with $S_i = \pm 1$.

Figure 3 shows a corresponding spin configuration during the reversal. The Ising spins are represented as light (spin up) and dark (spin down) grey boxes. The reversal process is initiated by many droplets at the boundary of the system.

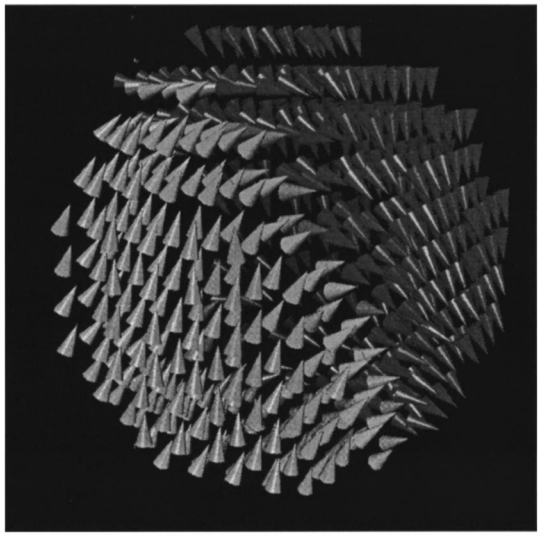

FIG. 2. Snapshot of a simulated spin system as in Fig. 1 but for single-droplet nucleation. The z component of the spin is color coded (lighter grey corresponds to spins up, dark to spin down). $B=0.7$ J, $d=0.7$ J/spin, and $T=0.45$ J.

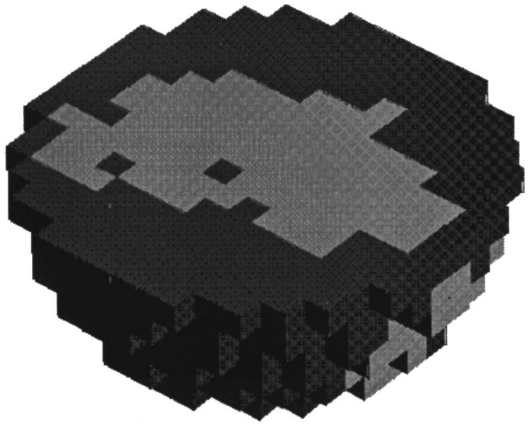

FIG. 3. Snapshot of a simulated spin system at the lifetime τ for multidroplet nucleation. Shown is an Ising system of size $R=8$ spins. In order to show the interior of the system we have cut the sphere and show only one half of the system. $B=0.5$ J and $T=2.8$ J.

Later all these droplets join each other so that the outer shell of the particle is reversed while the inner parts have still the initial magnetization direction.

Figure 4 shows the temperature dependence of the metastable lifetime following from simulations for two different fields. Each data point is an average over 100 independent runs. The data show a linear behavior with different slopes for low and high temperatures, respectively. For low temperatures single-droplet nucleation occurs and we can compare the corresponding data with the theoretical prediction, Eqs. (3) and (4). The slopes of the straight lines shown are the energy barriers ΔE_n obtained from Eq. (3) which have the theoretical values 40.4 ($B=0.5$ J) and 23.5 J ($B=0.8$ J) for the system size used here ($R=4$ spins) and for σ $=1.2$ J/bond[8] showing very good agreement between the numerical data and the theoretical predictions.

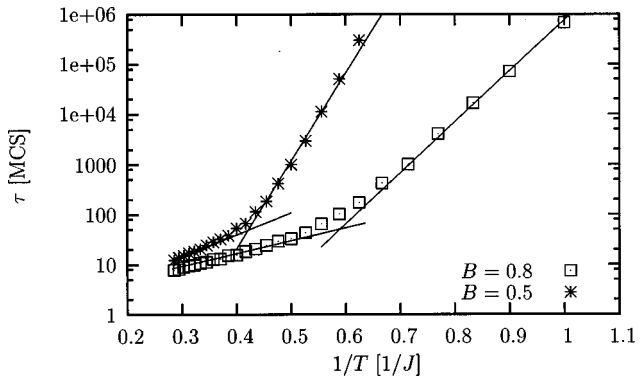

FIG. 4. Metastable lifetime τ vs $1/T$ for two different magnetic fields. System size $R=4$ spins.

For higher temperatures we find a crossover to multidroplet nucleation in which case theory predicts a reduction of the energy barrier by a factor of $(D+1)=4$, Eq. (6). The slopes of the straight lines shown are the energy barriers $\Delta E_n/(D+1)$ obtained from theory showing again very good agreement with the simulated data. Note that the position of all lines are fitted since we do not know the prefactors in Eqs. (4) and (6).

To conclude we found very good agreement between the energy barriers obtained from the numerical data and the predictions obtained from both single- and multidroplet nucleation theory. Especially, the general result that the effective energy barriers for single- and multidroplet nucleation are related by the D-dependent factor is confirmed. A corresponding behavior concerning the field dependence of the metastable lifetime was also observed recently.[15,16]

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