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The response of magnetic particles with mixed anisotropy at different frequencies

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Abstract

The response of magnetic particles at different frequencies is important for different applications ranging from mobility magnetic particle imaging in the lower kHz range up to a few hundred kHz for applications like magnetic fluid hyperthermia. In addition, realistic particles have different magnetic anisotropies contributing to the observed response. In this work, the response of particles with mixed cubic and uniaxial anisotropy in the frequency range from 1 kHz to 1 MHz are simulated by solving the corresponding Langevin equations for the mechanical and magnetic rotation of the particles. It is shown that even small ratios of cubic to uniaxial anisotropy visibly influence the response of the particles.

I. Introduction

Magnetic (nano-)particles (MNPs) are of great interest for applications like magnetic particle imaging (MPI) or magnetic fluid hyperthermia (MFH). The applications leverage the response of the MNPs in certain ways. In MPI, the nonlinear response of magnetic materials is used in conjunction with a spatially encoding external field to retrieve a spatially encoded signal [1]. This signal is then reconstructed into a spatial distribution of the trace concentration within the encoding area and MPI has shown great potential for different applications such as vascular imaging or cell tracking [2,3]. In MFH, on the other hand, the hysteretic behavior is used, and the opening of the hysteresis and the frequency of the external field determine the specific absorption rate (SAR), which is a measure for the power the particles absorb and subsequently proportional to the heat the particles generate. In both cases the response of the MNPs is of importance. One characteristic of the mentioned application is that the frequency of the external field can vary widely. While MPI typically uses excitation field frequencies in the range from 10-100 kHz with 25 kHz being mostly used, MFH uses frequencies exceeding 100 kHz with typically frequencies being around 500 kHz since the SAR scales linearly with frequency, if the area of the hysteresis is considered constant. Other techniques such as vibrating sample magnetometry, AC susceptibility or mobility MPI [4] utilize frequencies also below 10kHz as such the response of the particles is optimally known for every frequency range of interest.

In addition to the frequency of the applied field, the response of the magnetic particles depends on the physical properties of the particles, like e. g. the magnetic anisotropy and size, as well as physical properties of the embedding matrix like e. g. the temperature, the viscosity, or the amplitude of the applied field. The particle parameter which strongly influences the response is the magnetic anisotropy energy (MAE) of the particle. The MAE can be modeled in different ways. The mostly used anisotropy model for the MAE is that of uniaxial anisotropy, which only depends on the angle between one energetically preferred body axis and the particle magnetization. The model of uniaxial anisotropy is the

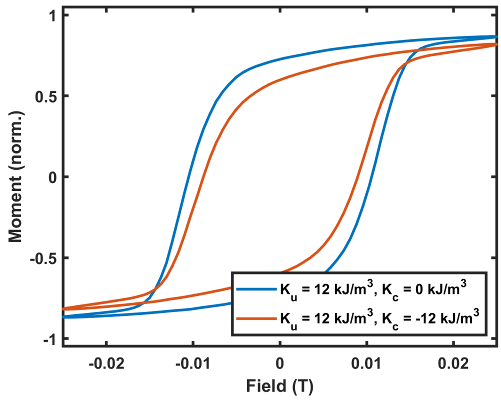

Figure 1: Simulation of 1000 particles with the parameters given in section II.II at a frequency of 100 kHz and varying cubic anisotropy constant K_c.

simplest and allows modeling real particles to a certain degree, if the particles exhibit a strong uniaxial behavior [5]. Unfortunately, this only covers a small amount of particle classes since particles exhibit different effects on the nanoscale (e.g. different surface anisotropies due to the particle geometry) which makes the total magnetic anisotropy energy a sum of different magnetic anisotropy energies. Experimental measurements of single particles also reveal more complex magnetic anisotropy energies [6] such as biaxial anisotropy.

This work will investigate the effect of the excitation frequency on the response of magnetic particles with different mixtures of uniaxial and cubic anisotropy.

II. Material and methods

II.I. Theoretical Model

The model used to describe the particle rotation and the magnetization dynamics are all based on the Yolk-Egg model [7, 8] and consists of coupled Langevin equations for the magnetization movement (a modified Landau-Liftschitz-Gilbert equation) and the mechanical rotation (a modified Euler equation) of the particle.

In the model, the state of the particle is described with Euler angles $\vec{\Phi}_n = (\phi_n, \theta_n, \psi_n)$ for the orientation of the particle and spherical coordinates $\vec{\Phi}_m = (\theta_m, \phi_m)$ for the magnetization direction, yielding:

$$\frac{\partial \vec{\Phi}_n}{\partial t} = \mathbf{E}_{313}(\vec{\Phi}_n)\vec{\omega}_n \text{ and } \frac{\partial \vec{\Phi}_m}{\partial t} = \mathbf{E}_{\mathbf{Sphere}}(\vec{\Phi}_m)\vec{\omega}_m$$

with $\mathbf{E}_{313}$ and $\mathbf{E}_{\mathbf{Sphere}}$ being projection matrices to map the angular velocities onto the change of state [9]. The corresponding angular velocities for the mechanical rotation $\vec{\omega}_n$ (ignoring the inertia of the particle and any vorticity of the surrounding medium) and the rotation of the magnetization vector $\vec{\omega}_m$ are given as [10]

$$\vec{\omega}_n = \frac{1}{6\eta V_H}(M_S V_M \vec{m} \times \vec{B}_{\text{eff}} + \vec{\tau}_{\text{eff}}) \text{ and}$$
$$\vec{\omega}_m = -\frac{\gamma}{1+\alpha^2}\vec{B}_{\text{eff}} + (\frac{|\gamma|\alpha}{(1+\alpha^2)}(\vec{m} \times \vec{B}_{\text{eff}}) + \frac{1}{6\eta V_H}(M_S V_M(\vec{m} \times \vec{B}_{\text{eff}}) + \vec{\tau}_{\text{eff}})).$$

Here, η is the viscosity of the surrounding medium, $V_H(V_M)$ is the hydrodynamic (magnetic) volume, $\vec{m}$ is the unit magnetisation vector, M_S is the saturation magnetization, γ is the (electron) gyromagnetic ratio, α is the damping constant, $\vec{B}_{\text{eff}}$ is the effective magnetic field given as $\vec{B}_{\text{eff}} = \frac{1}{M_S V_M}\frac{\partial U}{\partial \vec{m}} + \vec{B}_{\text{noise}}$ and $\vec{\tau}_{\text{eff}}$ is the effective torque given as $\vec{\tau}_{\text{eff}} = -\frac{\delta U}{\delta \phi} + \vec{\tau}_{\text{noise}}$. $\vec{B}_{\text{noise}}$ and $\vec{\tau}_{\text{noise}}$ are Gaussian white noise terms describing the thermal influence on the motion. U is the total energy or potential of the particle consisting of the Zeeman energy $M_S V_M \vec{m} \cdot \vec{B}_{\text{ext}}$ and the MAE. See [11] for details how to implement the MAE for arbitrary anisotropies. $\delta\phi$ is the infinitesimal rotation operator as derived in [12].

II.II. Simulation parameters

For the simulations particles with the following parameters where used: magnetic radius $r_M = 10$ nm, hydrodynamic radius $r_H = 20$ nm (volumes are assumed to be spherical), $M_S = 460$ kA/m, $\eta = 1$ mPa·s, $T = 295$ K, $\gamma = 1.76 \cdot 10^{11}$ (s·T)$^{-1}$, $\alpha = 0.1$. The particles have been simulated with different mixtures of uniaxial anisotropy constant K_u and cubic anisotropy constant K_c with random alignment of the uniaxial axis to the cubic axes. The amplitude of the external field is $B_0 = 25$ mT with frequencies f ranging from 1 kHz up to 1 MHz. The simulations are performed with a timestep of 5 ps and time averaging (oversampling) depending on the simulation frequency. The total simulation time is at least 10 periodes of the excitation signal.

III. Results and discussion

Figure 1 shows the result of two of the simulations with a constant uniaxial anisotropy constant of $K_u = 12$ kJ/m^3 and a varying cubic anisotropy constant of $K_c = 0$ and $K_c = -12$ kJ/m^3 at a frequency of $f = 100$ kHz. The value for the uniaxial anisotropy is selected because it reflects the shape anisotropy of a prolate sphereoid with an axis ratio of approximate 1.2 while the value for cubic anisotropy constant is approximatly the value found for magnetite in literature [13].

As can be seen from Fig. 1 the hysteresis of the two simulations is quite different. Comparing the simulations with cubic anisotropy to the ones without, it is observed that the hysteresis in general shows a lower

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remanent magnetization, a lower moment at 25 mT and a lower coercivity across the whole simulated frequency range. The main difference observed regarding changes to frequency is that the hysteresis opens for higher frequencies. The circumstance that there is a significant effect at an anisotropy ratio of $|K_c|/K_u = 1.0$ is unexpected since it is commonly believed that effects due to cubic anisotropy are dominated by even small values of uniaxial anisotropy. The reasoning behind this is that (thermally activated) switching is controlled by the height of the energy barrier ΔE. For uniaxial anisotropy the energy barrier is proportional to K_u while for cubic anisotropy the energy barrier scales with $K_c/12$ (for $K_c < 0$) or $K_c/4$ (for $K_c > 0$). Current data indicates that cubic anisotropy has affects on the hysteresis for aniostropy ratios of $|K_c|/K_u \geq 0.5$.

IV. Conclusions

Simulations have been carried out demonstrating that even small contributions of cubic anisotropy change the response of the magnetic particles significantly. As such, these simulations are required to obtain a ground truth for the particle properties and response. Considering the changes of the hysteresis, it is for example interesting to study if a similar effect can be achieved using a lower uniaxial anisotropy constant because it seems that the random superposition of cubic anisotropy has an angular average, which reduces the overall energy barrier ΔE. If the random superposition is switched to an aligned superposition of the energy minima, it is generally observed that the hysteresis shows higher coercivity and saturation values, which indicates a higher overall energy barrier ΔE. As such, modeling with an effective uniaxial $K_{\text{eff}} < K_u$ could yield similar results, but it needs to be investigated whether the hystresis is similar in all aspects. This work focused on particles with an axis ratio of 1.2 and uniaxial anisotropy due to shape anisotropy. For an ensemble of particles there will be a lot of particles with an axis ratio lower than that and only a few with a higher ratio. As such, the effects of cubic anisotropy are expected to be more pronounced in particle ensembles and will be investigated in future studies.

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