HPC Algorithms for Calculating Properties of Magnetic Nanostructures

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Abstract. *The critical phenomena on cobalt monolayer and submonolayer films and the properties of nanodots were studied by means of computer simulation and using HPC-algorithms. The proposed approach on the base of data of scanning tunneling microscopy gives the possibility estimate of the critical concentration needed for concentration transition to ferromagnetic state. An assumption about the presence of a critical switching field allowed the simulated hysteresis loops for the given 1.5, 2.0, 2.5, and 3.0 ML cobalt samples in frame of the Ising model, which have qualitative agreement with magnetometric data. Author's developed approaches to simulation of magnetic phenomena in nanostructures require using of supercomputers.*

Keywords

Parallel Monte Carlo method, Ising model, magnetic states, hysteresis, scanning tunneling microscopy, parallel tempering.

1 Introduction

It is assumed that, serious changes in information technologies are related with the successful studies on magnetic particles [1], and a further magnetic logic and MRAM development will be associated with magnetic nanostructures. The theoretical and experimental studies on the physical properties of ultrathin ferromagnetic films, ensembles, and single particles caused by the existence of the fundamental problems in the physics of magnetic phenomena are needed because of its details for nanoarchitecture construction [2–4].

The computer processing of experimental data and the subsequent simulation of the behavior of the surface of the ultrathin ferromagnetic films allow the development of new information about the physical nature of ferromagnetism and ferromagnetic anisotropy, which visualizes the processes of magnetization reversal in external fields. Research on the physical properties of thin ferromagnetic films is needed from the point of view of their practical applications in microelectronics and computer technology because magnetically nanostructured soft thin films are currently the main materials for the manufacture of the components of the magnetic random access memory [5–10]. The development of computing and supercomputer technology enables new classes of algorithms to solve complex problems of numerical modeling and to handle large and superlarge volumes of data. Thus, the discretization level of elements in the computer model now determines the resolution of a scanning tunneling microscope (STM) or a magnetic force microscope (MFM). This work was aimed at the creation of computer models and software for data processing STM and MFM data as well as the calculation of the magnetic and structural properties and numerical of magnetic materials.

2 Theoretical background

2.1 Simulation on the base of STM data

The methods of obtaining samples and experimental magnetometric data were published by Ivanov et al. [11,12]. The pixels on the STM images, see figure 1 (a-f), were differentiated into clustered atomic levels of Ising spins

over brightness, see figure 1 (e). It is assumed in the program model that all the underlying atomic steps are formed completely as solid, that is, without pores and vacancy defects in the process of the epitaxial growth. Therefore, clusters were constructed by means of filling a 3-D space face centered cubic (fcc) lattice. The computer model of STM image, see figure 1 (e), corresponds to the STM image on figure 1 (c) (numbers of atomic levels are the same on both figures). Before you start main topics of you paper, it is worth to provide overview of previous and related works, show motivation, why results presented in the paper are better, or author get further in investigation of paper topic.

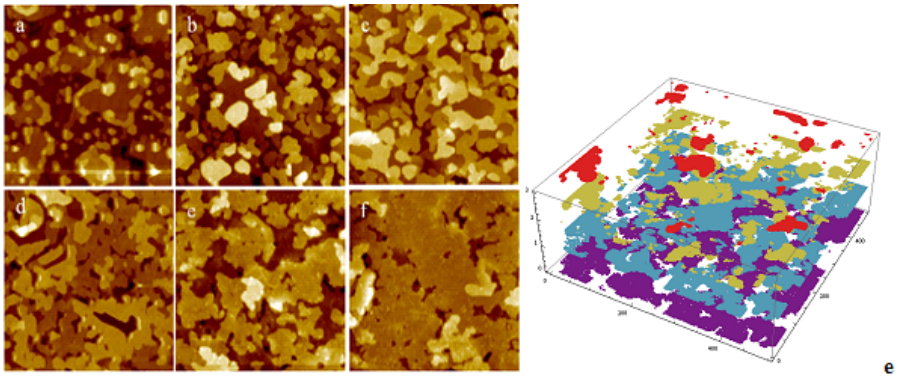

Figure 1. STM images of epitaxial Co(111) film at Co coverage: (a) 0.5 ML, (b) 1.0 ML, (c) 1.5 ML, (d) 2.0 ML, (e) 2.5 ML, and (f) 3.0 ML. Scale: 100 100 nm [11, 12], (e) The computer model of extracted field on STM Co (1.5 ML).

Each pixel, and consequently each point of the model sample, is approximately 1.443 atoms of fcc cobalt, with a lattice parameter of 4,089 Å. The total number of atoms (N) in the sample of 100 × 100 nm 1.5 ML of Co(111) is approximately $2.7 \cdot 10^5$. We used ranges of the pixel brightness values (0-80, 81-120, 121-150, 151-200, and 201-255) corresponding to the various heights of the atomic layers, see figure 2. The simulations

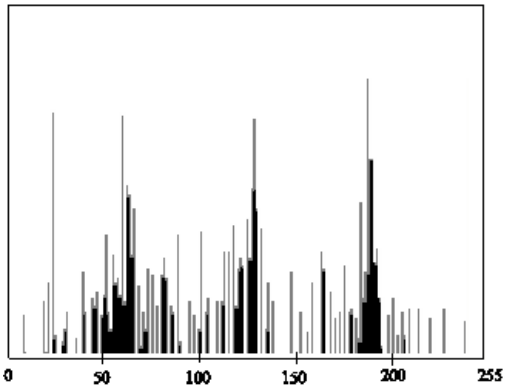

Figure 2. Histogram of the distribution of the pixel brightness.

are performed in the fcc lattice with the highest possible number of nearest neighbors ($z = 12$) using the famous Monte Carlo method. Each Ising spin in lattice point of simulated sample interacts with the nearest neighbor by means of the direct exchange. The number of Monte Carlo steps for the simulation of the temperature dependence of magnetization was approximately 10 times more than the number of points in a model system.

In the lattice sites are-spins S_i-whose values have changed abruptly from -1 to $+1$. In principle, the simulation can occur within any known model, such as the Ising model or the Heisenberg exchange integral of a certain value. We used the Ising model in which each spin in the lattice model of the nanofilm interacts via direct exchange with its nearest neighbors (up to 12 neighbors). In the Metropolis algorithm, we used dimensionless units for the Boltzmann constant, $k = 1$, and the exchange integral, $J = 1$. The transition from reduced units

to the measured physical quantities in the experiment is performed in accordance with the following expression [13]:

$$T_c = \frac{zJS(S+1)}{3k} \tag{1}$$

where z is the number of nearest neighbors, T_c is the Curie temperature, and S is the spin of the ion.

For the Ising spin system interacting with a direct exchange in an external magnetic field, we used the following equation:

$$\mathcal{H} = -J \sum_{n,n_0} S_n S_{n+n_0} - h \sum_n S_n \tag{2}$$

where n_0 is the number vector neighbor crystalline site n. The partition function is computed as follows:

$$Z_N(h,T) = \sum_{S_1} \sum_{S_2} \cdots \sum_{S_n} \cdots \sum_{S_N} Exp[-\sum_{n,n_0} \frac{\mathcal{H}}{kT}] \tag{3}$$

The probability of one of the 2^N configurations is defined by the Gibbs factor as follows:

$$P_i(h,T) = \frac{Exp[-\sum_{n,n_0} \frac{\mathcal{H}}{kT}]}{\sum_{S_1} \sum_{S_2} \cdots \sum_{S_n} \cdots \sum_{S_N} Exp[-\sum_{n,n_0} \frac{\mathcal{H}}{kT}]} \tag{4}$$

From the point of view of statistical physics, if the system $(+J)$ spins, as described by the Hamiltonian (equation 2) located in an external magnetic field h, coinciding with the sign of the spin excess at $T = 0$, then the system must be in the global minimum energy that corresponds to the magnetic state of complete ordering (ferromagnetism), and the probability of this event is equal to 1, according to equation 4, where the denominator can be left the most important term of the sum, which is equal to the numerator. The instantaneous change in the sign of the external field on the $-h$ should lead to the instantaneous change in the sign of the spin excess to reduce the Zeeman energy and, therefore, the transition to a symmetric configuration; as in this case, the degeneracy of the most likely state (here the ground state) of the system is 2.

At finite temperature $T \neq 0$ and $T < T_c$, the changes in the sign of the external magnetic field from h to $-h$ should also lead to a reversal of the spin excess. For an infinite number of spins (N) at finite temperature, there are an unlimited number of magnetic configurations with the same spin excess and energy, that is, with the same probability of realization. The changes in the sign of the field at $T < T_c$ should increase the probability of symmetric configurations with the opposite value of the spin excess. Currently available methods for Monte Carlo simulations to achieve equilibrium-in particular, the Metropolis-Hastings algorithm-imply the motion of the system in state space similar to a Markov process, where the probability of each successive configuration depends on the previous implementation:

$$P(E_0) \to P(E_1, e_0) \to P(E_2, E_1) \to \cdots \to P(E_{n-1}, E_n) \tag{5}$$

The movement toward equilibrium in this approach is due to the serial reversal of individual spins in accordance with equation 5.

The Ising model is used for simulation hysteresis phenomena, and the Monte Carlo method can introduce a positive anisotropy field (h_{an}), supporting the sign of the spin excess,

$$\mathcal{H} = -J \sum_{n,n_0} S_n S_{n+n_0} - h \sum_n S_n - h_{an} |\sum_n S_n| \tag{6}$$

then a magnetization reversal happens in case of equality in the energy of the spin system in the external magnetic field and the anisotropy energy.

The study of the phenomenon of magnetic hysteresis in the model takes into account the spin-flip probability, which depends on the average field of switching and temperature, as shown in figure 3. The transition to a state corresponding to the minimum energy is possible only after overcoming a potential barrier of anisotropy.

2.2 Simulation on the base of STM data

The algorithm of the processing of STM images is discussed in paper [11,12]. The number of rows of three-dimensional array equals the height of the STM-image, and the number of columns, the width of the picture, besides the "depth" is set equal to the number of layers in the sample (based on experimental data).

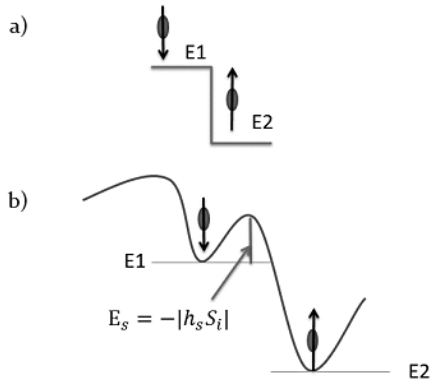

Figure 3. Variants of the transition to a state of minimum energy: (a) without field of switching; (b) with the field of switching.

The parallelism of the algorithm is implemented by splitting the three-dimensional array of spins on the parts (planes), for their subsequent distribution used the MPI library, and, accordingly, processing the each from a planes in the separate computation process. Pass (MC step) on the spin system and the implementation of Monte Carlo (MC) steps in the algorithm of Metropolis produced in the "checkerboard decomposition". This is done to avoid the problem of boundary conditions calculated for the configurations of planes handled, see figure 4. The initial values did not change during the MC, i.e. in this case, for each step of temperature or field, half of MC steps is initially for one half of the spins figure 4(b), and then for the second half figure 4(c). Parallel Metropolis algorithm is as follows:

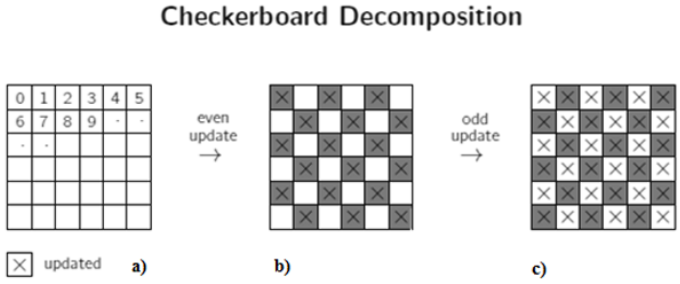

Figure 4. Distribution of the matrix on the process in a checkerboard pattern.

1. The number of rows (planes) of three-dimensional array of spins was send in the each process. This number was proportional to the number (braces on the right in figure 5). We used the approach, in which the maximum number of processes for the execution of the program equals to one form two of the linear dimensions of the STM (AFM) image in pixels;

2. Since each spin of the cobalt samples, see [11,12], the highest possible number of nearest neighbors $z = 12$, then for the correct accounting for spin neighbors standing on a block boundary rows (figure 5, marked by a white cross spin) the additional boundary rows of the neighboring processes sent in each process, which ones are located in different processes (braces on the left in figure 5);

3. The distribution of blocks of rows by using in-line functions MPI Scatterv, and the assembly, respectively, with the help of MPI Gatherv.

The search of the equilibrium configuration for each part is performed using usual Monte Carlo (Metropolis algorithm). Within the frame the model hysteresis magnetic phenomena were explained as the effect of nonequilibrium in the Ising spin lattice model. For the simulation of nonequilibrium processes in the monolayer samples were used only surface points of model sample, and used the number of MC steps used proportionally increased with the number of lattice sites. For this reason, the system of correlated spins cannot go into a state

of equilibrium during the time of field changing altering, which in our case leads to the phenomenon of magnetic hysteresis in the used model. The absence of an exact match of simulated and experimental data is due to the simplicity of the model.

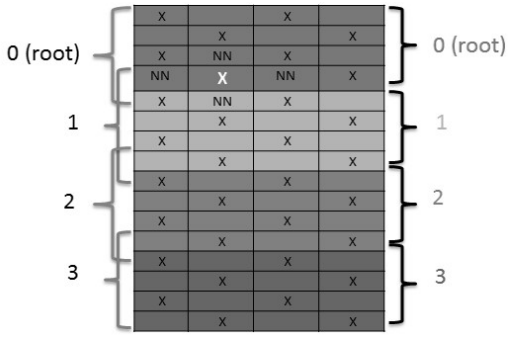

Figure 5. Distribution of the rows of blocks to process.

For systems of a large number of Ising spins N, movement toward equilibrium may be slow, especially at low temperatures T. Therefore, in order to speed up getting the most probable configuration with a given energy and spin excess was used in parallel computing scheme. Figure 6 shows dependencies of time from the number of processes for the sample 2.5 ML.

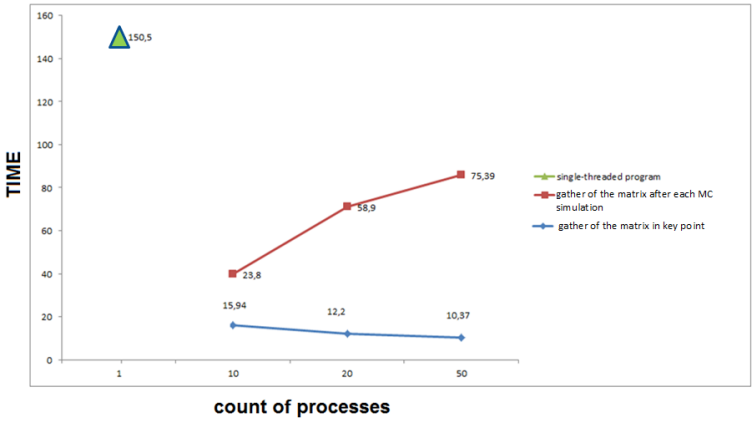

Figure 6. The plot of dependence of the execution time from the number of processes. The time in seconds.

The increase in time for the case when we are following each Monte Carlo simulations explain the fact that you want to collect a matrix with a large number of processes. The other is the schedule for the case when we collect the matrix only at key points. Reduce the time because the larger number of processes, the less processed of the matrix and so the time is reduced.

2.3 Simulation on the base of STM data

Since the calculation of the magnetization levels in described lattices is a very algorithmic-difficult task due to large number of possible configurations of the system, it was applied some acceleration algorithms. The methods to accelerate of the calculation of the ground state of previously described systems of magnetic particles, are also have been used. These methods could be applied as to lattice-ordered particles systems and to systems with random distribution of the particle positions.

Ground state (GS) – the state of the system with energy less than all other possible. According to theory of thermodynamics, a system at absolute zero temperature comes to GS state, so the properties of the system with will be determined by probability of all possible GS.

The simplest method of GS finding is the Brute-force method (BF). To find the GS, all states of the system should be calculated. Obviously, the amount of computation increases exponentially with the increase in the number of particles in the system. For this reason, it is very difficult to calculate the GS for a system.

The Metropolis algorithm could be applied. The main point of the method is randomly changes the directions of the magnetic moments of the particles in the system, with the condition that each step must be accompanied by a decrease of the energy. If energy is increased or not changed, the iteration is canceled with probability:

$$P = 1 - Exp[-\frac{\Delta E}{t}] \tag{7}$$

where ΔE - the energy difference between the last and current system state, t - temperature of system. However, this method is not able to give GS in 100% cases, since only one of the spins have been turned at the one step. This in most cases is not enough to get down to the global minimum energy state. An example of this behavior is shown in figure 7.

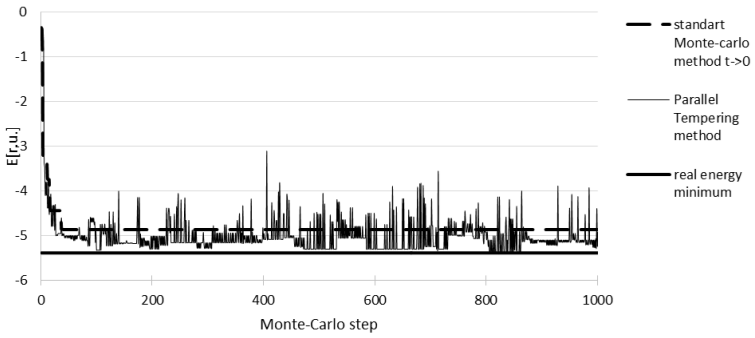

Figure 7. Comparison of the minimum energy getting speed: Monte Carlo method with $t = 0$ and Parallel Tempering with 5 replicas. The system consist of 20 particles is on the example.

Parallel Tempering method is the numerical simulation of multiple copies (replicas) of particle system, and their parallel annealing at different temperatures [15-17]. Difficult aspect of applying of this method is the correct selection of replicas count, their temperature and exchange moments of their temperatures.

Replicas exchange was made in accordance with [16] algorithm. Replicas exchange probability depends on energy difference between this replicas:

$$P = \min(1, Exp[-\Delta\beta]) \tag{8}$$

$$\beta = \frac{1}{k_B T_i} \tag{9}$$

Where k_B is a Boltzmann constant and equals 1, T_i - temperature of i replica, in relative units. Figure 7 shows that the PT method allows to reliably obtain GS unlike MC method, at list one for small number of particles. The use of PT method for a large number of particles in the system requires further research.

3 Results

3.1 Critical concentration and ferromagnetism

Belokon et al. [18] presented a method to calculate the critical concentration, which required a phase transition to ferromagnetic state in the crystal lattices with different numbers of nearest neighbor z. In this work, we determined the critical concentration of magnetic atoms for the transition to the ferromagnetic state for the monolayer and submonolayer samples of experimental data, which are given by Ivanov et al. [11]. The critical concentration, p_c, of the transition to the ferromagnetic state at T was determined from the following relation:

$$p_c = \frac{2}{z} \tag{10}$$

Table 1 shows the critical concentrations required for a phase transition to the ferromagnetic state, which implies that the sample of 1.5 ML at low temperatures should be in a state of the cluster ferromagnetism as far as $p < p_c$.

Table 1. Obtained concentrations of atoms in comparison with the critical concentrations and Curie temperature for different samples.

Number of monolayers	Number of nearest neighbors	T_c	p (at %)	p_c
1.5 ML	3.615	3.00	0.38	0.55
2.0 ML	6.984	6.15	0.50	0.29
2.5 ML	8.177	7.80	0.63	0.24
3.0 ML	9.308	8.70	0.76	0.21

3.2 Critical concentration and ferromagnetism

The critical field of switching of a magnetic particle (macrospins) needs to be overcome to change the magnetization of the magnetic particles. The effective field of switching was introduced to account for the spin-orbit interaction, which leads to the well-known phenomenon of anisotropy in the macroscopic scale. In the ultrafine materials, the distribution of the values of critical fields, the so-called coercive spectrum, could be observed. In our model of epitaxial nanostructures, all the spins interact with some field of switching, which preserves the direction of the spin. The reversal of the spin occurs when there is equality in the Zeeman energy (energy of the spin in an external field) and the energy of the spin in the field of switching. The greater the probability of switching, the higher the temperature; as temperature increases the probability of thermodynamic fluctuations, the probability of overcoming the energy barrier created the field of switching and, thus, the probability of local minimum energy. We used the following values of the field shift for the samples with different numbers of monolayers: 1.5 ML—2 reduced units (r.u.), 2.0 ML—8 r.u., 2.5 ML—4 r.u., and 3.0 ML—2 r.u. The different values of the field of switching are due to the need to provide qualitative agreement with the experiment, see figure 8.

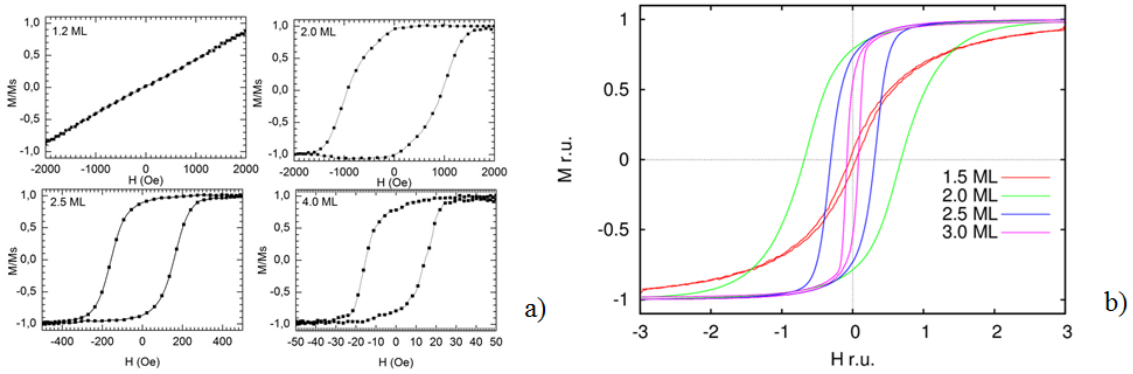

Figure 8. (a) Experimental hysteresis loops [11,12]. (b) Simulated hysteresis loops taking into account the field of switching.

4 Conclusion

This article discussed a model for supercomputer simulation on the base of a STM and an AFM data. The calculation of the magnetic and structural properties of the quasi-nanocluster magnets and the simulation of magnetic hysteresis phenomena were performed.

The concentration phase transition to ferromagnetic state at $T = 0$ was calculated as the critical concentration, pc. The simulation results of nanostructures and theoretical estimations are in qualitative agreement with the experiment for determining the concentrations of phase transitions in the ferromagnetic state.

The simulation results showed that the best method for finding the GS in two-dimensional magnetic particles system with the dipole-dipole interaction of randomly distributed on the plane particles is the PT method. However, this method requires high precision of replica and temperatures. Also, it was developed an accelerated method of system energy calculation. Calculation speed is increased at several times and is almost independent of the number of particles in the system, which allows almost without performance cost to implement the method in the algorithms of GS searching. The disadvantage of this method is big occupied RAM size.

5 Acknowledgments

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