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Thermal switching field distribution of a single domain particle for field-dependent attempt frequency

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We present an analytical derivation of the switching field distribution (SFD) at finite temperature for a single domain particle from the Néel-Brown model in the presence of a linearly swept magnetic field. By considering the field dependence of the attempt frequency f_0 in the rate equation, we find enhancement of coercivity compared to models using constant f_0. The contribution of thermal fluctuations to the standard deviation of the switching field H_C derived here reaches values of 10% H_C. Considering this contribution, which has been neglected in previous work, is important for the correct interpretation of measurements of switching field distributions.
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I. INTRODUCTION

Magnetic single domain particles are found in various applications working at room temperature such as the grains of magnetic recording media in hard disk drives or nanoparticles used for medical applications, e.g., drug delivery and hyperthermia. The switching behavior of a single domain magnetic particle with uniaxial anisotropy is strongly influenced by the presence of thermal fluctuations, which help the magnetization to overcome the energy barrier that is separating the two stable magnetization states. This leads to an effective reduction of the coercive field at finite temperatures, which depends on the time scale of the experiment. The detailed knowledge of coercivity as a function of measurement time and temperature is important for extracting material properties from experimental data. Sharrock[1] gave an analytical expression for a pulsed field experiment

$$H_C(t) = H_K\left[1 - \sqrt{\frac{1}{\beta}\ln(f_0 t)}\right], \tag{1}$$

where $\beta = KV/k_BT$ (with anisotropy constant K, sample volume V, Boltzmann's constant $k_B = 1.38 \times 10^{-23}$ J/K, and temperature T) is the thermal stability ratio, f_0 is the attempt frequency at zero external field, and t is the measurement time. Others[2–5] have also succeeded in deriving expressions for experiments in which an external field is swept at a constant rate. In the following, we present an explicit analytical derivation of the probability density function (PDF) describing the switching field distribution (SFD) arising from the presence of thermal fluctuations exclusively. Knowing the SFD and its relevant parameters is of great importance for the optimization of recording media as well as sensing technologies for magnetic fields as described in a former publication.[6]

According to the Néel-Brown model,[7,8] the magnetization's spatial orientation fluctuates due to random magnetic fields present at finite temperature. This results in thermal instability and forces the magnetization to switch between its two stable orientations separated by an energy barrier ΔE at a rate[9]

$$f = f_0 \exp\left(-\frac{\Delta E}{k_BT}\right). \tag{2}$$

Equation (2) is known as the Arrhenius-Néel law with the attempt frequency f_0, which is usually treated as a constant. However, as already shown by Brown,[8] even for the very simple case of a single domain particle with uniaxial anisotropy and a field H applied parallel to its easy axis, the attempt frequency (in Hz) depends on several material parameters

$$f_0 = \frac{\alpha\gamma}{1+\alpha^2}\sqrt{\frac{H_K^3 J_S V}{2\pi k_B T}}\left(1 - \frac{H}{H_K}\right)\left(1 - \frac{H^2}{H_K^2}\right), \tag{3}$$

where α is the dimensionless damping parameter from the Landau-Lifshitz-Gilbert (LLG) equation, $\gamma = \gamma_e/\mu_0 = 2.21 \times 10^5$ m/(As) is the electron gyromagnetic ratio divided by the permittivity, H_K [A/m] is the anisotropy field, and J_S [T] is the saturation magnetization. Expressions for a field applied at an arbitrary angle to the easy axis were derived, for example, by Coffey *et al.*[10] and Kalmykov.[11]

In the first part, following the work of Kurkijärvi,[12] we derive the switching field distribution from a master equation and the Arrhenius-Néel Law under consideration of the field dependence in the attempt frequency. In the second part, we compare results for a constant and field-dependent attempt frequency to Monte Carlo and Langevin simulation data. Furthermore, we discuss the rate dependence of the coercivity and its standard deviation and compare the results to the models described in literature.[2–5] Finally, we discuss the validity of the Néel-Brown model. This is closely connected to the understanding of the transition regime between thermally activated and dynamic switching of a single domain particle.

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II. ANALYTICAL MODEL

The energy landscape for the magnetization of a single domain particle with an external magnetic field H applied parallel to its easy axis has two stable minima separated by a barrier[13]

$$\Delta E = KV\left(1 - \frac{H}{H_K}\right)^2. \tag{4}$$

There exist similar expressions for more complex reversal paths of the magnetization, which essentially differ in the exponent. The exact shape of the minimum energy path can be calculated using, for example, the nugded elastic band method.[14]

When the field $H(t)$ is ramped up, the time dependent probability P_{not} that the particle has not switched until a certain moment t_0 is described by a master equation:

$$\frac{dP_{\mathrm{not}}}{dt} = -f\,P_{\mathrm{not}}, \tag{5}$$

where f is the transition rate from the Arrhenius-Néel law given in Eq. (2) and the contribution by particles that switch back is neglected. From Eq. (5), we get the following expression for P_{not}:[4]

$$\ln P_{\mathrm{not}} = -\int_{-\infty}^{t_0} f_0(H)\exp\left(-\frac{\Delta E}{k_B T}\right)dt. \tag{6}$$

By using Eq. (3) for $f_0(H)$, the integral on the right hand side of Eq. (6) is solved with the aid of the substitution

$$u = \sqrt{\beta}\left(1 - \frac{H(t)}{H_K}\right) \quad \beta = \frac{KV}{k_B T} \quad H(t) = Rt,$$

where R is the field rate in T/s for a linearly swept field. The probability of switching is then given by

$$P(u_0) = 1 - P_{\mathrm{not}}(u_0) = 1 - \exp\left\{-\frac{C}{2\sqrt{\beta}} \times\left[e^{-u_0^2}(1 - 2\sqrt{\beta}u_0 + u_0^2) + \sqrt{\pi\beta}\,\mathrm{erfc}(u_0)\right]\right\}, \tag{7}$$

with

$$u_0 = \sqrt{\beta}\left(1 - \frac{H_C}{H_K}\right) \quad \text{and} \quad C = \frac{\alpha\gamma}{1+\alpha^2}\frac{H_K^2}{\sqrt{\pi\beta}R}.$$

$P(u_0)$ with $u_0 = u_0(H_C)$ is the cumulative distribution function (CDF) which describes the likelihood for the particle to have switched at a field $H = H_C$. The switching field distribution is then given by the probability density function which is the derivative of Eq. (7)

$$\frac{dP}{dH_C} = \frac{d}{dH_C}(1 - P_{\mathrm{not}}) = P_{\mathrm{not}}\frac{C}{H_K}(2\sqrt{\beta}u_0^2 - u_0^3). \tag{8}$$

III. RESULTS

A. Switching field distribution

In Fig. 1, the analytical SFD from Eq. (8) is plotted together with the results of a Monte-Carlo simulation and a Langevin dynamics simulation, which solves the LLG equation in the presence of a random thermal field.[15] For comparison, we also show the result for the SFDs that is derived the same way as Eq. (8), but with $f_0 = \mathrm{const.}$

$$\frac{dP}{dH_C} = \frac{f_0}{R}\exp\left\{-\frac{f_0 H_K}{2R}\sqrt{\frac{\pi}{\beta}}[1 - \mathrm{erf}(u_0)]\right\}\cdot e^{-u_0^2}. \tag{9}$$

By taking into account the field dependence of the attempt frequency, we see that the peaks of the SFDs shift towards higher switching fields and the SFD is broadened. A similar result has been reported by Klik *et al.*,[16] who simulated the energy loss due to the dissipative parts of the LLG equation affecting the thermal reversal rate of the magnetization. For the Monte Carlo simulation, we assume a single macrospin switching between two magnetization states (up $= +1$, down $= -1$) in an external field $H(t)$ swept at a constant rate. When the external field is varied as a function of time, the switching probability is calculated by[14]

$$P = \exp\left\{-\Delta t f_0 \exp\left[-\beta\left(1 - \frac{H(t_i)}{H_K}\right)^2\right]\right\}, \tag{10}$$

where Δt denotes the time step of the simulation and $H(t_i)$ is the value of the swept field at a certain time t_i. Following the Metropolis algorithm, the values of P are then compared to a random number $x \in [0; 1]$. The value of H gets accepted as a switching field H_C as soon as $P > x$. At a value $H(t) \geq H_K$ the magnetization is automatically switched. We performed 1000 sweep cycles at field steps of 0.01 T and then computed the histogram of the obtained values for the switching field. The material parameters applied in the simulation are typical for modern perpendicular magnetic recording materials.

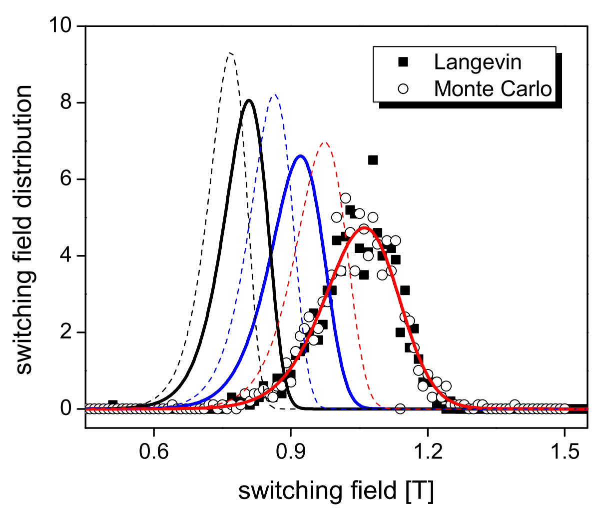

FIG. 1. Switching field distributions at 10^5 (black), 10^6 (blue), and 10^7 T/s (red) (left to right) for $K = 0.3$ MJ/m^3, $V = (8\,\mathrm{nm})^3$, $J_S = 0.5$ T, $\mu_0 H_K = 1.508$ T, $\alpha = 0.02$. Simulation results are for 10^7 T/s. The dashed lines denote the analytical SFDs for $f_0 = \mathrm{const.}$

The same parameters were used in the Langevin simulation. To keep computational times reasonably low, 10^7 T/s was the minimum field rate that was investigated with the Langevin simulation. The Monte Carlo simulation data agree perfectly with the analytical results at the lower field rates up to approx. 10^8 T/s.

B. Rate dependence of the coercivity

The coercivity of a magnetic recording medium is of special interest regarding the write process of a magnetic bit. Coercivity measurement methods usually employ very low field rates (<1 T/s in a vibrating sample magnetometer (VSM) measurement) in contrast to the high field rates of up to 1 T/ns used in modern hard disk drives for the write process. Various models have been proposed to extrapolate between the laboratory time scale and the actual time scale used in magnetic recording. An overview of the expressions is given in Table I.[2–5]

We calculate the switching field directly from the SFD. The mean value $\bar{H}$ of the variable H with the PDF dP/dH is given by

$$\bar{H} = H_C = \int_{-\infty}^{\infty} H \frac{dP}{dH} dH. \tag{11}$$

$\bar{H}$ is calculated by numerical integration. As it is shown in Fig. 2, the switching fields derived this way agree best with the model of El-Hilo *et al.*[5] up to a rate of approx. 10^8 T/s. This is because in contrast to the other models, El-Hilo's expression is also derived under consideration of a varying attempt frequency according to Eq. (3). It has been used successfully to fit data of coercivity simulations using a finite temperature micromagnetic method (FTM)[17] which are in good agreement with experimental data.

If the rate exceeds 10^7 T/s, the mean value of H_C starts to decrease according to our model. This is because with $H_C/H_K \approx 1$, the energy barrier (Eq. (4)) vanishes and a switching regime is entered here that is not properly described anymore by the Arrhenius-Néel Law (Eq. (2)).

At high field rates, the thermal fluctuations have less time to assist the switching. Therefore, the switching becomes dominated by the dynamics of the systems which is described by the LLG equation to which fluctuations are added by a thermal fluctuation field. For our model, we identify its limit of validity by calculating the numerical value of

TABLE I. Analytical expressions for rate-dependent coercivity.

Chantrell *et al.* [2]	$R(H_C) = H_K f_0 \frac{\exp[-\beta(1 - H_C/H_K)^2]}{2\beta(1 - H_C/H_K)}$
Feng and Visscher [4]	$R(H_C) = \frac{\pi f_0 H_K}{2 \ln 2\beta}\left\{1 - \mathrm{erf}\left[\sqrt{\beta}\left(1 - \frac{H_C}{H_K}\right)\right]\right\}$
El Hilo *et al.* [5]	$H_C(R) = H_K\left[1 - \sqrt{\frac{1}{\beta}\ln\left(\frac{f_0 H_K}{2R\beta}\right)}\right]$
Peng and Richter [3]	$H_C(t_{\mathrm{eff}}(R,\beta)) = H_K\left[1 - \sqrt{\frac{1}{\beta}\ln\left(\frac{f_0 t_{\mathrm{eff}}}{2\ln 2}\right)}\right]$

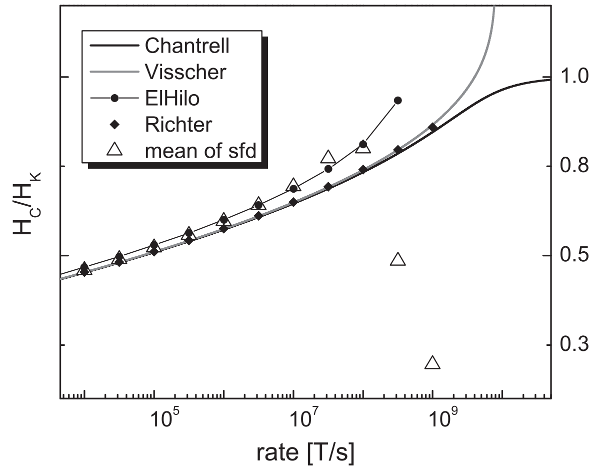

FIG. 2. Comparison of the models from Table I and Eq. (11) for the rate-dependent coercivity.

the integral over the SFD dP/dH_C (Eq. (8)). The normalization condition for a PDF

$$\int_{-\infty}^{\infty} \frac{dP}{dH} dH = 1,$$

is not fulfilled at field rates above 2×10^7 T/s (see Fig. 3). According to the general definition of a CDF, $P(u_0)$ has to fulfill

$$\lim_{u_0 \to \pm\infty} P(u_0) = \begin{cases} 0, & u_0 \to +\infty \\ 1, & u_0 \to -\infty. \end{cases}$$

We find

$$\lim_{u_0 \to -\infty} P(u_0) = 1 - \exp\left(-\frac{C\sqrt{\pi}}{2}\right) = 1,$$

only fulfilled if

$$\beta R \ll \frac{1}{2}\frac{\alpha\gamma}{1+\alpha^2} H_K^2. \tag{12}$$

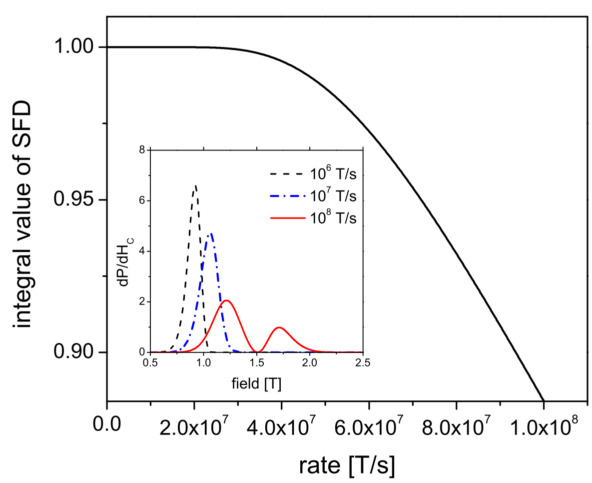

FIG. 3. Integral of Eq. (8) evaluated for varying field rate. The inset shows plots of the SFD at 10^6 (black), 10^7 (blue), and 10^8 T/s, where the last value is clearly beyond the limit of validity of the model.

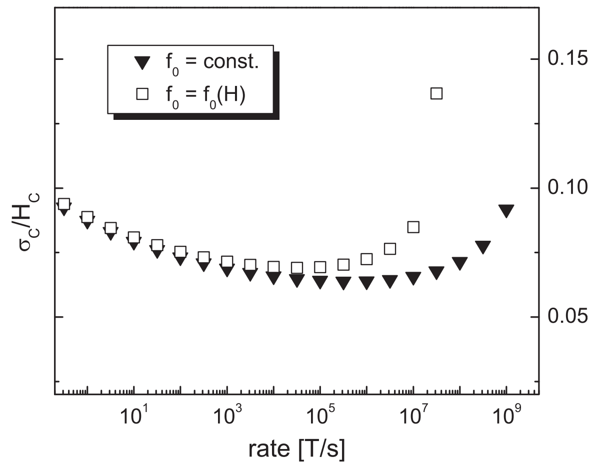

FIG. 4. Rate dependence of the standard deviation of the switching field.

For the parameters used here, the right hand side of Eq. (12) gives an upper bound for the field rate of 1.1×10^8 T/s.

C. Rate dependence of the standard deviation

Apart from a reduction of coercivity thermal activation also gives rise to a standard deviation of the switching field. This can be calculated from the second moment of the PDF, i.e., the variance,

$$\sqrt{\mathrm{var}(H)} = \sigma = \sqrt{\int_{-\infty}^{\infty} (H - \bar{H})^2 \frac{dP}{dH} dH}. \tag{13}$$

Fig. 4 shows the standard deviations σ_C normalized to the switching fields H_C plotted with respect to the field rate. It is interesting to see that σ_C/H_C first decreases slightly but then increases at higher field rates. Most importantly, σ_C/H_C has a minimum value at an intermediate field rate. The standard deviation in Eq. (13) is a different effect than the standard deviation described, e.g., by Hovorka *et al.*,[18] which arises from anisotropy and volume distributions of the grains in the magnetic medium. The switching field distribution we derive is an additional contribution to the SFD which originates solely from thermal activations acting on a single grain. Considering this fundamental contribution is important in order to extract accurate values for the intrinsic distributions of anisotropy values and grain volumes using the methods presented in literature.[18]

IV. CONCLUSION

We described an entirely analytical approach to derive the SFD of a single-domain particle with uniaxial anisotropy caused by thermal fluctuations under the consideration of a field-dependent attempt frequency. Unlike the SFDs derived from an underlying distribution of grain sizes and switching volumes, in our model the distribution originates from the thermal activation of the particle's magnetization for overcoming an energy barrier at a rate described by the Arrhenius-Néel Law. The effect exists independently of any other contribution to the SFD and therefore represents a fundamental limit to the accuracy of magnetization reversal at finite temperatures. The effect is important if distributions of intrinsic properties such as anisotropy values and grain volumes are extracted from magnetic property measurements such as VSM at finite temperature. An experimental evidence of the validity of the Néel-Brown model at low field rates was given by Wernsdorfer *et al.*[19] In this regime, the influence of the field dependence in the attempt frequency is small, but it becomes increasingly important at higher field rates where coercivity is notably enhanced. Our model is able to give an upper limit for the field rates where the assumptions of the Néel-Brown model are applicable. When the switching fields approach the value of zero temperature coercivity at high field rates, we find the limitation of the model determined by the loss of normalization of the PDF describing the SFD.

In the regime of magnetic recording above 10^8 T/s, the switching is dominated by the dynamics of the LLG equation. The corresponding Langevin equation can be solved on timescales up to 10^3 ns within a reasonable amount of computation time. To treat the long timescales of laboratory measurements, Monte Carlo methods based on the Arrhenius-Néel law are usually applied. However, we conclude they are not suitable for extrapolation towards magnetic recording field rates.

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