Computer simulation of nano-thin film condensation process in a vacuum

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Abstract. In this paper, the role of nano-thin film condensation process in thin film technology is shown. It was demonstrated by using the computer simulation method that the abovementioned process determines the quality of the thin film. Proprietary models were used in order to analytically calculate the condensation process of a particle on the potential field of ideal crystal substrate and to simulate the processes of condensation and growth for atoms with isotropic or anisotropic bonds with other atoms. The numerical method is based on the algorithm of a random chosen active atom, the direction of motion of this atom is calculated by the quasi-Newton method and the step of atom movement is considerably shorter than the optimal distance of two atoms.

1. Introduction

The process of obtaining thin films or coatings by utilizing advanced techniques can nowadays result in new materials with new characteristics and capabilities, which requires high technology to be applied and developed. To support this high technology, the parameters of technological regimes and operations need to be chosen based on qualitative and quantitative analysis and synthesis of all the occurring processes. Thin film condensation occurs in a nonlinear non-equilibrium dynamical system at an atomic level. Synthesis approach based only on experimental data will result in more time consumption accompanied with materials and solution that may not meet the optimal requirements. Today, with the development of computer engineering the approach based on computer simulation at the atomic level appears to provide a more promising solution.

The first application of computer simulation at an atomic level to solve the task in nanotechnology was in around 1950 years. The computer simulation based on some numerical methods and the choice of numerical method will depend on a compromise between the availability of a computing resource, the time of calculation, the accuracy and reliability of the numerical algorithm. In the opinion of authors, nowadays computer simulation in thin film technology by using of the existing software does allow for many modeling options, and the result does not provide quantitative estimation. However, based on the specifics of this process, a new computer simulation approach [1–3] for modeling the process of nano-thin film condensation, including a growing stage is shown in this paper.

2. Models of thin film condensation process for an atom having isotropic bonds with other atoms

Firstly, in order to understand the process, the condensation model of a particle on a substrate [4] is
used. The analysis of the model results in an analytical solution in the second stage when the whole process of condensation is observed.

In order to make predictions, a computer simulation utilizes a sufficient number of simulated particles. However, in the thin-film condensation process, more than a thousand atoms are needed to observe all steps of such a process like absorption, nucleation, growth of the nuclei and formation on larger islands, a coalescence of the islands and filling of the channels. Today the numerical methods used to simulate its behavior are molecular dynamic (MD) and kinetic Monte-Carlo (MC) methods or its modification. The first (MD) group is not appropriate to simulate the condensation process with growing on an ordinary computer, because with this numerical method one is able to conduct simulations in real-time for less than a nanosecond. The second numerical method is more appropriate to use in simulation, because this method does not conduct simulations in real time. However, by using this method one is able to find the local stable structure of the thin film.

In the opinion of authors, the second MC groups are not enough to get some quantitative estimation on influencing factors in processes, because this method has restrictions in the number of trial movement steps and the length of movement steps. To solve this problem, we suggested a new numerical algorithm based on the specific characteristics of nano-thin film condensation process [1]. The numerical method based on the algorithm of a randomly chosen active atom, the direction of motion of this atom calculated by the quasi-Newton method and the step of atom movement is even times less than the optimal distance of two atoms. To show the role of substrate and its structure in the simulation, we used two models of the substrate. In the first model, the structure of the substrate is unknown and the interaction of condensation particle depends just on its distance to the plate of the substrate. And the second one the structure of the substrate is known. The interaction between particles uses Lennard-Jones pair potential with the own parameters and depend on the approximation of the real interaction of simulation material.

![Figure 1](image1.png)

**Figure 1.** The top view of obtained films. The model on the left is the interaction of condensation particle with substrate depending on the distance to substrate plate and the model on the right is the active interactive length of condensation particle identical to the active interactive length of the substrate structure.

The new numerical method allow a researcher to conduct a large number of computer experiments [5]. In figure 1, the one on the left has shown the result of computer simulation in the first model of the substrate and the one on the right in figure 2 has shown the result on the second model of the substrate. Based on the result of computer experiments, we can obtain a quantitative estimate on each influenced factor or group of such factors.
Figure 2. Obtained film in the case where the active interactive length of condensation particle is twice the active interactive length of substrate structure, on the left – the left side view and on the right – the top view.

3. Models of thin film condensation process for an atom having anisotropic bonds with other atoms

In order to conduct simulations of the material with a covalent bond, it is impossible to use the pair potential as in the case of an atom with an isotropic bond. Based on the specific structure of the atom and the orbital theory, the new atom representation is shown in figure 3(a), as well as the interaction in an internal atom (figure 3(a)) and interatomic interaction (figure 3(b), (c)), which shows that the atom consists of two - parts external electron orbitals and internal nucleus. To accelerate the simulation process, we employ the distance of two atoms. There are two such cases as shown in figure 3(b), (c). Threshold distance usually assumes the value that is 3 times of active interactive length in Lennard-Jones potential.

Figure 3. A new model of one atom (a) and two cases of interatomic interaction: \( r \geq d_{\text{threshold}} \) (b) and \( r < d_{\text{threshold}} \) (c). These shows 11 various types of bonds in this model. The atomic diamond structure (d) is used in this work as a substrate.

The numerical method used in these models is identical to the one in the second models, however here we have two kinds of movement of the external electron of the atom - sliding and rolling movements. One is able to find a more detailed description of such processes is the following referenced research works [2, 3]. In figure 4, the result of computer simulation by applying this numerical method is
shown. These models allow us to study the influence of length, angle and strength (internal and external) of interaction inside an atom and between them.

4. Conclusion
Based on deep learning of the physical process on each technological stage by using computer simulation with own numerical algorithm will allow us to analyze and optimize the entire technological process. The numerical algorithm of the simulation was created based on the specific characteristics of nano-thin film condensation process and as a consequence will give a more quantitative estimation on influencing factors in processes and improve the accuracy of the calculation.

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Figure 4. 3D result of computer simulation of the growth process of 64 atoms (nucleus - blue) with sp3 hybridization type (green colours), on the left - in the vacuum condition, on the right - on the used model of the cover (with diamond structure - red and black).