Change the state of 2D nanofilms under the substrate influence

S V Belim$^{1,2}$ and I V Tikhomirov$^1$

$^1$Omsk State Technical University, 11 Mira ave., Omsk, 644050, Russia
$^2$Siberian State Automobile and Highway University, Omsk, Russia

E-mail: sbelim@mail.ru

Abstract. 2D films deformations under action of ferroelectric substrate by computer modeling method are performed in article. The film has a square lattice. We use harmonic law for the energy of interatomic interaction. The substrate effect on the film is simulated by the 2D Frenkel-Kontorova potential. The orientation of the film and the substrate do not match. Different cases for periods of film and substrate are considered. The Monte Carlo method is used for computer modeling. If the period of the film and the substrate coincide, the film atoms are placed at the minimum points of the substrate. The film on the substrate has a square crystal lattice. If the period of the substrate is less than the period of the film, the continuous film is converted into a film 2D nanoparticles. The substrate potential amplitude affects the filling of the space between particles. If the period of the substrate is longer than the period of the film, a superstructure in the form of a periodic lattice with an increased particle concentration is formed in the film. The distribution of atoms in the superstructure is determined by the substrate potential amplitude of the substrate potential.

1. Introduction

Ultra-thin films of ferromagnetic materials on the substrate are the basis for electronic devices using the effect of giant magnetic resistance. The main property these systems is the ability to control the film magnetic state through the influence an electric field on the substrate (magnetoelectric effect). The interaction between the substrate atoms and the film atoms causes a magnetoelectric effect in these systems. Deformation the substrate results in deformation the film. Changing the mutual arrangement of atoms affects the film magnetic properties. Substrate deformations are caused by an electric field. Ferroelectric materials are used for the substrate.

Magnetoelectric effect is actively studied experimentally. The substrate deformation leads to a change in distances between atoms. In article [1], the behavior of thin Ni-film on substrate BaTiO$_3$ is investigated. BaTiO$_3$ is ferroelectric materials. Article [2] examines deformations of Fe-Ga film on ferroelectric substrate. The magnetoelectric effect causes a compression 0.033%. X-ray diffraction shows non-uniform deformations. Article [3] examines the behavior the ferromagnetic film La$_{0.7}$Ca$_{0.3}$MnO$_3$ on ferroelectric substrate BaTiO$_3$. The deformations of the substrate affect the crystallographic, transport and nonlinear optical properties of the film. Compression and stretching strains result in a decrease in the phase transition temperature. The substrate deformations also affect the electrical conductivity of the film. The ferromagnetic film Co$_{86}$Fe$_{14}$B$_{20}$ on the ferroelectric substrate changes its magnetic properties [4]. The hysteresis loop of the film changes its shape. In article [5], an electric field controls the ferromagnetic-antiferromagnetic transition in the thin film CrI$_3$ on the ferroelectric substrate. Bilayer films BaTiO$_3$/GdFeO$_3$ are studied in article [6]. The influence of the
electric field leads to compression and tension deformations in these structures. Deformations cause high polarization values.

Theoretical studies the ultra-thin films properties on a substrate are carried out mainly based on the description the system from the first principles [7,8]. This article uses substrate modeling using the Frenkel-Kontorova potential. This approach allows us to describe the basic patterns of film interaction with the substrate [9,10]. We investigate 2D film on a deformable substrate by computer simulation in this paper.

2. Model

2D the film is modeled as a square lattice. Interatomic interaction is subject to harmonic law. The films intrinsic energy without the substrate influence is calculated as the sum of the interatomic interactions energies.

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

\((x_n, y_n)\) are the coordinates of the atom with the number \(n\). \(a_0\) is the period of the crystal lattice. \(g\) is the elastic constant. Minimization this potential energy leads to the location atoms in the nodes of the square lattice with the period \(a_0\).

We describe the interaction of film atoms with the substrate as a periodic potential. The Frenkel-Kontorova potential can be used in this problem [11].

\[
U_{\text{sub}} = \frac{A}{2} \sum_{n} \left( 1 - \cos \left( \frac{2\pi}{b} x_n \right) \cos \left( \frac{2\pi}{b} y_n \right) \right).
\]

\(b\) is the period for Frenkel-Kontorova potential. \(A\) is the amplitude for Frenkel-Kontorova potential. The minima of the substrate potential form a square lattice. The substrate potential lattice is oriented at an angle \(\pi/4\) to the film atom lattice. This form of potential provides two types deformation for the film on the side of the substrate: stretching and torsion. The substrate potential for \(b=1\) and \(A=1\) is shown in Figure 1.

**Figure 1.** The substrate potential for \(b=1\) and \(A=1\).

The equilibrium state of the film atoms is determined by minimizing the films energy.

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

The film energy is equal to the sum of the interatomic interaction energy and the substrate interaction energy.
We examine a film having $N$ atoms along each side. Interaction with the substrate is described by a potential having $M$ minima along each side. The concentration of atoms on the substrate is determined by the coating coefficient.

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

The atoms placement on the substrate depends on the boundary conditions. Atoms are placed in the nodes of the square lattice at fixed positions at the boundary of the region [12-15]. The period of the new lattice is determined by the coating factor.

$$a = \frac{b}{\theta}.$$ 

We model a system with periodic boundary conditions. For atoms located at points $(x_0, y_0)$, adjacent to the left are atoms located at points $(x_{N-1}, y_0)$. For atoms located at points $(x_0, y_n)$, adjacent to the left are atoms located at points $(x_0, y_{n-1})$. The same conditions are used along the $OY$ axis.

The algorithm for determining the equilibrium state of film atoms is based on the Monte Carlo method. The undeformed film is used as a zero approximation. Sequential atoms enumeration is performed in each iteration. The stable state of atoms is sought in each iteration. Atoms are shifted by a random vector. If this displacement reduces the energy of the film, then it is fixed, otherwise it is discarded. Iterations are performed until the system becomes equilibrium.

3. Computer experiment

In a computer experiment, films with $N = 50$ are examined. Substrate parameter $M$ is selected so that its geometric dimensions coincide with the film. The coating factor is calculated based on the ratio of the film and substrate periods.

$$\theta = \frac{b}{a_0}.$$ 

The dimensions of the substrate are determined from the coating factor.

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

We are considering three cases: $b=0.95a_0$, $b=a_0$ and $b=1.05a_0$. The coating factor for these cases is $\theta=0.95$, $\theta=1.00$, $\theta=1.05$. Influence of substrate is determined by amplitude ratio for substrate potential and elasticity coefficient. We are considering three cases: $A/g=0.1$, $A/g=0.5$ and $A/g=1.0$.

If the periods of the film and the substrate coincide, then the film rotates and the atoms form a square lattice at any ratio $A/g$ (Figure 2.)
If the substrate potential period is less than the film potential period ($b=0.95a_0$), then the film is separated into square areas. The separation results from compression against multiple centers. The distance between the nanoparticles increases as the amplitude of the substrate potential increases (Figure 3).

**Figure 2.** Position of film atoms at $b=a_0$.

**Figure 3.** The arrangement of atoms on the substrate at $b=0.95a_0$ and various values $A/g$. 

a) $A/g=0.1$  
 b) $A/g=0.5$  
 c) $A/g=1.0$
Film expansion near several centers occurs at $b=1.05a_0$. The result of this expansion is a square lattice with superstructure superimposed thereon (Figure 4). The superstructure is a square grid with an increased atoms density. The atoms density in the superstructure increases as the amplitude of the substrate potential increases.

![Figure 4](image_url)

4. Conclusion

We investigated 2D film deformations on a compressible substrate by computer simulations. Uniform deformations of the substrate cause non-uniform deformations of the film. If the substrate is uniformly compressed, regions with increased concentration of atoms appear in the film. The continuous film is transformed into a nanoparticle film. When the substrate is stretched, a superstructure in the form of a grid with an increased atoms concentration is formed in the film. New mechanical, electrical and magnetic properties in such films can be expected.

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