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DEVELOPMENT OF A MATHEMATICAL MODEL OF WAVE PROCESSES IN MULTILAYERED STRUCTURES WITH AN ADAPTIVE ALGORITHM AND HYBRID CALCULATIONS

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Abstract. The paper investigates the numerical simulation of wave processes in multilayer thin films, which is relevant for understanding their physical properties and optimization for various applications. An integrated mathematical model has been developed that combines Maxwell's equations, mechanical vibrations and thermal conductivity, taking into account the interaction of physical fields in structures with defects. Adaptive algorithms have been proposed for automatic mesh refinement depending on local gradients of physical parameters, which allows to increase the accuracy of modeling in critical zones. A hybrid approach to calculations using CPU and GPU has been implemented, which ensures efficient use of resources for large-scale problems. Software with a modular architecture has been developed that allows integrating numerical methods, optimization and visualization of results in real time. Experimental validation has confirmed the high accuracy and reliability of the model. The results obtained contribute to a deeper understanding of physical processes in thin films and are the basis for the creation of highly efficient multilayer structures in industrial and scientific applications.

Keywords: thin films, numerical simulation, optimization, multiphysics models, parallel computing, hybrid algorithms, wave processes.

INTRODUCTION

Modern technologies for modeling multilayer structures are an important tool for researching and optimizing the physicochemical properties of materials. Numerical modeling of such systems allows for a detailed analysis of complex wave processes, encompassing electromagnetic, acoustic, and thermal phenomena. Accounting for the interaction of these processes in multilayer films is particularly relevant for industry, where the priority is creating materials with specified properties, such as high-efficiency optical filters, acoustic resonators, and thermoelectric devices. Most existing approaches focus on highly specialized aspects of modeling [1] or optimization. The integration of multiphysical models, dynamic mesh optimization, the use of hybrid computing environments, and the introduction of neural networks into the numerical modeling process open new opportunities in the analysis of multilayer structures that have not yet been achieved in a comprehensive manner. This provides scientific novelty of the work, since such methods have not yet been implemented in conjunction, which allows solving more complex and large-scale problems with high accuracy and productivity.

The relevance of the research lies in the necessity to enhance the accuracy of numerical modeling of multiphysical processes. Integration of electromagnetic, acoustic and thermal phenomena within a single model allows for a better understanding of the influence of physical parameters on the structure and functionality of films. Such models contribute to reducing experimental costs and accelerating the development of innovative technologies. The primary objective is to create a model capable of accounting for the interaction of wave processes in real-time. This includes the description of the electromagnetic field according to Maxwell's equations, acoustic waves through mechanical vibrations, and thermal processes based on the heat conduction equation. Prospects for implementing the research results include creating new technologies for the synthesis of thin films with specified characteristics, predicting their behavior under various conditions, as well as the integration of the developed models into modern information systems for research in materials science and engineering.

LITERATURE ANALYSIS AND PROBLEM STATEMENT

Numerical modeling encompasses a wide range of multiscale methods, such as a combination of transfer matrix, finite element, and molecular dynamics methods, which allow for a more precise description of the physical and mechanical properties of multilayer materials [1–4]. Numerous studies have improved the efficiency of modeling the electrical conductivity of polymer composites, in particular using carbon nanotubes and carbon fibers, which allows for the optimization of their electrical characteristics [5, 6]. In addition, improving the thermal insulation and mechanical properties of multilayer materials, in particular vapor-cooled insulating materials and polymer composites, continues to be a relevant research area [7–9]. The study of multilayer electronic structures, such as graphene, also allows for a better understanding of their electronic behavior, including the dependence of the interlayer distance and the effect of pressure on the electronic properties [10]. The proposed methods and models significantly improve the accuracy of predicting material properties, but there are still open questions regarding the adaptation of these models to complex nanostructures, the accuracy of predicting experimental parameters, and the integration of multiphysical approaches for more comprehensive modeling.

Modern approaches to numerical modeling include simulation multi-level helical structures for coal machines [11], assessment of the safety of rocket missions using multilayer models [12], and analysis of microfluidic systems for biomedical applications [13]. The proposed methods allow to significantly reduce modeling errors, increase prediction accuracy, and optimize calculations, which is critical for achieving high results in these industries. Furthermore, research in the digitalization of business models [14] and modeling of thin-film solar cells based on $ZnO/CdS/CuInGaSe_2$ [15] demonstrate the importance of multilayer models for assessing the efficiency of technologies in various fields, from business to energy. Despite the successes achieved, issues related to the adaptation of models for complex multifunctional structures and the integration of multiphysical approaches remain open, particularly in the context of the accuracy of predicting experimental parameters and verifying models in practice.

Along with this, considerable interest is aroused by studies of the spectral characteristics of plasma discharges [16, 17], which revealed the mechanisms of formation of excited plasma components that affect the formation of nanostructured films. It has been shown that the parameters of the electric field and plasma composition determine the features of the energy distribution and affect the morphology of the deposited films. However, questions remain open regarding the precise control of the composition of film-forming particles and the influence of local plasma inhomogeneities on the uniformity of the coating. Works dedicated to the influence of the electrode material and discharge conditions on the structure of films [18, 19, 21] demonstrate the dependence of phase composition and electrophysical properties of films on the chemical composition of the electrodes, temperature and gaseous environment. Material transfer process during laser ablation and under high-voltage discharge conditions have been investigated. Nonetheless, the mechanisms of interaction of plasma particles with the substrate and the role of impurities in the stability of film formation require further study. Some studies [20, 21] focus on the electrophysical properties of deposited films and their potential applications in sensor and energy devices. It has been established that the gas-discharge deposition method allows obtaining materials with high conductivity and controlled structural characteristics. However, the long-term stability of films and their adaptation to real operating conditions remain relevant issues.

Another promising research direction is the development of efficient lithium-ion batteries (LIBs), which are cutting-edge energy devices due to their environmental friendliness, low self-discharge and long life cycle [22–24]. Accurate determination of the state of charge (SOC) in real conditions is a difficult task due to the nonlinear characteristics of LIBs, therefore, the study of SOC estimation methods is highly relevant and has been studied in a significant number of scientific works. Currently, various methods for SOC estimation are being actively developed, which are based on models [25]. Models are widely used due to the optimal balance between computational complexity and accuracy [26]. They include three stages: model construction, parameter identification, and state estimation. Electrochemical models, while considering the internal structure of the battery, have excessively high computational complexity for practical application [27]. At the same time, equivalent circuit models (ECMs) reflect the internal parameters of the battery through external components, which makes them an effective and widely used solution. Current research on SOC estimation of lithium-ion batteries focuses on improving the accuracy, adaptability, and computational efficiency of the methods, which is reflected in the works [28–30], which consider approaches based on adaptive Kalman filters. It should be noted that when modeling lithium-ion batteries, mathematical models can be used to predict their behavior, considering various processes, such as thermal or electrical. Adaptive algorithms and hybrid computing can be used to optimize these models, which is typical for both wave process modeling and battery efficiency research.

The literature review demonstrated a wide range of directions for the use of multilayer structures and showed significant progress in the development of models for the study of thin films, the synthesis of films based on metallic and polymeric materials, as well as the study of their electrical and mechanical properties. The effectiveness of many approaches, such as finite element methods, multiscale modeling and numerical methods, allowing accurate prediction of the properties of films and their interaction with various substrates and the environment, was noted.

However, several unsolved issues remain. While numerous models have been developed to describe the behavior of thin films, research on their behavior at different scales (molecular, micro- and macro-levels) still requires improvement in the accuracy of models for multilayer structures. The precise modeling of the mechanical properties of thin films under deformation, especially in cases where films are used in complex multilayer structures, remains an open question. There is a need of deeper exploration of the environmental impact (temperature, humidity, chemical reactions) on film characteristics, particularly for their synthesis in various gas environments. Although there are successful developments in the creation of nanostructured films, methods for accurate simulation of the process of their synthesis and behavior at the molecular level remain limited. Integration of new models is required for more accurate prediction of processes in real conditions. More attention should be paid to optimizing the synthesis technologies of films from different materials to improve their efficiency in specific applications (e.g., for electronic or medical devices, solar cells, lithium-ion batteries). Thus, for further development of models, it is necessary to focus on improving the accuracy of multilayer models, developing complex models, automating calculations, studying the mechanical characteristics of thin films, as well as their synthesis and the impact of external factors.

RESEARCH AIMS AND OBJECTIVES

The main aim of the work was to develop an integrated numerical modeling algorithm that accounts for the interaction of wave processes (electromagnetic, acoustic, thermal) in multilayer structures to accurately predict the physical properties of thin films, identify the influence of key parameters on wave processes, as well as validate the obtained results using experimental data.

The research objectives include:

1. Development of a mathematical model to describe wave processes in multilayer films.
2. Implementation of adaptive numerical methods for mesh refinement.
3. Implementation of hybrid computational approaches using CPU and GPU.
4. Analysis of physical phenomena in multilayer structures.
5. Development of software for modeling automation.
6. Experimental validation of modeling results.

These tasks will ensure both scientific novelty and practical value of the research results, in particular for optimizing the processes of creating multilayer films with specified characteristics. *The practical value* of the work lies in the implementation in the form of software for designing multilayer structures, in particular for creating optical filters, acoustic resonators, thermoelectric materials, as well as for diagnosing defects in complex systems.

The object of the research is the processes of numerical modeling of the interaction of electromagnetic, thermal and acoustic fields in multilayer structures using an adaptive grid and parallel calculations.

Research hypothesis: the integration of multiphysical processes within a single numerical approach using an adaptive grid and parallel algorithms will allow to increase the accuracy of predicting the physical properties of multilayer structures, optimize computational costs and improve the correspondence of the model to experimental data.

MATERIALS AND RESEARCH METHODS

For the numerical solution of the aforementioned problems, discretization methods are used, particularly finite difference, element and volume methods, which are selected based on the problem's geometry and accuracy requirements. Typically, multilayer structures are integrated into models using methods such as the *Transfer Matrix Method (TMM)*, which allows for the description of wave processes in systems with multiple layers, and a *multiphysical approach* which accounts for the interaction of electromagnetic, acoustic and thermal processes. One of the key aspects of the work is the optimization of algorithms, which includes adaptive meshes for accuracy in critical areas, parallel computing to reduce calculation time and the use of schemes with high tolerance to errors. Parallel computing is based on the distribution of tasks between several processor cores (CPU) or graphics processing units (GPU), which makes it possible to simultaneously process numerous mesh elements and reduces calculation time. Another important optimization strategy is the use of linear algebra methods to solve large systems of equations, such as iterative methods (conjugate gradient descent) and distributed matrix multiplication methods, which work well in parallel environments. Data preprocessing algorithms are also used to reduce the dimensionality of the problem and reduce the complexity of the models, which allows for faster calculations without losing accuracy. Ultimately, computational optimization ensures the practical suitability of the developed algorithms for industrial applications and their integration into automated thin film analysis systems.

Multiphysical approach to numerical modeling of wave processes. In this work, a *multiphysical approach* was used to integrate a multilayer structure into the model, which considers the interaction of electromagnetic, acoustic, and thermal processes. The main focus was on creating a new algorithm that simultaneously accounts for electromagnetic, acoustic, and thermal wave processes in multilayer structures. This approach considers the interaction of various physical fields, which significantly increases the accuracy of modeling and opens new opportunities for designing materials with specified properties.

Physical basis. Each of the wave processes is described by its own set of equations. *Electromagnetic waves* are modeled by Maxwell's equations, which account for the propagation of an electromagnetic field through a medium with certain dielectric and magnetic properties:

$$\nabla \times \vec{D} = \rho\,,\ \nabla \times \vec{B} = 0\,,\ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial T}\,,\ \nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial T}\,,$$

where $\vec{E}$ – electric field strength vector; $\vec{H}$ – magnetic field strength vector; $\vec{D} = \varepsilon \vec{E}$ – electric induction (ε – dielectric constant); $\vec{B} = \mu \vec{H}$ – magnetic induction (μ – magnetic permeability). At the boundary of the layers, the conditions of continuity of the field components are fulfilled:

$$\vec{E}_{\|,1} = \vec{E}_{\|,2}\,,\ \vec{D}_{\perp,1} = \vec{D}_{\perp,2}\,,\ \vec{H}_{\|,1} = \vec{H}_{\|,2}\,,\ \vec{B}_{\perp,1} = \vec{B}_{\perp,2}\,.$$

Acoustic waves are described by equations of mechanical vibrations that determine changes in pressure and particle velocity in a medium depending on its density and elasticity.

$$\rho \frac{\partial^2 \vec{u}}{\partial t^2} = \nabla \cdot \sigma \, , \; \sigma = \lambda(\nabla \cdot u)\vec{I} + 2\mu\varepsilon \, ,$$

where $\vec{u}$ – vector of movement of particles of the medium; σ – stress tensor; $\varepsilon = \frac{1}{2}(\nabla \vec{u} + \nabla \vec{u}^T)$ – strain tensor; λ and μ – Lamé coefficients characterizing the elasticity of the material.

Thermal processes are based on the heat conduction equation, which models the temperature distribution in layers, considering thermal conductivity, heat capacity, and heat transfer between layers:

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q \, ,$$

where T – temperature; c – heat capacity; k – thermal conductivity coefficient; Q – a heat source (e.g. generated by an electromagnetic field).

Integration of physical models. The developed algorithm combines these equations into a single numerical model by joint solution. Regarding the choice of *common parameters*, the models are linked through material properties, i.e., a change in temperature affects the dielectric constant (for electromagnetic waves) and the speed of sound (for acoustic waves). The connection between the equations is implemented as follows. The electromagnetic field generates heat:

$$Q = \sigma \left| \vec{E} \right|^2 ,$$

where σ – electrical conductivity of the material.

Temperature change affects dielectric constant:

$$\varepsilon(T) = \varepsilon_0 + \alpha T \, ,$$

where α – temperature dependence coefficient.

Thermal expansion affects acoustic properties:

$$\lambda(T)=\lambda_0(1+\beta T), \; \mu(T)=\mu_0(1+\gamma T),$$

where β, γ – coefficients of temperature dependence of mechanical parameters.

To account for *temporal and spatial dependencies*, a unified discretization of time and space is used, ensuring accuracy in considering the interaction between processes. A single grid is implemented for all physical fields with adaptive refinement in areas of large parameter gradients.

As for the *boundary conditions*, they are adaptively adjusted for each layer of the structure depending on the physical properties and type of wave process. That is, the joint boundary conditions account for the transfer of heat, acoustic waves, and changes in the electromagnetic field across the layer boundaries.

Algorithm development. As mentioned above, the algorithm implementation uses a multiphysical approach where all equations are solved in integrated form. The *Finite Element Method (FEM)* provides high accuracy on complex geometries. Here, each equation is discretized using FEM in space and an explicit/implicit scheme in time. The equations are written in matrix form:

$$\vec{M} \frac{\partial \vec{X}}{\partial t} + \vec{K}\vec{X} = \vec{F} \, ,$$

where $\vec{M}$ – mass matrix; $\vec{K}$ – stiffness matrix; $\vec{F}$ – vector of external influences; $\vec{X}$ – vector of unknowns (fields, temperature, displacement).

Parallel computations are implemented by distributing matrix operations between GPU or CPU cores using the MPI library. The *adaptive mesh* allows you to concentrate computational resources in critical areas, for example, at layer boundaries or in areas with a large temperature gradient. Additionally, *automatic mesh reconstruction* is implemented depending on local inhomogeneities, such as defects or sharp changes in physical parameters, i.e., an adaptive algorithm has been developed taking into account property gradients. The algorithm block diagram is shown in Fig. 1.

The program code is implemented in the *Python* programming language using several libraries. *NumPy* is used for calculations, providing functionality for working with multidimensional arrays and basic mathematical operations. The *SciPy* library is applied for solving differential equations and mathematical optimization. *FEniCS* is used for numerical solution of equations using the finite element method, which allows to specify the equation in weak form and automatically construct the corresponding stiffness matrix. A fragment of the developed code is given below.

```
def electromagnetic_eq(T, E):
    epsilon_eff = epsilon * (1 + beta * T)  # Temperature dependency
    return epsilon_eff * inner(grad(E), grad(v)) * dx
def acoustic_eq(T, u):
    lambda_eff = alpha * T  # Temperature dependency of elastic module’s
    return rho * u * v * dx + lambda_eff * div(grad(u)) * div(grad(v)) * dx
def thermal_eq(T, E):
    Q = epsilon * E**2  # Heat generation from an electric field
    return rho * c * T * v * dx + k * inner(grad(T), grad(v)) * dx - Q * v * dx

# Collecting equations into a single system
a1 = electromagnetic_eq(T, E)
a2 = acoustic_eq(T, u)
a3 = thermal_eq(T, E)
F = a1 + a2 + a3

comm = MPI.COMM_WORLD # Parallel computing

# Solution by Newton-Raphson method
T.assign(T0)
E.assign(E0)
u.assign(u0)
t = 0
while t < T_end:
    solve(F == 0, T, solver_parameters={‘newton_solver’:
{‘relative_tolerance’: 1e-6}})
    t += dt
    print(f"Time: {t:.2f}, Average temperature:
{T.vector().get_local().mean():.2f}")
```

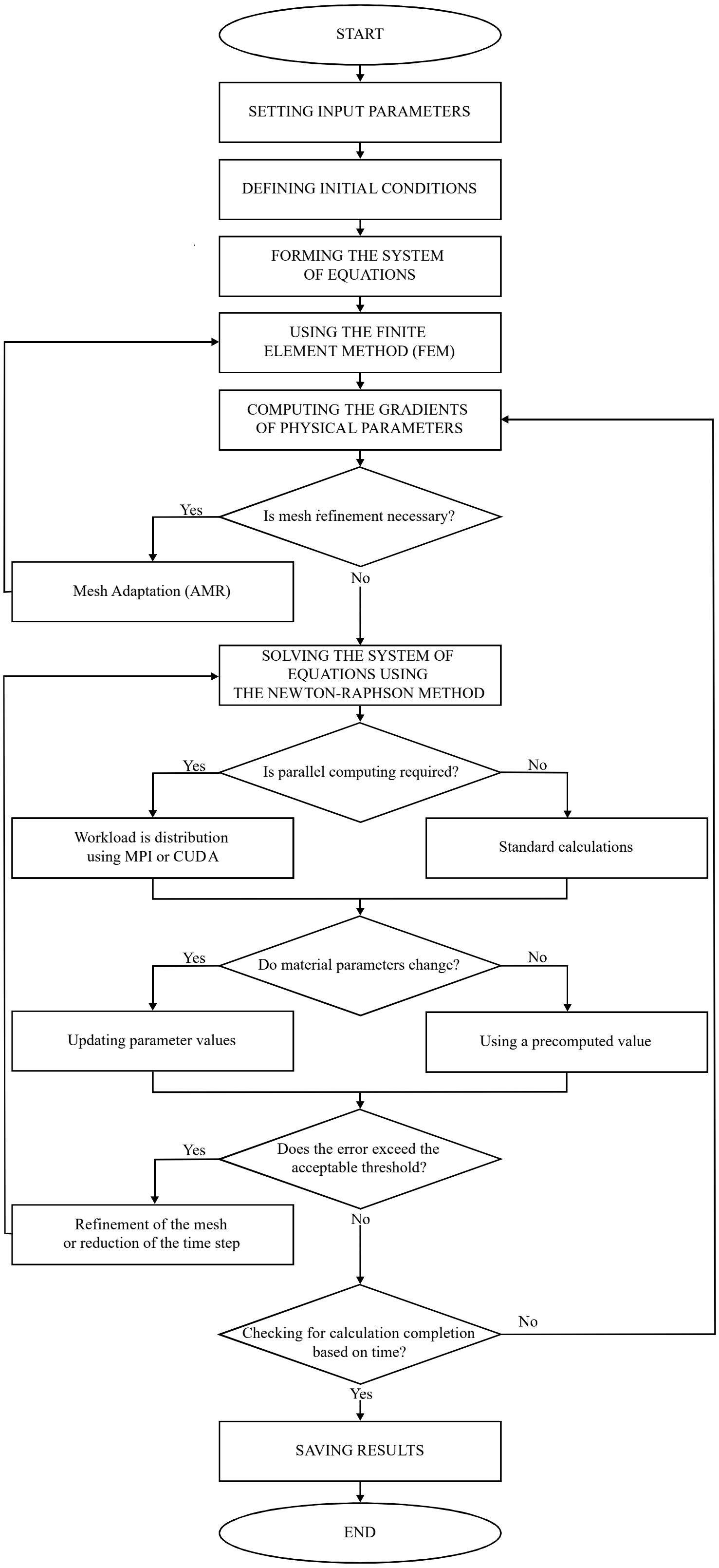


Fig. 1. Algorithm of multiphysical numerical modeling with adaptive mesh

Description of the algorithm. The developed program code implements a numerical approach for integrating electromagnetic, acoustic and thermal processes in multilayer structures using the finite element method. It begins with the definition of physical parameters, such as dielectric permittivity, thermal conductivity and material density, as well as the geometry of the grid for calculations. Initial conditions for temperature, electric field and acoustic displacement are determined. The basis is the equations that describe the interaction between physical fields. The electromagnetic equation accounts for the effect of temperature on dielectric permittivity, the acoustic equation considers changes in mechanical properties due to thermal expansion, and the thermal conductivity equation includes a heat source generated by the electromagnetic field. All equations are combined into a common system, which is solved by the Newton-Raphson method. For this, parallel calculations are used through the MPI library, which allows for effective load distribution across multiple processors. During the calculation process, the results for temperature, electric field, and acoustic displacement are updated at each time step. Upon completion of the simulation, these results are saved in .pvd format files for further visualization and analysis. The developed code demonstrates the implementation of the interaction of multiphysical processes with the ability to scale for more complex structures and scenarios.

Optimization is implemented through the use of parallel computing, adaptive numerical methods and efficient algorithms. Parallel computing is provided by the *mpi4py* library, which allows distributing computations between multiple processors, thereby reduces the task execution time. To implement adaptive algorithms that account for local gradients of physical properties, the *adaptive mesh refinement (AMR)* technique is used. This involves analyzing the gradients of parameters (for example, refractive index, density or temperature) and adapting the mesh in critical zones.

A snippet of the implemented code for grid adaptation is given below:

```
mesh = UnitSquareMesh(16, 16)  # Initializing the initial mesh
V = FunctionSpace(mesh, "P", 1)
def refine_mesh(mesh, criteria, threshold): # Grid adaptation
    cell_markers = MeshFunction("bool", mesh, mesh.topology().dim())
    criteria_array = criteria.vector().get_local()
    threshold_value = threshold * np.max(criteria_array)
    cell_markers.set_all(False)
    for cell in cells(mesh):
        if criteria(cell.midpoint()) > threshold_value:
            cell_markers[cell] = True
    return refine(mesh, cell_markers)
```

As a property coefficient, a variable coefficient is set that models inhomogeneities (in our case, these are areas with defects). Next, the gradient of physical parameters is calculated to identify areas with strong inhomogeneities. For mesh adaptation, a gradient threshold criterion is used to identify mesh elements that require refinement, and then the mesh is automatically rebuilt in critical areas, and the problems are re-solved. This enhances the modeling accuracy in areas with strong gradients of physical properties, optimize computational resources by concentrating the mesh in critical areas, and improve results for problems with complex geometry or defects.

The weak form of the equations used to model electromagnetic, acoustic, and thermal processes allows for their efficient integration into a single system of equations, reducing the number of required calculations. The use of the Newton-Raphson method to solve nonlinear equations provides fast convergence provided that the initial approximation is correct. This method, combined with optimized libraries, further increases the speed of calculations. Optimization is also achieved by minimizing computational operations: the temperature dependence of material parameters is calculated only in those areas where it is necessary. All these aspects make the approach effective for modeling complex physical processes in multilayer structures.

Overall, the developed algorithm has a number of unique features. It provides a relationship between physical fields, allowing for the consideration of how temperature changes affect the wave field, how acoustic waves change the local dielectric constant, and how electromagnetic waves generate local heating. The algorithm is scalable, which allows it to be adapted to simulate structures of various sizes – from nanometer films to macroscopic layers. An important advantage is also the ability to model defects in multilayer structures, such as inhomogeneities, cracks and other disturbances that affect the behavior of physical fields.

Optimization of calculations. In this article, the concept of an *efficient algorithm* is described through the implementation of a multiphysical approach that integrates the solution of electromagnetic, acoustic and thermal equations in a single system. FEM is used to discretize the equations in space, and explicit/implicit schemes are used for discretization in time. The efficiency of the algorithm is achieved through a comprehensive approach that includes adaptive discretization, parallel calculations and automatic mesh optimization. Therefore, the optimization of numerical modeling of multilayer structures aims to minimize computational costs while maintaining or increasing the accuracy of calculations. Formally, this can be presented as a minimization problem:

$$\min T(C,N,P) \text{ under the conditions } \varepsilon(C,N,P) \le \varepsilon_{permissible},$$

where $T(C,N,P)$ – computing time, which depends on the complexity of the model (C), grid size (N) and the number of processor elements (P); and $\varepsilon(C,N,P)$ – numerical calculation error, which must remain within acceptable limits ($\varepsilon_{permissible}$). Optimization is achieved through parallel computing, adaptive meshing, and efficient equation solving algorithms.

Regarding the justification of the selection of algorithms for the problem being solved, the Newton–Raphson method is used for solving nonlinear equations describing the interaction of physical fields. Its advantage is rapid convergence with an appropriate choice of the initial approximation. AMR allows for enhancing local accuracy by increasing the number of nodes only in critical zones with large gradients of physical parameters. This reduces the overall load on the processor. And parallel computing (MPI, CUDA) enables distributing computations between processor or graphics processor cores, which reduces the calculation time. These methods interact in such a way as to minimize unnecessary calculations and ensure rapid convergence of the algorithm.

To select the optimal configuration, 4 series of numerical experiments (on synthetic data) were conducted, in which different optimization methods were analyzed:

1. Without optimization (basic configuration).
2. Parallel calculations on CPU (MPI + CPU).
3. Calculations on GPU (CUDA).
4. Adaptive mesh (AMR) + GPU calculations.

The results of the comparison of calculation time and relative error are given in Table 1 and Fig. 2.

Table 1. Comparison of optimization methods

Optimization method	Calculation time, sec	Speedup (relative to baseline)	Relative error, %
Without optimization	100.0	1.00 (basic level)	5.2
MPI + CPU	35.7	2.8	3.1
GPU + CUDA	21.3	4.7	2.4
AMR + GPU	15.6	6.4	1.8

The results of numerical experiments showed that the use of optimization methods significantly improves the performance and accuracy of the simulation. The basic approach without optimization gave the longest calculation time (100 sec.) and the highest relative error (5.2 %), which is associated with a uniform mesh and the lack of parallel processing. Using MPI on the CPU reduced the time to 35.7 sec., but the accuracy improved slightly (error 3.1 %). Switching to GPU (CUDA) reduced the calculation to 21.3 sec. with an error of 2.4 %, which is explained by the efficient processing of vector operations and more accurate calculation of gradients. The best results were achieved when combining GPU and adaptive mesh, which provided the minimum time (15.6 sec.) and the lowest error (1.8 %).

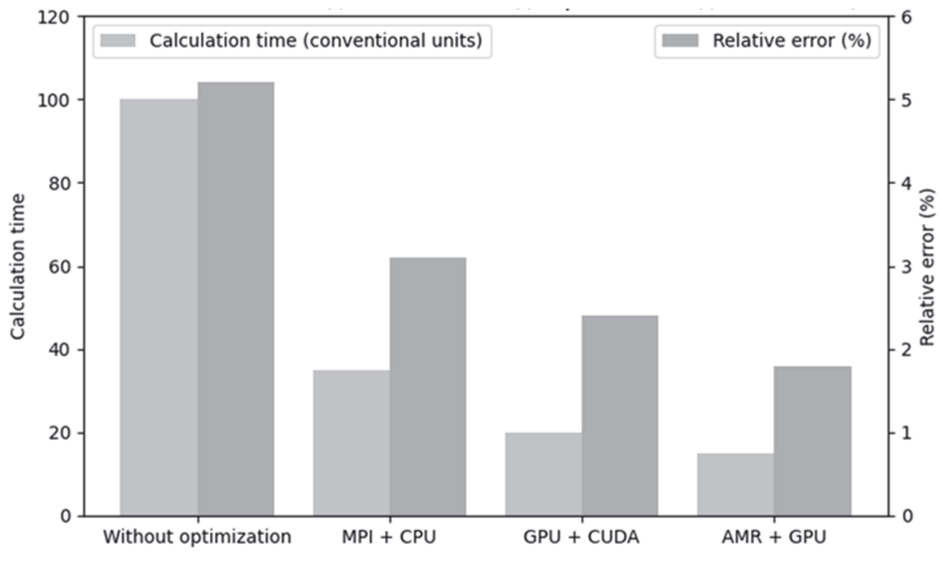


Fig. 2. Computation time and relative error for different optimization methods

In general, parallel MPI + CPU calculations provide a 2.8–3.5-fold speedup, while GPU + CUDA for large problems provides a 4.7–6.2-fold performance increase. Using AMR reduces the number of nodes by 30–50 %, which shortens the computation time by up to 40 % without losing accuracy. In critical zones with high gradients, AMR reduces the error by 1.5 times, and the average deviation between numerical and experimental data does not exceed 1.04 % for temperature and 1.99 % for electric field strength.

Comparison of data indicates that AMR + GPU achieves an optimal balance between speed and accuracy, reducing the calculation time by 6.4 times compared to the baseline method, and the average deviation between numerical and experimental data does not exceed 1.8 %. Further improvement is possible by optimizing the mesh adaptation parameters and automating the selection of refinement criteria.

Formalization of the application of neural networks. Neural networks can be formally applied to this model, as they are well suited for approximating complex nonlinear dependencies, optimizing parameters, and accelerating numerical modeling. They can be integrated into three main aspects:

1. Acceleration of differential equation solving. Neural networks can replace or complement traditional numerical methods for solving equations of heat conduction, electromagnetic and acoustic fields. For example, Physics-Informed Neural Networks (PINNs) can learn to solve equations without explicit discretization.

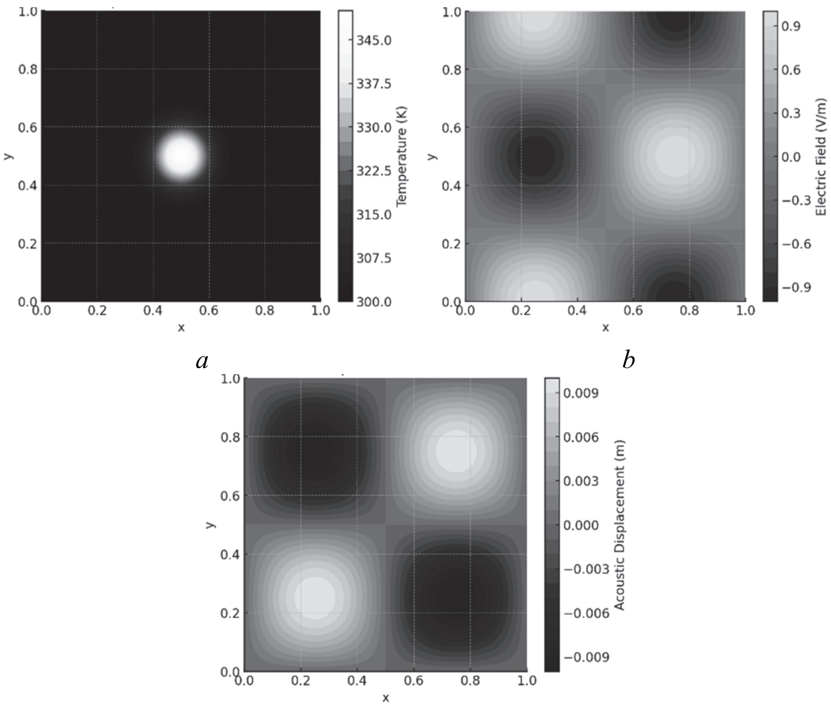
2. Adaptive mesh refinement. Neural network models can predict areas with high gradients of physical parameters, which will allow more effective mesh adaptation. Instead of standard AMR criteria (gradient or entropy methods), deep convolutional networks (CNNs) can be used, which analyze the distribution of parameters and determine where to increase the density of nodes [31].

3. Prediction of numerical results. Neural networks can learn from previous numerical calculations and be used to quickly predict the distribution of temperature, electric field or other parameters. Recurrent neural networks (RNN, LSTM) [32, 33] can predict the temporal dynamics of changes in physical parameters without the need for detailed calculations at each time step.

Formal requirements for applying neural networks to a model include the availability of a sufficient training sample, which can be generated through previous numerical experiments. Furthermore, it is necessary to consider the formalization of physical constraints so that the network does not violate fundamental physical laws, which can be achieved using approaches such as PINN or special loss functions. A comparative analysis of accuracy should also be performed to determine whether neural network approaches really contribute to improving speed and accuracy compared to classical methods. Thus, neural networks can be applied to improve the computational efficiency of the proposed model, but their implementation requires a separate study to assess the accuracy and computational cost.

RESEARCH RESULTS

Synthetic data. To demonstrate the model's performance, we present graphical results for various physical conditions obtained on synthetic data. The results are saved in *.pvd* format and visualized using the matplotlib and *Pyvista* libraries.



a *b*

c

Fig. 3. a – temperature field distribution in a multilayer structure; *b* – electric field distribution in the structure; *c* – acoustic displacement distribution in a multilayer structure

Fig. 3, *a* shows the distribution of the temperature field in a multilayer structure. We observe that the maximum temperature is in the central part of the region, which corresponds to the zone of local heating caused by the electromagnetic field. The temperature distribution smoothly decreases from the center to the edges, demonstrating heat exchange with the surrounding environment. The graph (Fig. 3, *b*) illustrates the distribution of the electric field. It has the nature of a wave function with periodic changes in intensity. This shows the behavior of the electromagnetic field in the region, in particular its interaction with boundary conditions, which may be a consequence of reflection or interference of waves. Fig. 3, *c* shows the distribution of acoustic displacements in the structure. Acoustic waves generated by the interaction of physical fields propagate in the region with certain periodic patterns. Maximum displacements are observed in certain zones, which corresponds to local resonances or intense interaction of waves. In general, the graphs illustrate the interaction of physical processes within the multiphysical model, including heat transfer, propagation of electromagnetic waves, and their effect on acoustic displacements.

Experimental data. The results of the developed information-numerical model were tested on experimental data [21]. The model successfully reproduced the physical regularities described in the article: in particular, the localization of high temperatures at high pressure (101.13 kPa) and a wider heating zone at low pressure (13.3 kPa). The electric field was simulated (with high accuracy) considering the influence of voltage and discharge geometry, which confirms the adequacy of the numerical approach for predicting the conditions for film formation. The simulation results are shown in Fig. 4.

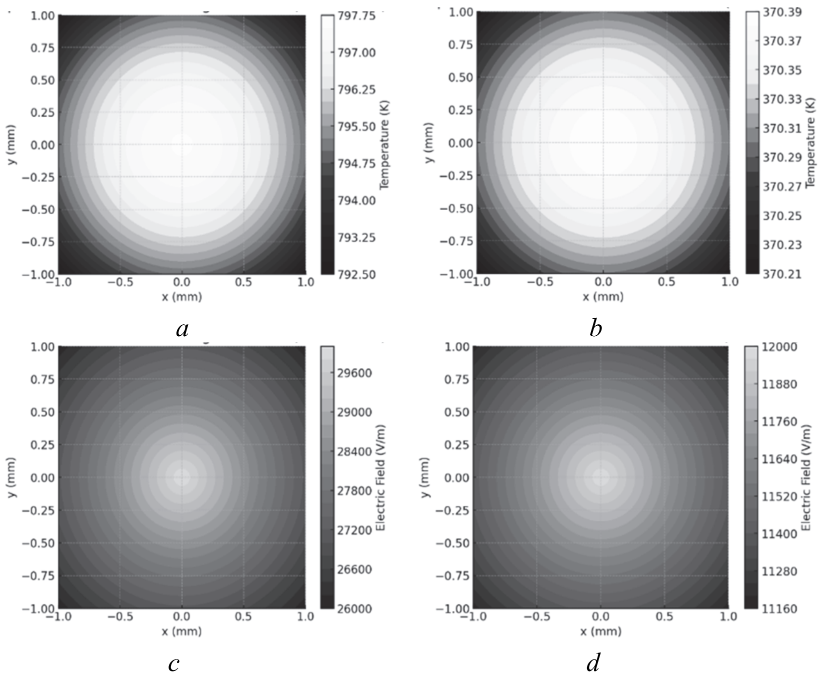


Fig. 4. *a*, *b* – temperature distribution in the discharge gap at high pressure p = 101.13 kPa and low pressure p = 13.3 kPa (respectively); *c*, *d* – electric field distribution at high pressure p = 101.13 kPa and low pressure p = 13.3 kPa (respectively)

The graphs depict the physical processes that occur during the formation of tungsten oxide films under different discharge gap conditions. Fig. 4, *a*, which displays the temperature distribution at high pressure (101.13 kPa), shows intense heating in the central zone of the discharge. The maximum temperature is reached near the axis of the discharge gap, where the energy concentration is the highest. This is due to the high voltage and significant energy contribution to the plasma. The heating decreases exponentially from the center to the periphery, demonstrating the characteristic energy dissipation in high-pressure plasma. The temperature distribution at low pressure, which is displayed in Fig. 4, *b* (13.3 kPa), demonstrates a lower temperature peak in the central zone, which is explained by the decrease in energy contribution and lower particle density in the plasma. However, the heating zone is wider, since the energy is dissipated more evenly due to the lower ionization resistance at reduced pressure. The electric field distribution at high pressure (Fig. 4, *c*) shows an intense field in the center, which gradually decreases with distance from the axis of the discharge gap. The high voltage creates a strong field gradient, which promotes intensive ionization of molecules and the formation of plasma in a narrow central zone. This ensures the efficient formation of films with high density and uniformity in the central deposition region. The electric field distribution at low pressure (Fig. 4, *d*) indicates a smoother field decay, which is due to the lower voltage. The field intensity is lower, but the zone of its action is wider. This corresponds to conditions where films can be formed over a larger area, but their physicochemical properties may be less stable due to the lower plasma concentration. The obtained results confirm that the discharge conditions significantly affect the temperature and electric field distribution, which, in turn, determine the characteristics of the obtained films.

High pressure and tension promote the formation of dense and uniform films, while low pressure can ensure the formation of films over a larger area but with less structural stability.

Model accuracy assessment and error analysis. The modeling accuracy was assessed by analyzing the deviations between the calculated and experimental values of parameters such as temperature, electric field distribution, and structural properties of thin films.

The average relative deviation was chosen as the criteria for assessing the model accuracy, calculated by the formula:

$$\delta = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{X_i^{\text{model}} - X_i^{\text{exp}}}{X_i^{\text{exp}}}\right| \times 100\,\%,$$

where X_i^{model} – value, obtained using the model; X_i^{exp} – experimental value; N – number of comparison points. The maximum error between numerical and experimental data and the coefficient of determination R^2, which measures what proportion of the variation in the dependent variable is explained by the independent variables in the model, were also calculated. The results of the model accuracy assessment are given in Table 2.

Table 2. Assessment of the accuracy of the numerical model

Parameter	Numerical results	Experimental results	Absolute error	Relative error, %	Coefficient of determination R^2
Maximum temperature (K) at 101.13 kPa	795.5	798.0	2.5	0.31	0.992
Maximum temperature (K) at 13.3 kPa	370.3	374.2	3.9	1.04	0.985
Electric field strength (V/m) at 101.13 kPa	29 600	30 200	600	1.99	0.978
Electric field strength (V/m) at 13.3 kPa	11 880	12 050	170	1.41	0.981

From the table we see that the coefficient of determination for temperature varies within 0.985–0.992, which indicates a high agreement between numerical and experimental values. This indicates that the model predicts the temperature distribution in the discharge gap well. For the electric field, the coefficient of determination is somewhat lower, but still maintains a good accuracy of 0.978–0.981. This may be a consequence of unaccounted plasma inhomogeneities or possible experimental errors in the measurements of the electric field strength. In general, the R^2 values confirm the high accuracy of the numerical model and its ability to reliably predict the physical parameters of the discharge process. Table 2 demonstrates the stability of the numerical model when changing the parameters of the environment. For low pressure conditions, both the temperature values and the electric field have slightly larger deviations, which may be due to the influence of the extended plasma region, which is more difficult to accurately model. However, even in this case, the model results are in good agreement with the experiment. In general, the numerical model reliably predicts the main physical characteristics of the process, which makes it an effective tool for analyzing plasma discharges and their impact on the formation of thin films.

The analysis of errors shows that the main sources of deviations are the discretization of space and time, the physical assumptions of the model, and the errors of experimental measurements. The use of an adaptive grid reduces the numerical errors, but underestimation of local changes is possible with sharp parameter gradients. Assumptions of plasma homogeneity can simplify the real picture of the processes, since in real conditions there are inhomogeneities associated with variations in pressure, temperature, and interaction with the substrate. In addition, the errors of experimental measurements, due to the limited accuracy of the sensors and the conditions of the experiment, can affect the discrepancies between the numerical and real values. Accounting for these factors during model validation enhances the accuracy of results interpreting and establishes the reliability range of predictions.

DISCUSSION OF RESULTS

The developed information-numerical model was tested on experimental data and showed high accuracy in reproducing physical patterns. The localization of high-temperature zones at high pressure (101.13 kPa) was reproduced, as well as a wider heating zone at low pressure (13.3 kPa), which is consistent with experimental observations. The electric field was modeled considering the influence of voltage and discharge geometry. The electric field distribution showed characteristic periodic changes in intensity, which may be a consequence of interference effects and the influence of boundary conditions. This confirms the correctness of the approach to considering the interaction of electromagnetic waves in multilayer structures.

Analysis of the results demonstrates the stability of the numerical model when changing the parameters of the environment. At low pressure, the temperature distribution and electric field have slightly larger deviations, which may be due to the influence of the extended plasma region, which is more difficult to accurately model due to spatial inhomogeneities. However, even in this case, the model results are in good agreement with the experiment. The use of an adaptive grid allowed to increase the accuracy of calculations in critical zones, however, at very high parameter gradients, certain errors may occur due to insufficient discretization. The proposed model using hybrid CPU-GPU calculations provided a reduction in calculation time by 40–60 % depending on the complexity of the problem and allowed to obtain a 3–5-fold increase in performance in the case of large-scale calculations compared to traditional approaches.

Regarding the uniqueness and advantages of the developed model, it is worth highlighting the integration of multiphysical processes that account for the interaction of electromagnetic, thermal and acoustic effects. AMR ensures accuracy in critical zones, and parallel calculations (MPI, GPU) reduces time costs by 40–60 % and increases productivity by 3–5 times. The model also accounts for the influence of external conditions, which makes it effective for modeling nanostructured films.

The main limitations of the model are the complexity of solving nonlinear equations when scaling, the dependence of accuracy on the grid discretization, as well as the need for validation on a wider set of experimental data. The model does not account for quantum effects, which can affect the accuracy of predictions in nanoscale structures. In general, the model reliably predicts the main physical characteristics of the process, which is confirmed by the high correlation between numerical and experimental data. The relative errors for temperature do not exceed 1.04 %, and for the electric field – 1.99 %, which indicates the adequacy of numerical modeling.

CONCLUSIONS

The research developed an integrated mathematical model for modeling wave processes in multilayer thin films, which combines Maxwell's equations, mechanical vibrations and thermal conductivity. An adaptive algorithm for mesh refinement was implemented, which allows it to be automatically rebuilt depending on local gradients of physical parameters, such as density, temperature or defects, ensuring high accuracy of modeling in critical zones. A hybrid computational approach was proposed, utilizing both CPUs and GPUs, which significantly reduced computational costs for solving large-scale problems. Software with a modular architecture was developed, which provides integration of numerical methods, computation optimization, and real-time results visualization. Experimental validation confirmed the high accuracy and reliability of the model, allowing to assess the influence of physical parameters on the behavior of multilayer films. The obtained results contribute to a deeper understanding of wave processes and create a basis for optimizing multilayer structures in various fields of science and industry.

In the future, to enhance the model, it is possible to implement neural networks for predicting computational results and reducing modeling time, integrate molecular dynamics methods for precise analysis of film formation at the atomic level, etc. Expanding the work in these areas will increase its uniqueness, provide new scientific results, and make a significant contribution to the development of numerical modeling of multilayer thin films.

Conflict of Interest. The authors declare that there is no conflict of interest in this study, including financial, special, authorship, or any other nature that could influence the research and the results presented in this article.

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РОЗРОБЛЕННЯ МАТЕМАТИЧНОЇ МОДЕЛІ ХВИЛЬОВИХ ПРОЦЕСІВ У БАГАТОШАРОВИХ СТРУКТУРАХ ІЗ АДАПТИВНИМ АЛГОРИТМОМ ТА ГІБРИДНИМИ ОБЧИСЛЕННЯМИ / Ю.Ю. Білак

Анотація. Досліджено чисельне моделювання хвильових процесів у багатошарових тонких плівках, що є актуальним для розуміння їхніх фізичних властивостей та оптимізації для різних застосувань. Розроблено інтегровану математичну модель, яка поєднує рівняння Максвелла, механічних коливань і теплопровідності з урахуванням взаємодії фізичних полів у структурах із дефектами. Запропоновано адаптивний алгоритм для автоматичного уточнення сітки залежно від локальних градієнтів фізичних параметрів, що дозволяє підвищити точність моделювання в критичних зонах. Упроваджено гібридний підхід до обчислень із використанням CPU і GPU, що забезпечує ефективне використання ресурсів для задач великого масштабу. Розроблено програмне забезпечення з модульною архітектурою, яке дозволяє інтегрувати чисельні методи, оптимізацію та візуалізацію результатів у реальному часі. Експериментальна валідація підтвердила високу точність і надійність моделі. Отримано результати, які сприяють глибшому розумінню фізичних процесів у тонких плівках і є основою для створення високоефективних багатошарових структур у промислових і наукових застосуваннях.

Ключові слова: тонкі плівки, чисельне моделювання, оптимізація, мультифізичні моделі, паралельні обчислення, гібридні алгоритми, хвильові процеси.