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THE MCAMC ALGORITHM IMPLEMENTATION (MONTE CARLO WITH ABSORBING MARKOV CHAINS) IN THE STUDY OF MAGNETIC RELAXATION PROCESSES IN NANOPARTICLE SYSTEM

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Due to the complexity of the magnetic nanoparticles systems, their study by simulation, requires more and more performant algorithms. This work represents an implementation of an advanced Monte Carlo algorithm, MCAMC (Monte Carlo with Absorbing Markov Chains) for the study of the magnetic relaxation processes in nanoparticles systems. The achieved results with stochastic model, based on MCAMC algorithm, are compared with the achieved results with Néel – Brown model for a diluted system of magnetic spherical nanoparticles, which is completed with a random distribution of dimensions, and a distribution of the effective anisotropy constants.

Key words: MCAMC algorithm; Relaxation process; Nanoparticle; Simulation.

1. INTRODUCTION

In nanomagnetism, the modeling and the simulation represent very important instruments, which are of help in exploiting very interesting phenomena in magnetic media that are interesting for technological applications [1], [2], [3]. As a strategy, it is necessary to realize simulation models as realistic as possible, using quicker and quicker algorithms for their implementation.

As dynamic Monte Carlo methods used till now for Ising physical models (with two metastable states), we note: the Glauber method [4] for a one-dimensional Ising chain dynamic or the Metropolis method [5]. Both methods offer us a correct statistic for Ising phenomenological model [6], [7], but it is necessary a long time if the state change probability is a small one. There were developed a lot of dynamic Monte Carlo performance algorithms [7], which can be very easy implemented in modeling of complex systems.

2. MAGNETIC RELAXATION IN NANOPARTICLES SYSTEMS AFTER NÉEL – BROWN MODEL

We consider a single domain spherical particles system with a lognormal distribution for anisotropy constants and diameters. The particles have a rigid catching, and do not interact. The particles are considered to exhibit uniaxial anisotropy.

For thermodynamics equilibrium in a zero magnetic field ($H = 0$), the magnetization medium of a particle is entirely zero ($M = 0$) due to the orientation of the easy magnetization axis, and, in the same time, due to the spontaneous magnetization of the particles, which are distributed with equal probability in all directions.

By applying a magnetic field, the spontaneously magnetized particles shift near the field direction, and become magnetized. Based on the model Néel-Brown [8], [9], where the magnetic field becomes zero, the whole remanent magnetization does not vanish, but suffers a gradual diminishing following an exponential law:

$$M_{rem}(t) = M(0) \cdot e^{-\frac{t}{\tau}} \tag{1}$$

where, M(0) is the remanence at t=0, i.e., in the moment of the field disconnection, the field which produced the saturation, $M_{rem}(t)$ is the remanence after the time interval t, and τ is the relaxation time (the time after which the system returns to the thermodynamic equilibrum). We define the reduced remanent magnetization at the moment t as the ratio between the remanence at the moment t and the remanence at the moment t = 0 (the moment of the disconnection of the external magnetic field) [8]:

$$M_r(t) = \frac{M_{rem}(t)}{M(0)} = e^{-\frac{t}{\tau}} \tag{2}$$

An estimation of the relaxation time is given by Néel and Brown [9], [10]:

$$\tau = \tau_0 \cdot \exp\sigma \tag{3}$$

with

$$\sigma = \frac{KV}{k_B T} \tag{4}$$

where K is the effective constant of particle anisotropy, k_B the constant of Boltzmann, and V is the volume of particles. τ_o was calculated by Stepanov and Shliomis [11]:

$$\tau_0 = \frac{\sqrt{\pi}}{2}\tau_a\left(\frac{KV}{k_B T}\right)^{-\frac{1}{2}} \tag{5}$$

where $\tau_a = \frac{M_s}{2\alpha\gamma K}$ is the relaxing time of the precession movement into the anisotropy field, M_s is the spontaneous magnetization, α is the relaxing adimensional constant and γ giromagnetic ratio.

3. STOCHASTIC MODELLING OF MAGNETIC RELAXATION PROCESS WITH A MCAMC ALGORITHM

In the following will be presented the essential of the algorithm MCAMC. One considers an absorbing Markov chain with s transient states and r absorbing states [7]. The system starts in one of the s transient states, and remains in the transient subspace of the s transient states until it is absorbed into one of the r absorbing states. One calculates the life of the system in the transient subspace.

One takes a monodomain spherical nanoparticle system with a lognormal distribution for diameters and for anisotropy constants, which does not interact, and have a rigid attachment into a solid matrix, under an external magnetization field. Let the nanoparticles have uniaxial anisotropy. We also consider an Ising system, with two metastable states (state 1- the magnetic moments of parallel nanoparticles with the magnetization field direction and state 2 - the magnetic moments at an angle of 180° as compared to the magnetization field direction). At the initial moment, we cancel the magnetization field and simulate dynamically the system.

For simulating the evolution of $M_{r,}$ reduced remanent magnetization, with the time, we used the MCAMC method [6],[7], where for transient subspace has only one state (the current state of system configuration).

By considering one nanoparticle of the system, primary, it is in state 1, then passes to state 2 (absorbing state), by one intermediate state - the current state. This i nanoparticle, has the E_i energy in each of these states. The transition probability is :

$$p_{ik} = \frac{\exp\left(-\frac{E_{bik}}{k_B T}\right)}{\exp\left(-\frac{E_i}{k_B T}\right) + \exp\left(-\frac{E_{bik}}{k_B T}\right)} \tag{6}$$

where: k=1 for state 1, k=2 for state 2. E_{bik} is the energy barrier for metastable states 1 and 2.

The algorithm steps are :

1. The initializing for reduced magnetizing for $M_r = 1$ system, the parallel magnetic moments with external magnetic field direction which cancel out.
2. The E_i nanoparticles of current energies;
3. Setting the t time at 0;
4. One repeates the next steps until $M_r = 0$;
   a. Incrementing the Monte Carlo time t=t+1.
   b. Generating a random number, r_1, having an uniform distribution in (0,1) interval, which is used for random selection of i nanoparticle from the system i =1+[$r_i N$] where $[x]$ is the complete part of x.
   c. Generating two random numbers, r_2 and r_3 for selected i nanoparticle.
   d. If *i* nanoparticle is not in state 1 and $r_2 \le \frac{1}{2}$, the *i* nanoparticle can pass in state 1, otherwise it passes in state 2
   e. The transition probabilities calculation for *i* nanoparticle (p_{i1} - transition in state 1, p_{i2} - transition in state 2), according to the relation (6).
   f. If $r_2 \le 1/2$ and $r_3 \le p_{i1,}$ the *i* nanoparticle passes in state 1,l with the reduced magnetization $M_r = M_r + \frac{1}{N}$.
   g. If $r \rangle 1/2$ and $r_3 \le p_{i2}$, the *i* nanoparticle passes in state 2, on making topical the reduced magnetization $M_r = M_r - \frac{1}{N}$ and the nanoparticle energy;
   h. If we have not any of these two sets of conditions, the i nanoparticle has no transition on.

A Monte Carlo step is connected by a possible random transition of a nanoparticle, of the system, in one Monte Carlo unity. As a real time, the period of time associated to a Monte Carlo step, can be connected to a real time unity in the Langevin dynamic sense $[12]$, t(MCS)=$10^{-12} s$.

In Fig. 1 it is represented the time dependence of reduced remanent magnetization, after the law (2)- continuous line, simulated with MCAMC algorithm - with * for a 1000 magnetite spherical nanoparticle system with $M_s = 4.7 \cdot 10^5 A/m$ spontaneous magnetization with a lognormal distribution of diameters (the average diameter is 10 nm), and, for effective anisotropy constants, at 300 K .

A good agremeent can be seen in Fig. 1.

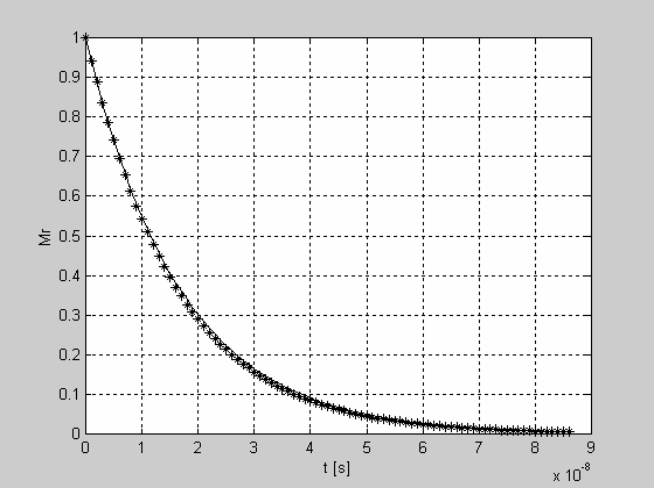

Fig. 1 The reduced remanent magnetizing depending on a Néel-Brown law (continuous line) and simulated with MCAMC algorithm (with *) for magnetic nanoparticles system (with an average diameter of 10 nm) with a lognormal distribution of diameters of anisotropy constants at 300 K.

4. CONCLUSIONS

The work represents an implementation of an advanced Monte Carlo algorithm (MCAMC) in real time with only one transient state in the study of the magnetic relaxation processes in nanoparticle superparamagnetic systems.

The results obtained by simulation are in good agremeent with the results obtained by Néel – Brown model. This algorithm can be used, with minor modifications (adding classes of microparticles to transient states) for studying the dynamics of the nanoparticle system with dipolar interactions at low temperatures.

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