# Simulation of Control Processes for Deposition of Nanofilms on Porous Alumina Substrates

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*Abstract:* - The results of the investigation of deposition processes of nanofilms formation on amorphous aluminum oxide substrates are presented in the article. The study was carried out by mathematical modeling. The equations of molecular dynamics and the modified embedded atom method were used in solving the problem. The required temperature and pressure were maintained using a Nose-Hoover thermostat and barostat. The simulation was performed using the software package LAMMPS. In the work, the precipitation of molecular zinc sulphide in both pure form and addition of alloying elements was investigated. In all cases, the picture of overgrowing of porous substrates was obtained in a similar way. The pores were not completely filled with the deposited atoms, they only partially penetrated it. Directly above the pores a layer of zinc sulphide was formed, which began to form from the sides of the porous structures. Alloying additives processes of formation of nanofilms did not significantly change. To investigate the possibility of controlling the processes of deposition and formation of nanofilms and burying of porous templates, the angle to the normal line of the porous template in which the epitaxial atoms and molecules move to the deposition surface was selected as one of the modeling control parameters. The angle from the normal varied from 0 to 60 degrees. Another controlling parameter was the preheating temperature of the already formed film. The nanofilms were heated at elevated temperatures in the range 293-593 K and the result of the modification of the nanofilm was considered. Investigations of the possibility of controlling the growth processes of nanofilms, overgrowing porous substrates, and the formation of nanostructured coatings have shown that the epitaxial deposition angles and heating of the nanosystem to temperatures do not lead to a significant change in the formation of nanostructures. At the same time, there is a slight restructuring of the structure and internal organization of nanoelements, but there are no certain filling of the pores and changes in the properties of the nanofilms.

*Key-Words:* - epitaxy, nanofilms, simulation, porous substrates, LAMMPS, molecular dynamics, zinc sulphide, optical films.

# 1 Introduction

Due to its hexagonal-ordered arrangement of pores vertically-aligned to the film surface, porous anodic aluminum oxide is quite often used as a template to synthesize different nanostructures: nanopoints, nanowires, nanorings, nanotubes, etc. [1, 2]. The anodic aluminum oxide can also be successfully used as a carrier of catalytically active nanoparticles [3], as well as nanostructures of semiconductors [4]. This gives the possibility to form the ordered aggregates of nanostructures of semiconductor fluorescent material of the same size and shape that allows representing each nanostructure as a separate light emitter. The coherent addition of radiation from each light source results in significant light intensity increase [5].

As it was pointed out before, the lighting properties of electroluminescent light sources depend on the fluorescent material layer thickness and its structure. In case of electroluminescent light sources formed as nanocomposites of the type "semiconductor / dielectric matrix", the template thickness also plays an important role since the precipitated material penetrates the matrix pores to the depth of up to 10 mcm. That is why the mechanism of nanostructure growth in matrixes of different thickness can differ, and the distribution of alloying element and structure of the fluorescent material obtained by the method of thermal precipitation of powder mixture can differ as well [6].

Despite of the wide application of nanofilms, the questions of detailed investigation of their composition, structure and processes flowing in them still arise. The problems of studying electrochemical and magnetic effects [7] in porous anodic aluminum oxide and application of similar templates as optic sensors [8] are topical. Similar problems are actively studied and solved by other authors both experimentally [9] and, to decrease the costs, with the help of theoretical methods and mathematical modeling apparatus [10-11]. Monte Carlo algorithms [12], condensation models, equations of liquid and gas motion, finite-element analysis [13], as well as molecular dynamics with different types of potentials are used as theoretical investigation methods. The application of molecular dynamics apparatus is often the most justified as it allows observing the structure evolution in materials in detail and registering the whole set of phenomena and processes in nanofilms. The understanding of mechanisms and multilayer examination of nanofilm forming and functioning, interaction of nanostructures and nanoparticles they contain, as well as the development of engineering ideas and approaches to managing and using these processes, will give the possibility to properly design nanocomposites and find perspective areas of their application.

The work objective is to develop the algorithms and methods for modeling the processes of precipitation of nanosized films onto the templates of porous aluminum oxide and to study the kinetics of the foregoing processes and structure of nanosized films with the help of mathematical modeling methods. An important task was to study the possibility of controlling the growth processes of nanofilms and nanostructures on porous substrates. The regulation of growth mechanisms makes it possible to control the obtaining of the required material and to form the target parameters of the nanocomposite.

# 2 Theoretical basis and statement of the problem

The problem of precipitating nanofilms onto porous templates of aluminum oxide was solved by molecular dynamics method [14]. The molecular dynamics method has been widely used when modeling the behavior of nanosystems due to the simplicity of implementation, satisfactory accuracy and low costs of computational resources. The solution of Newton's differential equation of motion for each particle forms the basis of this method.

The problem of deposition of nanofilms on porous substrates was solved using various interaction potentials. The most proven potential fields were the modified embedded atom method and the molecular potential with the use of individual contributions to energy in the form of bonded, angular and other interactions. More detailed theoretical foundations are set forth in previously published papers [15, 16]. In addition, the obtained results were the development of earlier studies in adjacent areas where the properties of nanoparticles, nanosized aerosol systems and nanocomposites were examined [17-19].

Software package for parallel computational processes LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is applied to conduct theoretical research. LAMMPS has been developed by the group of Sandia National Laboratories and is free software for mathematical models of different levels, including classical molecular dynamics [20].

The problem of modeling the formation of nanofilm coatings was solved in several steps. At the first stage, the template from amorphous

aluminum oxide was formed. Aluminum and oxygen atoms are put into the computational cell in the required proportion (2:3) with periodic boundary conditions on each side. The template stabilizes and comes to rest under the action of potential forces under normal thermodynamic conditions. At the same time, heat fluctuations and diffusion are present in the range of the set temperature in the template formed, but there is no essential reconstruction of its structure, the atoms slightly oscillate near the positions they occupy. The hole is cut in the template at the second stage – the pore with the required radius and depth. Later this pore will be silted with atoms of different types. The general pattern of the problem of forming heterogeneous electro-optical coatings is given in Fig. 1.

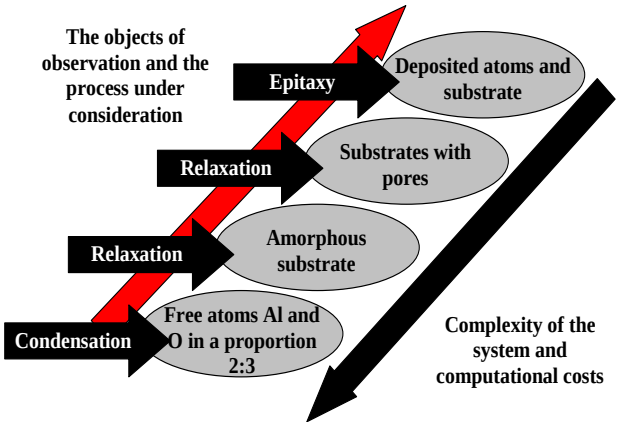


Fig. 1. Steps of solving the problem of forming nanofilm coatings based on porous aluminum oxide

The boundary conditions and appearance of the system being modeled are demonstrated in Fig. 2. Due to the periodic boundary conditions in the directions x and y, only one pore was considered in this work. In horizontal directions the periodic boundary conditions envisage the parallel transfer of the computational cell. The system being modeled was affected by rigid boundary conditions from the top and bottom. When the atoms were approaching the upper boundary of the system investigated, their bounce from the rigid wall was imitated. The positions of atoms in the thin layer near the boundary of the computational cell were rigidly fixed from the bottom. This type of boundary conditions did not allow the nanosystem atoms to leave the computational area in case of deviation from the main precipitation trajectory.

The convergence of numerical solution of the problem set frequently depends on the selection of the corresponding integration step. The step needs to be small enough to correctly reflect the system behavior. When using the methods of molecular dynamics, the value of the mass of substances being modeled influence the integration step value. It is selected in the range from 0.5 up to 2 fsec. In this work the integration step by time is 1 fsec.

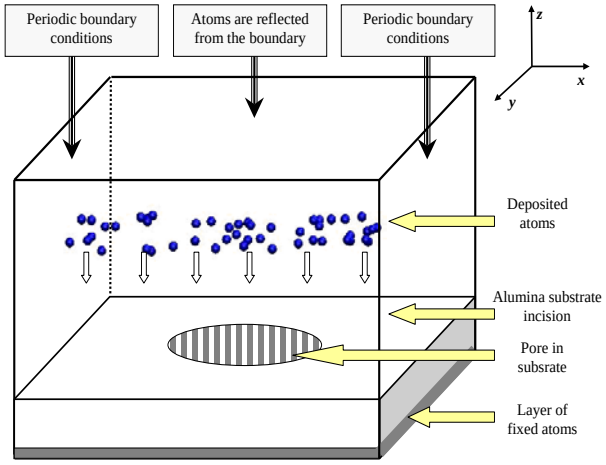


Fig. 2. Boundary conditions and appearance of the system being modeled

The porous template was silted by homogenous precipitation of atoms along the normal against the template. The atoms being precipitated were added in the region above the template during the siltation stage. Their position above the template was determined by the uniform random distribution law. The number of atoms added in a time unit and their total number were the process control parameters. The initial velocity of the precipitated atoms was constant. The velocity parameters were changed only under the interaction of the precipitated atoms with the template. To conduct the test calculations, the single nanostructure was considered in the air-free atmosphere and its dynamics during the relaxation self-organization of atoms.

## 4 Results of simulation and discussions

In continuation of the investigations of nanofilm formation on porous templates, the deposition of molecular zinc sulfide (ZnS) was considered in this work. In multi-particle potentials, such as Abel-Tersoff, Stillinger-Weber, embedded atom method, the bond formation and breakage occur due to the principles of force field performance. Nevertheless, for multi-particle potentials rather large number of empirical parameters is required. Especially for alloys and complex compounds it is necessary to obtain additional characteristics of force fields, adapting the action of energy fields for multi-molecular nanostructures.

Nanofilms based on ZnS are actively used in optical systems of IR band. For industrial purposes zinc sulfide is produced by chemical deposition from zinc gases and vapors onto the template. ZnS is not always applied in the pure state, the material is frequently added to admixtures and additives. The introduction of silver admixture into the composition results in the luminescence in the blue light region. The addition of copper as an alloying metal allows using the luminescence of green color, which is applied in display boards, panels, luminophores, oscillograph tubes.

When investigating luminophore properties, the luminescence brightness is usually the determining parameter. However, to find out main physical mechanisms underlying luminescence, it is necessary to investigate both spectral and kinetic characteristics of electroluminophors that confirms again the importance of theoretical studies of processes of nanofilm deposition onto porous templates.

In order to obtain realistic results maximally fitting the experimental data, the sizes of the modeling region were significantly increased. The amorphous aluminum oxide templates with the following dimensions: length – 19.1 nm, width 19.1 nm, height – 11.6 nm were used in the modeling process. The total number of atoms in the template after the pore formation was about 122 thousands. Before the precipitation process the template was at rest, at the beginning its temperature was 293 K and it was further maintained at the same level. The pore with the radius of 5 nm and 10 nm deep was cut in aluminum oxide template. The lower template layer was fixed to avoid its vertical movement at the precipitation stage. The rest of the atoms were not fixed and could freely move in any direction.

The number of precipitated ZnS molecules was 200,000. The proportion of alloying elements increased in proportion to its composition increased the percentage of epitaxial atoms. The precipitation was uniform along the whole template surface and with the same intensity in time. The atom velocity at epitaxy was 0.05 nm/psec.

The evaporation process of nanofilms from pure zinc sulfide is demonstrated in Fig. 3. The duration of the complete deposition stage was 0.6 nsec. Analysis of the graphical results indicates that a pore is gradually buried with nanofilm. Initially, the neck starts forming on the sides above the hole (Fig. 3 a), which is gradually covered later on. Zinc sulfide molecules partially get into the pore, but its complete dense filling does not occur (Fig. 3 b and c). Nevertheless, practically all internal surface of the porous hole appears to be covered with ZnS molecules by the deposition stage completion. The gradual pore filling results in the emergence of rounded overgrowths above the pore region.

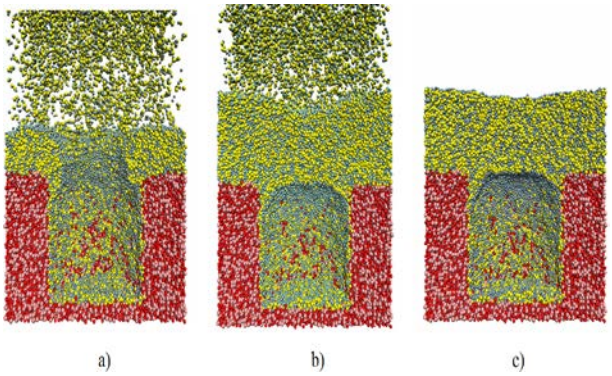


Fig. 3. Result of burying the porous template of aluminum oxide with zinc sulfide for the deposition time: a) 0.2 nsec, b) 0.4 nsec and c) 0.6 nsec

In general, the surface of ZnS nanofilm formed is rather even with slight flash above the pore region. The formation of molecular agglomerates above the template during epitaxy is not registered, therefore, the resultant film does not have considerable relief changes in the surface. The nanofilm intensity growth was even. The resultant thickness of the nanofilm formed for pure zinc sulfide was 6.6-6.8 nm.

To investigate the possibility of controlling the processes of deposition and formation of nanofilms and burying of porous templates, the angle to the normal line of the porous template in which the epitaxial atoms and molecules move to the deposition surface was selected as one of the modeling control parameters.

The percentage of atoms in the pore relative to the total number of particles being deposited for different time moments of the condensation stage and nanofilm growth and different angles relative to the normal line of epitaxy direction is given in Fig. 4. The graph analysis demonstrates that the deposition process only slightly depends on the angle, at which the atoms are evaporated, and it is practically identical in time. Slight deviations of the atom share in the pore are observed at the time moments of 200-400 psec, when the active rearrangement of the internal structure of nanofilms and nanoformations in the pore takes place. Afterwards, the dependencies under consideration are stabilized and reach the stationary regime. The stationary behavior of the atom percentage in the pore relative to the total amount of the particles being deposited (time moments of 450-600 psec) still has a slight difference for different deposition

angles. The deviation from the normal line to the template surface results in slight increase in the area onto which the atoms are deposited that is explicitly confirmed in the graph considered. The deposition angles for all graphs are given in degrees.

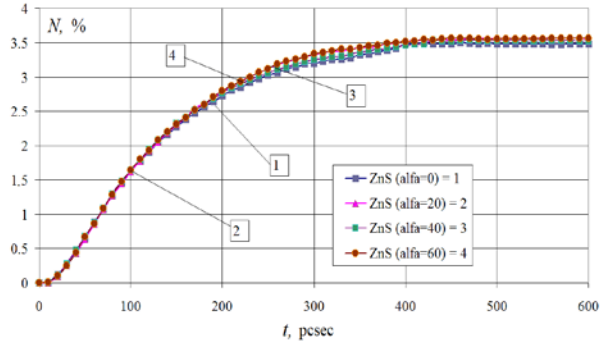


Fig 4. Percentage of atoms in the pore relative to the total number of particles being deposited for different deposition angle

Similar behavior is observed for the position of mass center of nanostructure being formed inside the pore shown in Fig. 5. As we can see from the behavior of the graphs in Fig. 5, the change in the height of mass center of the deposited atoms and molecules inside the pore also only slightly depends on the deposition angle.

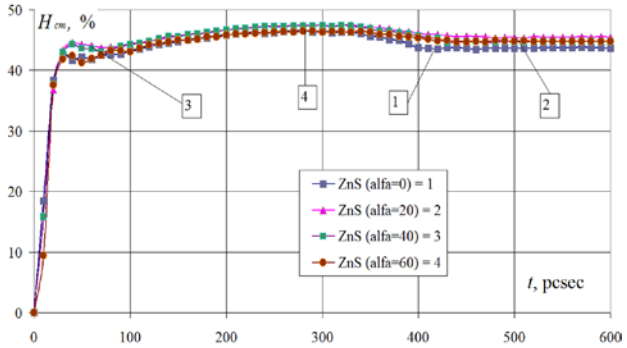


Fig. 5. Relative depth of the mass center of nanoformations in the pore for different deposition angle

Slight deviations in the behavior of dependencies occur for the time moment of 30 psec of the condensation stage. The height of nanostructures for the deposition angles of 20 and 40 degrees is a bit lower. After the time moment of 400 psec the situation changes and the mass center for the epitaxy angle of 0 degrees has the least height. Thus, for the case of deposition along the normal line to the template surface the mass center of atoms and molecules inside the pore is the lowest. Nevertheless, the deviations between the graphs in Fig. 5 are slight and do not exceed 5 %.

To continue with the analysis, the thickness of the nanofilm being formed above the template surface was considered. The computational algorithm of the nanofilm thickness considers its layer-by-layer structure at each time moment. The numeration of layers starts from the template surface and increases at the distance from it. The thickness of layers in the algorithm can vary, but it should depend on the crystalline structure type of the material being formed and lattice parameters, in particular, distances to the nearest neighbors. In the prevailing majority of cases, the thickness of the nanofilm intermediary layers of 0.2-0.3 nm provides the satisfactory accuracy of calculations. For each layer, starting from the first, the number of particles in the layer and atomic density are calculated. These values are compared with similar values on the previous layer. If the spatial layers become much rarer, the computational process stops. The nanofilm final thickness will comprise all layers previously considered. The level of atomic density is a variable algorithmic value, the value of 50 % was used in this work.

The nanofilm thickness growth on the template surface for different deposition angles is presented in Fig. 6. For the initial time moments (0-400 psec) practically linear growth of the nanofilm thickness is characteristic. At the time moments of 400-600 psec the deposited atoms and molecules are compacted and the internal structure is rearranged, so, the film average thickness slightly decreases.

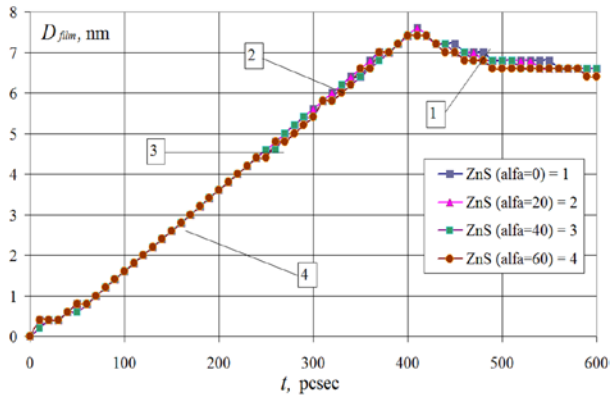


Fig 6. Nanofilm average thickness on the template surface for different deposition angles

The material sintering is the next possibility to control the processes of nanofilm formation and burying of porous templates. Sintering is carried out in relation to the already dusted film and is aimed at denser filling of the pore with deposited atoms. From the point of modeling, sintering is a short-duration heating of material. Due to the temperature elevation, atoms and molecules start moving more

actively and the migration of particles and filling of free spaces in the internal structure can take place.

To investigate the mechanisms of nanofilm sintering on porous templates of aluminum oxide, the coatings of molecular zinc sulfide from the previous series of computational experiments, already evaporated, were considered. The total duration of the heating period of the substrate-nanofilm nanosystem was 200 ps. The temperature in the modeling area was maintained using a Noze-Hoover thermostat. The dimensional parameters of the alumina substrate and the pore, which cut into it, remain unchanged, as in the previous series of calculations.

To compare the results and coverage of several potential development scenarios, the nanosystem at the warm-up phase was simulated at the temperatures 293 K, 493 K and 593 K. The temperature 293 K is normal. The nanosystem is at this temperature at the initial time of the heating stage and it is given to compare the various obtained data. As expected, at normal temperature the system is calm, there are no significant driving forces, no significant potential differences between structural nanoelements and atoms.

Visually, atoms, nanofilms and other composite nanostructural objects in the system behave identically for all considered temperatures (293 K, 493 K and 593 K). There no major modifications in the nanofilms and the substrate, the pore inside the substrate is not denser filled. The obtained results are confirmed by numerical data and graphically. Figure 7 presents the percentage of atoms in the pore relative to the total number of deposited particles for different heating temperatures of the nanosystem.

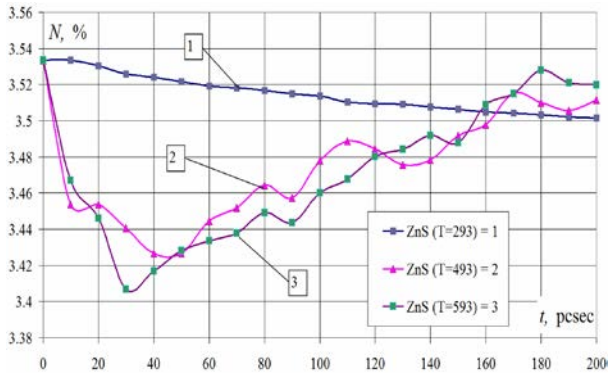


Fig 7. The percentage of atoms in the pore relative to the total number deposited particles for different heating temperatures of the nanosystem

Analysis of the graphs shows that the functional dependencies in Figure 7 differ insignificantly and vary slightly. In contrast to the expected results, there no the additional pore overgrowth when the temperature rises. Noticeable is the restructuring of the internal organization and structure of atoms and molecules, which are in the aperture of the substrate. At the initial moments of time, the percentage of atoms in the pore decreases, and then gradually increases. For the case of the normal temperature of the nanosystem, the restructuring of the atomic-molecular structure is minimized and practically linear in time.

The relative depth of the center of mass of the nano-formations in the pore for different heating temperatures of the nanosystem is shown in Fig. 8. The behavior of the constructed dependencies co-correlates with the distribution of the percentages of atoms in the pore relative to the total number of deposited particles shown in Fig. 7. The mass center of the nanostructures inside the pore changes insignificantly during heating. Initially, the atoms and molecules that filled the pore begin to move upward to the surface of the substrate and the formed nanofilm. At subsequent times, the position of the center of mass is corrected and tends to the initial state. It should be noted that the general dynamics and fluctuations of the quantities in Fig. 7 and Fig. 8 are insignificant. The most stable behavior of the center of mass is observed for a non-heated nano system, that is, for a temperature of 293 K.

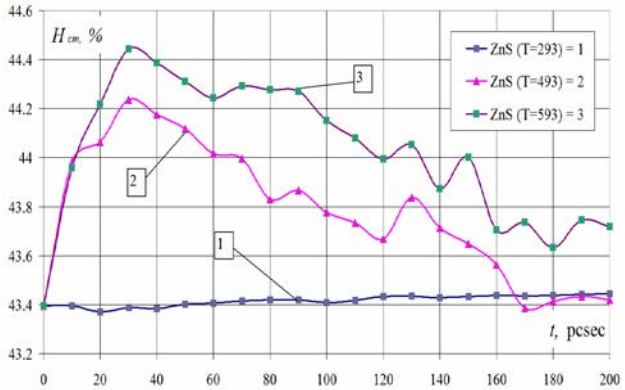


Fig 8. Relative “depth” of the center of mass of nanostructures in a pore for different heating temperatures of a nanosystem

In addition to the analysis of nano-formations within the pore for the heating stage, the behavior of the formed nanofilm from zinc sulfide was considered. The average thickness of the nanofilms on the surface of the substrate for different heating temperatures of the nanosystem is shown in Figure 9.

By the results of the constructed dependences of the film thickness on the temperature, it can be

asserted that heating the nanosystem to the chosen temperatures does not lead to a restructuring of the nanofilm. The thickness of the nanocoating does not increase or decrease in this case.

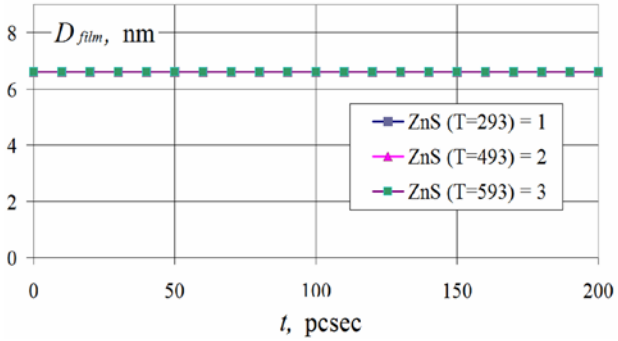


Fig 9. The average thickness of the nanofilm on the substrate surface for different heating temperatures of the nanosystem

Investigations of the possibility of controlling the growth processes of nanofilms, overgrowing porous substrates, and the formation of nanostructured coatings have shown that the epitaxial deposition angles and heating of the nanosystem to temperatures of 293-593 K do not lead to a significant change in the formation of nanostructures. At the same time, there is a slight restructuring of the structure and internal organization of nanoelements, but there are no certain filling of the pores and changes in the properties of the nanofilms.

## 5 Conclusion

The results of modeling the processes of precipitation of pure molecular sulphide of zinc and with the addition of additives in the form of copper atoms and manganese sulphide molecules have shown that the addition of uniformly distributed alloying elements to the nanofilms does not significantly affect the process of pore contraction. The process of incubation proceeds with partial filling of the cavity in the substrate. The growth of the nanofilm proceeds evenly, without sudden jumps and shifts.

When adding alloying elements, there are no visual changes in the growth processes, there is an insignificant deviation of functional dependencies within the limits of not more than 0.3%. The introduction of additives leads to an increase in the number of deposited atoms and a regular increase in the thickness of nanostructured coatings of substrates. The highest nanofilms were detected in the cases of 10% alloying additives, which led to the appearance of an additional 0.2-0.6 nm layer-by-layer deposition.

Investigations into the possibility of controlling the growth processes of nanofilms, overgrowing porous substrates, and the formation of nanostructured coatings have shown that the epitaxial deposition angles and heating of the nanosystem to temperatures of 293-593 K do not lead to a significant change in the formation of nano-formations. At the same time, there is a slight restructuring of the structure and internal organization of nanoelements, but there is no certain filling of the pores and changes in the properties of the nanofilms.

Right now, the modeling results are used for developing and optimizing of technological processes of optic coating formation.

To get acquainted with the detailed information about the theoretical and experimental studies of the authors, with modeling methods and experimental devices for filling processes of nanopores into templates aluminum oxide by atoms of various materials we recommend to the interested reader a new book of the authors [21].

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*References:*

[1] J.Y. Ying, Nanoporous Systems and Templates the Unique Self-Assembly and Synthesis of Nanostructures, *Science Spectra*, Vol. 18, 1999, pp. 56–63.

[2] A.P. Li, F. Muller, A. Birner, K. Nielsch, and U. Gosele, Hexagonal Pore Arrays with a 50-420 nm Interpore Distance Formed by Self-Organization in Anodic Alumina, *Journal of Applied Physics*, Vol. 84, NO. 11, 1998, pp. 6023–6026.

[3] C. Mu, Y. Yu, W. Liao, X. Zhao, D. Xu, X. Chen, and D. Yu, Controlling Growth and Field Emission Properties of Silicon Nanotube Arrays by Multistep Template Replication and Chemical Vapor Deposition, *Appl. Phys. Lett.*, Vol. 87, NO. 11, 2005, pp. 1–3.

[4] A.E. Nikolaev, Yu.V. Melnik, N.I. Kuznetsov, A.M. Strelchuk, A.P.Kovarsky, K.V. Vassilevski, and V.A. Dmitriev, GaN pn-Structures Grown by Hydride Vapor Phase Epitaxy, *Mat. Res. Soc. Symp. Proc.*, Vol. 482, 1998, pp. 251–256.

[5] H.J. Xu, and X.J. Li, Structure and Photoluminescent Properties of a ZnS/Si Nanoheterostructures Based on a Silicon Nanoporous Pillar Array, *Semicond. Sci. Technol.*, Vol. 24, Issue 7, 2009, p. 075008.

[6] H. Masuda, *Highly Ordered Nanohole Arrays in Anodic Porous Alumina. Chapter in book: Ordered Porous Nanostructures and Applications. Part of the Series Nanostructure Science and Technology*. US: Springer. 2005, pp. 37–55.

[7] D. Lysenkov, J. Engstler, A. Dangwal, A. Popp, G. Muller, J.J. Schneider, V.M. Janardhanan, O. Deutschmann, P. Strauch, V. Ebert, and J. Wolfrum, Nonaligned Carbon Nanotubes Anchored on Porous Alumina: Formation, Process Modeling, Gas-Phase Analysis, and Field-Emission Properties, *Small*, Vol. 3, Issue 6, 2007, pp. 974–85.

[8] C. Toccafondi, R.P. Zaccaria, S. Dante, and M. Salerno, Fabrication of Gold-Coated Ultra-Thin Anodic Porous Alumina Substrates for Augmented SERS, *Materials*, Vol. 9, Issue 6, 2016, pp. 403.1–403.12.

[9] W. Zaghdoudi, M. Gaidi, and R. Chtourou, Microstructural and Optical Properties of Porous Alumina Elaborated on Glass Substrate, *Journal of Materials Engineering and Performance*, Vol. 22, Issue 3, 2013, pp 869–874.

[10] H.N.G. Wadley, X. Zhou, R.A. Johnson, and M. Neurock, Mechanisms, Models and Methods of Vapor Deposition, *Prog. Mater. Sci.*, Vol. 46, Issue 3–4, 2001, pp. 329–377.

[11] H. Song, O.J. Ilegbusi, and L.I. Trakhtenberg, Modeling Vapor Deposition of Metal / Semiconductor-Polymer Nanocomposite, *Thin Solid Films*, Vol. 476, Issue 1, 2005, pp. 190–195.

[12] L. Bruschi, G. Mistura, P.T.M. Nguyen, D.D. Do, D. Nicholson, S.J. Parkd, and W. Lee, Adsorption in Alumina Pores Open at One and at Both Ends, *Nanoscale*, Issue 7, 2015, pp. 2587–2596.

[13] O. Amsellem, F. Borit, D. Jeulin, V. Guipont, M. Jeandin, E. Boller, and F. Pauchet, Three-Dimensional Simulation of Porosity in Plasma-Sprayed Alumina Using Microtomography and Electrochemical Impedance Spectrometry for Finite Element Modeling of Properties, *Journal of Thermal Spray Technology*, Vol. 21, Issue 2, 2012, pp. 193–201.

[14] J.E. Lennard-Jones, On the Determination of Molecular Fields. II. From the Equation of State of a Gas, *Proc. Roy. Soc. A*, Vol. 106, 1924, pp. 463–477.

[15] A.V. Vakhrushev, A.Yu. Fedotov, A.V. Severyukhin, and R.G. Valeev, On the Structure and Properties of Nanofilms Deposited on Porous Aluminum Oxide Substrates, *Nanoscience and Technology: An International Journal*, Vol. 8, Issue 3, 2017, pp. 167–192.

[16] A.V. Vakhrushev, A.Yu. Fedotov, A.V. Severyukhin, and R.G. Valeev, Influence of Pore Size Parameters on the Mechanisms of Formation of Nanofilms Coatings on Porous Alumina Substrates, *Bulletin of the South Ural State University. Series Mathematical Modeling and Programming*, Vol. 10, Issue 2, 2017, pp. 83–97.

[17] A.V. Vakhrushev, R.G. Valeev, A.Yu. Fedotov, and A.V. Severyukhin, "Control of nanosensors forming on base of aluminum template", Proceeding of the 3rd International Workshop on Dynamics and Control of Advanced Structures and Machines, Perm, Russia, 18-22 September 2017, Springer, 2019, pp. 185-192

[18] A.V. Vakhrushev, A.Yu. Fedotov, A.A. Vakhrushev, V.B. Golubchikov, and A.V. Givotkov, Multilevel Simulation of the Processes of Nanoaerosol Formation. Part 2. Numerical Investigation of the Processes of Nanoaerosol Formation for Suppression of Fires, *International Journal of Nanomechanics Science and Technology*, Vol. 2, Issue 3, 2011, pp. 205–216.

[19] Vakhrushev A.V. Computational Multiscale Modeling of Multiphase Nanosystems. Theory and Applications. Waretown, New Jersey, USA: Apple Academic Press, 2017-402p.

[20] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, *Journal of Computational Physics*, Vol. 117, Issue 1, 1995, pp. 1–19.

[21] Valeev R.G., Vakhrushev A.V., Fedotov A.Yu., Petukhov D.I. Functional Semiconductor Nanostructures in Porous Anodic Alumina Matrices: Modeling, Synthesis, Properties, *Apple Academic Press, Waretown, USA:* 2019 September (ISBN: 9781771887700) - in print