Journal of Non-Crystalline Solids 354 (2008) 5224–5226

Contents lists available at ScienceDirect

Journal of Non-Crystalline Solids

journal homepage: www.elsevier.com/locate/jnoncrysol

Interplay between the magnetic field and the dipolar interaction on a magnetic nanoparticle system: A Monte Carlo study

D. Serantes [a,b,*], D. Baldomir [a,b], M. Pereiro [a,b], J.E. Arias [a], C. Mateo-Mateo [c], M.C. Buján-Núñez [c], C. Vázquez-Vázquez [c], J. Rivas [b]

[a] Instituto de Investigacións Tecnolóxicas, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Galiza, Spain
[b] Departamento de Física Aplicada, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Galiza, Spain
[c] Departamento de Química Física, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Galiza, Spain

A R T I C L E   I N F O

Article history:
Available online 22 October 2008

PACS:
75.20.−g
75.40.Mg

Keywords:
Magnetic properties
Modeling and simulation
Monte Carlo simulations
Nanoparticles, colloids and quantum structures
Nanoparticles

A B S T R A C T

We have studied the influence of the applied magnetic field on the blocking temperature (T_B) of a fine magnetic particle system. By means of a Monte Carlo technique we have simulated zero field cooling (ZFC) curves under different applied fields, obtaining the respective T_B as a function of *H*. We have focused our study on the limit $H \to H_K$ (where H_K is the anisotropy field), since the results found in the literature usually lack a detailed study of this range. The simulations were done at different sample concentration of the nanoparticles, with the purpose of observing how the magnetic dipolar interaction affects the field dependence of T_B. The classical expression predicts T_B to disappear for $H \geqslant H_K$, independently of the dipolar interaction strength. Our simulations show that at strong interacting conditions T_B exists even for fields $H > H_K$.

1. Introduction

Fine magnetic particle systems constitute a research field of main interest nowadays based on its promising qualities for the field of biomedicine [1], magnetic recording [2], or magnetocaloric effect [3]. The interest on these systems lays on the different magnetic properties that current materials exhibit at the nanometer scale [4], which strongly depend on both the intrinsic characteristics of the particles (shape, anisotropy, size) and on external parameters (applied magnetic field, dipolar interaction). In the literature it has been widely studied the role played by the magnetic field [5] and the magnetic dipolar interaction [6], although as separate influences. We present in this work a numerical approach to the interplay between the magnetic field and the dipolar interaction on the superparamagnetic properties of a magnetic nanoparticle system. We have focused our study on the behavior of the blocking temperature (T_B) of the system as a function of both parameters. By means of a Monte Carlo technique, we simulate zero field cooling (ZFC) processes under different magnetic field/sample concentration conditions, and approximated T_B as roughly defined as the maximum of the ZFC curves. We observe that large values of the dipolar interaction allow the existence of the superparamagnetic phenomena even for fields larger than the anisotropy field (H_K), where the classical theory for superparamagnetic nanoparticles predicts T_B to disappear [7].

2. Monte Carlo simulation conditions

The physical model used for the simulations is the same described in Ref. [6], a system of single-domain magnetic nanoparticles exhibiting superparamagnetic behavior. It resembles the experimental situation of a frozen ferrofluid without aggregations where the positions of the particles are kept fixed. The only energies considered are the anisotropy (uniaxial), dipolar, and Zeeman, and the total energy is computed over a whole temperature range under different physical processes.

The results are presented in reduced units that allow the result to be generalized. The total magnetization is normalized with the saturation magnetization (M_S). The simulation is done over $N = 64$ particles, and averaged over 500 configurations. The temperature is shown in reduced units of $t = k_B T/2\,KV$, where *T* is the temperature and k_B is the Boltzmann constant. The parameters varied in our simulation are the sample concentration, *c*, and the applied magnetic field, *H*. The sample concentration directly

* Corresponding author. Address: Instituto de Investigacións Tecnolóxicas, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Galiza, Spain. Tel.: +34 981563100x13960; fax: +34 981520829.
E-mail addresses: david.serantes@usc.es, david.serantes@gmail.com (D. Serantes).

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doi:10.1016/j.jnoncrysol.2008.07.040

accounts for the strength of the dipolar interaction [8], and is defined as the ratio between the volume occupied by the particles and the volume of the sample. It is treated by means of the reduced parameter c/c_0, where $c_0 = 2K/M_S^2$ is a unitless constant that characterizes the material. The magnetic field is introduced by means of the reduced field $h = H/H_K$, where $H_K = 2K/M_S$.

3. Results and discussion

We simulated the ZFC processes for different sample concentrations $c/c_0 = 0.064$, 0.128, 0.192, and 0.256, and the values of the reduced field vary between 0.05 and 1.20 for each value of c/c_0. We have simulated also the non-interacting limit case $c/c_0 = 0.000$ for the sake of the comparison with the aforementioned sample concentrations.

The temperature variation ratio was $0.00613\,KV/k_B$ every 1000 Monte Carlo steps. In Fig. 1(a) are represented the ZFC curves for the increasing values of reduced field for the $c/c_0 = 0.064$ case. It is observed the expected trend for the magnetic nanoparticle assembly: the overall increase of the magnetization for increasing values of the reduced applied field, together with the shift of the maximum of the curves to lower temperatures. We show also in Fig. 1(b) the ZFC curves obtained for the different interacting conditions under the same applied field. It is observed the overall shift of the blocking temperature (T_B) to higher values as the concentration increases, in agreement with previous works [6].

From the maximum of the curves of Fig. 1(a) we obtain the blocking temperature as a function of the applied field. Analogously, we obtain this dependence for the different interacting conditions of Fig. 1(b). The results are shown in Fig. 2.

The overall shape of the curves in Fig. 2 shows that at low fields the blocking temperature is quite close for the different interacting conditions, and gradually separates as the field grows. This situation shows that at low fields the more important energy is the anisotropy, and that the low Zeeman energy does not affect much the superparamagnetic behavior. With regards to the influence of the dipolar interaction energy at these low fields we cannot infer a clear tendency, since more detailed calculus should be done for this purpose. Experimental works in 2D systems report negligible effect of the magnetic field on T_B at low concentrations below magnetic percolation [9], and so it remains as an interesting task the comparison between the 2D and the 3D arrangements. However, the purpose of this work was not to study this low-field scenario, but instead the whole-field spectra, and in particular the values around the anisotropy field of the particles, where for this sake the calculus show enough precision.

For increasing fields the curves progressively separate. For dilute conditions the curves decay rapidly to lower temperatures, while this tendency is attenuated and shows a plateau-like shape for increasing concentrations. This behavior is expected, in the sense that for larger concentrations the dipoles are more tighten and therefore the same field produces a less noticeable effect. This is the reason why, though at low sample concentrations t_B disappears for fields quite below H_K, for large concentrations t_B exists even for fields larger than H_K. This result contradicts the equation usually assumed to describe this dependence [7], which describes T_B as proportional to $(1 - H/H_K)^{1.5}$.

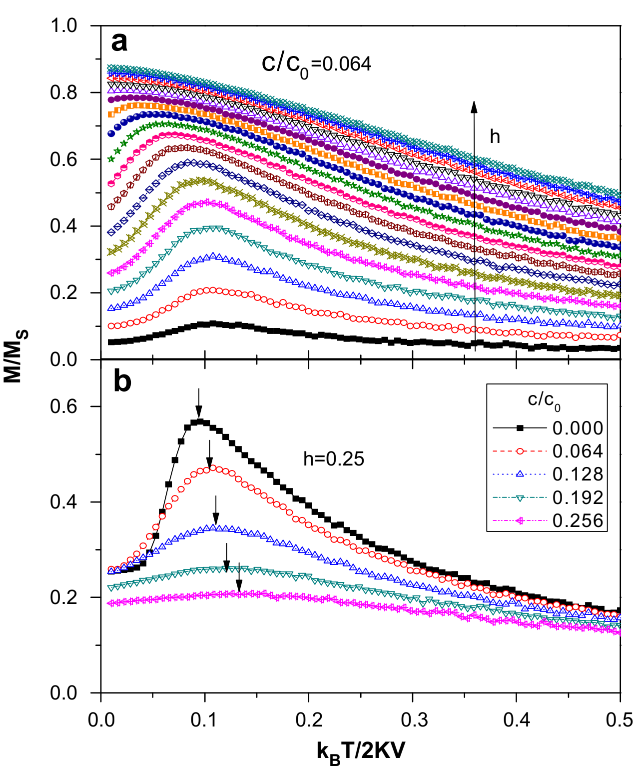

Fig. 1. (a) ZFC curves for increasing fields at $c/c_0 = 0.064$. The arrow signals the direction of increasing fields. (b) ZFC for increasing interacting conditions at a fixed reduced field $h = 0.25$. The arrows point the corresponding maxima of the curves.

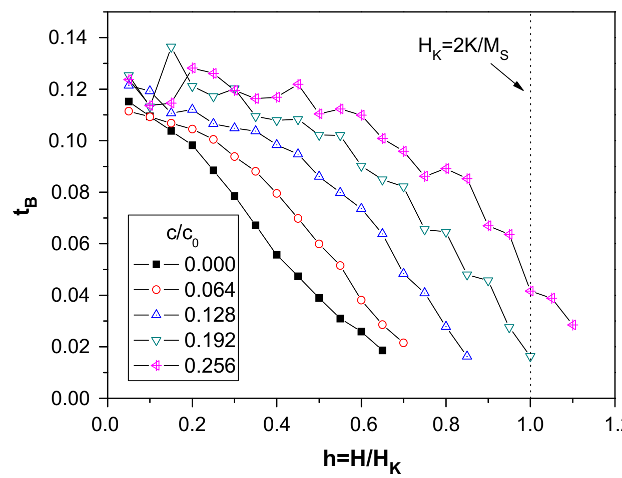

Fig. 2. Reduced blocking temperatures for different interacting conditions plotted against the reduced applied field. The dotted line shows the reduced field that corresponds to the anisotropy field (H_K) of the particles.

4. Conclusions

We have used a Monte Carlo technique to observe how the magnetic dipolar interaction affects the field dependence of T_B for a fine magnetic particle system. We observed that for large concentrations T_B exists even for $H > H_K$, and we showed therefore that the classical expression [7] that predicts T_B to disappear when $H \to H_K$ must be improved.

Acknowledgements

The authors acknowledge the Centro de Supercomputación de Galicia (CESGA) for computational assistance. D. Serantes and M. Pereiro acknowledge financial support from the Xunta de Galicia ("Maria Barbeito" and "Isabel Barreto" programs, respectively). This work was supported by the Spanish Ministry of Education and Science under the Project No. NAN2004-09203-C04-04 and by the Xunta de Galicia under the Project No. INCITE08PXIB236052PR.

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