Modeling of thin films growth processes in the early stage for atoms with covalent bonds

V A Tupik, V I Margolin and Chu Trong Su
Department of Radio Microelectronics and Radio Equipment Technology, Electrotechnical University “LETI”, Saint Petersburg 197376, Russia
E-mail: chusu171@mail.ru

Abstract. Computer simulation for obtaining thin film’s growth process at an early stage with the proposed model of atoms with isotropic and anisotropic interactions been considered. Carrying out the procedure for analyzing the problem on the basis of the program being implemented, computer simulation of thin film growth processes has been carried out on several examples. The results of computer simulation of the growth process of thin film on a given substrate and an aggregate in a vacuum condition are shown. Some characteristic distributions of the obtained structure have been carried out to evaluate the proposed adequate model and to reflect the high complexity of thin films growth process.

1. Introduction
Nowadays, with the advancement in nanotechnology, one of the high promising directions is the application of computer modeling with an approach that allows taking into account features at the atomic level, which for human cognition, is always indirectly accessible. And using the computer approach for the optimization and synthesis of the processes of formation of these thin films at the early stage also plays a big role. The work was designed so that from the beginning the optimization of configuration setting and the process macroparameters are based on the macroparameters of the final function of the resulting thin film, like the film thickness, deposition rate, distribution of thin film thickness etc., then we proceed to optimize microparameters thin film such as surface roughness, atomic structure, defect structures, etc. Based on previous studies [1–4, 6, 8], many particular feature processes were shown for simple atoms which had an isotropic bond which is described by a pair potential interaction.

In this study, we would take a look on most of the described computer approach for more complex atoms wherein the bond is anisotropic, which means we can expand the range of applications, for example, the semiconductor material atoms.

2. Description of new models
As shown in [1, 7] we can observe that at present it is more important to use an empirical approach in the description of interatomic interaction. Also, due to restrictions on the available power of computing techniques and the number of simulated atoms (in the order of 100 atoms in the approach based on the first principles of quantum mechanics), the new idea, using in this work, was such that all the particles (atoms) were represented as described in figure 1(a), (b), (c) [1]. The atom has two parts, namely the external electron orbitals (often referred to as electron, and denoted as \( e \) in figure 1) and
the nucleus (more precisely, the inner part of the atom, excluding the outer electronic orbital). The electrons repel each other and form an angle $\varphi_0$ (figure 1), they also attract the electrons to the optimal distance $r_1$ in figure 1.

Atoms are related to each other depending on the distance between them ($r_2$), and if this distance is greater than the threshold value, we then use an isotropic potential bond to simplify the computational load and accelerate the modeling process. Otherwise, when atoms related to each other at a close distance is less than the threshold value; we use an anisotropic potential bond, separating the electrons into bound (connected) and unbound (unconnected) ones. A more detailed description is given in [1].

![Figure 1](image.png)

**Figure 1.** 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). There are shown 11 various types of bonds in this model [1]. The atomic diamond structure (d) used in this work as a substrate.

![Figure 2](image.png)

**Figure 2.** Computer simulation of thin film growth process without thermal noise (a) and with thermal noise (b) [2].

As shown in this paper [2, 3], we also considered the same problem, but for complex atoms with $sp^3$ type of hybridization. For example, figure 2 shows the result of computer simulation of thin film growth on a substrate with a body-centered cubic lattice with an equal lattice parameter. The left diagram, figure 2(a) shows the process without thermal noise on the substrate, and in the other diagram figure 2(b) we took into account the parameter of thermal noise in the average energy order of $10^{-1}$, and also the optimal interaction energy of two particles in Lenard-Jones pair potential [2]. As shown in figure 2, the thermal
noise will affect the size of the nucleus and the roughness of the resulting thin film. We want to note here that all the linear dimensions used in this paper were normalized by \( r = r_n / \sigma_0 \). Where \( d_{\text{threshold}} \), \( \sigma_0 \) are adjustable parameters for the working material and each type of bonding (in Lenard-Jones pair potential), as usually offered as the distance is longer than \( 3 \sigma_0 \).

\[
\sigma_0 / r = \theta
\]

3. Two computer simulations with new algorithm

Using the new approach (anisotropic model), we conducted two experiments, in the first computer experiment, the deposited structure is obtained without a substrate in the vacuum condition (figure 4(a)), and in the second experiment, on the selected structure of the substrate as shown in (figure 4(b)) as the substrate parameter, we use a structure where \( r_1 = 1 \) and it consists of two layers (figure 3) of diamond structures with the orientation shown as in figure 1(d). This structure only creates a potential impact and is a fixed structure in the thin films growth process. The growth process proceeds according to this algorithm, the particle is randomly generated at a distance \( r \) from the substrate with random coordinates \( (x, y) \), and then the growth process, the system of deposited particles behaves this way so that the energy of the system (deposited particles with the substrate) becomes minimum. Numerical
methods were used by the Monte Carlo method for random particle selection and a quasi-Newtonian method was used for selecting the optimal direction of particle motion [3, 4]. After that, we calculated its analytical statistical characteristics and we compared it with the structure of the film deposited on the substrate.

![Distribution of angles between two orbitals](image1)

![Radial distribution function](image2)

![Distribution of orbital length](image3)

![Distribution of distances between two bonded atoms](image4)

Figure 5. Some characteristic distributions of the obtained structure (figure 4). F(1−4) – the number of atoms or orbitals having a given distance or angle between two orbitals: l – analysis for internal atoms (φ₀); 2 – analysis only for bonded atoms (φ₁); a – analysis for obtained film on a substrate (figure 4 (b)); b – analysis for the obtained aggregate, which was growth in a vacuum condition (figure 4 (a)).

4. Results and discussion

Based on the results obtained with the aid of the calculation model in [1], in figure 5, F1 – it shows the angle between two orbitals φ₀ inside one particle it also changes (not constantly), and most particles have an optimal angle of 109° (acos(−1/3)), the angle between two connected particles φ₁ also changes, as shown on the image. In figure 5, F2 it is shown that the orbital length inside one particle (r₁) and the distance between two particles (r₂) vary. And in figure 5, F3 – the character of the crystallization of the obtained structure is shown (if the number of simulated particles is sufficient), as a result, it is seen that the structure obtained is likely to have an amorphous structure, as shown in figure 4.

As for the process of obtaining single crystals of SiC, it shows there is a lot of different polytypes and polymorphs [9, 10], which implies that the system which consists of two parts could go one in a lot of directions of system development, and the distribution of sp², sp³ [5] reflects the complexity (nonlinear dynamics) occurring at this stage. Our model which will assist in showing our understanding at this stage is really the first approximate calculation closest to reality. But the use of this approach from first principles is still a bit far from implementation due to the complexity and loaded work [11].

5. Conclusions

In this paper, we presented the result of studying the process of condensation of thin films on the potential field of an ideal substrate structure for complex atoms with sp³ type of hybridization. The procedure for the movement of computer simulation into synthesis and optimization of simple to
complex models were suitably shown for different types of interatomic potential. It has been estimated that in spite of the first approximate results, the model can account for an anisotropic bond, change bond lengths and angles between the two particles in the condensation process. These are very significant steps to the modeling of atoms with an anisotropic bond as discussed and shown.

References
[1] Tupik V A et al. 2017 IEEE Conference of Russian Young Researchers in Electrical and Electronic Engineering (EIConRus) 1209–12
[2] Tupik V A et al. 2016 J. Phys.: Conf. Ser. 729 012025
[3] Chu Trong Su 2016 Proceeding of the Russian Universities: Radioelectronics 6 22–31
[4] Tupik V A et al. 2016 IEEE NW Russia Young Researchers in Electrical and Electronic Engineering Conference (EIConRusNW) 93–6
[5] Osswald S et al. 2006 Journal of the American Chemical Society 128 (35) 11635–42
[6] Tupik V A et al. 2016 IEEE V Forum Strategic Partnership of Universities and Enterprises of Hi-Tech Branches (Science. Education. Innovations) 42–5
[7] Tersoff J 1988 Phys. Rev. B 37(12) 6991–7000
[8] Tupik V A et al. 2015 Proceeding of the Russian Universities: Radioelectronics 5 15–9
[9] Ching W Y et al. 2006 Materials Science and Engineering: A 422(1–2) 147–56
[10] Wasylik J et al. 2010 Materials Science Forum 645-648 359–62
[11] Lee J G 2016 Computational material science (CRC Press)