Critical behavior of a two-dimensional ferromagnetic film on a non-magnetic substrate

S V Belim¹², I V Bychkov³⁴ and I V Maltsev³

¹ Physics Department, Omsk State Technical University, Omsk, Russia
² Applied Informatics Department, Siberian State Automobile and Highway University, Omsk, Russia
³ Faculty of Physics, Chelyabinsk State University, Chelyabinsk, Russia
⁴ Laboratory of functional materials, South Ural State University, Chelyabinsk, Russia

E-mail: sbelim@mail.ru

Abstract. In this paper, we investigate the behavior of a ferromagnetic (FM) film on a nonmagnetic substrate near the Curie point by the computer simulation. The influence of the substrate is specified using the two-dimensional Frenkel-Kontorova (FK) potential. The study is carried out for a two-dimensional film described by the Ising model. At the first step, we calculate the positions of the substrate's atoms in the ground state depending on the parameters. The parameters are (i) the ratio of the substrate periods and the crystal lattice of the film; and (ii) the ratio of the substrate potential amplitude to the elasticity coefficient of interatomic interaction. The period ratio determines the system coverage ratio. Minimization of the system's total energy determines the ground state. Calculations show that the ground state has a periodic structure that differs from a square lattice with a coverage coefficient not equal to unity. We calculate the displacements of atoms from the equilibrium position for systems with a different linear scale.

1. Introduction

Nowadays, FM thin films are widely using in spintronic devices. Deposition on a substrate is the base technology for thin-film formation. Monolayer FM films are of extreme interest due to their demonstrate new physical properties. Studying the properties of these films, one should take into account the effect of the substrate. The materials of film and substrate are different. The substrate performs the external periodic potential function. The film atoms change their position due to the substrate, and the film structure changes, which causes changes in its physical properties. In particular, it causes the Curie point shift. The film becomes FM at higher or lower temperatures. This phenomenon is called a substrate-induced phase transition.

The behavior of the ferromagnetic thin MnAs films on a nonmagnetic substrate has been investigated in papers [1-3]. In this system, the substrate has a crystal lattice different from the film. In addition, the substrate imposes constraints on the film size. Additional stresses related to the difference in the film and substrate thermal expansion appear under heating. It was shown in [4] that tensile deformation in 0.5% MnAs film leads to a change in the phase transition temperature by 50 K.

2. Description of the system

The effect of substrate on the critical behavior of the two-dimensional (2D) Ising model is due to a change in the relative positions of the spins. Atoms are displacing from the square lattice sites by the...
substrate potential. This shift leads to a change in the exchange integral. As a result, both the phase transition temperature and the critical exponents of the system change.

We take the 2D Ising model on a simple square lattice with $a_0$ period as an unperturbed system. To simulate the influence of the substrate, we use the 2D FK potential [5] with a period $b$. If the period of the unperturbed spin-lattice coincides with the period of the substrate, atoms locate at the potential minima, and the lattice deformation does not occur. The Curie temperature and critical exponents remain unchanged. Contrary, if the periods of the unperturbed spin-lattice and the substrate potential are not equal, the lattice deforms. We restrict ourselves to the case of a small period difference. As shown in the experiment [4], a significant change in the phase transition temperature is observed even in this case.

To study the phase transition in the system, we need first to determine the geometry of the atom distribution on the substrate. For this, we calculate the ground state of a 2D system with FK potential.

The potential energy of the atoms will include two terms [6]

$$U = U_{\text{sub}} + U_{\text{int}}$$

where $U_{\text{int}}$ is the energy of the film atoms interaction. Since we restrict ourselves to small values for the period difference, the harmonic approximation can be used for $U_{\text{int}}$

$$U_{\text{int}} = \frac{g}{2} \sum_n \left( (x_{n+1} - x_n - a_0)^2 + (y_{n+1} - y_n - a_0)^2 \right).$$

Here $g$ is the stiffness coefficient, $a_0$ is the interatomic distance without the substrate influence. The energy of interaction with the substrate $U_{\text{sub}}$ is described by the 2D FK potential

$$U_{\text{sub}} = \frac{A}{2} \sum_n \left( 2 - \cos \left( \frac{2\pi}{b} x_n \right) - \cos \left( \frac{2\pi}{b} y_n \right) \right).$$

where $A$ is the amplitude of the potential, $b$ is the substrate period. The total potential energy of the system can be found as follows

$$U = \frac{g}{2} \sum_n \left( (x_{n+1} - x_n - a_0)^2 + (y_{n+1} - y_n - a_0)^2 \right) + \frac{A}{2} \sum_n \left( 2 - \cos \left( \frac{2\pi}{b} x_n \right) - \cos \left( \frac{2\pi}{b} y_n \right) \right).$$

The ground state of the system is calculated from the minimum potential energy condition

$$U \rightarrow \min$$

If the periods of the unperturbed lattice and the FK potential are different ($a_0 \neq b$), the atomic arrangement depends on the boundary conditions. Let the lattice has $N \times N$ atoms, and it is placed on the sector of $L \times L$ size. There are $M$ substrate potential minima on a segment of length $L$. Let us introduce the coverage parameter

$$\theta = \frac{N}{M}.$$  

If the outermost lattice atoms are fixed along the sector boundary, the rest atoms are located at the sites of a square lattice with a new period, as shown in [7-11]
Systems with free edges are more interesting [10, 11]. Let us consider a system with atoms fixed only along two boundaries described by the equations \( x = 0 \) and \( y = 0 \). For the remaining two boundaries, we impose periodic boundary conditions. For atoms with coordinates \((x_0, y_0)\), the atom with coordinates \((x_{N-1}, y_0)\) is neighbor to the left. While for atoms with coordinates \((x_{N-1}, y_n)\), the atom with coordinates \((x_0, y_n)\) is neighbor to the right. We imposed similar conditions on the \( OY \) axis.

Let’s consider the problem of finding the ground state for a 2D system with a coverage coefficient \( \theta \). The magnetic phase transition in a FM film is described by the 2D Ising model. The Hamiltonian of this system is

\[
H = J(a) \sum_i S_i S_j.
\]

Here \( S_i \) is the spin value at \( i \) site, \( J(a) \) is the exchange integral depending on the distance between atoms. Summation is performed over the nearest neighbors only. We consider just small deviations from the equilibrium position. Therefore, we use a linear approximation for the exchange integral in Taylor expansion form

\[
J(a) = J_0 - B(a - a_0).
\]

Here \( J_0 = J(a_0) \) is the exchange integral of the initial undeformed film. Coefficient \( B \) shows the rate of exchange integral decrease with distance

\[
B = -\left. \frac{dJ(a)}{da} \right|_{a=a_0}
\]

We used magnetization as an order parameter to describe the magnetic behavior of the system. It is calculated as the total spin per particle

\[
m = \sum S_i / N^2.
\]

The critical behavior near the Curie point was simulated using the Wolf cluster algorithm [12]. The phase transition temperature was determined as the intersection of the fourth-order Binder cumulants [13] for systems with different linear sizes

\[
U_4 = 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2}
\]

Angle brackets are used to denote averaging over the thermodynamic states of the system. The Curie temperature \( T_C \) was calculated in units of the exchange integral of the undeformed film \( J_0 \).

We used the fluctuation relations to calculate the susceptibility

\[
\chi = NK \left( \langle m^2 \rangle - \langle m \rangle^2 \right).
\]
where $K = |J|/(k_B T)$ and $k_B$ is the Boltzmann constant.

Near critical point, the susceptibility satisfies the following relationship

$$\chi \sim L^{\gamma / \nu}.$$  

Using this equation, we can find the ratio of the critical indexes $\gamma / \nu$. The critical index $\nu$ can be determined from the following relation

$$\frac{dU_{\Delta}}{dT} \sim L^{-\nu}.$$  

The rest of the critical indexes are determined from the scaling relations

$$\eta = 2 - \gamma / \nu, \quad \beta = \frac{\nu}{2}(D - 2 + \eta), \quad \alpha = 2 - D\nu.$$

3. **Computer experiment**

Computer simulation is performed for systems with linear sizes for $L$ from 8 to 24 with a step $\Delta L = 4$. The initial lattice period of the 2D film is 1. The period of the substrate potential varies from 0.9 to 1.1 with a step $\Delta b = 0.01$. With a change in the substrate potential period, the coverage parameter also changes from 0.9 to 1.1. The stiffness coefficient is equal to 1. We carried out our calculations for the substrate potential amplitude $A = 0.1$. Firstly, we determine the dependence of the phase transition temperature on the substrate potential period. The results are shown in Fig. 1. After that, we calculate the dependence of the critical exponents’ ratio $\gamma / \nu$ on the identical parameters of the substrate potential.

One can see three intervals of different critical temperature behavior depending on the substrate period. The dependence is linear in the interval $0.95 < b < 1.05$. The substrate makes the atom's lattice stretch or contracts linearly in this range. The exchange interaction changes linearly in the approximation we select. The critical temperature is directly proportional to the exchange integral and also varies linearly. In this interval, the critical exponents match the values specific to the 2D Ising model. Crystal lattice structure changes in intervals $b < 0.95$ and $b > 1.05$. This change occurs due to the large difference between the free lattice and the substrate period. Structural phase transition takes place at $b = 0.95$ and $b = 1.05$. These two points are the intersection of the ferromagnetic and structural phase transition lines. The equilibrium structures of atoms at $b = 0.91$ and $b = 1.10$ are shown in Figs. 2 and 3.
4. Conclusion
We investigated the phase transition in a two-dimensional lattice on a substrate with periodic potential. The periodic potential has a linear effect on the lattice with small differences in the lattice and substrate periods. There are two critical values of the substrate period. Passing through these critical values leads to a crystal lattice rearrangement and change in the phase transition temperature.

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