Langevin Dynamics of Small Ferromagnetic Particles and Wires

W. Scholz* J. Fidler† D. Süss‡ T. Schrefl§

Abstract

Thermally induced magnetization reversal of small particles is studied using Langevin dynamics. The deterministic Gilbert equation of motion transforms to a stochastic partial differential equation adding a random thermal field to the effective field. The space discretization leads to a system of stochastic differential equations with multiplicative noise which is interpreted in the sense of Stratonovich and solved using the method of Heun. The ellipsoids and wires reverse by rotation if the length of the particle is $l \leq 16$ nm. In longer wires, a nucleus of reverse magnetization forms at one end of the particle. The activation volumes associated with the different reversal modes are calculated from the field dependence of the energy barrier. The calculated activation volume is $v = (2.1 \text{ nm})^3$ for Co-wires with $l > 20$ nm.

Key words: Numerical micromagnetics, Langevin equation, thermal activation, ...

AMS subject classifications: 65C30, 82D40, ...

1 Introduction

The basic structural units of magnetic recording media are particles or grains in the nanometer range. Data is stored in small regions consisting of several grains or particles which have their magnetization oriented in two allowed directions. With increasing recording density the grain size as well as the number of grains or particles forming a bit becomes smaller. With decreasing size of the elementary storage volumes, thermally activated magnetization reversal becomes an important issue in magnetic recording [1]. Thermal activation governs the time dependence of the magnetization. Therefore, thermal effects are relevant to the high speed switching of the magnetization in the write process and to the long term thermal stability of the written bit. The irreversible switching of the particle occurs either by the rotation of the magnetization or by the expansion of a nucleus of reverse magnetization. Both processes are associated with activation energy and may be described using the Arrhenius-Néel model. At finite temperatures, random magnetic field fluctuations help to overcome the reversal barrier [2, 3]. The stochastic fluctuation field arises from the interplay of the lattice vibrations and the magnetization. The probability of irreversible switching is given by the probability per unit time of crossing the energy barrier

$$p = f_0 \exp(-E/k_\mathrm{B}T), \tag{1}$$

where f_0 is a thermal attempt frequency for barrier crossing, k_B denotes the Boltzmann factor, and T is the temperature. The reciprocal of the switching probability is the relaxation time

$$\tau = f_0^{-1} \exp(E/k_\mathrm{B}T). \tag{2}$$

*Institute of Applied and Technical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, A-1040 Vienna Austria, scholz@atp330.tuwien.ac.at

†fidler@tuwien.ac.at

‡suess@atp330.tuwien.ac.at

§thomas.schrefl@tuwien.ac.at

16th IMACS World Congress (© 2000 IMACS)

The attempt frequency f_0 depends on material parameters, like anisotropy, particle shape, and damping [4]. Its value, which ranges from $f_0 = 10^9$ Hz to $f_0 = 10^{12}$ Hz, sets the time scale for thermally assisted magnetization reversal $\tau_0 = f_0^{-1} \approx 1$ ns.

The activation energy and the attempt frequency can be estimated for coherent rotation of the magnetization in single domain particles [3] and the nucleation of reversed domains in thin ferromagnetic wires [4]. The theoretical treatment of thermally activated magnetization reversal for particles with nonuniform demagnetizing field requires to solve the Langevin equation numerically. The Langevin equation follows from the Gilbert equation of motion by adding a random thermal fluctuation field to the effective magnetic field. The deterministic Gilbert equation [5] is believed to describe the physical path of the magnetization towards equilibrium, taking into account gyromagnetic precession and damping. In real systems, thermal fluctuations changes the deterministic motion of the magnetization into a random walk. A theoretical description must treat magnetization reversal as stochastic process. The magnetic properties like the coercive field and the switching time follow from averages over many numerical realizations of the reversal process. Garcia-Palacíos and Lázaro [6] numerically solved the Langevin equation for a single magnetic moment. They reported important phenomena like crossing-back or multiple crossing of the energy barrier which are attributed to the gyromagnetic nature of the system. Zhang and Fredkin [7] used the finite element method to study thermally activated reversal in ellipsoidal particles large enough to show an inhomogeneous reversal process.

Time dependent effects in magnetic media may be described in terms of an activation volume [8]. The activation volume is a parameter to characterize the time dependent and thermal effects and is in general no identifiable physical entity. For coherent rotation, the activation volume is much smaller than the particle size. For nucleation process, the activation volume may be associated with the volume of the nucleus of reverse magnetization [9, 10]. This work estimates energy barriers and activation volumes from numerical results obtained from the simulation of irreversible switching of ellipsoidal and cylindrical particles. A finite element method is used to discretize the Langevin equation. The resulting system of stochastic differential equations with multiplicative noise is interpreted in the sense of Stratonovich [11] and solved using the method of Heun [6]. Section 2 of the paper reviews the micromagnetic and numerical background. Section 3 presents finite element micromagnetic simulations of thermally activated magnetization reversal in ellipsoidal Co-particles and Co-nanowires.

2 Micromagnetic and numerical background

2.1 Langevin micromagnetics

The Langevin equation [5]

$$\frac{\partial \mathbf{J}}{\partial t} = -|\gamma| \mathbf{J} \times (\mathbf{H}_{\text{eff}} + \mathbf{H}_{\text{th}}) + \frac{\alpha}{J_{\text{s}}} \mathbf{J} \times \frac{\partial \mathbf{J}}{\partial t} \tag{3}$$

describes the random motion of the magnetic polarization vector $\mathbf{J} = (J_1, J_2, J_3) = \mu_0 \mathbf{M}$ at finite temperatures. The first term on the right hand side of equation (3) accounts for the gyromagnetic precession, the second term arises from viscous damping. γ is the gyromagnetic ratio of the free electron spin $\gamma = 2.21 \times 10^5$ m/(As); α is the Gilbert damping constant. The critical value of α which minimizes the relaxation time was found to $\alpha = 1$ for athermal [12] and thermally activated reversal [13]. The effective field, $\mathbf{H}_{\text{eff}} = -\delta E_{\text{t}} / \delta \mathbf{J}$, is the variational derivative of the total magnetic Gibbs free energy

$$E_{\text{t}} = \int_{\Omega_{\text{int}}} dV \left\{ \frac{A}{J_{\text{s}}^2} \sum_{i=1}^{3} (\nabla J_i)^2 - \frac{K_{\text{u}}}{J_{\text{s}}^2} (\mathbf{J} \cdot \mathbf{u})^2 - \frac{1}{2} \mathbf{J} \cdot \mathbf{H}_{\text{d}} - \mathbf{J} \cdot \mathbf{H}_{\text{ext}} \right\}. \tag{4}$$

E_{t} is the sum of the exchange energy density, the magneto-crystalline anisotropy energy density, the magnetostatic energy density, and the Zeeman energy density. A is the exchange constant, $J_{\text{s}} = |\mathbf{J}|$ is spontaneous magnetic polarization, K_{u} is the uniaxial anisotropy constant, and $\mathbf{u}$ is the anisotropy direction. $\mathbf{H}_{\text{ext}}$ is the external field. The demagnetizing field $\mathbf{H}_{\text{d}}$ follows from the magnetic scalar potential $\mathbf{H}_{\text{d}} = -\nabla U$ which which satisfies the following boundary value problem

$$\nabla^2 U(\mathbf{r}) = \nabla \cdot \mathbf{J}(\mathbf{r}) / \mu_0 \quad \text{for } \mathbf{r} \in \Omega_{\text{int}}, \tag{5}$$

$$\nabla^2 U(\mathbf{r}) = 0 \quad \text{for } \mathbf{r} \in \Omega_{\text{ext}}, \tag{6}$$

where $\Omega_{\rm int}$ and $\Omega_{\rm ext}$ denote the space within and outside the magnet, respectively. At the boundary Γ the boundary conditions

$$U^{\rm int} = U^{\rm ext}, \quad \left(\nabla U^{\rm int} - \nabla U^{\rm ext}\right) \cdot \mathbf{n} = \left(\mathbf{J} \cdot \mathbf{n}\right)/\mu_0 \tag{7}$$

hold. Here $\mathbf{n}$ denotes the outward pointing normal unit vector on Γ. The magnetic scalar potential is regular at infinity

$$U \propto 1/\mathbf{r} \quad \text{for } \mathbf{r} \to \infty. \tag{8}$$

In order to treat thermally activated processes a stochastic, thermal field, $\mathbf{H}_{\rm th}$, is added to the effective field, $\mathbf{H}_{\rm eff}$. The thermal field is assumed to be a Gaussian random process with the following statistical properties:

$$\langle H_{{\rm th},i}\left(\mathbf{r},t\right)\rangle = 0, \tag{9}$$

$$\langle H_{{\rm th},i}\left(\mathbf{r},t\right) H_{{\rm th},j}\left(\mathbf{r}',t'\right)\rangle = D\delta_{ij}\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right). \tag{10}$$

The average of the thermal field, taken over different realizations, vanishes in each direction i in space. The thermal field is uncorrelated in time and space. The strength of the thermal fluctuations follow from the fluctuation-dissipation theorem [11]:

$$D = \frac{2\alpha k_{\rm B} T}{\gamma J_{\rm s}}. \tag{11}$$

2.2 Space and time discretization

The Cartesian components of the magnetic polarization vector, $\mathbf{J}$, and the magnetic scalar potential, U, are interpolated with piecewise linear functions on a tetrahedral finite element mesh. A hybrid finite element / boundary element method [14] is used to solve equations (5)–(8). The effective field at the node k of the irregular finite element mesh may be approximated using a box scheme:

$$\mathbf{H}_{\rm eff}^{(l)} \approx -\frac{1}{V^{(l)}} \frac{\partial E_{\rm t}\left(\ldots,\mathbf{J}^{(l-1)},\mathbf{J}^{(l)},\mathbf{J}^{(l+1)},\ldots\right)}{\partial \mathbf{J}^{(l)}} \tag{12}$$

where $V^{(l)}$ is the volume associated with the node l. The following conditions hold for the box volumes

$$\sum_l V^{(l)} = \int_{\Omega_{\rm int}} dV \quad \text{and} \quad V^{(l)} \cap V^{(m)} = 0 \quad \text{for } l \neq m. \tag{13}$$

The Langevin equation (3) reduces to three stochastic differential equations for each node of the finite element mesh, using the box scheme (12) to approximate the effective field. The resulting system of $3N$ Langevin type equations with multiplicative noise reads [6]

$$\frac{\partial J_i^{(l)}}{\partial t} = A_i^{(l)} + \sum_k B_{ik}^{(l)} H_{{\rm th},k}^{(l)}\left(t\right), \tag{14}$$

$$A_i^{(l)} = \left[-\frac{|\gamma|}{1+\alpha^2}\mathbf{J}^{(l)} \times \mathbf{H}_{\rm eff}^{(l)} - \frac{\alpha|\gamma|}{1+\alpha^2}\mathbf{J}^{(l)} \times \left(\mathbf{J}^{(l)} \times \mathbf{H}_{\rm eff}^{(l)}\right)\right]_i, \tag{15}$$

$$B_{ik}^{(l)} = -|\gamma| \sum_j \epsilon_{ijk} J_j^{(l)} - \frac{\alpha|\gamma|}{1+\alpha^2}\left(J_i^{(l)} J_k^{(l)} - \delta_{ik} J_{\rm s}^2\right), \tag{16}$$

where the indices i, j, k run over the three space directions, and the index $l = 1, \ldots, N$ runs over the number of nodes. The drift term $A_i^{(l)}$ is the right hand side of the deterministic Landau-Lifshitz-Gilbert equation. The noise term of equation (14) is multiplicative, since the factor, $B_{ik}^{(l)}$, for the stochastic process $H_{{\rm th},k}^{(l)}\left(t\right)$ depends on $\mathbf{J}^{(l)}$. The Heun

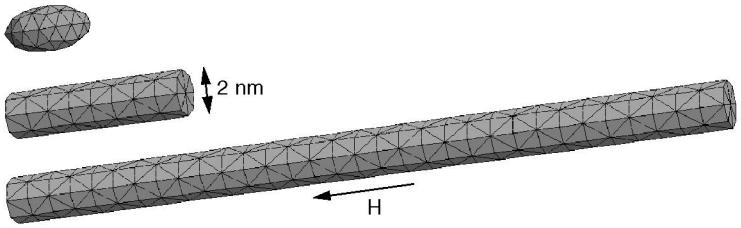

Figure 1: Finite element models of the particles used for the simulation of thermally activated switching.

scheme for equation (14), interpreted in the sense of Stratonovich, reads:

$$\bar{J}_i^{(l)} = J_i^{(l)}(t) + \Delta t A_i^{(l)}\left(\ldots, \mathbf{J}^{(l-1)}, \mathbf{J}^{(l)}, \mathbf{J}^{(l+1)}, \ldots\right) + \sqrt{D^{(l)}\Delta t}\sum_k B_{ik}^{(l)}\left(\mathbf{J}^{(l)}\right)\eta_k^{(l)}, \tag{17}$$

$$J_i^{(l)}(t+\Delta t) = J_i^{(l)}(t) + \frac{\Delta t}{2}\left[A_i^{(l)}\left(\ldots, \mathbf{J}^{(l-1)}, \mathbf{J}^{(l)}, \mathbf{J}^{(l+1)}, \ldots\right) + A_i^{(l)}\left(\ldots, \bar{\mathbf{J}}^{(l-1)}, \bar{\mathbf{J}}^{(l)}, \bar{\mathbf{J}}^{(l+1)}, \ldots\right)\right] + \frac{\sqrt{D^{(l)}\Delta t}}{2}\sum_k\left[B_{ik}^{(l)}\left(\mathbf{J}^{(l)}\right) + B_{ik}^{(l)}\left(\bar{\mathbf{J}}^{(l)}\right)\right]\eta_k^{(l)}, \tag{18}$$

$$D^{(l)} = \frac{2\alpha k_\mathrm{B} T}{\gamma J_\mathrm{s} V^{(l)}}, \tag{19}$$

where $\eta_k^{(l)}$ are independent Gaussian variables of mean 0 and variance 1.

The time step, $(\gamma J_\mathrm{s}/\mu_0)\,\Delta t = 10^{-3}$, was used for the calculations. The mesh size was $h \leq 0.3\, l_\mathrm{ex}$, where l_ex is the exchange length, $l_\mathrm{ex} = \sqrt{2\mu_0 A/J_\mathrm{s}^2}$.

3 Numerical examples

Thermally activated reversal was simulated for ellipsoidal and cylindrical particles. The intrinsic magnetic properties of Co ($J_\mathrm{s} = 1.76$ T, $A = 1.3 \times 10^{-11}$, $K_\mathrm{u} = 6.8 \times 10^5$ J/m^3) and a Gilbert damping constant $\alpha = 1$ were assumed for the calculations. The particles have a diameter $d = 2$ nm and an aspect ratio of 2:1, 4:1, and 16:1, respectively. Figure 1 shows the surface of the finite element mesh for the different particles.

The extension of the ellipsoid is comparable with the exchange length, l_ex. Thus it is expected to reverse by coherent rotation. According to the Stoner-Wohlfarth theory the field dependence of the activation energy, $E(H)$, is [8]:

$$E(H) = KV\left(1 - \frac{H}{H_\mathrm{K}}\right)^2, \tag{20}$$

$$K = K_\mathrm{u} + \frac{J_\mathrm{s}^2}{2\mu_0}\left(N_\perp - N_\parallel\right), \tag{21}$$

$$H_\mathrm{K} = \frac{2K}{J_\mathrm{s}}. \tag{22}$$

K is the effective anisotropy constant taking into account the shape of the particle; V is the particle volume; $N_\parallel$ and $N_\perp$ are the demagnetizing factors parallel and normal to the symmetry axis. A fit of the calculated relaxation time τ using equation (2) provides the energy barrier from numerical experiments. Figure 2 shows that $\ln\tau$ versus $1/(k_\mathrm{B}T)$ forms a straight line in the investigated field and temperature range. The cylindrical particle with an aspect ratio of 4:1 shows a similar behavior.

The formation of a nucleus of reverse magnetization at the end starts the reversal process in the nanowire with aspect ratio 16:1. Using an analytical model, Braun [15] estimated the energy barrier for the nucleation in a nanowire

$$E(H) = (8/3)r^2\pi\sqrt{AK}\left(1 - \frac{H}{H_\mathrm{K}}\right)^{3/2}, \tag{23}$$

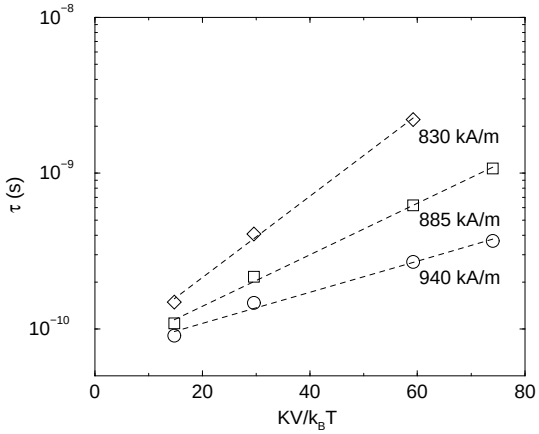

Figure 2: Relaxation time as a function of $KV/(k_{\mathrm{B}}T)$ for different applied fields.

where r is the radius of the wire. Figure 3 gives the energy barriers, $E(H)$, as a function of the field for the ellipsoid and the nanowire with the aspect ratio 16:1. For the ellipsoid, the numerical values for the activation energy agree perfectly with the analytical results given by equation (20). For the nanowire, the energy barriers according to equation (23) exceed the numerical results by about a factor of 2 to 3. This may be attributed to inhomogeneous magnetic states across the wire, which are neglected in the analytical model. These magnetic inhomogeneities arise from thermal fluctuations and the highly nonuniform demagnetizing field near edge at the ends of the wire.

An effective activation volume can be derived under the assumption that the activation energy corresponds to the energy of the nucleus of reverse magnetization

$$E(H) = -vJ_{\mathrm{s}}H. \tag{24}$$

Then the activation volume, v, can be derived from the slope of $E(H)$

$$v = -\frac{1}{J_{\mathrm{s}}}\frac{\partial E}{\partial J}. \tag{25}$$

Figure 3 clearly shows that the activation energy for the wire depends linearly on the applied field within the investigated field range. This behavior indicates that magnetization reversal occurs by the formation of a nucleus of reverse magnetization [8]. The analysis of the calculated magnetization configurations as a function of time confirms a nucleation mechanism. The magnetization starts to reverse within a finite volume at one end of the wire. Once a reversed domain has formed, it expands over along the entire wire. The calculated activation volume, $v = (2.1\ \mathrm{nm})^3$, was found to be independent of the length of the nanowire. Li and co-worker [10] obtained a similar result from magnetic measurements on α-Fe nanowires.

4 Summary

The Langevin equation describes the random motion of the magnetization towards equilibrium. A finite element method and the method of Heun are applied to discretize the stochastic partial differential equation in space and in time. The numerical results obtained for elongated Co-particles show that magnetic nanowires which exceed a critical length switch via a nucleation mechanism. Magnetization reversal starts at one end and proceeds along the entire wire. The volume of the initially formed nucleus is independent of the length of the wire.

5 Acknowledgements

The authors thank Denise Hinzke, Ulrich Nowak, and Andreas Lyberatos for helpful discussions. This work was supported by the Austrian Science Fund (Y132-PHY, 13260 TEC) and the European COST P3 action.

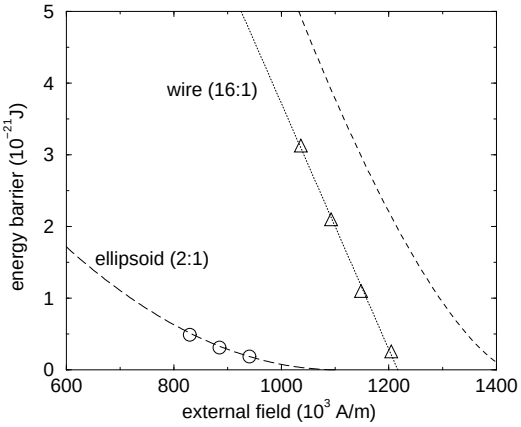

Figure 3: Activation energy as a function of the applied field. The open symbols give the numerical values. The dashed lines give the analytical results according to equation (20) and (23). The dotted line is linear fit of the numerical values for the nanowire.

References

[1] D. Weller, A. Moser, *Thermal effect limits in ultrahigh-density magnetic recording*, IEEE Trans. Magn., 35 (1999), pp. 4423–4439.

[2] L. Néel, *Théorie du trainage magnétique*, Ann. Geophys., 5 (1949), pp. 99–136.

[3] W. F. Brown, Jr., *Thermal fluctuations of a single-domain particle*, Phys. Rev., 130 (1963), pp. 1677–1686.

[4] H.-B. Braun, *Kramers's rate theory, broken symmetries, and magnetization reversal (invited)*, J. Appl. Phys., 76 (1994), pp. 6310–6315.

[5] W.F. Brown, Jr., *Micromagnetics*, Wiley, New York, 1963.

[6] J. L. García-Palacios, F. J. Lázaro, *Langevin-dynamics study of the dynamical properties of small magnetic particles*, Phys. Rev. B, 58 (1998), pp. 14937–14958.

[7] K. Zhang, D. R. Fredkin *Stochastic dynamic micromagnetic study of fine particles*, J. Appl. Phys., 85 (199), pp. 5208–5210. 1999

[8] R. Street, D.C. Crew, *Fluctuation aftereffects in magnetic materials*, IEEE Trans. Magn., 35 (1999), pp. 4407–4413.

[9] E.D. Boerner, H.N. Bertram, *Dynamics of thermally activated reversal in nonuniformly magnetized single particles*, IEEE Trans. Magn., 33 (1997), pp. 3052–3054.

[10] F.L. Li, R.M. Metzger, W.D. Doyle, *Influence of particle size on the magnetic viscosity and activation volume of α-Fe nanowires in alumite films*, IEEE Trans. Magn., 33 (1997), pp. 4423–4439.

[11] N.G. van Kampen, *Stochastic processes in physics and chemistry*, Norh-Holland, Amsterdam, 1992. VCH, Basel, 1990.

[12] R. Kikuchi, *On the minimum of magnetization reversal time*, J. Appl. Phys., 27 (1956), pp. 1352-1357.

[13] D. Hinzke, U. Nowak, *Magnetization switching in nanowires: Monte Carlo study with fast Fourier transformation for dipolar fields*, J. Magn. Magn. Mater., to appear.

[14] D.R. Fredkin, T.R. Koehler, *Hybrid method for computing demagnetizing fields*, IEEE Trans. Magn., 26 (1990), pp. 415–417.

[15] H.-J. Braun, *Nucleation in ferromagnetic nanowires—magnetostatics and topology*, J. Appl. Phys., 85 (1999), pp. 6172–6174.