Fine-grid Simulations of Thermally Activated Switching in Nanoscale Magnets

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Abstract. Numerical integration of the Landau-Lifshitz-Gilbert equation with thermal fluctuations is used to study the dynamic response of single-domain nanomagnets to rapid changes in the applied magnetic field. The simulation can resolve magnetization patterns within nanomagnets and uses the Fast Multipole method to calculate dipole-dipole interactions efficiently. The thermal fluctuations play an essential part in the reversal process whenever the applied field is less than the zero-temperature coercive field. In this situation pillar-shaped nanomagnets are found to reverse through a local mode that involves the formation and propagation of a domain wall. Tapering the ends of the pillars to reduce pole-avoidance effects changes the energies involved but not the fundamental process. The statistical distribution of switching times is well described by the independent nucleation and subsequent growth of regions of reversed magnetization at both ends of the pillar.

Magnetic nanoparticles are important components of nanotechnology. Previously, Ising models, which describe only highly anisotropic materials, have been used to understand thermally activated switching in single-domain magnets [1,2]. Single-domain magnets with dimensions of only a few nanometers are being manufactured and measured, for instance, using scanning microscopy techniques [3]. We have chosen these nanomagnets as a specific system in which to investigate magnetization switching with more realistic computational models.

Here magnetic materials are modeled by position-dependent magnetization density vectors $\boldsymbol{M}(\boldsymbol{r})$ with fixed length M_s, that precess around the local field $\boldsymbol{H}(\boldsymbol{r})$ according to the Landau-Lifshitz-Gilbert equation [4,5]

$$\frac{\mathrm{d}\boldsymbol{M}(\boldsymbol{r})}{\mathrm{d}t} = \frac{\gamma_0}{1+\alpha^2}\boldsymbol{M}(\boldsymbol{r}) \times \left[\boldsymbol{H}(\boldsymbol{r}) - \frac{\alpha}{M_s}\boldsymbol{M}(\boldsymbol{r}) \times \boldsymbol{H}(\boldsymbol{r})\right] , \tag{1}$$

where $\gamma_0 = 1.76 \times 10^7\,\mathrm{Hz/Oe}$ is the electron gyromagnetic ratio and α is a phenomenological damping parameter. The value $\alpha = 0.1$ was chosen to give an underdamped system. The saturation magnetization $M_s = 1700\,\mathrm{emu/cm^3}$ and the exchange length $\ell_x = 2.6\,\mathrm{nm}$ were chosen to match those of bulk iron.

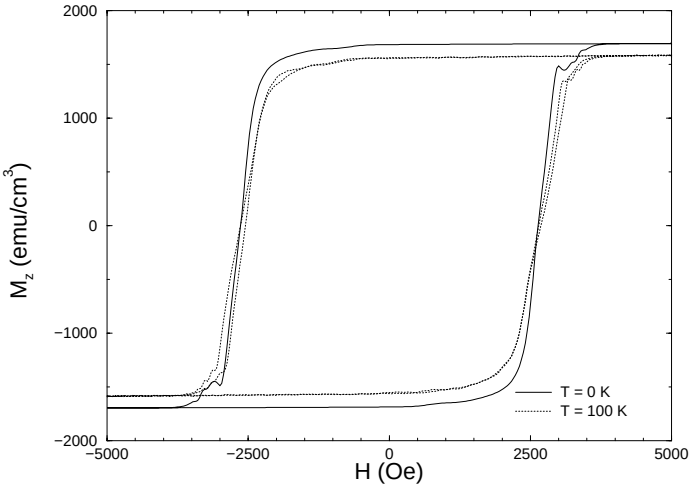

Fig. 1. Hysteresis loops of period 4 ns for flat-ended nanoscale pillars described in the text. One is at $T = 0\,\mathrm{K}$ (solid) and two at $T = 100\,\mathrm{K}$ (dotted)

Numerical integration of (1) was carried out using a finite-differencing scheme with $\Delta r = 1.5\,\mathrm{nm}$ and $\Delta t = 5 \times 10^{-5}\,\mathrm{ns}$. The local field includes exchange interactions, dipole-dipole interactions, and thermal fluctuations. Details of the numerical approach are given in Ref. [6].

Here we consider nanomagnets with square cross sections of side 9 nm. One geometry has flat ends, and is 150 nm along the z-direction [7]. A simulated hysteresis loop at $T = 0\,\mathrm{K}$ with a period of 4 ns for this system is shown in Fig. 1. There is no crystalline anisotropy included in the model, but the shape anisotropy is quite strong, giving a coercive field of about 1980 Oe [6]. Even for these extremely fast loops, for a significant amount of time the magnet experiences a field just below the coercive field, and thermal fluctuations can carry the magnetization through the configuration associated with the energy barrier. Two hysteresis loops simulated at $T = 100\,\mathrm{K}$ are also shown in Fig. 1 to illustrate the extent of this effect.

A more dramatic way to see the effects of thermal fluctuations on the reversal of the magnetization is to hold the applied field fixed just below the coercive field. This traps the magnetization in a shallow metastable energy well, and thermal fluctuations become an essential part of the reversal process. Snapshots of the z-component of the magnetization separated by 0.05 ns are shown in Fig. 2(a). The end caps associated with pole avoidance become strong in an antiparallel field, and thermal fluctuations affect their volume. The reversal starts when thermal fluctuations make one of these regions supercritical [7], after which it propagates at a constant rate towards the other end of the magnet. (A discussion of the saddle point associated with the nucleation process is found in Ref. [8].) Tapering the ends of the magnet reduces the pole-avoidance effects, and hence affects the end caps. However, the switching is still characterized by nucleation

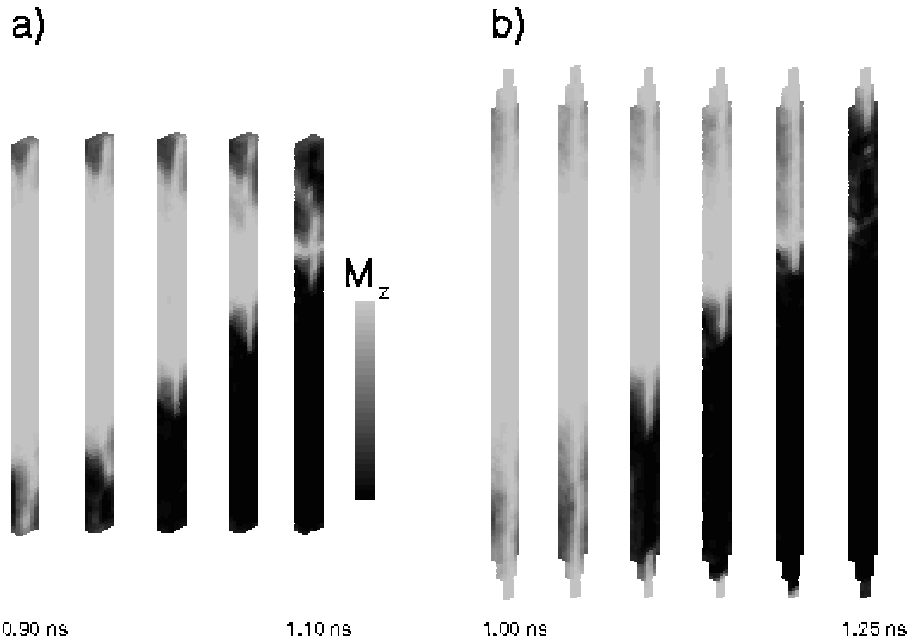

Fig. 2. Snapshots of the z-component of the magnetization, M_z, at equally spaced times for (a): pillars with square ends and $H_{\rm app} = 1800\,{\rm Oe}$ (b): pillars tapered at both ends and $H_{\rm app} = 1975\,{\rm Oe}$. All are identical cutaway views with only half of the pillar shown. Light shades indicate magnetization pointing in the unfavorable direction while the darkest shades indicate magnetization pointing in the favorable direction. Both simulations are for $T = 20$ K

at the ends; an example is shown in Fig. 2(b) for pillars 227 nm tall. The major effect we have observed of the tapering is an increase in the coercive field.

A simple model based on independent nucleation at the ends, followed by constant growth, allows calculation of the probability of not switching before time t to be [6,7]

$$P_{\rm not}\,(t) = \begin{cases} 1 & t < t_0 \\ e^{-2\mathcal{I}(t-t_0)}\,[1 + 2\mathcal{I}(t-t_0)] & t_0 \le t < 2t_0 \\ e^{-2\mathcal{I}(t-t_0)}\,[1 + 2\mathcal{I}t_0] & 2t_0 \le t \end{cases}, \qquad (2)$$

where t_0 is the earliest time at which a pillar can switch (when both ends start growing at t=0) and $\mathcal{I}$ is the nucleation rate for each end. This form is compared to the simulation results for both pillars with flat and tapered ends in Fig. 3. The biggest obstacle to testing (2) is generating sufficient statistics at fields well below the coercive field [6,7].

In summary, thermal fluctuations and dipole-dipole interactions have been included in a three-dimensional model of single-domain nanoscale magnetic pillars. Simulated dynamics using the Landau-Lifshitz-Gilbert equation with thermal noise show that magnetization switching in the pillars occurs as the end caps

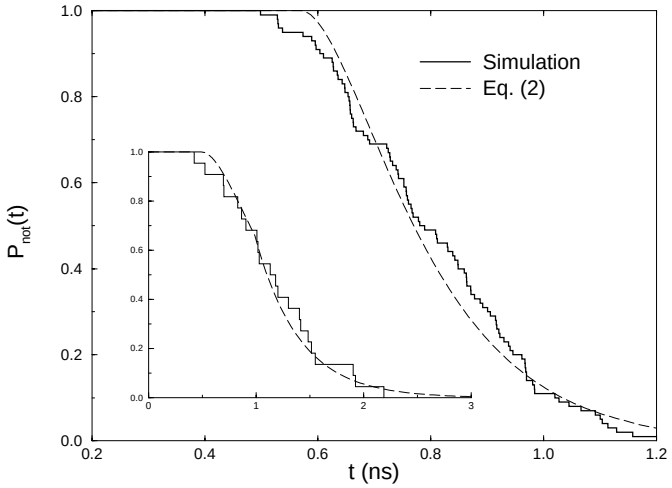

Fig. 3. Probability of not switching, $P_{\rm not}(t)$, for 100 simulations of the flat-ended pillars at $H_{\rm app} = 1800\,{\rm Oe}$ and $T = 20\,{\rm K}$, along with a fit to (2). The inset shows similar results for 22 trials with the tapered-end pillars at $H_{\rm app} = 1975\,{\rm Oe}$ and $T = 20\,{\rm K}$

nucleate, grow, and eventually coalesce. A simple model based on the thermally-activated nucleation of end caps for subcoercive fields gives a reasonable description of the simulation results for $P_{\rm not}(t)$.

Supported by NSF Grant Nos. DMR-9871455 and DMR-0120310, U.S. DOE, NERSC, and by FSU/SCRI, FSU/CSIT, and FSU/MARTECH.

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