

# Computer Simulation of Two-Dimensional Film Placement on Crystalline Substrate

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## Abstract

The paper discusses computer simulation the process of forming a 2D film under the ferroelectric substrate influence. The film is formed from randomly arranged atoms. The interaction between the film atoms is described by the Lennard-Jones potential. Substrate is modeled by periodic potential. Cases of different values for substrate potential amplitudes and periods and different atoms density are considered. For computer modeling, the Monte Carlo method is used. An equilateral triangular atoms lattice is formed without the influence of the substrate. When considering the potential of the substrate, nanoparticles with a triangular crystal lattice are formed. At long periods of the substrate, the nanoparticles are located in the minimum potential of the substrate. At small periods of the substrate, a crystalline film with substrate symmetry is formed. As the density of atoms increases, the size of the nanoparticles increases. The substrate potential amplitude affects the shape of the nanoparticles.

## 1 Introduction

Computer modeling of two-dimensional films is relevant in connection with their active use in electronics devices. Computer modeling of such systems is mainly carried out from the first principles [1, 2]. Calculations from the first principles are substance-specific. An alternative approach is to computer model these systems from common principles [3, 4].

Of particular interest are ultrathin ferromagnetic films on a ferroelectric substrate. These composites are actively used in spintronics devices. The interaction between the substrate atoms and the film makes it possible to control the films magnetization. The ferroelectric substrate is controlled by an electric field. In these systems, the magnetization is controlled by an electric field. This phenomenon is called magnetoelectric effect.

The magnetoelectric effect is observed in a large number of experiments. Re-magnetization of thin films on a ferroelectric substrate is described in several works: *Ni* film on a substrate *BaTiO<sub>3</sub>* [5], Fe-Ga on various

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ferroelectric substrates [6],  $La_{0.7}Ca_{0.3}MnO_3$  on a ferroelectric substrate  $BaTiO_3$  [7]. The substrate deformations alter the physical films properties. Interaction of film atoms with substrate allows controlling phase transitions in film [9]. Electric field causes deformation of substrate and film simultaneously [10].

This article purpose is to computer simulate the effect of the substrate on the formation of 2D films.

## 2 System description

We're looking at a two-dimensional atoms' system. The interaction between atoms is described by the Lennard-Jones potential. We record the potential energy for atoms' system in the absence interaction with the substrate.

$$U_{int} = 4\varepsilon \sum_{ij} \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right].$$

$r_{ij}$  is the distance between atoms numbered  $i$  and  $j$ .  $\varepsilon$  and  $\sigma$  are constants.  $\sigma$  is the distance between atoms at which the energy of their interaction is zero.  $\varepsilon$  is the depth of the potential hole. Atoms repel at  $r_{ij} < \sigma$ . Atoms are attracted at  $r_{ij} > \sigma$ . If this energy is minimized without the influence of the substrate, then the atoms are located at the nodes of an equilateral triangular lattice with a period  $\sigma$ .

The influence of the substrate is modeled as a two-dimensional periodic potential. We use the generalized Frenkel-Kontorova potential formula for the substrate potential [11].

$$U_{sub} = \frac{A}{2} \left( 1 - \cos \left( \frac{2\pi x}{b} \right) \cos \left( \frac{2\pi y}{b} \right) \right).$$

$b$  is the substrate potential period.  $A$  is the amplitude of the substrate potential. The potential of the substrate in this form has a periodic structure. Main directions of substrate are oriented at angle  $\pi/4$  to axes  $OX$  and  $OY$ . The general view of the potential  $U_{sub}$  is shown in Figure 1.

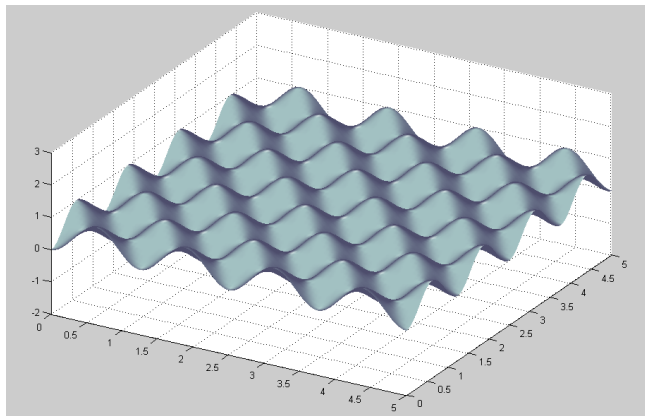


Figure 1: General view of substrate potential.

The minimum potential energy of the system is to calculate the atoms position in the ground state. The total potential energy for the system consists of the energies for interaction between atoms and the interaction atoms with the substrate.

$$U = 4\varepsilon \sum_{ij} \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right] + \frac{A}{2} \left( 1 - \cos \left( \frac{2\pi x}{b} \right) \cos \left( \frac{2\pi y}{b} \right) \right).$$

$N$  atoms are placed on a substrate with dimensions  $L \times L$ . The coating factor indicates the number of atoms per minimum.

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

$M$  is the number of minima for the substrate potential. We calculate the number of minimums on the  $L \times L$  film for the selected substrate potential.

$$M = 2 \left( \frac{L}{b} \right)^2.$$

If the average distance between atoms is less than  $\sigma$ , then one atom accounts for a large energy. This effect is associated with the overlap the electron shells of atoms. The initial position of the atoms is chosen randomly. The distance between atoms in the initial state must be greater than  $\sigma$ . The maximum density of atoms for this condition is achieved in an equilateral triangular lattice with a period  $\sigma$ .

$$n_{max} = \frac{N}{L^2} = \frac{2}{\sqrt{3}\sigma^2}.$$

We consider systems with an average density of atoms not exceeding this value.

The Monte Carlo method is used to calculate the ground state of the system. The system is simulated with periodic boundary conditions. The random offset for each atom is given in each iteration. If random displacement reduces the energy of the system, then the new position of the atom is taken. If random displacement increases the potential energy of the system, then the atom remains in its original position. This algorithm corresponds to finding the ground state of the system at zero temperature. The number of iterations is an algorithm parameter. A computer experiment shows that the position of atoms does not change after a certain number of iterations. The systems energy is constant.

### 3 Computer experiment

In a computer experiment, a square substrate region with a side  $L = 10$  is examined. Calculations showed that increasing the size of the study area does not lead to a qualitative change in the atoms arrangement. The  $\sigma$  and  $\varepsilon$  parameters specify the length and energy scales.  $\sigma$  is set to 0.3. The  $\sigma$  parameter can be interpreted as the average atom radius. We use the value  $\varepsilon = 1$ . Dependence the ground state on parameters  $A$ ,  $N$ ,  $b$  is investigated in numerical simulation.

The dependence of the ground state on the amplitude of the substrate potential  $A$  was carried out for  $N = 500$  atoms and the value  $b = 3$ . We look at four cases:  $A = 0$ ,  $A = 5$ ,  $A = 10$ ,  $A = 15$ . The results are shown in Figure 2. When parameter  $A$  is increased, separate nanoparticles are formed. Atoms are located in the nodes of an equilateral triangular lattice in each nanoparticle. The orientations of crystal lattices in nanoparticles are different. The location of the nanoparticles is ordered according to the substrate potential.

The dependence of the ground state for the system on the number of atoms  $N$  is shown in Figure 3. We select the substrate potential amplitude  $A = 10$ . Substrate period is  $b = 3$ . We are considering four cases:  $N = 300$ ,  $N = 450$ ,  $N = 600$ ,  $N = 750$ . Atoms localize near the minima of the substrate potential, forming separate nanoparticles at low density. As the density of atoms increases, a continuous film is formed. Crystal lattices of nanoparticles are oriented in one direction during fusion. The order of filling the film with atoms is defined by substrate symmetry.

A study of the ground state dependence for the system on the substrate period  $b$  was carried out. We select the substrate potential amplitude  $A = 10$ . The calculation is made for 700 atoms. We are considering four cases:  $b = 0.5$ ,  $b = 1.0$ ,  $b = 1.5$ ,  $b = 2.0$ . The results are shown in Figure 4. At approximation substrate period  $b$  to parameter  $\sigma$  for Lennard-Jones potential, film with substrate square symmetry is formed. When the parameter  $b$  is increased, an intermediate distribution of atoms between the square and triangular symmetries occurs. With a further increase in the parameter  $b$ , the atoms line up in an equilateral triangular lattice.

### 4 Conclusion

We studied the effect of the substrate potential period and amplitude on the atoms system ground during the formation the 2D film by computer modeling. Calculations showed that when taking into account the influence of the substrate, the film is divided into 2D nanoparticles. As the number of atoms increases, the nanoparticle film changes to a continuous film. As the period of the substrate in the film decreases, the symmetry of the crystal lattice changes. Films with symmetrically arranged nanoparticles can be expected to exhibit new mechanical, electrical and magnetic properties.

### 5 Acknowledgements

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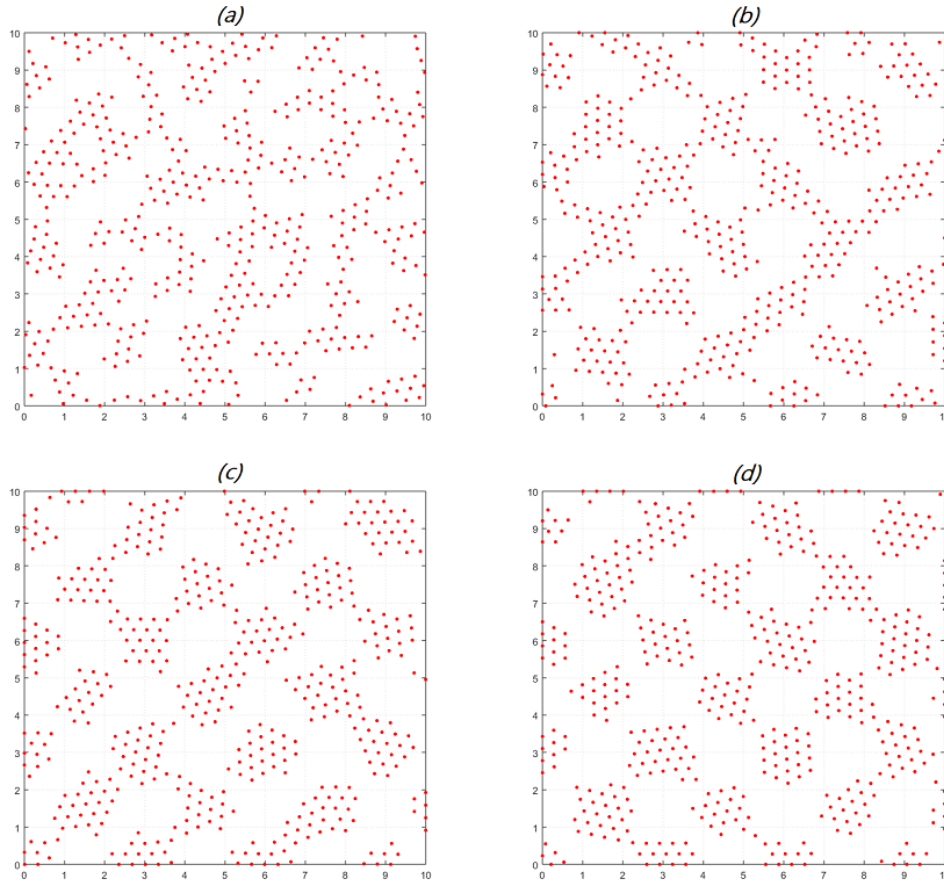


Figure 2: Dependence of the ground state on the the substrate potential amplitude. (a)  $A = 0$ . (b)  $A = 5$ . (c)  $A = 10$ . (d)  $A = 15$

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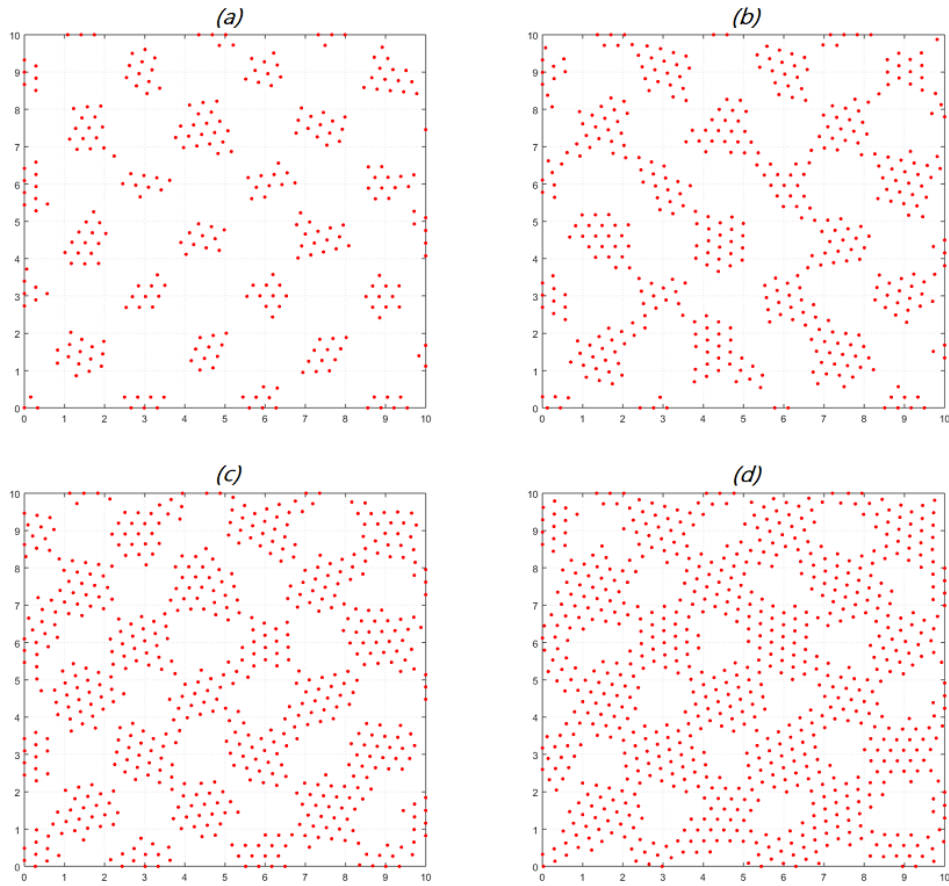


Figure 3: The dependence of the ground state on the number of atoms. (a)  $N = 300$ . (b)  $N = 450$ . (c)  $N = 500$ . (d)  $N = 750$ .

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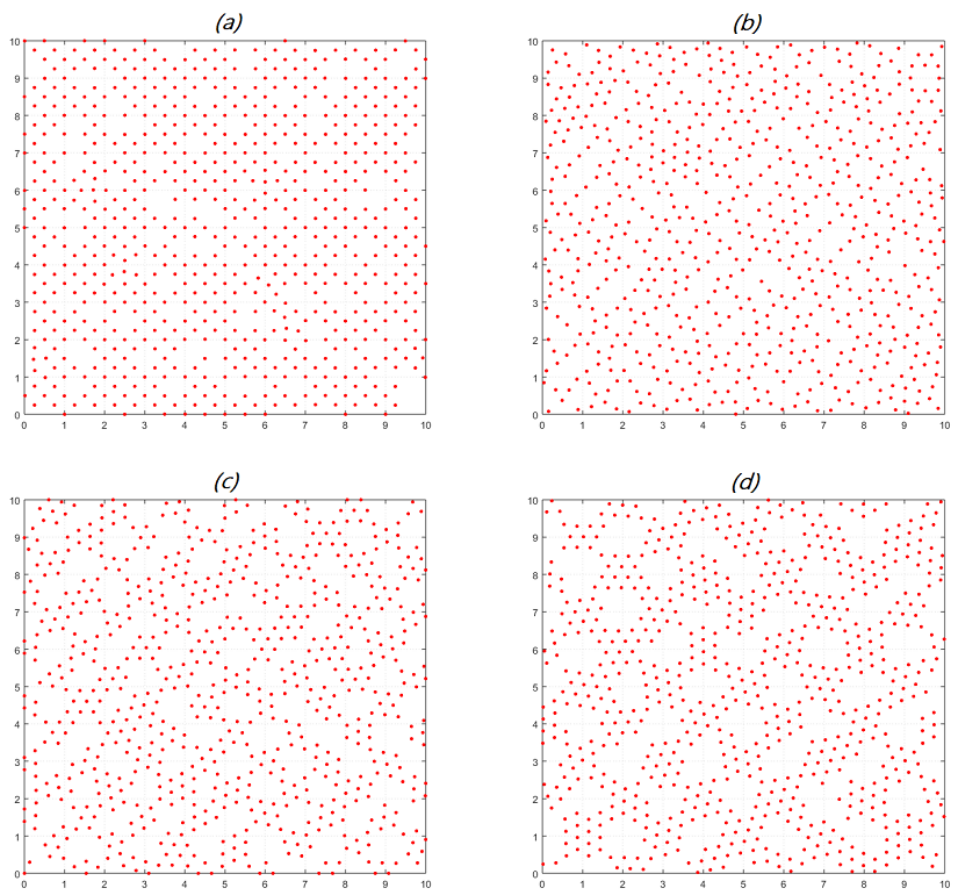


Figure 4: The dependence of the ground state on the substrate period. (a)  $b = 0.5$ . (b)  $b = 1.0$ . (c)  $b = 1.5$ . (d)  $b = 2.0$ .