Monte Carlo simulation of critical properties of ultrathin anisotropic Heisenberg films

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The dimensional crossover of magnetic properties from two-dimensional to three-dimensional character in magnetic multilayers has currently attracted much interest as a result of both technological and fundamental importance [1]. Of particular interest is the critical behavior of magnetic thin films for which the dimensionality d is not well established. It is interesting to consider how magnetic properties such as the magnetization m, magnetic susceptibility χ, and critical temperature T_c depend on the thickness of the film.

The anisotropic Heisenberg model studied is described by the following Hamiltonian [2]:

$$H = -J\sum_{ij}[(1-\Delta)(S_i^x S_i^x + S_i^y S_i^y) + S_i^z S_i^z], \qquad (1)$$

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, $J > 0$ being the exchange constant, and Δ characterizes the amount of anisotropy. $\Delta = 0$ is the isotropic Heisenberg case, $\Delta = 1$ the Ising case. In order to study the critical properties of anisotropic Heisenberg magnets we thus made Monte Carlo calculations, studying cubic lattice with periodic and free boundary conditions are used for the in-plane and out-plane directions, respectively. The anisotropy constant for different sizes of the film is chosen from experimental studies of thin films of Ni(111)/W(110) [3]. The anisotropy constant is chosen proportional to the temperature corresponding to the critical temperatures of films to different thickness.

The simulation are carried out for simple cubic films of size $N_s = L \times L \times N$ where $L \times L$ represents the number of sites (spins) in each layer of the film and N is the number of layers. The spin configurations of the films are updated using the Swendsen-Wang algorithm. As a starting configuration we always used a completely ordered ferromagnet. We measured the total magnetization $m = \langle (1/N_s)|\sum \mathbf{S}_i|\rangle$, out-plane magnetization $m_z = \langle (1/N_s)\sum S_i^z\rangle$, the in-plane magnetization $m_{||} = \langle (m_x^2 + m_y^2)^{1/2}\rangle$ where angle brackets denote the statistical averaging. To estimate the critical temperature T_c was calculated temperature dependence of the susceptibility $\chi \sim [\langle m^2\rangle] - [\langle m\rangle]^2$ for different lattice size. The position of the susceptibility maximum allowed to estimate range of values of the critical temperature. To clarify the critical temperatures were calculated temperature dependence of the forth order Binder cumulant.

In this work from the temperature dependence of the magnetization near the critical point $m \sim (T_c - T)^\beta$ values have been estimated the critical exponent β for different thickness of the magnetic film. From this dependence was found the crossover from two-dimensional Ising model to three-dimensional Heisenberg model with increasing film thickness. For a strong anisotropy we observed the spin reorientation transition. In the experimental and theoretical studies devoted to the study of single-layer magnetic materials, it is predicted that the orientation of the spin transition is a weak first-order transition.

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