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Monte Carlo simulation of hysteresis loops of single-domain particles with cubic anisotropy and their temperature dependence

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Abstract

By means of Monte Carlo simulation the hysteresis of non-intereacting single-domain magnetic particles presenting cubic crystalline anisotropy are studied. Both signs of the anisotropy constant are considered, and relevant properties, such as remanence and coercivity, are obtained as a function of temperature. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Monte Carlo simulation; Hysteresis loop; Anisotropy; Remanence; Coercivity

1. Introduction

The hysteresis loop of a non-interacting system of randomly aligned single-domain particles presenting uniaxial anisotropy has been known since the publication of the classical paper by Stoner and Wohlfarth [1]. They obtained the values $H_c = 0.479H_a$ for the coercive field and $M_r = 0.5M_s$ for the remanence, where M_s is the saturation magnetization and $H_a = sK/M_s$ is the anisotropy field. They assumed a coherent magnetization reversal model, which is a good approach for a restricted range of particle sizes, such as the micromagnetic model [2,3] predicts.

Particles presenting cubic crystalline anisotropy, such as iron or nickel, are also very important in the experimental magnetism however, until very recently, their theoretical hysteresis loop was unknown. It has been possible to obtain the value of the remanence analytically [4] ($M_r = 0.831M_s$ for the case $K_1 > 0$ and $M_r = 0.866\,M_s$ for the case $K_1 < 0$), and also the reversible part of the hysteresis loop has been studied [5] but it is not possible to follow the same process of Stoner and Wohlfarth for the whole cycle due to the fact that the magnetization can jump to any of the several local minima [5].

Recently, Usov and Peschany [6] presented the first advance for the complete hysteresis loop of cubic anisotropy particles using a dynamical approach. They described the following upper and lower limits for the coercitivity: $0.320H_a < H_c < 0.335H_a$ when $K_1 > 0$ and $0.180H_a < H_c < 0.200H_a$ when $K_1 < 0$. Essentially following the method of Stoner and Wohlfarth, the problem of the indetermination of the discontinuous jumps was solved by a dynamical model of evolution, in which there are different probabilities to each adjacent energy minimum. In this work we have chosen a different way. Using the Monte Carlo (MC) simulation technique (see e.g. Ref. [7]), we study in detail the hysteresis loops of particles presenting cubic cristalline anisotropy (assuming also homogeneous rotation of magnetization). An extended approach using the micromagnetic model directly should give valid results for a wider range of particles sizes, but it would result in a huge computational effort. The MC approach has the advantage that extensions to nonzero temperature are straightforward. In addition, the method can be used for any kind of

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distribution of particle orientations, and it allows the study of interparticle interactions.

2. Model, numerical simulation, and results

Usually the cubic anisotropy energy is written as

$$E_a = K_1 V(\alpha^2\beta^2 + \alpha^2\gamma^2 + \beta^2\gamma^2) + K_2 V\alpha^2\beta^2\gamma^2,$$

where (α, β, γ) are the direction cosines of the magnetization with respect to the crystal directions and K_1 and K_2 are the anisotropy constants, whose values are taken from the experiments and are usually sensitive functions of temperature. Since no interaction between particles is considered, each particle is completely defined by a set of six angles (θ_1, ϕ_1), (θ_2, ϕ_2), and (θ, ϕ). The first four angles defining the orientation of the easy axes are kept constant during the simulation of a single configuration. The two remaining angles which define the magnetization direction will be variable throughout the MC simulation.

Taking into account both anisotropy and the interaction with an external field in z direction, the total energy (with $\gamma^2 = 1 - \alpha^2 - \beta^2$ and divided by $2|K_1|V$ in order to compare the results with the Stoner–Wohlfarth model) reads as

$$e_{tot} = \pm\frac{1}{2}\left(\alpha^2 + \beta^2 - \alpha^4 - \beta^4 - \alpha^2\beta^2 + \frac{K_2}{K_1}\alpha^2\beta^2(1 - \alpha^2 - \beta^2)\right) - h\cos\theta,$$

where $h = H/H_a$ and $H_a = 2/K_1/M_s$ are as defined for uniaxial particles. The plus sign corresponds to the case when K_1 is positive, the minus sign to the case when K_1 is negative. Furtheron, we restrict ourselves to the $K_2 = 0$ case only.

The MC algorithm is as follows: In every MC step an attempted orientation $\boldsymbol{\mu}_{att}$ of the magnetization is generated. The attempted direction is chosen in a spherical segment around the present orientation $\boldsymbol{\mu}$, which is used as azimuthal axis, with $\bar{\phi} \in [0, 2\pi]$ and $\bar{\theta} \in [0, \delta\theta]$. Thus the energy difference Δe between the attempted and the current state is calculated. If $\Delta e \leqslant 0$ the magnetization is changed to μ_{att}. If $\Delta e > 0$ the magnetization is changed with probability $\exp(-\Delta e/t)$ and remains unchanged with probability $1 - \exp(-\Delta e/t)$. Here, $t = k_B T/(2|K_1|V)$ is the reduced temperature. In any case the variable counting the MC steps is increased and the process is continued. Varying the aperture angle $\delta\theta$, i.e. the maximal jump angle, it is possible to modify the range of acceptance in order to optimize the simulation. Using this kind of local dynamics allows us to detect the confinement in metastable states responsible for the hysteresis. Choosing a non-local algorithm and drawing the attempted direction independently to the current one, the system would always be superparamagnetic since it would be possible to explore the whole phase space independently of the temperature. To perform the complete hysteresis loop a very high field is applied initially at very high temperature. Then the system is carefully thermalized to the desired temperature, and the loop is started by slowly varying the reduced applied field in steps of 0.05 (0.02 if $h \in [-0.5, 0.5]$ for better accuracy) every 2000 MC steps. The process is repeated for a large number of independent configurations to perform an ensemble average.

The resulting reduced hysteresis loops for both $K_1 > 0$ and $K_1 < 0$ at $T = 0$ are shown in Fig. 1. The loop for uniaxial particles is also represented for comparison. For $K_1 > 0$, the obtained reduced remanence $M_r = M_r/M_s$ is $m_r = 0.831 \pm 0.004$, which is in perfect agreement with the theoretical value [4]. The reduced coercive field is $h_c = 0.316 \pm 0.002$, which is within the lower limit of the range given by Usov [6]. The reduced coercivity is lower for $K_1 < 0$, than in the case with the positive constant, the reduced remanence on the contrary is slightly larger. The obtained value $m_r = 0.865 \pm 0.004$ is again in good agreement with the exact result [4], and $h_c = 0.183 \pm 0.002$ is within the limits given by Usov [6].

The evolution of the reduced hysteresis loops and coercitivity with temperature for $K_1 > 0$ and $K_1 < 0$ are shown in Figs. 2–4 respectively. As in the actual experiments the time of measurement plays an important role. More time between changing field and measurement means more time to relax. All the loops shown in the present study are carried out with 2000 MC steps between measurements, this sets the blocking temperature T_B when $K_1 > 0$ around $k_B T_B/(2K_1 V) = 0.02$ in reduced units. A comparison of simulations done with a different

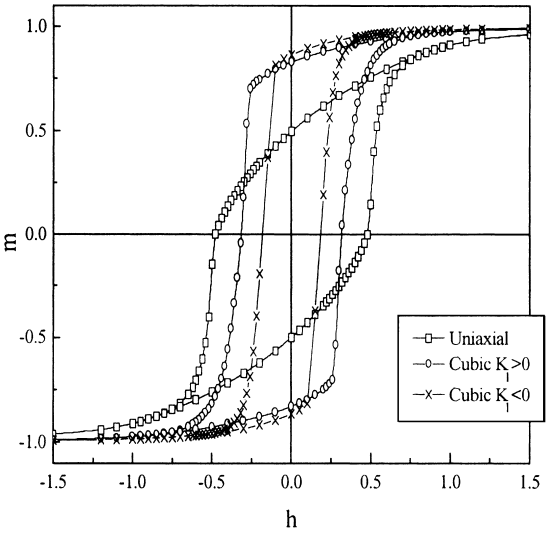

Fig. 1. Reduced hysteresis loops of non-interacting randomly aligned single-domain particles. In the figure the cases for uniaxial anisotropy (Stoner–Wohlfarth model) and for cubic anisotropy with both signs of the anisotropy constant are shown.

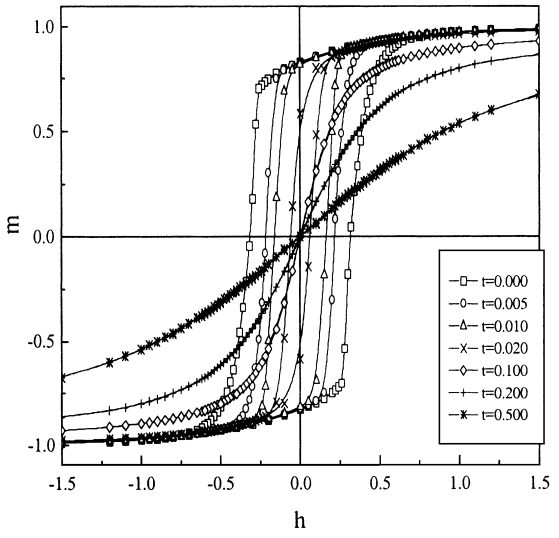

Fig. 2. Effect of temperature on the hysteresis loops of non-interacting randomly aligned single-domain particles with cubic anisotropy, case $K_1 > 0$. At high temperatures the loops become superparamagnetic.

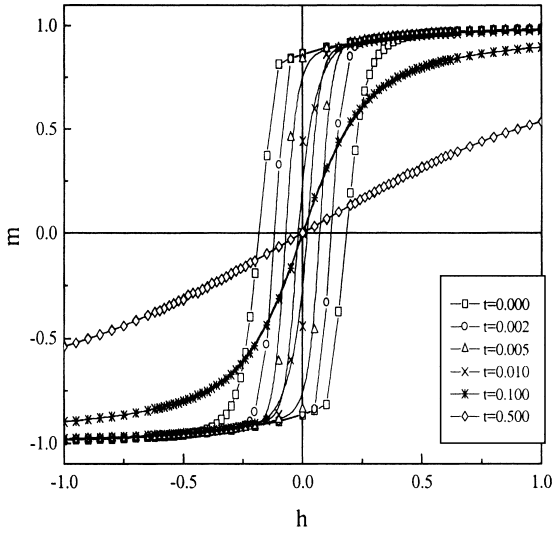

Fig. 3. Effect of temperature on the hysteresis loops of non-interacting randomly aligned single-domain particles with cubic anisotropy, case $K_1 < 0$. At high temperatures the loops become superparamagnetic.

number of MC steps between measurements can be carried out by rescaling the temperature with the blocking temperature. In whichever case, the functional dependence of the magnetic parameters will be the same, as will be the shape of the loops.

Finally, it should be kept in mind that the parameters which enter in the definition of the reduced magnitudes, e.g., M_s and especially K_1, depend strongly on temperature, and consequently so does the anisotropy field H_a.

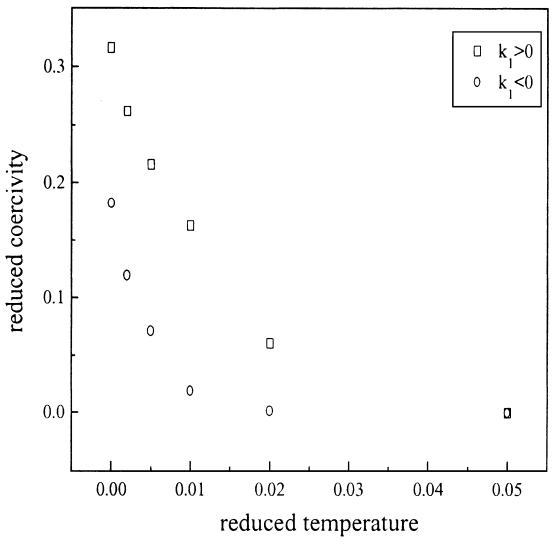

Fig. 4. Temperature dependence of the reduced coercivity for both signs of the first constant of cubic anisotropy.

Thus, taking this additional dependence into account, obtaining the measured parameters for a given material is straightforward.

The simple model studied does not take into account interparticle interactions, but can be of interest in the case of very diluted systems of single-domain particles. The influence of dipolar interactions will be our next objective.

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