Monte-Carlo investigation of competition between uniaxial anisotropy, exchange and dipolar interactions in critical behavior of ultrathin magnetic films

Anna P. Soldusova†, Pavel V. Prudnikov‡, Vladimir V. Prudnikov§
Department of Theoretical Physics, Omsk State University, Omsk 644077, Russia
E-mail: †anka.omsk@mail.ru, ‡prudnikp@univer.omsk.su, §prudnikv@univer.omsk.su,

Abstract. The investigation includes the observation of ferromagnetic-paramagnetic phase transition for a weak dipolar interaction. The system with strong dipolar interaction reveals the striped domain structure. Bilayer model with dipolar interlayer interaction demonstrates its effective antiferromagnetic character. Memory effects in ultrathin magnetic films are studied on basis of analysis of non-equilibrium relaxation of the autocorrelation function and magnetization.

1. Introduction
Ultrathin magnetic films are used in different applications such as storage and high-density record devices [1], high-sensitivity magnetic fields sensors [2], optical research of spin transmission [3], etc. The theoretical and experimental investigations of their properties become of great importance.

Competition between short-range exchange interaction, uniaxial anisotropy and long-range dipolar interaction results in appearance of different domain structures and in occurrence of the phase transitions. The strong enough dipolar interaction can provide the appearing of striped domain structures. Stripe phases are experimentally observed in high-temperature superconductors [4], and some computer studies are devoted to simulate these phenomena [5, 6, 7, 8].

This study includes the Monte-Carlo simulation of the critical behavior of ultrathin magnetic films. Memory effects can be observed in the non-equilibrium critical behavior of these systems.

2. Model and simulation
Magnetic film is constructed as a spin lattice with linear size $L$ and thickness of the film $N$. The model is described by the Hamiltonian in the following form:

$$H = -J \sum_{<i,j>} S_i \cdot S_j - A \sum_i S_{i,z}^2 - h \sum_i S_i + D \sum_{i \neq j} \left( \frac{S_i \cdot S_j}{r_{ij}^2} - 3 \frac{(S_i \cdot r_{ij})(S_j \cdot r_{ij})}{r_{ij}^5} \right),$$

(1)
where $\mathbf{S}_i$ is a three-dimensional spin in the lattice cite $i$, $J$ is exchange constant, $A$ characterizes uniaxial anisotropy in out-of-plane direction, $\mathbf{h}$ is applied magnetic field, $D$ characterizes the strength of dipolar interaction and $r_{ij} = r_i - r_j$ is the distance between cites $i$ and $j$.

Magnetization of the system and its projections is determined by

$$m = \left\langle \frac{1}{N_s} \sum_i \sqrt{S_{i,x}^2 + S_{i,y}^2 + S_{i,z}^2} \right\rangle, \quad m_z = \left\langle \frac{1}{N_s} \sum_i S_{i,z} \right\rangle, \quad m_{xy} = \left\langle \frac{1}{N_s} \sum_i \sqrt{S_{i,x}^2 + S_{i,y}^2} \right\rangle,$$

where $N_s = NL^2$ represents the number of spins in the film and $\langle ... \rangle$ denotes the statistical averaging.

For critical temperatures evaluation it was used Binder’s cumulant method determined by

$$U_\alpha = \frac{1}{2} \left( 3 - \frac{\langle m_{\alpha}^4 \rangle}{\langle m_{\alpha}^2 \rangle^2} \right).$$

Orientational order parameter which characterizes striped domain structure with spins oriented in the direction $\alpha$ is determined by Eq. 4, where $n^h_\alpha = \frac{1}{2} \sum_r \{1 - \text{sgn}[S_\alpha(r_x, r_y) \cdot S_\alpha(r_x + 1, r_y)]\}$ and $n^v_\alpha = \frac{1}{2} \sum_r \{1 - \text{sgn}[S_\alpha(r_x, r_y) \cdot S_\alpha(r_x, r_y + 1)]\}$ represent the number of nearest spins with antiparallel alignment in the horizontal and vertical directions respectively.

$$O_\alpha = \left\langle \sqrt{n^h_\alpha n^v_\alpha} \right\rangle.$$

Susceptibilities of magnetization projections $\chi_m$ and that of the order parameter $\chi_O$ are calculated with following equations

$$\chi_m = \frac{\langle m_{\alpha}^2 \rangle - \langle m_{\alpha} \rangle^2}{N_s T}; \quad \chi_O = \frac{\langle O_{\alpha}^2 \rangle - \langle O_{\alpha} \rangle^2}{T}.$$

3. Results of modeling
Simulation of the system with $A = 0.1J$, $D = 0.01J$ results in observing phase transition from the paramagnetic state to the ferromagnetic state with all spin aligned in the out-of-plane direction. Temperature dependencies of magnetization projections $m_z$ and $m_{xy}$ and their susceptibilities are demonstrated in Fig. 1 for the system with linear size $L = 32$.

![Figure 1](image-url)

**Figure 1.** Temperature dependencies of magnetization projections $m_z$, $m_{xy}$ and their susceptibilities $\chi_z$, $\chi_{xy}$ for ultrathin film with $A = 0.1J$, $D = 0.01J$, and $N = 1 \div 4$.
Temperature dependence of the orientational order parameter $O_z$ and its susceptibility $\chi_O$ is shown in Fig. 2. There is no striped domain structure in this case. Dipolar interaction is too weak to form such a structure.

Figure 2. Temperature dependencies of orientational order parameter $O_z$ and its susceptibility $\chi_O$ for ultrathin film with $A = 0.1J, D = 0.01J$, and the number of layers $N = 1 \div 4$.

Binder’s cumulants $U$ provide calculating critical temperatures of ultrathin films with $A = 0.1J, D = 0.01J$: $T_c = 0.713(11)$ for $N = 1$; $T_c = 1.034(13)$ for $N = 2$; $T_c = 1.175(25)$ for $N = 3$; $T_c = 1.272(12)$ for $N = 4$.

3.1. Striped spin configurations for ultrathin film with strong dipolar interaction

The simulation was conducted for the system with $N = 2$ and strong dipolar interaction $D = 1.0J, 10.0J, 100.0J$. The system with $D = 1.0J$ demonstrates no striped domain structure. Instead, ferromagnetic order was observed between spins in the same layer and antiferromagnetic order between spins in neighboring layers at a low temperature. An example of such a configuration for $T = 0.7$ is shown in Fig. 3. In this figure colors show spin projections in the out-of-plane direction for both layers of the film. Spins has antiparallel alignment in neighboring stripes and in neighboring layers. At a high temperature paramagnetic state is observed.

For the system with $D = 10.0J$ and $D = 100.0J$ striped domain structure is appeared. Typical spin configurations are shown in Fig. 4 for $T = 0.7$. The increase of temperature leads to gradual destruction of stripes and transition to paramagnetic state. When the dipolar constant $D$ becomes larger it leads to increase of the critical temperature.

Figure 3. Striped spin configuration for ultrathin film with $N = 2, A = 0.1J, D = 1.0J, T = 0.7$

Figure 4. Striped spin configuration for ultrathin film with $N = 2, A = 0.1J, D = 10.0J, T = 0.7$
3.2. Bilayer structure with dipolar interlayer interaction
The study of bilayer structure was carried out. The scheme of such structure is presented in Fig. 5. The system consists of two films with thickness \( N \) and dipolar interaction between them. At low temperature antiferromagnetic order is observed between two layers. Temperature dependence of out-of-plane layer magnetization \( m_z \) is demonstrated in Fig. 6. This order can be changed to ferromagnetic by applying of external magnetic field in the out-of-plane direction. Temperature dependence of out-of-plane layer magnetization \( m_z \) is shown in Fig. 7 for the case of \( h_z = 1.0 \).

4. Memory effects
Memory effects were revealed by analysis of non-equilibrium critical relaxation of the autocorrelation function \( C(t, t_w) = \left\langle \frac{1}{N} \sum_i S_i(t) S_i(t_w) \right\rangle \) and the magnetization from low- and high-temperature initial states. Time dependencies of these functions for low-temperature initial state (\( m_0 = 1 \)) and waiting times \( t_w = 20, 40 \) MCs/s are shown in Fig. 8.

Time dependencies of autocorrelation function and magnetization for high-temperature initial state (\( m_0 \ll 1 \)) and waiting times \( t_w = 20, 100 \) MCs/s are shown in Fig. 9. It were concluded
Figure 9. Non-equilibrium critical relaxation of autocorrelation function $C$ and magnetization $m$ for waiting times $t_w = 20, 100$ MCs/s. At the moment $t_{start} = t_w$ it were produced cooling (blue color) or heating (red color) cycling procedure for $\Delta T = 0.2$ during $\Delta t = t_w$ MCs/s. Evolution starts with high-temperature initial state with $m_0 = 0.01$

that memory effects brightly appear in cooling cycling procedure with relaxation from the low-temperature initial state.

5. Conclusions
The competition between exchange interaction, uniaxial anisotropy and dipolar interaction leads to appearance of wide range of phenomena. The phase transition from ferromagnetic to paramagnetic state is observed in systems with weak dipolar interaction with out-of-plane spin alignment in ferromagnetic phase. The increase of dipolar interaction strength leads to antiferromagnetic ordering between spins in adjacent layers with conserve of the ferromagnetic order in the same layer at a low temperature. Further increasing of dipolar interaction strength leads to striped domain structure phase.

The modeling of the bilayer film with dipolar interlayer interaction demonstrates the effective antiferromagnetic character of this interaction. Dipolar interaction is resulted in antiparallel orientations of adjacent ferromagnetic layers. This spin configuration may be changed by application of the external magnetic field.

The study of memory effects in thin magnetic films shows that these effects brightly appear in non-equilibrium relaxation from low-temperature initial state with cycling procedure of cooling.

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