Consideration of the condensation processes of thin films in the crystal substrate’s potential field

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Abstract. The condensation process of a single particle in an ideal crystal substrate’s potential field is considered. The optimal deposition path and the potential barrier of deposited particle’s motion are shown. Some computer modeling examples of thin film’s growth process were carried out on the basis of the implemented programs. A fractal analysis of obtained thin films was made, on the basis of which the possibility of estimating the performance of thin film’s growth process will be discussed.

1. Introduction
Obtaining thin films of high quality today is constantly required, especially for micro-nanoelectronics industries and the formation of various functional coatings. A major problem in the way of improving the quality of thin films has to do with the analysis of the conditions and the processing of how the films are obtained. In this paper, the process of film condensation will be examined as one of the possible ways of obtaining high quality thin films.

2. Assumption
The theories adopted in this work, are as follows:
a) material consists of spherical particles (atoms, molecules), having isotropic interactions with other particles through the Lenard–Jones pair potentials (LJ) [1]. This approach characterizes a simple model calculation but has some limitations [2];
b) substrate has an ideal structure and does not change with time of calculation.

3. A procedural analysis of the process
The analysis of the process is done by three successive calculation models, which are as follows.

3.1. Condensation process of single particle on substrate
In considering the condensation process the firstly we want to examine the process for a single particle on the potential field of an ideal crystal (without taking into account the deposited particle’s kinetic energy). The potential bond \( U(x, y, z) \) of deposited particles with substrate was calculated by the following equation:

\[
U = U_{1\text{-layer}} + U_{2\text{-layer}} + U_{3\text{-layer}} + \ldots, \tag{1}
\]

where
The number of particles: 1409 | Radius of substrate: 20
The partitioning number of substrate: 40
Thin film’s surface

Figure 1. The optimal condensation path \( x(z) \) and \( y(z) \), and the potential interaction of deposited particle with ideal substrate.

3.2. Computer modelling of thin film growth process

In order to visually consider the process of condensation and growth of thin films on potential field substrate was built a designated program \([3]\), the foundations of which are based on the Monte Carlo method, to select a number of particles and quasi-Newton lattice’s method in determining the optimal direction of motion of the particles, such that the potential energy of the system (consist of deposited particles) was minimal. As you know, this process is random (using the Monte Carlo method) and the self-organizing nature of the (using quasi-Newton lattice’s method) with a phase transition \([4]\).
Figure 3. Topology relief: (a) \( U(x, y, z = z_0) \); (b) \( U(x, y, z = z_0 / \sqrt{2}) \); (c) \( U(x, y, z = z_0 / 2) \). Profile potential relief in two cases (d).

Below are shown the results of computer modeling for such data, 1409 particles randomly generated and successively dropped onto a substrate (the structure and properties of the particles were already set up in the calculation model A). This is the number of particles selected as sufficient to cover the substrate with a radius of 20; precipitated by lowering the particle flow rate chosen so that during lowering of a particle on a substrate is realized 500 + 8N steps traffic \( (N – \) number of particles in a real-time simulation) in lattice grid calculating coordinates (the step-size selected is \( r_{opt}/10 \) – the lesser the step-size the more precise the calculation, but the calculation time is longer). Figure 4 shows the result of computer simulation of the particle deposition process parameters \( \sigma \) and \( V \) are same as the parameters of the particles on the substrate, the left takes into consideration thermal noise while the right excludes it, and the noise level is from \( 10^{-1} \) to \( V_0 \). It can be seen that the thermal noise allows the particles to remove a potential barrier (which we calculated in the calculation model A) and formed larger clusters; however the number of defects (disorder) in the picture is more.

3.3. Fractal analysis for obtained thin film

The basis of fractal analysis of obtained thin film structure; as is known, the fractal dimension of the physical objects may take on different values depending on the method of calculation and for different regions (volume surface or section) may be different (result confirmed in table 1 and figure 5). The fractal dimension of the resulting thin film was calculated in this paper using three known methods [5, 6].

The first method: box counting method, (Hausdorff–Besicovitch) fractal dimension \( D_b \) of obtained structures was estimated by the formula: \( N(\delta) \sim \delta^{-D_b} \), where \( N(\delta) \) – the number of filling elementary cubes with the number of partitions of calculation area (see figure 3) (for three directions \( x, y, z \) ) \( \delta \).
The second method: fractal analysis of the surface, the surface fractal dimension $D_f$: 

$$S_{fact}(\delta) \sim \delta^{D_f}$$

where $S_{fact}(\delta)$ – the surface area of the resulting thin film when the number of partitions of calculation area (for two directions $x, y$) $\delta$.

The third method: fractal analysis of the vertical section, the fractal dimension (profile) is calculated using the formula: 

$$L(\delta) \sim \delta^{D_L}$$

where $L(\delta)$ – the length of the profile of a cross section through the center of the resulting thin film with the number of its partitions (one direction) $\delta$.

Below in table 1 and figure 4 are shown the result of calculating the fractal dimension of the resulting thin film in the scope of investigation (figure 3) at different moment in a thin film growth process, and for the two cases when the length of the Lenard–Jones parameters of the deposited particles ($\sigma_{dep}$) and particles on a substrate ($\sigma_{sub}$) are equal (epitaxial growth, figure 3(a)) and different ($\sigma_{dep}:\sigma_{sub} = 2:1$) According to the calculation results the fact (statistical law) that fractal dimension is increased with the thin film growth process for the three calculation methods. The longer and more complex the growth process, the greater the value of the fractal dimension.

**Table 1.** Result of fractal dimension’s calculate for three different methods.

| Fractal dimension | $D_b$ | $D_f$ | $D_L$ |
|-------------------|-------|-------|-------|
| Ratio of $\sigma_{dep}:\sigma_{sub}$ | 1:1   | 2:1   | 1:1   | 2:1   |
| Thin film consisting of 1409 particles | 1.61  | –     | 0.58  | –     | 0.40  | –     |
| Thin film consisting of 939 particles  | 1.48  | –     | 0.36  | –     | 0.23  | –     |
| Thin film consisting of 705 particles  | 1.43  | 1.69  | 0.27  | 1.05  | 0.16  | 0.81  |
| Thin film consisting of 282 particles  | 1.10  | 1.30  | 0.11  | 0.47  | 0.06  | 0.31  |

**4. Conclusion**

This paper presents the result of studying the condensation process of thin films in the potential field of an ideal structure of the substrate. By considering the model of the condensation process of single particle it was shown that motion path of a condensed particle is complex, interaction potential’s topography changes, and the presence of potential barrier in particle’s motion on the substrate.
The calculation area for $D_b$

The calculation area for $D_f$ and $D_L$

**Figure 5.** The dependences of $\ln(S)$, $\ln(L)$, $\ln(N)$ on $\ln(n)$ for obtained thin films in different moments of its growth process.

Thanks to the efficiency of the computer simulation of thin films growth process these facts have been confirmed, and it is also shown that the potential barrier can be removed with the thermal noise (thermal treatment). According to the results of fractal analysis of the obtained thin film structure, it can be concluded that this thin film has a fractal structure and moreover, by the value of fractal dimension the difficulty and time of their growth process can be determined.

**References**

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