

Physical-Technical Institute









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Multi-level modeling of the functional nanostructures Vakhrushev Alexander



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Outline:

Introduction Problems statement and modeling technique

Nanotechnological Processes Calculation results and analyses (A brief overview of the results of modeling)

> Future trends Conclusions Acknowledgment

Introduction

TYPES OF THE FUNCTIONAL NANOSTRUCTURES

Condensed (nanopowder and nanostructural materials, nanocomposites, nanomechanisms, nanodevices ...) **Gaseous and liquid** (currents in nanochannels, in the closed nanovolumes Multiphase (complex), Self-organizing Controlled









The Main Stages of the Nanotechnological Processes Development

Multilevel and Multiphysical Modeling

Formation of Nanostructures

Investigation of Structures and Properties of Nanostructures



Why the mathematical modeling is so useful for manufacture?

- **1.** Reduction of time to prepare for the production
- 2. Acceleration of technological processes is several times(10 times)
- **3.** Automation of technological processes
- 4. **Reducing the cost of production (2-3 times)**
- 5. Improving the quality of materials and products
- 6. Improving ecology

Problem's statement and modeling technique



Methods of modeling

Problems statement and modeling technique



The main methods of modeling and indicates their state ofthe-art capabilities regarding time, space and the number of calculated atoms.

The main goals of multiscale modelling

1. Formation of nanoelements (the form, structure and properties depend on size of nanoelements).

2. Interaction of separate elements of nanosystem (static and dynamics interaction with and without loading).

3. Definition of structure of isolated nanosystem in static and dynamic conditions.

4. Calculation of nanosystem parameters at interaction with an environment.

5. Calculation of macroparameters of nanosystem.

6. Determination of parameters technological processes for making nanostructures and conditions of use. Identification of ranges of external parameters and process parameters that provide the creation and existence of nanosystems.

7. Control and optimization of the processes of formation of nanosystems.

The main problems of multiscale modeling

- 1. Multiscale nature and connectedness of problems.
- 2. Large number of variables.
- **3.** Variation of scales both over space and in time. Characteristic times of processes at different scales differ by orders of magnitude.
- 4. Variations of the problems change at different scales of modeling.
- 5. Matching of boundary conditions at the transition from one modeling scale to another.
- 6. Stochastic behavior of nanoscale systems.
- 7. The instability of nanoscale systems.

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Classification of quantum-mechanical methods for modeling and investigating properties of nanosystems.

Fedotov, A.; Vakhrushev, A.; Severyukhina, O.; Sidorenko, A.; Savva, Y.; Klenov, N; Soloviev, I. Theoretical Basis of Quantum- Mechanical Modeling of Functional Nanostructures. *Symmetry 2021, 13, 883. https://doi.org/10.3390/ sym13050883* Modeling of Nanotechnological Processes The calculation results and analyses



Formation of nanowhiskers



- 1. Thin layer of the active catalyst (Au) on a surface of a silicon substrate is rendered.
- 2. System is warmed up to temperature above a point at which formation of drops of the catalyst is possible.
- **3.** "Bombardment" of drops of the catalyst by atoms of silicon (Si) is carried out.
- 4. There is a formation of nanowhiskers under drops of gold.



International Journal of Nanomechanics Science and Technology. 2012. T. 3. Nº 3. C. 193-209.





Change of structures of nanowhiskers



Diffusion of gold from a drop into nanowhisker

Silicon nanoedge generated during modelling (in a right corner – in practice)



Comparison of the results of simulation with the model proposed by Schubert et al. (2004)

SIMULATION OF THE PROCESSES OF FORMATION OF QUANTUM DOTS ON THE BASIS OF SILICIDES OF TRANSITION METALS





Chemical bonds

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Changing of the number of bonds in various amounts of deposited chromium.



Comparison of results of modelling with experimental data (Galkin N.G.)



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Self made experimental setup



ZnS:Cu(Mn) deposition in high (10⁻⁵ Pa) vacuum



 1 – MBE type evaporators,
2 – evaporators cooling system,
3 – deposition chamber,
4 – window,
5 – ion pump,
6 – substrate holder rotator,

Samples classification

S_D_M S – substrate (AAO1, AAO2, glass1) D – AAO matrix pores diameters (nm) M – impurity type (Cu, Mn)





Steps of solving the problem of forming nanofilm coatings based on porous aluminum oxide: a) initial state of the system; b) template relaxation without the pore; c) template relaxation with the pore; d) precipitation



Boundary conditions and appearance of the system being modeled



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

Nanofilm formation from silver atoms



Results of silver atom precipitation onto the template of porous aluminum oxide

Horizontal section of nanofilm coating surface after the precipitation of silver atoms along the template surface



Siltation of the template of porous aluminum oxide with palladium atoms: a) top view, b) vertical section along the pore center, precipitation time – 0.2 nsec



The dependence of the potential and total energy of the deposited atoms on the condensation stage



Siltation of the template of porous aluminum oxide with iron atoms: top view

Simulation of Multilayer Nanosystems Interface Formation Process for Spintronics

Molecular dynamics modeling of the influence forming process parameters on the structure and morphology of a superconducting spin valve Alexander Vakhrushev, Aleksey Fedotov, Vladimir Boian, Roman Morari and Anatolie Sidorenko Beilstein J. Nanotechnol. 2020, 11, 1776–1788. https://doi.org/10.3762/bjnano.11.160 The development of nanotechnology has led to the emergence of a special section of quantum electronics - spintronics. Systems in spintronics are based on <u>multilayer nanosystems</u> consisting of ferromagnets, superconductors, and normal metals.







Real multilayer nanosystems formed from various materials. The structure of real nanosystems is far from ideal:

- 1. The surface separating the various nanolayers of the system is not perfectly flat (the surface has noticeable irregularities that are directed towards the contacting layers);
- 2. Mutual penetration of atoms of one contacting layer into another is observed (the interface of the layers has a certain (not zero) thickness);
- 3. The atomic structure of each layer does not form an ideal one-piece nanocrystal (a system is formed that combines nanocrystals).





Scheme of the multilayer nanosystems formation modeling processes. The nanosystem contains a material evaporation zone, atoms deposition area, a substrate with a fixed lower layer of atoms. During the first nanofilm formation, the deposition is carried out directly onto the substrate; for the subsequent ones, onto the substrate with previously formed nanofilms.



Figure 5: Multilayer nanosystem of niobium and cobalt. The

contact points of the nanofilms are indicated by (b) and (c). At the indicated contact points, the distribution of coordination numbers is given in Figure 6. The substrate temperature was fixed at 300 K.



Figure 6: Change in coordination (CN) number along the *z*-axis (shown in Figure 5) in Nb and Co layers of the nanostructure. The contact points of the nanofilms are shown by the dashed vertical lines. The distribution is plotted for substrate deposition at 300, 500, and 800 K.





Future trends

Approximation in size of nanosystem, process time and technological parameter





The dependence of relative Young's modulus on the relative radius for nanoparticles from different materials: 1 – cesium, 2 – calcium, 3 – zinc and 4 – magnesium



Changing the number the 0 nanoparticles formed from 3component metal mixture in а calculating cell during the condensation phase





The weight content of nanoparticle on current density

Conclusion

- 1. Application of multilevel modelling for research of nanosystems is the powerful tool for the analysis, designing and development of technology of their creation.
- 2. Machine learning can efficiently combine calculations at separate structural levels using the method of exact multilevel modeling, and also combine the results of experiments and theoretical calculations into a single block of data necessary for training a neural network.
- 3. High accuracy of exact multilevel mathematical modeling combined with significant acceleration of machine learning modeling is a prerequisite for successfully solving the problems of designing new nanomaterials for the modern industrial revolution "Production 4.0".

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