ABSTRACT

We present Monte Carlo and Langevin micromagnetic calculations to investigate thermal switching of single-domain ferromagnetic particles. For the Monte Carlo study we place particular emphasis on the probability that the magnetization does not switch by time $t$, $P_{\text{not}}(t)$. We find that $P_{\text{not}}(t)$ has different behaviors in different regimes of applied field, temperature, and system size, and we explain this in terms of different reversal mechanisms that dominate in the different regimes. In the micromagnetic study of an array of Ni pillars, we show that the reversal mode is an ‘outside-in’ mode starting at the perimeter of the array of pillars.

INTRODUCTION

All facets of the dynamics of nanoscale magnetic materials are currently active areas of research. The ability to construct single-domain nanoparticles via various methods and to measure the properties of individual nanoparticles and small arrays of nanoparticles [1—4] provides clean experiments compared with previous studies of mixtures of magnetic particles. One of the driving forces for applications is the rapid increase in density of magnetic recording devices, and the associated need to store each bit of information on a smaller number of grains [5]. On the theoretical and simulational side, a detailed understanding of nucleation and growth mechanisms that lead to the decay of a metastable state in finite systems has led to the identification of different decay modes in different parameter regimes [6—10]. In addition, new simulation algorithms are becoming available that may allow microscopic simulations at the inverse phonon frequency to extend to the technologically important time scales of years [11, 12].

In this brief paper we concentrate on using the thermal activation picture of nucleation and growth in simple metastable systems to better understand the reversal mechanisms for more realistic models of magnetism. We present Monte Carlo simulations for $P_{\text{not}}(t)$, the probability that the metastable magnetization has not yet reversed at time $t$. We show how well this simulation of a heterogeneous system fits our theoretical description for $P_{\text{not}}(t)$. We also present Langevin micromagnetic results for an array of Ni pillars. In the Langevin micromagnetic calculations the switching mechanism involves escape over a saddle point driven by random thermal fluctuations at constant field, rather than the deterministic disappearance of the metastable state as the field increases [13, 14]. Consequently, the Langevin micromagnetic calculations have the ability to measure $P_{\text{not}}(t)$ directly.

MODELS AND METHODS

We have preformed two types of computer calculations. The first consists of Monte Carlo...
Simulations [15] of the square-lattice Ising model with Hamiltonian

\[ \mathcal{H} = -J \sum_{\langle i,j \rangle} s_is_j - \sum_i H_is_i , \]  

(1)

where \( s_i = \pm 1 \) and the local fields \( H_i \) are random numbers uniformly distributed between a maximum and a minimum value. This work uses periodic boundary conditions and a Glauber Monte Carlo update at randomly chosen sites. The initial state has all spins up, and at \( t=0 \) a negative field \( \{ H_i \} \) is applied. The unit of time is Monte Carlo Steps per Spin (MCSS). A rigorous derivation of the stochastic Glauber dynamic for Ising models from microscopic quantum Hamiltonians has been established under certain conditions in the thermodynamic limit [16], with the Monte Carlo time unit related to heat-bath phonon frequencies. This simulation has been performed to test our prediction for the forms of \( P_{\text{not}}(t) \) in a system with quenched bulk randomness.

In order to simulate models with realistic spin degrees of freedom, we have programmed a Langevin micromagnetics code similar to that reported in [17]. We have used a phenomenological damping parameter \( \alpha \), and classical spins of constant length given by the bulk saturation magnetization \( M_s \). Then at each lattice site \( i \) there is a scaled magnetization \( \vec{m} = \vec{M}/M_s \). The standard Ginzburg-Landau-Lifshitz micromagnetic equation [13, 14] is

\[ \frac{d\vec{m}_i}{dt} = -\frac{1}{1 + \alpha^2} \vec{m}_i \times \left( \vec{h}_{i,\text{eff}} + \alpha \vec{m}_i \times \vec{h}_{i,\text{eff}} \right) . \]  

(2)

The scaled effective field at each site, \( \vec{h}_{i,\text{eff}} \), contains contributions from terms including the exchange interaction, the dipole-dipole interaction, the interaction due to crystalline anisotropy, the applied field, and a scaled noise term proportional to the the Langevin fields \( \zeta(t) \) [14, 17]. The Langevin noise term \( \zeta \) and the integration time step \( \Delta t \) are related by \( \zeta \propto \sqrt{\Delta t} \). Even though the set of equations used in this Langevin micromagnetics simulation are approximations to the actual equations [18], the approximation should be reasonable far below the critical temperature. We have used a fourth-order Runge-Kutta algorithm as the integration scheme in order to keep the length of the \( \vec{m}_i \) constant.

RESULTS

In the Ising simulation, we used 100×100 lattices at \( T=0.8T_c \approx 1.815J \). As in the case of homogeneous nucleation [7], homogeneous nucleation for single-domain Ising particles with demagnetizing fields [8], and for single-domain Ising particles with different boundary conditions [9], we have identified different decay regimes [6 — 10]. The functional form for quantities such as \( P_{\text{not}}(t) \) are different in the different decay regimes. In particular, in the single-droplet (SD) regime of a single-domain magnetic particle, \( P_{\text{not}}(t) = \exp \left( -t/\tau \right) \). Here \( \tau \) is the average lifetime for the decay of the metastable magnetic state due to thermal fluctuations. However, in the multi-droplet (MD) regime for single-domain particles the functional form for \( P_{\text{not}}(t) \) is given by

\[ P_{\text{not}}(t) = \frac{1}{2} \text{erfc} \left( \frac{t - \tau}{\Delta} \right) , \]  

(3)

where \( \text{erfc} \) is the complementary error function, and the width \( \Delta \) depends on the system size. This form for \( P_{\text{not}}(t) \) results from the assumption that many independent droplets nucleate and grow in different parts of the system, collectively leading to the magnetization reversal.
Figure 1: The probability $P_{\text{not}}(t)$ in the multidroplet (MD) regime for a $100 \times 100$ Ising model with periodic boundary conditions at $T = 0.8T_c$. The data (open circles) are for 1000 escapes from the metastable state. The random fields $H_i$ are uniformly distributed, and centered on $-0.34725$ with a width of $0.34725$. Two different one-parameter fits to the data are shown. The solid line is a fit to the complementary error function given by Eq. (3). The dashed curve is a one-parameter fit to a stretched exponential. In both of these fits the average lifetime was set at the measured value of $\tau = 54.4$ MCSS. (So that the solid line can be seen, only a small number of the 1000 data points are shown.)

Figure 2 shows an example of the type of thermal switching simulations [19] that can be performed using Langevin micromagnetic calculations. This figure represents a square array of magnetic Ni pillars. Similar arrays of Fe pillars have been built and measured experimentally [1, 2]. The simulation was started with all spins pointing up, and at $t=0$ a field parallel to the spins was applied for 1 nsec to allow the system to come to thermal equilibrium. Then the field was reversed to point opposite to the average magnetization, leaving the spins in a metastable state. However, the magnitude of the applied field would not have been sufficient to switch the system at zero temperature, and the switching event depicted in Fig. 2 is enabled by the thermal fluctuations included in Eq. (2). The random thermal field has its strongest effect at the edges of the array, where the demagnetizing field is...
weakest. In particular, an ‘outside-in’ switching mode is seen, in which the decay towards the stable magnetization direction starts from the pillars at the edge and subsequently propagates to the pillars in the interior of the array.

It is important to note that both the Monte Carlo and the Langevin micromagnetic simulations were conducted for applied fields sufficiently weak that a free-energy barrier against decay of the metastable state remained, and that this barrier had to be overcome by the thermal fluctuations in order for the magnetization switching to occur.

CONCLUSIONS

Realistic simulations of models for magnetic materials have been carried out. The form for the probability of not switching, \( P_{not}(t) \), is shown to fit the form of a complementary error function. The reversal mode for arrays of single-domain magnetic pillars has been identified as reversal of pillars on the boundary, followed by reversal of interior pillars.

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Figure 2: A series of snapshots of a Langevin micromagnetic calculation for magnetization reversal in a square array of Ni pillars that are 200 nm tall, 200 nm apart, and each have a diameter of 40 nm. Each pillar is discretized using 5 lattice points. (For clarity of presentation, the vertical scale of this figure is enhanced compared with the horizontal scale.) The temperature is 300 K, the spins are initially up, and the applied field is down with a magnitude of 1225 Oe. The integration time step is $\Delta t=1$ psec. The time sequence following field reversal, (reading line by line – left to right and top to bottom) is 4 nsec, 8 nsec, 12 nsec, 16 nsec, 20 nsec, and 24 nsec. This reversal mode is different from coherent rotation [5, 20].