Determining the Saddle Point in Micromagnetic Models of Magnetization Switching

Gregory Brown\(^{1,2}\) and M.A. Novotny\(^{3}\) and Per Arne Rikvold\(^{2,4}\)

\(^{1}\) Center for Computational Sciences, Oak Ridge National Laboratory, P.O. Box 2008 Mail Stop 6114, Oak Ridge, TN 37831-6114, USA
\(^{2}\) School of Computational Science and Information Technology, Florida State University, Tallahassee, FL 32306-4120, USA
\(^{3}\) P.O. Box 5167, Department of Physics and Astronomy, Mississippi State University, Mississippi State, MS 39762-5167, USA
\(^{4}\) Center for Materials Research and Technology and Department of Physics, Florida State University, Tallahassee, FL 32306-4351, USA

A numerical model of single-domain nanoscale iron magnets fabricated using scanning-microscope-assisted chemical vapor deposition is simulated using finite-temperature micromagnetics. A Projective-dynamics method is used to determine the magnetization at the saddle point as a function of temperature. This magnetization is found to decrease linearly as the temperature is raised.

An interesting problem in nonequilibrium statistical mechanics, with numerous applications in condensed-matter physics and materials science, is how a system approaches the global minimum of the free energy. One simple, but common, situation is that of a local free-energy minimum which is separated from the global minimum by a free-energy barrier. In other words, any path between the metastable local minimum and the equilibrium global minimum involves an initial increase in the free energy. The most probable path between the minima involves the minimum free energy increase since spontaneous increases in free energy are improbable. The maximum free energy along that most probable path corresponds to the saddle point. Often, the behavior of the nonequilibrium dynamics are dominated by properties near the minima and the saddle point. While the minima can be determined by examining histograms of the state of the system, the saddle point is much harder to determine. In this paper we present a technologically important example of finding the saddle point using a projective-dynamics technique.

The results described here are for a numerical model of single-domain nanoscale iron magnets that have been fabricated using chemical vapor deposition directed by a scanning-tunneling microscope. These magnetic pillars have cross-sectional dimensions on the order of 10 nm and extend on the order of 100 nm perpendicular to the substrate. The magnetic pillars are modeled by a one-dimensional array of magnetization density vectors \(\vec{M}(r)\) with fixed length \(M_s\). Each vector precesses around a local field \(\vec{H}(\vec{r})\) according to the Landau-Lifshitz-Gilbert equation \(2\)

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

where the electron gyromagnetic ratio \(\gamma_0 = 1.76 \times 10^7\) Hz/Oe. The phenomenological damping parameter \(\alpha = 0.1\) was chosen to give underdamped dynamics. Properties of bulk iron were assumed with the saturation magnetization \(M_s = 1700\) emu/cm\(^3\) and the exchange length \(\ell_x = 2.6\) nm. The model pillar has a square cross section with area \(4\ell_x^2\), and is \(34\ell_x\) long. Details of the numerical approach, including the inclusion of thermal fluctuations in the local field, are given in Ref. \(\text{[4]}\).

These nanopillars have a strong shape anisotropy, and the magnetization is most favorably oriented along the long axis of the magnet, which is taken to be the \(z\) direction. The nanopillars are prepared in a metastable state via equilibration in an externally-applied magnetic field \(+H_0z\), which is subsequently varied rapidly in magnitude (without changing its orientation) to \(-H_0z\). If the field \(H_0\) is less than the coercive field, here \(H_c \sim 1500\) Oe \(\text{[1]}\), a free-energy barrier separates the positively-oriented magnetization from the equilibrium negative orientation. Previous simulations \(\text{[7]}\) suggest that the saddle point in these pillars corresponds to the nucleation of a region of reversed magnetization at one of the ends of the pillar. The nucleated region grows until the entire magnetization is reversed.

A useful technique for determining the magnetization corresponding to the free-energy maximum of the barrier, also called the saddle point, is the projective-dynamics technique \(\text{[6]}\). The essence of this technique is projecting the original dynamics described in a high-dimensional phase space onto a probabilistic dynamic in a phase space of much lower dimension. A specific example is helpful. The dynamics of an Ising model can be projected onto the number of overturned spins, a measure of the global magnetization. The dynamics of the one-dimensional model are then described in terms of the probability that the number of overturned spins increases or decreases. Thinking in terms of the number of spins in the stable orientation, these probabilities are referred to as the probability of growing \((P_{\text{grow}})\) and shrinking \((P_{\text{shrink}})\), respectively \(\text{[6]}\).

Projective dynamics for the model nanopillars is more complicated than that for the Ising model for two reasons. First, the magnetization is a continuous, three-dimensional variable. This is handled by projecting the \(z\)-component of
the global magnetization into uniformly sized bins. Then $P_{\text{grow}}$, the probability of the region of stable magnetization “growing,” is the probability that during an integration step the magnetization moves into a bin corresponding to a smaller magnetization. Similarly, $P_{\text{shrink}}$ is the probability that the magnetization moves into a bin corresponding to a larger magnetization. The second complication involves the persistent, subcritical regions of reduced magnetization that develop at each end of the pillar. To accommodate this, during the projective-dynamics analysis the pillar is divided into its top and bottom parts with the normalized, “global” magnetization $M_z$ of each half considered separately.

The measured $P_{\text{grow}}$ and $P_{\text{shrink}}$ at $H_0=1000$ Oe are shown in Fig. 1 for temperatures of 20 K, 50 K, and 100 K. For each temperature the results represent averaging over more than $10^9$ integration steps and on the order of $10^4$ switches. Consider the probabilistic dynamics at $M_z=0.85$ for $T=100$ K. Here $P_{\text{shrink}}>P_{\text{grow}}$ and on average the magnetization moves to the right. For $M_z=0.98$ the situation is reversed, and on average the magnetization moves to the left. The crossing point where $P_{\text{shrink}}=P_{\text{grow}}$ corresponds to a locally stable fixed point since, on average, here the magnetization moves towards the crossing. In this case the crossing is the metastable local free-energy minimum. For the crossing near $M_z=0.74$ the magnetization moves away from the point on average, and it corresponds to an unstable local maximum in the free energy. This is the saddle point. Measuring the value of $M_z$ for which $P_{\text{shrink}}=P_{\text{grow}}$ is a convenient method for finding the saddle point.

From Fig. 1 it is obvious that $M_z$ at the saddle point is different for magnetization reversal at different temperatures. The value of $M_z$ at the saddle point is presented vs temperature in Fig. 2. The point where $P_{\text{shrink}}=P_{\text{grow}}$ is estimated using lines fit via a least-squares method to each probability in the region near the crossing. The error bars are taken large enough to include nearly all $M_z$ for which the difference in the probabilities is less than the fluctuations in their estimates.

There is a clear linear trend in $M_z$ at the saddle point with respect to the temperature. The solid line in Fig. 2 is an unweighted least-squares fit to the data. This fit indicates that $M_z(T \to 0)=0.860$ at the saddle point. The dependence on temperature is quite strong, since $M_z(100 \text{ K})=0.72$.

In summary, micromagnetic simulations at finite temperature have been used to investigate magnetization reversal in single-domain nanoscale magnets. The saddle point in the free energy was determined using the projective-dynamics technique, and the magnetization at the saddle point was found to depend linearly on the temperature for all the temperatures investigated, $T \leq 100$ K.

This work was supported in part by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725, and by the Ames Laboratory, which is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-82. This work was also supported by NSF grant No. DMR-0120310 and by FSU/CSIT. Computer resources were provided by the FSU Department of Physics.

[1] S. Wirth, M. Field, D.D. Awschalom, S. von Molnár: Phys. Rev. B 57, R14028 (1998); J. Appl. Phys. 85, 5249 (1999)
[2] W.F. Brown: Phys. Rev. 130, 1677 (1963)
[3] A. Aharoni: Introduction to the Theory of Ferromagnetism (Clarendon, Oxford, 1996)
[4] G. Brown, M.A. Novotny, P.A. Rikvold: Phys. Rev. B 64, 134422 (2001)
[5] M. Kolesik, M.A. Novotny, P.A. Rikvold: Phys. Rev. Lett. 80, 3384 (1998)
[6] M.A. Novotny: Int. J. Mod. Phys. C 10, 1483 (2000); M.A. Novotny: Annual Reviews of Computational Physics IX, D. Stauffer (ed), (World Scientific, Singapore, 2001), p. 153
[7] S.J. Mitchell, M.A. Novotny, J.D. Muñoz: Int. J. Mod. Phys. C 10, 1503 (2000)
FIG. 1. Probability of “growing” and “shrinking” as functions of the magnetization of one half of the pillar for three temperatures: 100 K, 50 K, and 20 K. The left-most crossing shown for a given temperature indicates the saddle point, while the right-most crossing indicates the metastable local free-energy minimum. The crossings associated with the equilibrium global free-energy minimum lie near −1 and are not shown.

FIG. 2. Magnetization along the pillar, $M_z$ at the saddle point as a function of temperature (circle). The magnetization at the saddle point decreases with increasing temperature, and the solid line is a least-squares fit with intercept at 0.860. The error bars are estimated from the range of $M_z$ where $P_{\text{grow}}$ and $P_{\text{shrink}}$ are nearly equal.