Computer simulation of substrate effect on 2D ferromagnetic film state

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Abstract. In the article computer simulation of ground state for two-dimensional film on the substrate is performed. The influence of the substrate is modeled using a periodic potential. The potential contains a parameter defining the width of the maxima and minima. The film has a simple square crystal lattice. The substrate potential structure models a square lattice. We consider the case of different film coating ratio ratios. The lattice and substrate periods are also different. If the coating coefficient is different from one, mechanical stresses are present in the film. The case with one fixed edge for the film and periodic boundary conditions was investigated. The film atoms do not form a square lattice in this case. The displacements of atoms are periodic. The period depends on the coating factor. A superlattice is present in such film.

1. Introduction

Thin ferromagnetic films are actively used in spintronics devices. The main technique for forming thin films consists in spraying them on a substrate. Monolayer ferromagnetic films are of increased interest. These films have new physical properties. The influence of the substrate should be taken into account when studying the properties these films. Substrate is made of crystalline material. The substrate crystal lattice differs from the film's lattice. The substrate acts as an external periodic potential. Film atoms change mutual position under action of substrate. The films structure changes. The ferromagnetic film physical properties also vary. The Curie point is offset when the film structure changes. The film becomes ferromagnetic at a higher or lower temperature. This phenomenon is called substrate induced phase transition.

The behavior of ferromagnetic thin films MnAS on a non-magnetic substrate has been investigated in the works [1-3]. The substrate in this system has a crystal lattice other than the film. The substrate also imposes a limitation on the film size. Additional mechanical stresses are created when the system is heated. These stresses are related to the difference in thermal expansion of the film and substrate. Article [4] shows that the strain of the stretch in the film MnAS by 0.5% leads to a change in the phase transition temperature by 50 K.

The study of phase transitions induced by the substrate requires the calculation the film atoms equilibrium arrangement under the influence of the substrate potential. Thermal fluctuations in the position of atoms are not taken into account. This is a task to find the ground state of the system. Today, the basic states for one-dimensional chains are quite well studied. Analytical expressions for the atoms position in the ground state can be obtained only in the case of fixed chain ends [5-8]. If one chain ends is free or both ends are free, then the calculation the ground state is possible only using computer simulation [9-10].
This paper examines the ground state of a two-dimensional film on a substrate with periodic potential by computer simulation.

2. Description of the system
We are looking at a two-dimensional the magnetic atoms lattice on a non-magnetic substrate. Atoms are located in the nodes of a square lattice without external influence. The influence of the substrate is taken into account using an external potential. The presence of the substrate results in a change in the ground state the magnetic atom system. Atoms are displaced from the nodes of the square lattice under the substrate influence. The period of placement for the film atoms becomes irregular.

We record the potential energy of the film atoms to calculate the ground state for the system. It consists of two terms [11].

\[ U = U_{\text{sub}} + U_{\text{int}} \]

We use harmonic approximation for the interaction energy between the film atoms \( U_{\text{int}} \).

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

where \( g \) is stiffness coefficient, \( a_0 \) is interatomic distance between magnetic atoms excluding substrate potential.

We describe the influence of the substrate with a two-dimensional potential. Our potential is obtained as a generalization of the one-dimensional potential [11] into two-dimensional systems.

\[ U_{\text{sub}} = A \sum_n \frac{(1 + s)^2 \left( 1 - \cos \left( \frac{2\pi}{b} x_n \right) \cos \left( \frac{2\pi}{b} y_n \right) \right)}{1 + s^2 - 2s \cos \left( \frac{2\pi}{b} x_n \right) \cos \left( \frac{2\pi}{b} y_n \right)}, \quad |s| < 1. \]

The parameter \( s \) defines the general appearance of the potential. This potential coincides with the well-known Frenkel-Kontrova potential [12] at \( s = 0 \). The potential is characterized by narrow potential barriers and flat potential pits at \( s < 0 \). Potential pits are narrow and barriers are wide and flat at \( s > 0 \) (Figure 1). \( A \) is the height of potential barriers. \( b \) is the substrate potential period.

We record the full potential energy of the system.

\[ U_{\text{int}} = \frac{g}{2} \sum_n \left( (x_{n+1} - x_n - a_0)^2 + (y_{n+1} - y_n - a_0)^2 \right) + \frac{A}{2} \sum_n \frac{(1 + s)^2 \left( 1 - \cos \left( \frac{2\pi}{b} x_n \right) \cos \left( \frac{2\pi}{b} y_n \right) \right)}{1 + s^2 - 2s \cos \left( \frac{2\pi}{b} x_n \right) \cos \left( \frac{2\pi}{b} y_n \right)}. \]

The systems ground state is determined from the minimum potential energy condition.

\[ \frac{\partial U}{\partial x_n} = 0, \quad \frac{\partial U}{\partial y_n} = 0. \]
Figure 1. Substrate potential at different values of parameter $s$.

If the lattice and potential periods coincide with $a_0 = b$, then the atoms form a square lattice with period $a_0$. If the periods are different $a_0 \neq b$, the placement of atoms depends on the boundary conditions. The lattice has dimensions $N \times N$ atoms. This lattice is placed on a site with size $L \times L$. The length $L$ is $M$ of the substrate minima. We record the coverage parameter.

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

If the extreme lattice atoms are fixed along the boundary of the site, then the remaining atoms are placed in the square lattice nodes with a new period [13-17].
Systems with free ends are of interest [16,17]. We consider a system in which atoms are fixed only along two boundaries. These two boundaries are described by equations $x=0$ and $y=0$. We apply periodic boundary conditions to two other boundaries. For atoms with coordinates $(x_0, y_n)$, the adjacent to the left is considered an atom with coordinates $(x_{N-1}, y_n)$. For atoms with coordinates $(x_{N-1}, y_n)$, the adjacent to the right is considered an atom with coordinates $(x_0, y_n)$. Similar conditions were applied along the $OY$ axis. We solve the problem of finding the ground state for a two-dimensional system with a coverage factor $\theta$. Period of substrate is selected close to period for film lattice. Periodic boundary conditions can lead to additional deformation for the lattice.

3. Computer experiment
The ground state of the system is determined by computer simulation. Stable atoms states are determined by searching for a minimum of potential energy. The minimum potential energy is determined by the Monte Carlo method. The initial state is a state without an underlay. Each atom is sequentially shifted from the equilibrium position by a random vector. Offset vector value does not exceed $0.1a_0$. If the new position of the atom is energetically advantageous, then it is accepted, otherwise it is discarded. After that, the transition to another atom is performed. An attempt to move all atoms is made in one pass along the lattice. Successive passes on the lattice are performed until the atoms assume a stable state. The system state is stable if the passage along the lattice does not shift any atoms.

The ground state is examined with different sets of parameters. Systems with coverage factor $\theta=0.9$, $\theta=1.0$ and $\theta=1.1$ are studied. The film is not deformed at the coverage factor $\theta=1.0$. Coverage factor $\theta=0.9$ corresponds to film stretching strain. Coverage factor $\theta=1.1$ corresponds to compression strain of the film. The initial period of the lattice is taken as one $a_0=1$. Stiffness factor value is selected equal to unit $g=1$. Amplitude of substrate potential is measured in relative values. We selected $A=0.1$ for the amplitude of the substrate potential. For the period of the substrate, the values $b=0.9$, $b=1.0$ and $b=1.1$ are sequentially used. The potential parameter is $s=-0.9; -0.5; 0.0; 0.5; 0.9$.

The number of atoms and minima of the substrate potential must be integer. This principle is used to select system dimensions. The number of substrate minimums is constant $M=10; 20; 30$. The number of film atoms is determined by the coverage factor. Systems with different linear dimensions are considered. For the coverage factor $\theta=0.9$, systems have the number of atoms $N=9; 18; 27$ are considered, for $\theta=1.0$ system have $N=10; 20; 30$, for $\theta=1.1$ system have $N=11; 22; 33$.

Film atoms are located in potential pits of substrate at coverage factor $\theta=1.0$. Atoms form a square lattice with a period $b$. The result is independent of the substrate period $b$. This result coincides with the predictions of the theory. Position of atoms for potential parameter $s = 0.5$ and $s = -0.5$ are shown in Figure 2.
A new ordering of atoms occurs at the coverage factor $\theta=0.9$. His structure differs from a simple square lattice. A new periodicity in the placement of atoms is observed. The displacement of atoms is repeated with a period $T=9$. The graph for the atom’s displacement from the initial position at $s = 0$ and various values of $b$ is shown in Figure 3. For atoms numbered $n = 9k$ ($k = 0, 1, 2, ...$), the offset is zero. Similar situation is observed for other values $s$. The position of atoms with respect to the substrate for the coverage factor $\theta=0.9$ at $b = 0.9$ for $s = 0.9$ is shown in Figure 4.

Figure 2. Position of film atoms at $\theta=1.0$ N=M=10: a) $s=0.5$, b) $s=-0.5$.

Figure 3. Graph for the relation of the atom’s displacement $\Delta x$ from the initial position $n$ at $\theta=0.9$, $s=0.0$ and various values $b$. 

Figure 4.
Figure 4. The position of atoms with respect to the substrate for the coverage factor $\theta=0.9$ at $b=0.9$ for $s=0.9$.

A similar pattern is observed with a coverage factor $\theta=1.1$. The new structure of atoms has a period equal to $T=11$ and does not depend on the values $b$ and $s$. The graph for the displacement of atoms from the initial position at $s=0$ and various values $b$ is shown in Figure 5. For all atoms numbered $n=11k$ ($k=0,1,2,...$), the offset is zero. The position of atoms with respect to the substrate for the coverage factor $\theta=1.1$ at $b=1.1$ for $s=-0.5$ is shown in Figure 6.

Figure 5. Graph for the relation of the atom’s displacement $\Delta x$ from the initial position $n$ at $\theta=1.1$, $s=0.0$ and various values $b$. 
4. Conclusion

We studied the basic state for a two-dimensional film on a substrate with a periodic structure. The computer simulation method is used for calculations. The substrate is modeled with a periodic potential. The formula for potential has a parameter. This option allows you to vary the type of potential. The coverage parameter and lattice and substrate period ratios are also parameters of the system. We found the ground state with different sets of parameters. The ground states for the system have a periodic arrangement of atoms. The period of the ground state structure is determined by the coverage parameter and the potential parameter.

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Acknowledgments

The reported study was funded by RFBR, project number 20-07-00053.