Sweep-rate dependent coercivity simulation of FePt particle arrays

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(Dated: October 16, 2003)

We present a simple method for parameterizing the sweep-rate dependence of the coercivity. We use it to fit data obtained from Landau-Lifshitz dynamic simulation, to extrapolate them to experimental time scales. The method is a generalization of the Sharrock theory in which all the data fall on a single universal curve if the coercivity and sweep-rate are scaled properly.

I. INTRODUCTION

In characterizing particulate assemblies and evaluating their potential as magnetic storage media, the time-scale-dependent coercivity is frequently measured. This can be done in a hysteresis loop, in which case the relevant time scale is the reciprocal of the sweep rate $R \equiv dH/dt$, or in response to a constant field, in which case the relevant time scale is the duration t of application of the field. In the constant-field case, it has been found by several groups[1][2] that the resulting coercivity $H_c(t)$ can be fit very accurately by Sharrock's Law (Eq. 5 below) by varying two or three parameters. Sharrock's Law can be derived in a very simple way from very simple assumptions. We assume that the particles of an assembly are identical and switch by a thermally activated mechanism that is described by an Arrhenius law

$$r = f_0 e^{-E/k_B T} \tag{1}$$

where the constant f_0 is called the "attempt frequency" and E is an activation energy given by

$$E = KV(1 - H/H_0)^n \tag{2}$$

with K the uniaxial anisotropy energy and H_0 the field at which the activation energy vanishes. The parameter H_0 is equal to the anisotropy field $H_K = 2K/M_s$ (M_s is the saturation magnetization) if the particles are aligned along the field axis, but will be smaller if the particles are not aligned. The exponent n is equal to 2 in the simplest case (particles aligned along the field direction) but other values such as 3/2 have been used [3][2]. In this paper, we will give results for $n = 3/2$.

The application envisioned in the present paper is the determination of the fundamental anisotropy parameter K from experimental coercivity data on particle arrays. Extensive work on this problem has been done by a number of groups using the Monte Carlo[4] and master-equation[5][6] methods. However, these methods require assuming an Arrhenius law for the switching rate of an individual particle, i.e. assume that the reversals are independent and that transition state theory is valid. Although these assumptions may often be justifiable, in the present paper we will take a more microscopic approach to the dynamics and use the Landau-Lifshitz equation to evolve the system. This has the advantage of describing precessional phenomena and collective switching correctly, but the disadvantage of being limited to very short time scales.

Thus we have the problem of extrapolating our simulated coercivities from the nanosecond scale to a scale of seconds. To do this, we will fit our results to a Sharrock-like formula based on transition state theory. Note that this approach does not require assuming the detailed validity of the theory behind the fitting formula – it is only used to fit a result obtained from a more fundamental theory. Because it is experimentally easier to measure the sweep-rate dependent coercivity[7] than the time-dependent coercivity modeled by Sharrock's law, we have done simulations of hysteresis loops and determined the sweep-rate dependent coercivity from LL simulation with known H_K, and wish to extrapolate these results to low sweep rates. Thus we would like a sweep-rate analog of Sharrock's law.

Several adaptations of Sharrock's law to sweep-rate dependent coercivity have been discussed previously. Flanders and Sharrock[7] have made a graphical argument, based on the approximate history-independence of the switching rate, that one can simply identify the sweep rate R with the derivative $dH_c(t)/dt$ with respect to the pulse-duration t. Chantrell *et al*[10] have calculated the R-dependent coercivity in the small-R limit (see Eq. 12 below). Unfortunately, not all of our simulations are in the small-R limit, so we would like a result valid for all R. We have found that it is possible to calculate the relationship between R and H_c analytically in terms of error functions, for all values of R, and this provides a very convenient way of fitting our data and extrapolating to the small-R limit. Our new result reduces to that of Chantrell *et al* in the appropriate limit.

II. SWEEP-RATE DEPENDENT COERCIVITY

As in the original Sharrock theory of pulse-duration-dependent coercivity, we assume that the probability $P_u(t)$ that a particle is still unswitched at time t obeys

$$\frac{dP_u}{dt} = -rP_u \tag{3}$$

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Using Eqs. 1 and 2 for the rate r, and $P_u(-\infty) = 1$,

$$\ln P(t) = -f_0 \int_{-\infty}^{t} r dt' = -f_0 \int_{-\infty}^{t} e^{-\frac{KV}{k_B T}(1-H(t')/H_0)^n} dt' \tag{4}$$

Since the coercive state is achieved when $P(t) = 1/2$, the left hand side is $-\ln 2$.

If we now assume that $H(t)$ is constant over a time interval of length t, we immediately obtain the standard Sharrock law[1]

$$\ln 2 = f_0 t e^{-\frac{KV}{k_B T}(1-H_c/H_0)^n} \tag{5}$$

However, if we instead assume the field is swept linearly with time, with a sweep rate $R \equiv dH/dt$, we can again solve the problem analytically. To do this, convert to the dimensionless variable $y \equiv s(1 - H(t')/H_0)$ where

$$s \equiv (\frac{KV}{k_B T})^{1/n} \tag{6}$$

so that

$$\ln 2 = \frac{H_0 f_0}{Rs} \int_{s(1-H_c/H_0)}^{\infty} e^{-y^n} dy \tag{7}$$

In the case $n = 2$, this integral is a well-known function, the complementary error function defined by[9]

$$\mathrm{erfc}(y) \equiv \frac{2}{\pi^{1/2}} \int_{y}^{\infty} e^{-y'^2} dy' \tag{8}$$

For other values of n, we can define a generalized error function

$$\mathrm{erfg}_n(y) \equiv \frac{2}{\pi^{1/2}} \int_{y}^{\infty} e^{-y'^n} dy' \tag{9}$$

so that $\mathrm{erfc}(y) = \mathrm{erfg}_2(y)$. [For simplicity, we use the standard normalization constant chosen so $\mathrm{erfc}(0) = 1$, though in general $\mathrm{erfg}_n(0) \neq 1$.] This is easy to compute by numerical integration.

Thus we obtain a very simple relation between the sweep rate R and the coercivity H_c:

$$R = R_0 \ \mathrm{erfg}_n(s(1 - H_c/H_0)) \tag{10}$$

where the sweep-rate scale is set by

$$R_0 \equiv \frac{\pi^{1/2}}{2\ln 2} \frac{f_0 H_0}{s} \tag{11}$$

When the rate R is very small, the argument of the error function is very large, and one can use the asymptotic form

$$\mathrm{erfg}_n(y) \rightarrow \frac{2}{\pi^{1/2}} \frac{e^{-y^n}}{n y^{n-1}} \tag{12}$$

In this limit, our results are equivalent to those of Chantrell *et al*[10].

Note that Eq. 10 has a simple universal form

$$x = \mathrm{erfg}_n(y) \tag{13}$$

in terms of rescaled rate and field variables,

$$x = R/R_0 \text{ and } y = s(1 - H_c/H_0) \tag{14}$$

The universal function erfg_n is shown in Fig. 2 below, for $n = 2$ and $n = 3/2$; x and y increase to the left and down, for consistency with plots in which the variables are time and coercive field H_c.

In Sec. IV below, we will fit this formula to our simulation results.

III. SIMULATION

We have simulated an infinite 2D hexagonal array of FePt particles using the Landau-Lifshitz equations[11]. We have used periodic boundary conditions with a 4×8 array of particles, and include all magnetostatic interactions using a fast multipole method recently adapted to periodic boundary conditions[12]. We assume the particles are 4 nm in diameter with a 6 nm center-to-center distance, so there is no exchange interaction. We used a program that was written for micromagnetics with cubic cells, but at this separation the multipole field of a sphere is indistinguishable from that of a cube (they differ only at the fourth order or hexadecapole level).

To check that the stochastic Landau-Lifshitz simulation program worked correctly, at least without interactions, we computed the equilibrium magnetization at several values of the field and checked that they agreed with the Langevin formula for the magnetization of non-interacting particles.

We have determined the coercivity from a hysteresis loop at field sweep rates $R = 2.5, 5, 10, 20$, and 40 kOe/ns, for each of three values of anisotropy: H_K = 4, 15, and 50 kOe. An animated visualization of the hysteresis simulation is at http://bama.ua.edu/∼visscher/mumag, showing the evolution of the particle magnetizations while the hysteresis loop is drawn. The coercivity shown in the figures has been averaged over 10 simulations.

IV. FITS

The simulation data points are shown in the H_c *vs.* R plane in Fig. 1. To fit them to our model (Eq. 3), we must choose the three parameters H_0, s, and R_0. It is apparent from Fig. 1 that the data fall very close to a straight line, and hence determine only two parameters (the height and slope of the line). The curvature of the available data is too small to determine the third parameter reliably. The parameter about which we can make the best guess is H_0, related to the static switching

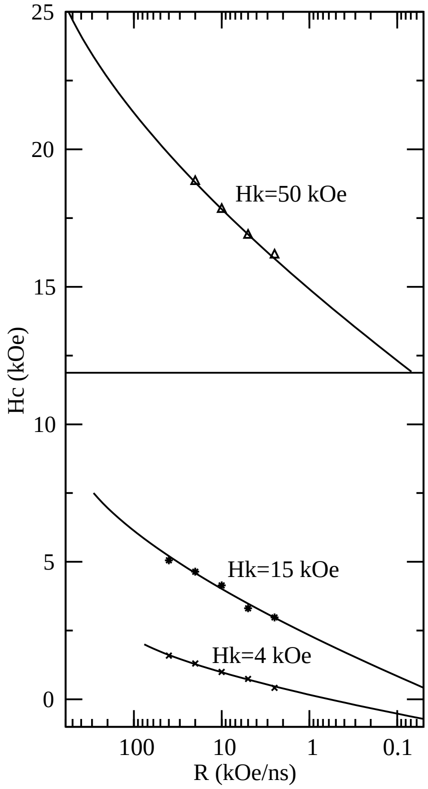

FIG. 1: Hysteresis vs. sweep-rate data, fitted to Eq. 10.

field, which is known to be about $0.5H_K$ for 3D random anisotropy. So we will constrain $H_0 = H_K/2$. The remaining two variables can actually be fit without a numerical fitting program, because changing these variables just rigidly translates the points in a plot of $\ln y$ *vs.* $\ln x$ (like Fig. 2 but with a logarithmic vertical axis). Changing s shifts the points vertically by shifting $\ln y$, whereas changing R_0 shifts them horizontally. Thus we need only find a point where the universal $\ln y$ *vs.* $\ln x$ curve has the correct slope, and translate the center of the data segment to that point. Then all the points lie near the universal curve in Fig. 2, in terms of dimensionless variables x and y. As a reminder that all the curves in Fig. 1 differ only by rescaling, we have scaled Fig. 1 so that the top part (above the horizontal line) is identical with Fig. 2 except for axis scaling.

V. ACKNOWLEDGEMENTS

This work was partially supported by DOE grant No. DE-FG02-98ER45714 and NSF grant DMR-0213985, and by the DOE Computational Materials Sciences Network. We thank J. W. Harrell for useful conversations.

[1] M. P. Sharrock and J. T. McKinney, IEEE Trans. Magn. **17**, 3020 (1981).
[2] J. W. Harrell, IEEE Trans.Magn. **37**, 533 (2001).
[3] R. H. Victora, Phys. Rev. Lett. **63**, 457 (1989).
[4] R. W. Chantrell, D. Weller, T. J. Klemmer, S. Sun, E. E. Fullerton, J. Appl. Phys. **91**, 6866 (2002).
[5] C. Papusoi, Jr., and T. Suzuki, IEEE Trans.Magn. **38**, 1687 (2002).
[6] J. J. Lu, H. L. Huang, and I. Klik, J. Appl. Phys. **76**, 1726 (1994).
[7] P. Flanders and M. Sharrock, J. Appl. Phys. **62**, 2918 (1987).
[10] R. W. Chantrell, G. N. Coverdale, and K. O'Grady, J. Phys. D **21**, 1469 (1988); A. M. de Witte, M. El-Hilo, K. O'Grady, and R. W. Chantrell, J. Mag. Mag. Mat. **120**, 184 (1993).
[9] M. Abramowitz and I. Stegun, "Handbook of Mathematical Functions, AMS55", National Bureau of Standards, 1964.
[10] R. W. Chantrell, G. N. Coverdale, and K. O'Grady, J. Phys. D **21**, 1469 (1988); A. M. de Witte, M. El-Hilo, K. O'Grady, and R. W. Chantrell, J. Mag. Mag. Mat. **120**, 184 (1993).
[11] Xuebing Feng and P. B. Visscher, Physical Review B 65, 104412, 2001.
[12] D. M. Apalkov and P. B. Visscher, IEEE Trans. Mag. **39** No. 6, Nov. 2003.

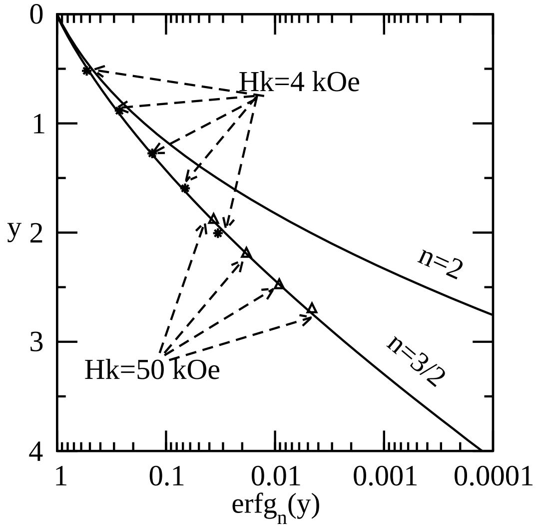

FIG. 2: Universal curves for $n = 3/2$ and $n = 2$, showing that the scaled data points (x,y given by Eq. 14) for $H_K = 4$ kOe and $H_K = 50$ kOe (as well as $H_K = 15$ kOe, which is not shown to avoid clutter) all fall on the universal curve, if choose the right scaling parameters R_0 and s. Horizontal (x) axis is logarithmic.