

## THE INFLUENCE OF THE EFFECTIVE ANISOTROPY CONSTANT ON THE RELAXATION PROCESS IN INTERACTING NANOPARTICLE SYSTEMS

Mihaela OSACI

Hunedoara Engineering Faculty, Revolutiei no.5, 331128, Romania  
e-mail: [mihaela.osaci@fih.upt.ro](mailto:mihaela.osaci@fih.upt.ro)

The most challenging problem in physics of disordered systems of magnetic nanoparticles is the investigation of their dynamical properties. The major difficulty here is due to the long – range and dipolar inter particle interaction. Some experimental and theoretical researches of last period on the relation between the dipolar magnetic interaction strength and the relaxing time give inconsistent results. This study introduces a feigning parameter for the effective anisotropy constant. Thus, a description of the influence of the parameter on the energy barrier distribution density in interacting magnetic nanoparticle systems, is given as a possible interpretation of the mentioned inconsistent results.

*Key words* :Relaxation process; Nanoparticles; Dipolar interaction; Simulation.

### 1. INTRODUCTION

Experimental measurements show us, on one side, that the relaxing time in such systems, increases with the nanoparticle concentration increase, that means, it increases with the interaction strength [1], [2], [3], [4], and in some cases [5] shows a decreasing relaxing time when the interaction strength increases.

In this paper we try an interpretation for this contradiction.

The most direct theoretical method to study the corresponding dynamics is based on numerical solution of stochastic Langevin equations [8]. Our study originates from the three – dimensional simulation model for the relaxation process in ultra fine magnetic particle systems presented in [7]. The  $z_{med}$  parameter connected with the effective anisotropy constant by means of the anisotropy shape constant is investigated.

### 2. THE LANGEVIN – DYNAMICS SIMULATION OF INTERACTING ULTRA FINE MAGNETIC PARTICLE SYSTEM

In this paragraph we present novel results obtained using a method based on numerical solution of stochastic Langevin equation [8]. In this work one simulates a system of randomly placed non-overlapping spherical single-domain magnetic particles. To calculate  $\chi(T)$  they integrate numerically the stochastic Landau – Lifshitz – Gilbert equation [6] for the motion of the nanoparticle magnetic moments  $\mu_i$  in the deterministic  $H_i^{eff}$  and random  $H_i^n$  fields. The field  $H_i^{eff}$  includes the external and interparticle interaction fields. One assumes that all nanoparticles possess uniaxial anisotropy with the reduced anisotropy constant  $\beta = \frac{2K}{M_s^2}$ , where K is the effective anisotropy constant and  $M_s$  the saturation magnetization. The real  $\chi'(\omega, T)$

and the imaginary  $\chi''(\omega, T)$  part of the ac-susceptibility are calculated in a standard way applying an oscillating field  $h_z = h_0 \cos \omega t$  and measuring in – and out-of-phase magnetization components. The low

temperature used below is defined in units of the stray field energy as  $T = \frac{kT}{M_s^2 V}$  ( $V$  being the nanoparticle

volume), the low frequency is  $w = \frac{\omega}{\gamma M_s}$ , ( $\gamma$  is the gyromagnetic ratio). The most interesting question

concerning the behavior of the system under study is the influence of the interparticle interaction on its ac – susceptibility  $\chi(T)$ . To study this problem one performs simulations for various particle volume concentrations  $c$ . Typical results [8] show that changes in the  $\chi(T)$ - curves with increasing concentration depend qualitatively on the single particle anisotropy  $\beta$ . For high and moderate anisotropies ( $\beta > 1$ ) the peak on the  $\chi(T)$ - dependencies shifts towards lower temperatures when the particle concentration (and the interaction strength) increase.

This means that the dipolar interaction leads to the decrease of the free energy barriers in systems of nanoparticles with high and moderate anisotropies. This result is in agreement with the Mössbauer experiments of Morup et al. and his theoretical predictions [5], [9] (where the interaction is treated as a small perturbation) and our recent numerical results for the energy barrier distribution density in such systems [7]. For sufficiently small anisotropy values (how small – depends on  $\lambda$ ) the  $\chi(T)$  - peak shifts towards higher temperatures with increasing concentration. This can be easily understood, because the low anisotropy  $\beta$  means that already for moderate particle concentration the interparticle interaction is the dominant contribution to the energy barrier height. Hence the average barrier height increases when the particle concentration increases. Such behavior (shift of the  $\chi(T)$  – peak towards higher temperatures with increasing concentration) was founded in most experiments on standard magnetite or maghemite ferrofluids [10], [11].

### 3. THE INFLUENCE OF THE EFFECTIVE ANISOTROPY CONSTANT PARAMETER ON THE RELAXATION PROCESS

We discuss this problem using the three-dimensional simulation model for the relaxation process in magnetic nanoparticle systems presented in [7]. In this model, we suppose that the nanoparticles are randomly distributed in the considered volume. The overall magnetic dipolar energy of the nanoparticle  $i$  will be:

$$E_{id} = -\frac{\mu_0}{4\pi} M_i \cos \theta_i \sum_j \frac{M_j}{r_{ij}^3} (3z_{ij}^2 - 1) \cos \theta_j \quad (1)$$

where  $\vec{M}_i$  is the magnetic moment of the nanoparticle  $i$ ,  $\vec{M}_j$  is the magnetic moment of the nanoparticle  $j$ ,  $\vec{r}_{ij}$  is the vector which joins the centers of the two nanoparticles and where  $z_{ij}$  is the component of the unit vector on the axis  $Oz$ , in the direction which joins the two nanoparticles. We consider that the easy magnetization direction of the particle  $i$  is the direction of the axis  $Oz$  (figure 1).

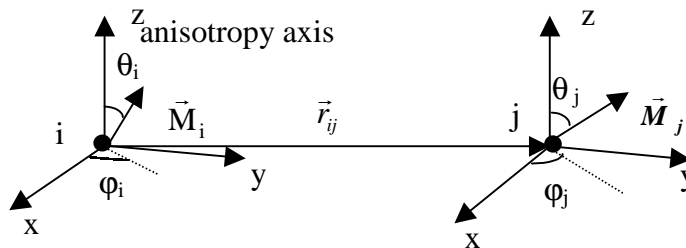


Fig. 1 The scheme of the simulation model.

Considering that the nanoparticle system exhibits an uniaxial anisotropy, the overall energy of the  $i$  nanoparticle is:

$$E_i = -\frac{\mu_0}{4\pi} M_i \cos \theta_i \sum_j \frac{M_j}{r_{ij}^3} (3z_{ij}^2 - 1) \cos \theta_j - K v \cos^2 \theta_i \quad (2)$$

where  $K$  is the nanoparticle uniaxial anisotropy constant. We also assume that the  $z$  - components of the unit vectors along the direction between  $i$  nanoparticle and another nanoparticle have a gaussian distribution in  $(0,1)$  domain with  $z_{med}$  mean. We generate this distribution with the Box Mueller transform [12].

$$z_{ij} = z_{med} + \sigma_{zz} \sqrt{-\ln(rand1)} \cdot [\cos(2\pi \cdot rand2) + \sin(2\pi \cdot rand2)] \quad (3)$$

where  $rand1$  and  $rand2$  are two random numbers with uniform distribution in  $(0,1)$  domain and  $\sigma_{zz}$  is the variance of the  $z_{ij}$  variable. The value of  $z_{med}$  parameter is related to the arrangement mode for the nanoparticles around of a given nanoparticle. The conclusions of the study are related to the  $z_{med}$  influence on the relaxing process for dense systems. The  $z_{med}$  parameter is possible related to the shape anisotropy of the nanoparticles. For explaining the relation we shall consider an ultra dense spherical nanoparticle system. Taking into account that the first-order neighbors of the nanoparticle  $i$  (the tangent spheres at  $i$  sphere) are 12 for  $z_{med}=0$ . Using the Garcia formula [13] we get the volume fraction of the nanoparticles:

$$F = 0.32 \cdot \frac{8\pi K}{\mu_0 M_s^2} \quad (4)$$

If the nanoparticles shape is not perfectly spherical, the effective anisotropy constant value grows, the volume fraction, the number of the first order neighbors with the nanoparticle  $i$  grows and the arrangement mode of the nanoparticles gives a value non zero for  $|z_{med}|$  parameter.

In Fig. 2 it is presented the reduced remanent magnetization with time for ultra fine ( $v=5 \times 10^{-25} \text{ m}^3$ ) magnetite particles with  $|z_{med}|=0$  and  $\sigma_{zz} = 0.5$  for different temperatures (300 – 420 K).

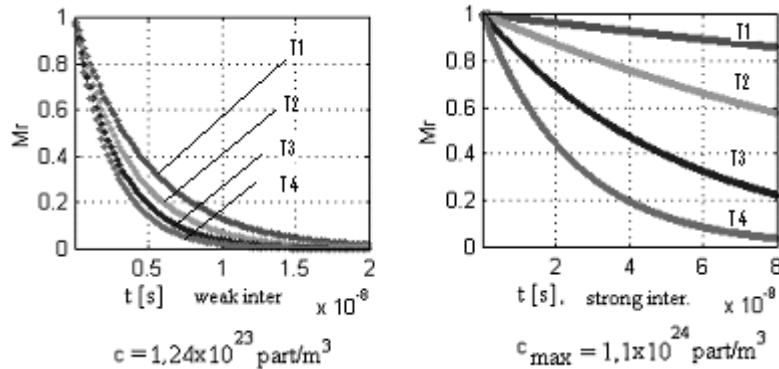


Fig. 2. The time dependence of the reduced remanent magnetization for an ultrafine identical spherical magnetite particles system (1622 particles) without shape anisotropy ( $|z_{med}|=0$  and  $\sigma_{zz} = 0.5$ ) for different temperatures (T1 = 300K, T2 = 340K, T3 = 380K, T4=420 K).

In Fig. 2, it is seen that the relaxing time increases when the interaction strength increases in agreement with the Dormann – Bessais - Fiorani theory [1] and by numerical integration of the stochastic Landau – Lifshitz – Gilbert [8] equation for small anisotropy values.

In case of the non-zero value for  $|z_{med}|$  parameter ( $|z_{med}|=0.5$  and  $\sigma_{zz} = 0.01$ ), for moderate and high effective anisotropy constant (particles with shape anisotropy) we find (Fig. 3) a decreasing of the relaxing time when the interaction strength increases in agreement with Morup [5] theory and with numerical integration of the stochastic Landau – Lifshitz – Gilbert equation [8] for moderate and high anisotropy values.

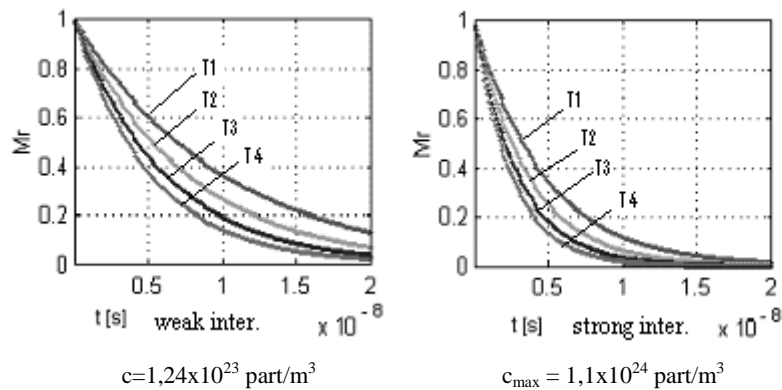


Fig.3

Fig. 3. The time dependence of the reduced remanent magnetization for an ultra fine identical spherical magnetite particles system (1622 particles) with shape anisotropy ( $|Z_{med}|=0.5$  and  $\sigma_{zz} = 0.01$ ) for different temperatures (T1 = 300K , T2 = 340K, T3 = 380K, T4=420 K).

#### 4. CONCLUSIONS

Using the 3D model for simulation of the relaxation process in ultra fine magnetic particle systems we got a decrease of the relaxation time when the interaction strength increases in agreement with Morup theory and by numerical integration of the stochastic Landau – Lifshitz – Gilbert equation for moderate and high anisotropy value and an increasing of the relaxation time when the interaction strength increases in agreement with the Dormann – Bessais - Fiorani theory, and with numerical integration of the stochastic Landau – Lifshitz – Gilbert equation for small anisotropy values.

#### REFERENCES

1. DORMANN, J.L., BESSAIS, L., FIORANI, D., J. Phys. C. 21, 2015, 1988.
2. ZHANG, P., ZUO, F., URBAN III, F.K., KHABARI, A., GRIFFITHS, P., HOSSEINI-TEHRANI, A., J. Magn. Magn. Mat. 225 337, 2001.
3. DORMANN, J.L., SPINU, L., TRONC, E., JOLIVET, J.P., LUCARI, F., D'ORAZIO, F., FIORANI, D., J. Magn. Magn. Mat. 183 (1998) L255 – L260
4. BARQUIN, L. F., GARCIA CALDERON, R., Journal of Physics (Conference Series) 17 (2005) 87 –100 Fifth International Conference on Fine Particle Magnetism
5. MORUP, S., TRONC, E., Phys. Rev. Lett. 72, 3278, 1994.
6. GARCIA – PALACIOS, J.L., LAZARO, F.J., Phys. Rev., B 58, 14937, 1998.
7. OSACI, M., PANOIU, M., HEPUT, T., MUSCALAGIU, I., Applied Mathematical Modelling 30, 545, 2006.
8. BERKOV, D.V., GORN, N.L., GÖRNERT, P., INNOVENT e.V., Felsbachstr.5,D-07745, Jena, Germany
9. HANSEN, M.F., MORUP, S., J. Magn. Magn. Mat. 184, 262, 1998.
10. JONSSON, T., MATTSO, J., DJURBERG, C., KHAN, F.A., NORDBLAD, P., SVENDLINDH, P., Phys. Rev. Lett., 75, 4138, 1995.
11. ZHANG, J., BOYD, C., LUO, W., Phys. Rev. Lett., 77, 390, 1996.
12. KOCH, R.G., s.a., *Modelling of Arc Furnace Flicker and SVC Compensation Requirements*, South African Universities Power Engineering Conference, 1994
13. GARCIA – OTERO, J., PORTO, M., RIVAS, J., BUNDE, A., Physical Review Letters, vol. 84, nr.1, 2000.

Received: January 21, 2007