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Dimensionality crossover in critical behaviour of ultrathin ferromagnetic films

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ABSTRACT

We propose the model which takes account of magnetocrystalline anisotropy effects in thin magnetic films. The dimensionality crossover from two-dimensional monolayer to three-dimensional system in multilayer magnetic films is studied using a Monte Carlo technique. Finite-size scaling is applied for the determination of the critical characteristics as a function of film thickness. The transition to intermediate planar phase is discussed.

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1. Introduction

The behaviour of ultrathin magnetic films has become of great technological importance due to the applications in magnetic storage devices [1]. 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 [2]. HAMR is the most appropriate technology to achieve magnetic recording densities 1 TBit/in^2 [3,4]. In this respect, it is important to understand the temperature evolution of magnetization in thin magnetic films, especially at temperatures close to or above the Curie temperature.

Magnetic order in thin ferromagnetic films is very complex due to a strong influence of the shape and the magnetocrystalline anisotropies of the sample. In the past decade, a considerable amount of experimental results on different aspects of magnetism in ultrathin films has appeared [5]. Nevertheless it is difficult to reach general conclusions even in seemingly basic things such as the kind of magnetic order at low temperatures. In view of this complexity, theoretical work on simplified models and computer simulations is essential for rationalizing and guiding new experimental work.

In the vicinity of the critical temperature T_c, the thermodynamic observables associated with statistical models display universal characteristics, which may be parametrized in terms of critical exponents. These quantities tend to zero or infinity at the transition and depend only on the spatial dimensionality of the system, the range of the interactions and the number of components of the order parameter.

The dimensionality aspects of magnetic and structural phase transitions represent one of the key problems of ultrathin film [6,7]. For magnetic systems, the spin dimensionality as well as the spatial extension determines the universality class, giving rise to a great number of ordering phenomena on different length scales. Furthermore, there are transition regions not represented by any universality class with corresponding critical exponents, but representing something in between. For example, the dependence of the critical exponents of thin magnetic films with thickness exhibit such a transition, in which the exponents are continuously changes with increasing film thickness of the layers, from two-dimensional (2D) Ising ($\beta=0.125$) to three-dimensional (3D) Heisenberg ($\beta=0.364$) [8] behaviour. The crossover from 2D to 3D critical exponents has been observed in thin films of Ni on W(110) [9] and of Co on Cu(111) [10] as their thickness is increased. Thus, studying the dimensional crossover of a system as its thickness is increased often provides a significant degree of insight.

It is well known now the fundamental role of competing interactions in the emerging features of low-dimensional systems. Among a wide number of numerical and theoretical investigations on equilibrium and dynamical properties of several model Hamiltonian of low-dimensional magnets, Heisenberg-like models are one of the most widely used to approach real magnetic

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materials. In fact, anisotropic versions of the Heisenberg model describe several compounds as K_2NiF_4 [11], $BaCo_2(AsO_4)_2$ [12], $CoCl_2$-GIC [13] and Rb_2CrCl_4 [14].

In early experiments on Fe/Cu(100) films [15,16], a spin reorientation transition (SRT) from a region with perpendicular magnetization to one with in-plane magnetization was observed. SRT transitions in films have actively been studied both theoretically [17,18] and experimentally [19–21], recently.

In this paper we investigate the magnetic phase transition in anisotropic Heisenberg thin films using extensive Monte Carlo (MC) simulations. We have found the dimensional crossover of magnetization m and susceptibility χ_m from 2D to 3D like with increasing film thickness. Estimated values of the critical exponents for different thicknesses demonstrate crossover from 2D Ising universality class to 3D Heisenberg through 3D Ising class.

The paper is organized in the following manner. The anisotropic Heisenberg model and the Monte Carlo simulation scheme are discussed in the next section (Section 2). The numerical results for universal dimensionality behaviour of thin films with increasing film thickness and for SRT transition are given in Section 3. The paper ends with concluding remarks and summary in Section 4.

2. Model and methods

We have performed Monte Carlo simulations of macroscopic spin system with crystalline structure of ultrathin film which is described by the anisotropic Heisenberg model [22] with Hamiltonian

$$H = -J\sum_{i,j}[(1-\Delta(N))(S_i^xS_j^x + S_i^yS_j^y) + S_i^zS_j^z], \tag{1}$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is a unit vector in the direction of the classical magnetic moment at lattice site i, the sum is extended over nearest-neighbor pairs on the cubic lattice, J being the exchange constant, and Δ characterizes the amount of anisotropy. Thus, $\Delta=0$ corresponds to the isotropic Heisenberg case, $\Delta=1$ – the Ising case.

The effective anisotropy constant $\Delta(N)$ as a function of film thickness N was chosen from experimental studies of the Curie temperature T_C for thin films of Ni(111)/W(110) [9] with different thicknesses of Ni film. Microscopic nature of anisotropy in films of Fe, Co, Ni and its dependence of film thicknesses N is determined by influence of crystalline field of substrate surface, magnetic single-ion anisotropy and dipole–dipole interaction of magnetic moments of atoms in film and their concurrence. Therefore, the calculation of anisotropy effects in magnetic films is very complicated task. It was proposed that Δ is proportional to the critical temperature for different film thicknesses. In approximation procedure the fact that Ni films with a large number of layers demonstrate bulk critical properties of 3D isotropic Heisenberg magnets was used [23,24].

The simulations were carried out for films with sizes $L\times L\times N$ with the use of periodic and free boundary conditions for the in-plane and out-plane directions, respectively. $L\times L$ represents the number of spins in each layer of the film and N is the number of layers. We considered films with $L=32$, 48, 64 and N ranging from a monolayer to 32 layers. Temperature T of system is changed in interval [0.01; 5.01] J/k_B with step $\Delta T_{\text{step}} = 0.02$. As a starting configuration we always used a completely ordered ferromagnetic state.

We measured the magnetization

$$m = \left\langle \frac{1}{N_s}\left[\left(\sum_i^{N_s} S_i^x\right)^2 + \left(\sum_i^{N_s} S_i^y\right)^2 + \left(\sum_i^{N_s} S_i^z\right)^2\right]^{1/2}\right\rangle, \tag{2}$$

out-plane magnetization

$$m_z = \left\langle \frac{1}{N_s}\sum_i^{N_s} S_i^z\right\rangle, \tag{3}$$

the in-plane magnetization

$$m_\parallel = \left\langle \frac{1}{N_s}\left[\left(\sum_i^{N_s} S_i^x\right)^2 + \left(\sum_i^{N_s} S_i^y\right)^2\right]^{1/2}\right\rangle, \tag{4}$$

and an orientational order parameter [25,26]

$$O_\alpha = \left\langle \left|\frac{n_h^\alpha - n_v^\alpha}{n_h^\alpha + n_v^\alpha}\right|\right\rangle, \tag{5}$$

where $N_s = NL^2$ is a total number of spins in film, angle brackets denote the statistical averaging, $\alpha\in\{x, y, z\}$, n_h and n_v are the number of horizontal and vertical pairs of nearest neighbor spins with antialigned $\{x, y\}$ components, respectively,

$$n_h^\alpha = \sum_{\mathbf{r}}\left\{1 - \text{sgn}[S^\alpha(r_x, r_y), S^\alpha(r_x+1, r_y)]\right\},$$
$$n_v^\alpha = \sum_{\mathbf{r}}\left\{1 - \text{sgn}[S^\alpha(r_x, r_y), S^\alpha(r_x, r_y+1)]\right\}. \tag{6}$$

We define the magnetic susceptibility χ_m as

$$\chi_m \sim [\langle m^2\rangle] - [\langle m\rangle]^2 \tag{7}$$

and orientational susceptibility χ_O as

$$\chi_O \sim [\langle O_z^2\rangle] - [\langle O_z\rangle]^2 \tag{8}$$

Temperature dependence of the susceptibility has been calculated for different lattice sizes to estimate the critical temperature T_c. The position of the susceptibility maximum allowed us to determine range of values of the critical temperature.

The spin configurations of the films are updated using the Swendsen–Wang cluster algorithm [27]. The spin-flip algorithm for $O(n)$ models was proposed in [28]. The spin system is divided into clusters. The bonds between sites in cluster are created with probability $1-\exp[-2J(\mathbf{S}_i\mathbf{r})(\mathbf{S}_j\mathbf{r})/T]$ only if the condition $(\mathbf{S}_i\mathbf{r})(\mathbf{S}_j\mathbf{r}) > 0$ is true, where $\mathbf{r}$ is a random unit vector. After that each cluster is flipped with probability 1/2.

The temperature dependencies of the Binder cumulant $U_4(T)$

$$U_4 = \frac{1}{2}\left(3 - \frac{[\langle m^4\rangle]}{[\langle m^2\rangle]^2}\right) \tag{9}$$

were calculated to clarify the critical temperatures of second-order phase transition in samples. The scaling dependence of the cumulant

$$U_4(L, T) = u[L^{1/\nu}(T - T_c)]. \tag{10}$$

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.

We consider finite size scaling form for film geometry [29] to find how m and χ scale with the size L and thickness N of the systems and use this to extract the effective critical exponents from our results. The basic finite-size scaling ansatz [30] rests on

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