Non-equilibrium critical behaviour of ultrathin magnetic and metamagnetic Ising films

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Abstract. Monte-Carlo simulations have used to observe both equilibrium and non-equilibrium critical behaviour of Ising thin films with simple cubic lattice structure. The thickness dependency of critical temperature was obtained for metamagnetic thin films. By exploring the short-time scaling dynamics, we have found critical exponents z and θ' for ferromagnetic thin film. Aging effects were discovered for non-equilibrium behaviour of thin ferromagnetic films.

1. Introduction

Magnetic multilayer films provide convenient model systems for studying the physics of antiferromagnetic films and surfaces. The new physical phenomena can be observed in thin films and some states can be realized, which are not observed in bulk samples. Possible application field of ultrathin magnetic films range from spintronics devices [1] to high-density recording technology [2, 3].

It has been theoretically suggested that the highest areal density advantage for Heat assisted magnetic recording (HAMR) can be achieved when the maximum heating temperature is closed to or exceed the Curie temperature [4]. HAMR is the most likely candidate technology to achieve magnetic recording densities 1 TBit/in^2 [5, 6]. In this sense, it is important to understand the evolution of magnetization in ultrathin magnetic films with temperature, especially at temperatures close to or above the Curie temperature.

Artificial antiferromagnets, formed of nanostructured superlattices that are coupled antiferromagnetically, have been the focus of many recent studies, due to their high potential for technological applications [7]. Artificial antiferromagnets are heterostructures composed of ferromagnetic layers that are coupled antiferromagnetically via spacers. This structure yields a high level of control over both the intra- and interlayer interactions, allowing for a tailoring of the physical properties.

Examples include [Co/Pt]/Ru, where ferromagnetic Co/Pt multilayers are periodically separated by Ru layers [8, 9]. [Co/Pt]/Ru, with strong perpendicular anisotropy have been called synthetic metamagnets [10], as they can exhibit a regime with an antiferromagnetic phase at low external magnetic fields and a paramagnetic phase at large fields. Metamagnetic systems are systems which present both ferromagnetic and antiferromagnetic couplings simultaneously. Metamagnetic materials are of great interest because it is possible to induce novel kinds of critical behaviour by forcing competition between these couplings, especially by applying a magnetic field. Critical behaviour in metamagnetic films can be differ from bulk behaviour. Both new

intermediate phase and critical end point exist for metamagnetic films (see the phase diagram from [11]) unlike bulk metamagnetics.

In this paper we study the equilibrium and non-equilibrium properties of Ising magnetic and metamgnetic films using Monte Carlo simulations by short-time dynamic method [12, 13].

The paper is organized in the following manner. The Ising metamagnetic model and the Monte Carlo simulation scheme are discussed in the next section (Section 2). The numerical results are given in Section 3. The paper ends with concluding remarks and summary in Section 4.

2. Model and simulation technique
In this study we consider the Ising hamiltonian

$$H = -J_{xy} \sum_{<i,j>} S_i S_j - J_z \sum_{(i,j)} S_i S_j - h \sum_i S_i, \tag{1}$$

where spins $S_i = \pm 1$, $J_{xy} > 0$ and J_z are intralayer and interlayer coupling strengths, respectively; $J_z > 0$ for ferromagnetic film and $J_z < 0$ for metamagnetic film; h is external magnetic field. The sums over $\langle i, j \rangle$ are the sums over nearest-neighbor pairs in the plane of film and (i,j) – along the z direction. The interaction is nearest-neighbor short-ranged in-plane and out-of-plane direction. Periodic and free boundary conditions are used for the in-plane and out-of-plane directions, respectively.

The simulations are carried out for systems of size $L \times L \times N$, where L is linear size of layer and N is number of layers. Metropolis algorithm was used for updating spin configurations.

The order parameter for ferromagnetic films ($J_z > 0$) can be defined as magnetization

$$m = \left\langle \frac{1}{N_s} \sum_i^{N_s} S_i \right\rangle, \tag{2}$$

where $N_s = NL^2$ is the number of spins, angle brackets denote the statistical averaging. The order parameter for metamagnetic films is the staggered magnetization

$$m_{stg} = |m_1 - m_2|, \tag{3}$$

where m_1, m_2 are the magnetization of odd and even layers, respectively.

The critical temperature of metamagnetic films T_c is located via fourth-order cumulant $U_4(L, T)$, defined as

$$U_4(L, T) = \frac{1}{2} \left[3 - \frac{\langle m^4(L, T) \rangle}{\langle m^2(L, T) \rangle^2} \right], \tag{4}$$

where T is temperature in J/k_B, the angle brackets denote the statistical averaging, fourth-order cumulant $U_4(L, T)$ is equilibrium characteristic of metamagnetic materials.

The cumulant $U_4(L, T)$ has a scaling form

$$U_4(L, T) = u \left[L^{1/\nu}(T - T_c) \right]. \tag{5}$$

The scaling dependence of the cumulant makes it possible to determine the critical temperature T_c from the coordinate of the intersection points of the curves specifying the temperature dependence $U_4(L, T)$ for different L.

For investigation non-equilibrium properties of critical behaviour of magnetic materials we were considered time dependencies of magnetization $m(t)$ and second-order Binder cumulant $U_2(t)$, where time t is measured in Monte-Carlo steps per spin (MCS/s). According to the

argument of Janssen et al. [15] obtained with the RG method and ε-expansion, one may expect a generalized scaling relation for the time dependence of k-th moment the magnetization

$$m^{(k)}(t, \tau, L, m_0) = b^{-k\beta/\nu} m^{(k)}(b^{-z}t, b^{1/\nu}\tau, b^{-1}L, b^{x_0}m_0), \qquad (6)$$

is realized after a time scale t_{mic} which is large enough in a microscopic sense but still very small in a macroscopic sense. In (6) b is a spatial rescaling factor, β and ν are the well-known static critical exponents, z is the dynamic exponent, the new independent exponent x_0 is the scaling dimension of the initial magnetization m_0 and $\tau = (T - T_c)/T_c$ is the reduced temperature.

When system evolving from a completely ordered state ($m_0 = 1$) magnetization have a scaling form $m(t) \sim t^{-\beta/z\nu}$. The cumulant $U_2(t)$ is defined on the basis of the magnetization and its second moment like

$$U_2(t) = \left[\frac{\langle m^{(2)}(t) \rangle}{\langle m(t) \rangle^2} - 1 \right] \sim t^{d/z}. \qquad (7)$$

When system evolving from high-temperature state ($m_0 \ll 1$) we can choose the scaling factor $b = t^{1/z}$ and applying the scaling form (6) for $k = 1$ to the small quantity $t^{x_0/z}m_0$, one obtains

$$m(t, \tau, m_0) \sim m_0 t^{\theta'} F(t^{1/\nu z}\tau, t^{x_0/z}m_0) = m_0 t^{\theta'} \left(1 + at^{1/\nu z}\tau \right) + O(\tau^2, m_0^2), \qquad (8)$$

where $\theta' = (x_0 - \beta/\nu)/z$ has been introduced. For $\tau = 0$ and small enough t and m_0, the scaling dependence for magnetization (8) takes the form $m(t) \sim t^{\theta'}$.

3. Results and discussion

3.1. Equilibrium critical behaviour

For research equilibrium critical behaviour we considered $L = 64, 96, 128$ and $N = 2, 4, 6, 8, 10, 14, 20$. To ensure equilibrium we wait at least 10^4 Monte-Carlo steps per spin (MCS/s) from its initial state before taking any measurements. Averages were calculated using 10^5 MCS/s for each sample and 100 samples with temperature's shift equaling 0.001.

The temperature dependencies of staggered magnetization m_{stg} and staggered susceptibility $\chi_{\mathrm{stg}} = \left(\langle m_{\mathrm{stg}}^2 \rangle - \langle m_{\mathrm{stg}} \rangle^2 \right)/T$ for metamagnetics films were presented in Fig. 1.

From calculating fourth-order cumulant $U_4(L, T)$ (Fig. 2) we have obtained critical temperature's values, which presented in Table 1. These values demonstrate a good agreement with results of [16] for $J_z = 1$. The values of critical temperature T_c evolve from 2D to 3D values with increasing film thickness N.

Whereas the phase diagram of the bulk system exhibits only one phase transition between the antiferromagnetic and paramagnetic phases, the phase diagram of thin Ising metamagnets includes an additional intermediate phase where one of the surface layers has aligned itself with the direction of the applied magnetic field. Transition from antiferromagnetic phase to intermediate phase ends at a critical end point with $T_{\mathrm{cr}} = 2.50(5)$ and $h_{\mathrm{cr}} = 0.98(1)$ [11] for $N = 8$. In Fig. 3 it is presented metamagnetic films behaviour in the magnetic field. For $T > T_{\mathrm{cr}}$ it demonstrates the transition from antiferromagnetic to paramagnetic phase only, but $T < T_{\mathrm{cr}}$ it demonstrates the discontinuous transitions from antiferromagnetic to intermediate and to paramagnetic phase.

3.2. Non-equilibrium properties

For study non-equilibrium critical behaviour we have considered $L = 32$ and $N = 2$ and 4. We consider evolution of thin ferromagnetic film both from high-temperature ($m_0 \ll 1$) and from low-temperature ($m_0 = 1$) initial states. Starting from initial configurations, the system was
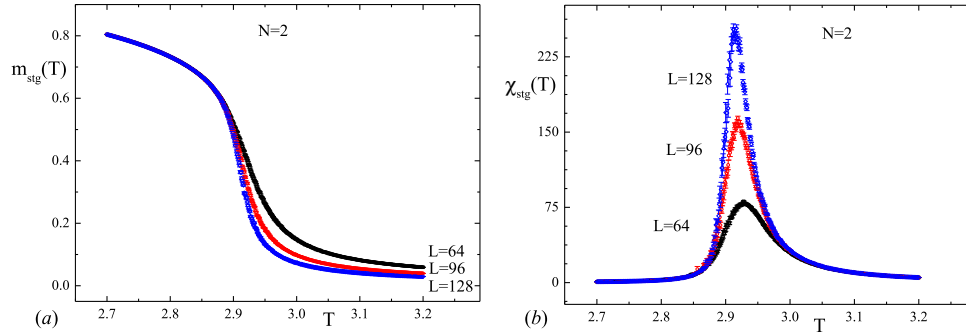
Figure 1. Temperature dependencies of staggered magnetization m_{stg} (a) and staggered susceptibility χ_{stg} (b) for $N = 2$, $J_z = -0.5$ and different L
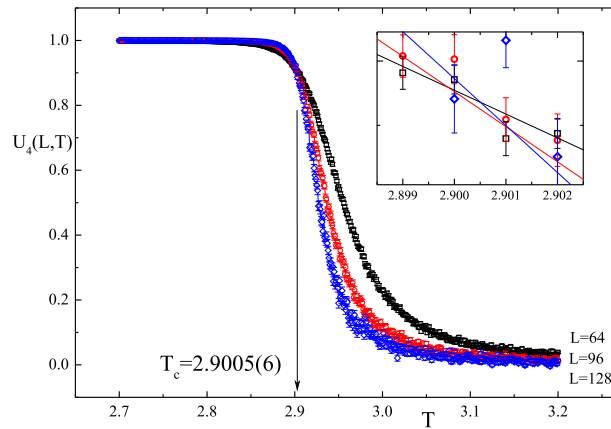

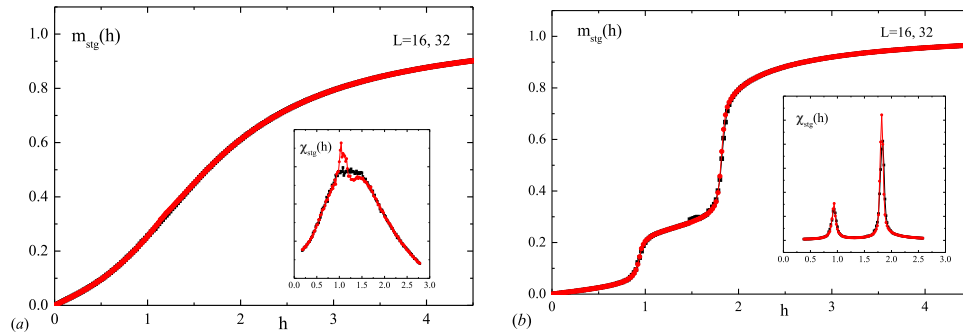**Figure 2.** Binder's cumulants $U_4(L, T)$ as function of T for $N = 2$, $J_z = -0.5$ and different L

Figure 3. Field dependencies of staggered magnetization m_{stg} and staggered susceptibility χ_{stg} (inset) for $T = 3.2 > T_{\text{cr}}$ (a) and $T = 2.5 < T_{\text{cr}}$ (b) for $N = 8$, $J_z = -0.5$

updated with Metropolis algorithm at the critical temperatures $T_c = 3.2076(4)$ for $N = 2$ and $T_c = 3.8701(3)$ for $N = 4$ [16]. In both cases simulations have been performed up to $t = 10000$ MCS/s.

We measured the time evolution of the magnetization $m(t)$, the second moment $m^{(2)}(t)$, which also allow to calculate the time-dependent cumulant $U_2(t)$. In Fig. 4 the magnetization is plotted for high-temperature initial state (Fig. 4a) and low-temperature initial state (Fig. 4b). The increasing of the magnetization $m(t)$ from a high-temperature initial magnetization $m_0 \ll 1$ at

Table 1. The critical temperatures $T_c(J_z, N)$ determined for magnetic films with different number of layers N and different interlayer coupling strength J_z.

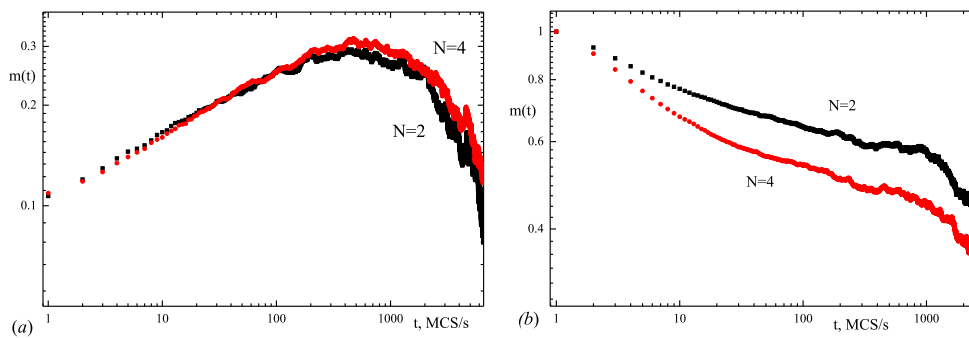| N	T_c		
	$J_z = -1$	$J_z = -0.5$	$J_z = 1$ [16]
2	3.2062(12)	2.9005(11)	3.2076(4)
4	3.8691(10)	3.3120(7)	3.8701(3)
6	4.1161(11)	3.4607(9)	4.1179(3)
8	4.256(17)	3.560(14)	4.2409(2)
10	4.344(50)	3.585(24)	4.3117(3)
14	4.412(20)	3.636(27)	—
20	4.481(16)	3.672(19)	4.4381(2)

Figure 4. The relaxation of magnetization $m(t)$ from non-equilibrium initial $m_0 \ll 1$ (a) and $m_0 = 1$ (b) states for $N = 2$: $T_c = 3.2076$ and $N = 4$: $T_c = 3.8701$

short-time regime $t < t_{\text{cr}} \simeq m_0^{-1/(\theta' + \beta/z\nu)}$ have form $m(t) \sim t^{\theta'}$. The initial rise of magnetization is changed to the well-known decay $m(t) \sim t^{-\beta/z\nu}$ for $t \gg t_{\text{cr}}$. From slope of magnetization at high-temperature initial state on $t \in [0; 100]$ we can estimate the value of critical non-equilibrium exponent θ'. From the slope of time dependence of the cumulant $U_2(t)$ on $t \in [0; 100]$ we can estimate the value of critical exponent z. The calculated values of θ' and z are presented in Table 2. A comparison of the obtained values with the results for 2D Ising model in various works show the very good agreement ie thin ferromagnetic film belong universality class non-equilibrium behaviour of 2D Ising model.

For study ageing effects from high-temperature initial state we calculated time dependencies of two-time autocorrelation function

$$C(t, t_w) = \left\langle \frac{1}{N_s} \sum_i S_i(t) S_i(t_w) \right\rangle - \left\langle \frac{1}{N_s} \sum_i S_i(t) \right\rangle \left\langle \frac{1}{N_s} \sum_i S_i(t_w) \right\rangle, \qquad (9)$$

where t_w ("waiting time") is time which characterizes the time elapsed since the preparation of the sample prior to measurement of its quantities.

Time dependencies of autocorrelation function $C(t, t_w)$ for $t_w = 10, 20, 30, 50$ MCS/s are presented in Fig. 5 for $N = 2$ and 4. The resulting curves presented in Figs. 4 and 5 have been obtained by averaging over 1000 samples.

Autocorrelation function have scaling form

$$C(t, t_w) \sim t_w^{-2\beta/\nu z} F_C(t/t_w). \qquad (10)$$

Table 2. Values of the critical exponents z and θ'.

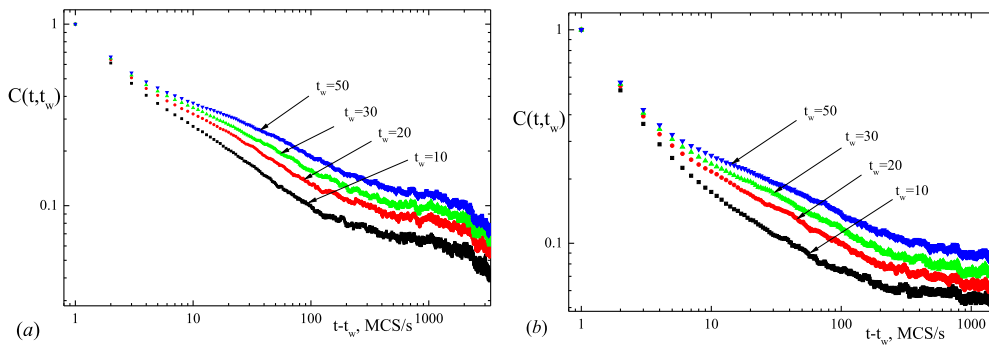| System	Method	z	θ'
Present report	MC	1.98(31)	0.188(30)
		2D Ising	
Okano et al, 1997 [17]	MC		0.191(1)
Prudnikov et al, 2006 [18]	RG	2.0842(39)	
Wang, Hu, 1997 [19]	MC	2.166(7)	
Nightingale and Blöte, 2000 [20]	MC	2:1667(5)	
Prudnikov, Markov, 1995 [21]	MC	2.24(7)	
Prudnikov, Vakilov, 1992 [22]	RG	2.277	
Kalle, 1984 [23]	MC	2.14(2)	
Jan et al., 1983 [24]	MC	2.12(6)	

Figure 5. Time dependencies of autocorrelation function $C(t; t_w)$ for $N = 2$ (a) and $N = 4$ (b) for different t_w $(m_0 \ll 1)$

Data presented in Fig. 5 clear demonstrates the presence of the two characteristics regimes: quasi-equilibrium regime at times $(t - t_w) \ll t_w$ and non-equilibrium regime at times $(t - t_w) \gg t_w$. At times $(t - t_w) \sim t_w$ there is a crossover regime with the dependence of correlation characteristics of the waiting time.

At quasi-equilibrium regime autocorrelation function have a scaling form $C(t) \sim t^{-c_a}$, where $c_a = \gamma/z\nu$. As we can see on Fig. 5 the increasing of system age t_w lead to decreasing of value c_a and consequently lead to amplification of critical slow-down and ageing effects.

4. Conclusions

We have studied the critical behaviour of Ising thin films on simple cubic lattice using extensive Monte Carlo simulations. We have found critical temperatures T_c of metamagnetic films for different thickness N and different coupling strength J_z. The film's T_c evolve from 2D to 3D values with increasing film thickness.

We have researched non-equilibrium behaviour of ferromagnetic thin film by short-time dynamics method. The obtained values of critical exponents z and θ' demonstrates that ultrathin ferromagnetic films with $N < 4$ belong to class of universal critical non-equilibrium behaviour of the 2D Ising model. Aging effects were discovered for non-equilibrium regime $(t - t_w) \gg t_w$.

Acknowledgments

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