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Micromagnetic simulation of thermally activated switching in fine particles

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Abstract

Effects of thermal activation are included in micromagnetic simulations by adding a random thermal field to the effective magnetic field. As a result, the Landau–Lifshitz equation is converted into a stochastic differential equation of Langevin type with multiplicative noise. The Stratonovich interpretation of the stochastic Landau–Lifshitz equation leads to the correct thermal equilibrium properties. The proper generalization of Taylor expansions to stochastic calculus gives suitable time integration schemes. For a single rigid magnetic moment the thermal equilibrium properties are investigated. It is found, that the Heun scheme is a good compromise between numerical stability and computational complexity. Small cubic and spherical ferromagnetic particles are studied. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Thermal activation; Langevin equation; Heun scheme; Micromagnetics

1. Introduction

Micromagnetic simulations of permanent magnetic materials reveal the details of the magnetization distribution and dynamic magnetization reversal processes. A knowledge of the dynamic behaviour is of great importance for the design of future magnetic recording media. When the desired magnetization switching frequencies reach an order of magnitude, which is comparable to the intrinsic relaxation time of the media, the switching dynamics have to be investigated in more detail.

The paper is organized as follows: In Section 2 we extend the theory to take into account thermal

perturbations and find a stochastic differential equation. In Section 3 stochastic calculus is summarized and we find the quantitative properties of the thermal field. For the numerical solution of our Langevin equation we develop suitable numerical integration schemes in Section 4. Then we study the behaviour of a rigid magnetic moment in Section 5 before we go on to cubic and spherical particles in Sections 6 and 7, respectively, which are discretized into smaller computational cells.

2. The stochastic Landau–Lifshitz equation

Thermal activation is introduced in the Landau–Lifshitz equation by a stochastic thermal field \mathbf{H}_{th} , which is added to the effective field. It accounts for

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the effects of the interaction of the magnetization with the microscopic degrees of freedom (e.g. phonons, conducting electrons, nuclear spins, etc.), which cause fluctuations of the magnetization. This interaction is also responsible for the damping, since fluctuations and dissipation are related manifestations of one and the same interaction of the magnetization with its environment.

Since a large number of microscopic degrees of freedom contribute to this mechanism, the thermal field is assumed to be a Gaussian random process with the following statistical properties

$$\langle H_{\text{th},i}(t) \rangle = 0. \quad (1)$$

This means, that the average of the thermal field taken over different realizations vanishes in each direction $i \in \{x, y, z\}$ of space. The second moment, or variance, is given by

$$\langle H_{\text{th},i}(t)H_{\text{th},j}(t') \rangle = 2D\delta_{ij}\delta(t - t'). \quad (2)$$

This equation is a manifestation of the fluctuation–dissipation theorem. It relates the strength of the thermal fluctuations (the variance $2D$ of the thermal field) to the dissipation due to the damping of our system [1]. The Kronecker δ expresses the assumption, that the different components of the thermal field are uncorrelated, whereas the Dirac δ expresses, that the autocorrelation time of the thermal field is much shorter than the response time of the system (“white noise”).

After adding the thermal field we get the *stochastic Landau–Lifshitz equation*

$$\frac{d\mathbf{M}}{dt} = -\gamma'\mathbf{M} \times (\mathbf{H}_{\text{eff}} + \mathbf{H}_{\text{th}}) - \frac{\alpha\gamma'}{M_s}\mathbf{M} \times (\mathbf{M} \times (\mathbf{H}_{\text{eff}} + \mathbf{H}_{\text{th}})), \quad (3)$$

where

$$\gamma' = \left| \frac{\gamma}{1 + \alpha^2} \right|, \quad \gamma = \frac{\mu_0 g |e|}{2m_e}.$$

Rearrangement to separate deterministic from stochastic contributions gives

$$\frac{d\mathbf{M}}{dt} = -\gamma'\mathbf{M} \times \mathbf{H}_{\text{eff}} - \frac{\alpha\gamma'}{M_s}\mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}}) - \gamma'\mathbf{M} \times \mathbf{H}_{\text{th}} - \frac{\alpha\gamma'}{M_s}\mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{th}}), \quad (4)$$

which reveals, that it is a Langevin type stochastic differential equation with multiplicative noise.

To keep the notation simple, we rewrite Eq. (4) by substituting

$$A_i(\mathbf{M}, t) = \left[-\gamma'\mathbf{M} \times \mathbf{H}_{\text{eff}} - \frac{\alpha\gamma'}{M_s}\mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}}) \right]_i \quad (5)$$

and

$$\begin{aligned} B_{ik}(\mathbf{M}, t) &= -\gamma'\varepsilon_{ijk}M_j - \frac{\alpha\gamma'}{M_s}\varepsilon_{ijn}M_j\varepsilon_{nmk}M_m \\ &= -\gamma'\varepsilon_{ijk}M_j - \frac{\alpha\gamma'}{M_s}(\delta_{im}\delta_{jk} - \delta_{ik}\delta_{jm})M_jM_m \\ &= -\gamma'\varepsilon_{ijk}M_j - \frac{\alpha\gamma'}{M_s}(M_iM_k - \delta_{ik}M^2), \end{aligned} \quad (6)$$

where we have written M^2 for $M_{jj} = M_s^2$. We have used the Einstein summation convention and we will do so in the following. The outer products have been rewritten with the totally antisymmetric unit tensor ε (Levi–Civita symbol).

Hence, we can simplify the stochastic Landau–Lifshitz equation (3) and get

$$\frac{dM_i}{dt} = A_i(\mathbf{M}, t) + B_{ik}(\mathbf{M}, t)H_{\text{th},k}(t). \quad (7)$$

This is the general form of a system of Langevin equations with multiplicative noise, because the multiplicative factor $B_{ik}(\mathbf{M}, t)$ for the stochastic process $H_{\text{th},k}(t)$ is a function of \mathbf{M} .

3. Stochastic calculus

As we have seen in Section 2, the effect of thermal activation can be introduced in the formalism of micromagnetics by adding a random fluctuation field to the effective magnetic field. A trajectory of the magnetization can be obtained by integrating the equation of motion. However, in addition to the well-known deterministic terms we also have a stochastic contribution.

It is assumed that the thermal activation is caused by perturbations of very high frequency. “Very high” means in this case that the frequency is well above the typical precession frequency of the magnetization vector. Thus, the fluctuating

field, which is used to simulate the effect of thermal activation, is represented by a stochastic process. It is assumed to be Gaussian white noise, because the fluctuations emerge from the interaction of the magnetization with a large number of independent microscopic degrees of freedom with equivalent stochastic properties (e.g. phonons, conducting electrons, nuclear spins, etc.) [2]. As a result of the central limit theorem, the fluctuation field is Gaussian distributed.

Let us assume a one-dimensional stochastic differential equation with *multiplicative* noise [3]

$$\frac{dX(t)}{dt} = a(X(t), t) + b(X(t), t) \eta(t). \tag{8}$$

The increment dX during a short time interval dt is given by

$$dX(t) = \int_t^{t+dt} a(X(t'), t') dt' + \int_t^{t+dt} b(X(t'), t') \eta(t') dt'.$$

The second term, which is a stochastic integral, has to be investigated in more detail. We can evaluate the integrand at the beginning of the interval $[t, t + dt]$, multiply it by the length of the interval and use the result as the increment for small dt . Thus, we obtain

$$dX(t) = a(X(t), t) dt + b(X(t), t) \eta(t) \sqrt{dt},$$

where $\eta(t)$ is a standard Gaussian random variable at each discrete time step with

$$\langle \eta(t) \eta(t') \rangle = \delta(t, t').$$

However, we could also evaluate the integrand b at any other time t' in the interval $[t, t + dt]$ and at

$$\begin{aligned} \bar{X}(t) &= (1 - \alpha)X(t) + \alpha X(t + dt) \\ &= (1 - \alpha)X(t) + \alpha(X(t) + dX(t)) \\ &= X(t) + \alpha dX(t). \end{aligned} \tag{9}$$

In this general case we get for the increment $dX(t)$ an implicit expression

$$dX(t) = a(\bar{X}(t), t) dt + b(X(t) + \alpha dX(t), t) \eta(t) \sqrt{dt}.$$

With the abbreviation $b' = \partial b(X, t) / \partial X$ we get

$$\begin{aligned} b(X(t) + \alpha dX(t), t) \eta(t) \sqrt{dt} &= b(X(t), t) \eta(t) \sqrt{dt} \\ &+ \alpha b'(X(t), t) dX(t) \eta(t) \sqrt{dt} + \dots \end{aligned} \tag{10}$$

$$\begin{aligned} b(X(t) + \alpha dX(t), t) \eta(t) \sqrt{dt} &= b(X(t), t) \eta(t) \sqrt{dt} \\ &+ \alpha b'(X(t), t) b(X(t), t) \eta^2(t) dt \\ &+ O(dt^{3/2}). \end{aligned} \tag{11}$$

Finally, we get for the increment $dX(t)$

$$dX(t) = [a(X(t), t) + \alpha b'(X(t), t) b(X(t), t) \eta^2(t)] dt + b(X(t), t) \eta(t) \sqrt{dt}. \tag{12}$$

In this equation we find an additional drift term, which contains α and $\eta^2(t)$. The latter can be replaced by 1 for terms up to the order of dt . Depending on the choice of α and the interpretation of the integral, we get different drift terms. If we set $\alpha = 0$, we get

$$dX(t) = a(X(t), t) dt + b(X(t), t) \eta(t) \sqrt{dt} \tag{13}$$

and we call it the *Itô interpretation* of the stochastic differential equation

$$\dot{X}(t) = a(X(t), t) + b(X(t), t) \eta(t). \tag{14}$$

For $\alpha = 1/2$, we get

$$dX(t) = \left[a(X(t), t) + \frac{1}{2} b'(X(t), t) b(X(t), t) \right] dt + b(X(t), t) \eta(t) \sqrt{dt} \tag{15}$$

and we call it the *Stratonovich interpretation*, which is indicated by writing

$$\dot{X}(t) = a(X(t), t) + b(X(t), t) \circ \eta(t). \tag{16}$$

Thus, we have to distinguish between the interpretation of a stochastic differential equation and the version, in which it is written. The stochastic differential equation (16) can be written in an Itô version using Eq. (15) as

$$\begin{aligned} \dot{X}(t) &= a(X(t), t) + \frac{1}{2} b(X(t), t) b'(X(t), t) \\ &+ b(X(t), t) \eta(t), \end{aligned} \tag{17}$$

where we find the noise induced drift term

$$\frac{1}{2}b(X(t), t)b'(X(t), t). \tag{18}$$

Reversely, Eq. (14) can be written in a Stratonovich version as

$$\begin{aligned} \dot{X}(t) &= a(X(t), t) - \frac{1}{2}b(X(t), t)b'(X(t), t) \\ &\quad + b(X(t), t) \circ \eta(t) \\ &= \bar{a}(X(t), t) + b(X(t), t) \circ \eta(t). \end{aligned} \tag{19}$$

Due to the different drift terms, the two interpretations yield different dynamical properties [3]. Itô calculus is commonly chosen on certain mathematical grounds, since rather general results of probability theory can then be employed. On the other hand, white noise is usually an idealization of physical (coloured) noise with short autocorrelation time, in which case the two time covariance function is given by

$$\langle \eta(t)\eta(t + \tau) \rangle = \frac{\sigma^2}{2m} e^{-m|\tau|}$$

with a short time constant m^{-1} .

The Wong–Zakai Theorem [4] then says, that in the formal zero-correlation-time limit

$$\sigma \rightarrow \sigma m, \quad m \rightarrow \infty$$

the coloured noise becomes white noise and we obtain the Stratonovich interpretation for the stochastic differential equation. The results coincide with those obtained in the limit of fluctuations with finite autocorrelation time. Therefore, Stratonovich calculus is usually preferred in physical applications.

4. Stochastic time integration

The mere translation of a numerical scheme valid for deterministic differential equations does not necessarily yield a proper scheme in the stochastic case. Depending on the selected deterministic scheme its unconditional translation might converge to an Itô solution, to a Stratonovich solution, or to none of them. Even if the scheme converges in the context of stochastic calculus, the order of convergence is usually lower than that of the deterministic scheme. This has to

be considered, when deciding for the discretization time step.

The stochastic Landau–Lifshitz equation (7) may be effectively solved using the Heun method. The improved Euler or Heun method [2] is an example of a predictor–corrector method. The predictor is given by a simple Euler type integration. If we consider the Langevin equation (7), the predictor is

$$\bar{M}_i = M_i(t) + A_i(\mathbf{M}, t)\Delta t + B_{ik}(\mathbf{M}, t)\Delta W_k, \tag{20}$$

where Δt is the discretization time step and

$$\Delta W_k = \int_t^{t+\Delta t} H_{\text{th},k}(t') dt'$$

are Gaussian random numbers, whose first two moments are given by

$$\langle \Delta W_k \rangle = 0, \quad \langle \Delta W_k \Delta W_l \rangle = 2D\delta_{kl}\Delta t,$$

where $2D$ is the variance of the stochastic thermal field (2). The Heun scheme is then given by

$$\begin{aligned} M_i(t + \Delta t) &= M_i(t) + \frac{1}{2}[A_i(\bar{\mathbf{M}}, t + \Delta t) + A_i(\mathbf{M}, t)]\Delta t \\ &\quad + \frac{1}{2}[B_{ik}(\bar{\mathbf{M}}, t + \Delta t) + B_{ik}(\mathbf{M}, t)]\Delta W_k. \end{aligned} \tag{21}$$

The stochastic Heun scheme converges in quadratic mean to the solution of the general system of Langevin equations (7) when interpreted in the sense of Stratonovich.

To conclude, there are two main reasons for the choice of the Heun scheme for the numerical integration of the stochastic Landau–Lifshitz equation: First, the Heun scheme yields Stratonovich solutions of the stochastic differential equations without alterations to the deterministic drift term. Secondly, the deterministic part of the differential equations is integrated with a second-order accuracy in Δt , which renders the Heun scheme numerically more stable than Euler type schemes.

The stochastic Landau–Lifshitz equation is discretized either with a finite difference or a finite element method depending on the particle geometry.

5. Rigid magnetic moment

The time step dependence of the numerical integration schemes has been investigated by simulating a single rigid magnetic moment. The material parameters were chosen as $M_s = 1\,281\,197\text{ A/m}$, $K_1 = 6.9 \times 10^6\text{ J/m}^3$, $\alpha = 0.1$, and $V = 1\text{ nm}^3$. The effective field, which is just the anisotropy field, is then given by

$$H_{\text{ani}} = \frac{2K_1}{\mu_0 M_s} = 8571\text{ kA/m}.$$

For the time for one full precession of the magnetization vector we obtain

$$T = \frac{1}{f} = \frac{2\pi}{\omega} = \frac{2\pi}{\gamma H_{\text{ani}}} = 3.32\text{ ps},$$

where $\omega = \gamma H$ is the Larmor frequency. The average magnetization in thermal equilibrium according to

$$\begin{aligned} \langle M_z \rangle &= \frac{\int_0^1 \exp(\chi z^2) z \, dz}{\int_0^1 \exp(\chi z^2) \, dz} \\ &= \frac{1/2\chi[\exp(\chi) - 1]}{\sqrt{\pi/2}\text{erf}(1)}, \end{aligned} \quad (22)$$

where $\text{erf}(x)$ denotes the error function and

$$\chi = \frac{K_1 V}{k_B T}$$

is given in Table 1. Eq. (22) follows from the probability density of the magnetization angle for a single-domain Stoner–Wohlfarth particle [2].

Fig. 1 compares the time step dependence of the average magnetization obtained with the Heun method and the Milshtein scheme. The Milshtein scheme [5] is the generalization of the deterministic Euler method taking into account the multiplicative noise term in Stratonovich interpretation.

Table 1

Average component of the magnetization parallel to the magneto-crystalline anisotropy axis for different temperatures calculated for a single spin

Temperature (K)	$\langle M_z \rangle / M_s$
10	0.98979
50	0.94268
200	0.71976

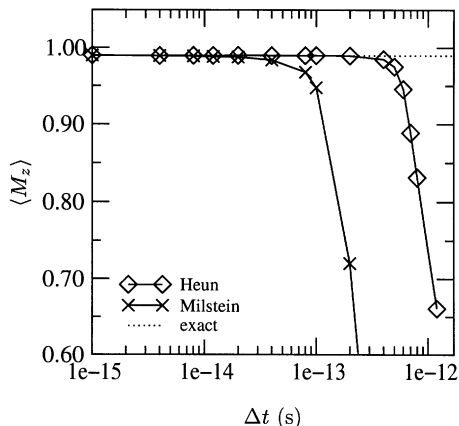


Fig. 1. Time step dependence of numerical integration schemes.

With the Milshtein scheme we find the correct values for time steps smaller than 0.01 ps, which is about 1/300 of the precession time. The Heun scheme is suitable for time steps, which are 10 times larger, because it has a higher order of convergence. As a rule, the discretization time step should be at most 1/30th of the precession time of the magnetization vector in the effective field.

6. Cubic particles

Cubes are easy to handle with finite difference packages, because they have no curved boundaries. The results are compared with those of Nakatani et al. [6], whose material parameters have been used. They are chosen as $M_s = 0.4 \times 10^6\text{ A/m}$ and $K_1 = 2 \times 10^5\text{ J/m}^3$, $A = 1 \times 10^{-11}\text{ J/m}$. In all simulations the number of switching events was counted for at least 100 ns up to 1 μs and the results extrapolated to 1 μs .

Figs. 2 and 3 show the time dependence of the magnetization for a cubic particle of 32 nm edge length at 300 K. The magnetization fluctuates in the energy minimum around ± 1 . From time to time reversal processes occur when the magnetization crosses the energy barrier and switches to the other energy minimum. The probability per unit time, that M_z jumps over the energy barrier E in

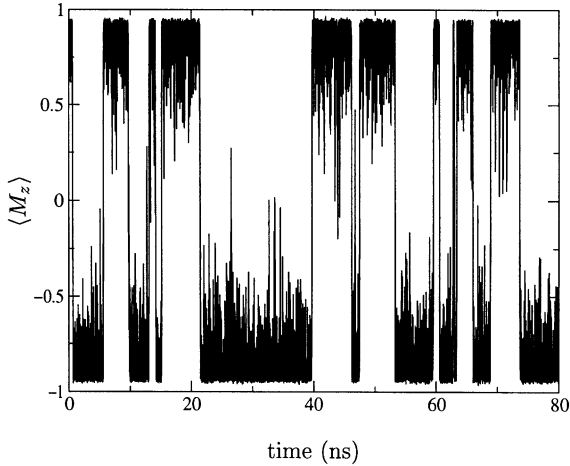


Fig. 2. Magnetization reversal of a cubic particle for $\alpha = 1$.

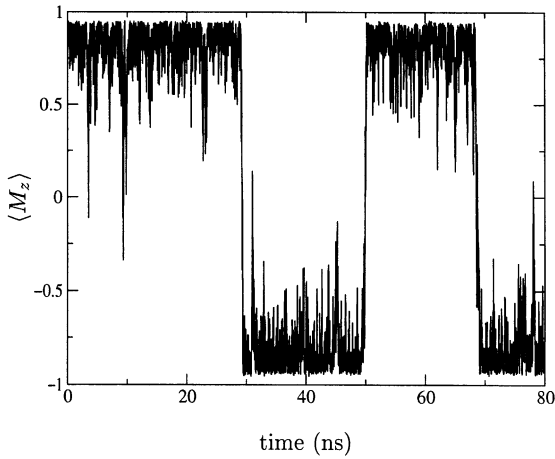


Fig. 3. Magnetization reversal of a cubic particle for $\alpha = 0.1$.

thermal equilibrium, is proportional to

$$\exp\left(-\frac{E}{k_B T}\right).$$

We consider a single energy barrier model and take only the anisotropy into account. The reciprocal of the switching probability is the relaxation time τ which can thus be written in the form of the Arrhenius–Néel law [7]

$$\frac{1}{\tau} = f_0 \exp\left(-\frac{K_1 V}{k_B T}\right), \quad (23)$$

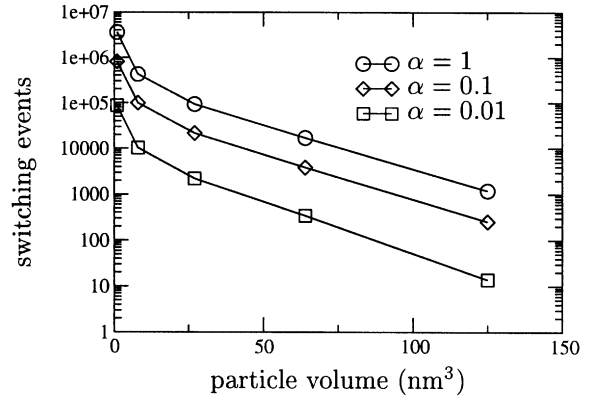


Fig. 4. Dependence on damping constant for different particle sizes.

where f_0 is the characteristic dynamic frequency. The original estimation of Néel was $f_0 \approx 10^9 \text{ s}^{-1}$, but recently it has become more customary to take $f_0 \approx 10^{10} \text{ s}^{-1}$ up to $f_0 \approx 10^{12} \text{ s}^{-1}$. Fig. 4 gives the number of switching events as a function of the particle size calculated for different damping constants α .

If we fit the data of the smallest time step in the linear region of Fig. 4 ($\alpha = 1$) with the Arrhenius–Néel law, we find a characteristic dynamic frequency of $f_0 = 3.5 \times 10^{11}$. The exponent is $-4.7 \times 10^{25} \text{ V}$ and it is in good agreement with the value

$$-\frac{K_1}{k_B T} = -4.8 \times 10^{25} \text{ m}^3$$

which we would expect for a single (anisotropy) energy barrier.

Brown [8] has derived an analytic expression for the high-energy-barrier approximation of the attempt frequency (here for SI units)

$$f_0 = \frac{\alpha \gamma \mu_0}{1 + \alpha^2} \sqrt{\frac{H_k^3 M_2 V \mu_0}{2\pi k_b T}} \times (1 - (H/H_k)^2)(1 + H/H_k). \quad (24)$$

For the material parameters given above we find with

$$\gamma = 1.7588 \times 10^{11} \text{ 1/Ts}, H_k = \frac{2K_1}{\mu_0 M_s} = 795 \text{ kA/m}$$

at zero external field $H = 0$ an attempt frequency of 1.97×10^{12} . This result differs by a factor of 4

from the numerically found value given above. The reason is that the cubic particle has internal degrees of freedom and the energy barriers might not be high enough for the approximation to be valid.

7. Spherical particles

The mechanism of thermally activated magnetization switching in small spherical ferromagnetic particles has been investigated using the finite element method. The material parameters have been chosen as $M_s = 0.4 \times 10^6$ A/m, $A = 3.64 \times 10^{-12}$ J/m, $\alpha = 1$, and a radius $R = 11.5$ nm, which gives a volume of 6.37×10^{-24} m³. The finite element mesh consists of 115 nodes and 440 elements. The mean diameter of the finite elements is 3 nm. This discretization is sufficient, if we assume a rather low magnetocrystalline anisotropy. For $K_1 = 2 \times 10^5$ J/m³ we find a typical domain wall width of

$$\delta = \pi \sqrt{\frac{A}{K_1}} \approx 57 \text{ nm.}$$

The initial magnetization is homogeneous and parallel to the easy axis of the particle. Its magnetization distribution is destabilized by an external magnetic field, which is parallel to the easy axis but antiparallel to the initial magnetization. Since this is a metastable state, we can expect the particle to overcome the energy barrier, which is called the *activation energy*, and reverse its magnetization after some time. In contrast to Monte Carlo simulations [9,10], we obtain not only information about the dynamical behaviour, but also about the switching times. The metastable lifetime (or relaxation time) τ is defined as the time, which passes from the initially saturated state $M_z(\tau) = M_s$ until $M_z(\tau) = 0$.

In order to measure the metastable lifetime a large number of simulations have been performed for each set of parameters. After 200 measurements a waiting time histogram was obtained. The integral of this histogram is proportional to the switching probability $P(t)$, that is the probability, that the particle has switched after a certain time. However, it is more common to draw graphs for

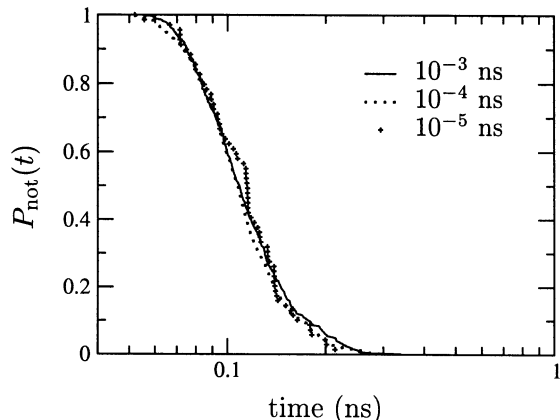


Fig. 5. Probability of not switching for different time step sizes.

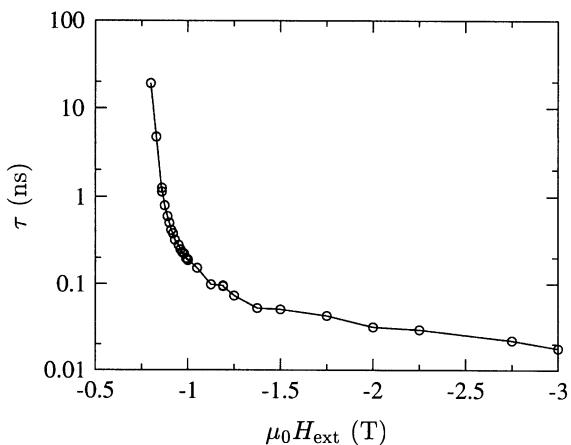


Fig. 6. Dependence of the metastable lifetime on the external field.

the (rescaled) probability of not switching (Fig. 5) $P_{\text{not}}(t) = 1 - P(t)$.

The magnetization reversal process can happen in different reversal modes. In a particle with low anisotropy (or at low external fields) the magnetization rotates coherently, which means, that the magnetization remains almost homogeneous during the reversal process except for small thermal fluctuations. If the anisotropy (or the external field) is increased, it becomes favourable to form a nucleus of reverse magnetization. Thus, a droplet nucleates near the surface and expands until the magnetization is completely reversed.

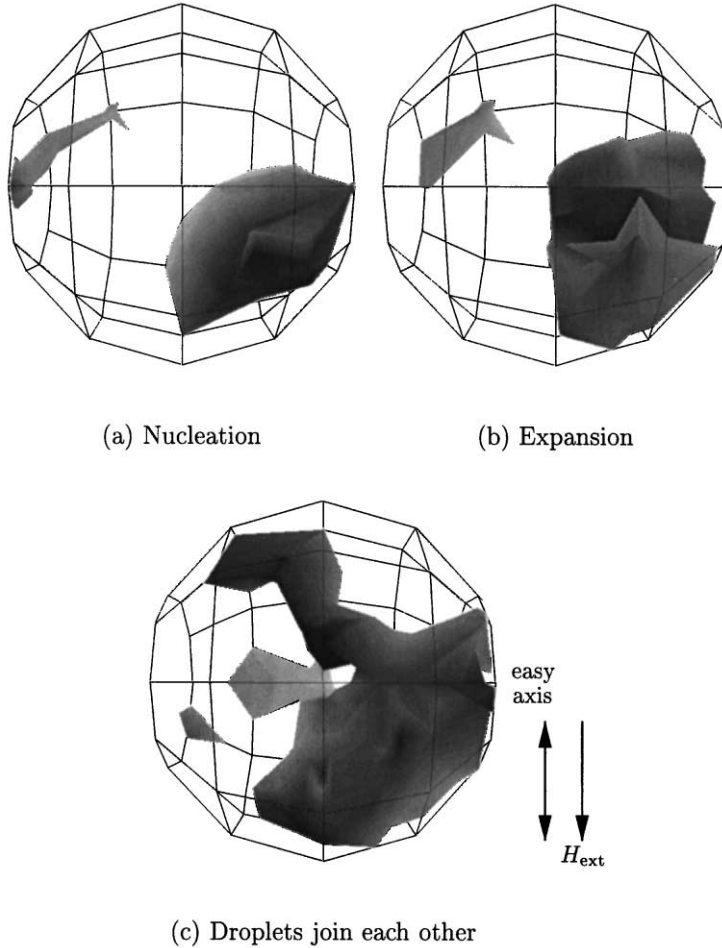


Fig. 7. Nucleation of a reverse domain at an external field of -1.5 T .

The external field has been chosen to be comparable to the anisotropy field

$$H_{\text{ani}} = \frac{2K_1}{\mu_0 M_s}$$

Fig. 6 shows, how the metastable lifetime decreases, when the external field is increased (the solid line is only a guide to the eye). $K_1 = 2 \times 10^5 \text{ J/m}^3$ and $\mu_0 H_{\text{ext}} = \mu_0 H_{\text{ani}} = 1 \text{ T}$ have been used at a temperature of 500 K .

Two different regimes, characterized by different magnetization reversal processes can be identified. For external fields lower than the anisotropy field ($|H| < H_{\text{ani}}$), magnetization reversal by coherent rotation is found. For high external fields

($|H| \gg H_{\text{ani}}$), the reversal process is driven by the expansion of a nucleus of reverse magnetization.

Since the external field is higher than the anisotropy field, there is no energy barrier any more. The system approaches the global energy minimum in a random walk. This happens by the nucleation and expansion of a reverse domain (Fig. 7).

8. Conclusions

The Langevin dynamics approach proved to be a suitable method to model the effects of thermal activation in magnetic materials.

- Simulations of a single rigid magnetic moment showed, that the Heun scheme is a suitable time integration method, which allows a time step size one order of magnitude larger than that for the Milshtein scheme. Moreover the stochastic Landau–Lifshitz equation of motion in Stratonovich interpretation leads to the correct thermal equilibrium properties.
- The magnetization switching behaviour found for a small cubic particle is identical for the finite difference and finite element model, even though their method of calculating the effective field is substantially different. The finite element method is better suited for the simulation of particles with curved or very complex surfaces and allows the modeling of polycrystalline grain structures.
- For a small cubic ferromagnetic particle, magnetization reversal by coherent rotation has been found. As a result, its switching dynamics is well described by the Arrhenius–Néel law for reversal over a single energy barrier.
- Complex magnetization reversal mechanisms have been found for small spherical magnetic particles. The magnetocrystalline anisotropy and the strength of the external field determine the switching mechanism and two different regimes have been identified. For fields, which are smaller than the anisotropy field, magnetization by coherent rotation has been observed.

If the external field is significantly higher than the anisotropy field nucleation is the driving reversal process.

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