MODERN PROBLEMS IN MODELING MATERIALSFOR MECHANICAL, MEDICAL AND BIOLOGICAL APPLICATIONS (MPMM&A-2024)

Abstracts of the Fourth International Conference
(November 18–22, 2024, Rostov-on-Don)

Rostov-on-Don
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The conference focused on the results of work in the following areas: contact problems of elasticity theory for media with complex mechanical properties; modelling of hard and soft biological tissues; modelling of composite materials; modelling of piezoactive materials; actual problems of computer engineering; training of modern engineering personnel.

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INVESTIGATION OF BUCKLING OF LATTICE STRUCTURES

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In this paper, an experimental and numerical study of lattice structures of 502 species was carried out. Two kinds of lattice structures were taken from [1], 500 kinds were determined using Monte Carlo method in order to find the optimal set of dimensionless parameter λ.

Lattice structures were a set of blocks connected in longitudinal direction. Each block consisted of seven unit cells (edges of a hexagonal bipyramid). The geometry of a unit cell was described by a dimensionless parameter. The first type of construction was a set of unit cells with the same and constant value of the dimensionless parameter. The second type of construction had a nonconstant distribution of the dimensionless parameter.

Three types of experiments were performed: numerical calculations using the ANSYS Mechanical APDL software package, in-situ testing on a testing machine, and loading inside the CT using patented tooling [2].

Two types of boundary conditions were considered for numerical calculations. Boundary conditions of the 1st type corresponded to a rigid embedment with a loaded free edge. Boundary conditions of the 2nd type corresponded to a hinged immobile support on one side and a movable hinge with applied load on the other side.

For the experiments inside the CT, the lattice structures were loaded by longitudinal compressive loading. X-ray computed tomography (XCT) imaging was performed in cooperation with the loading of the specimens. Thus, four imaging points were obtained in one experiment: one imaging without loading and three with applied external loading. In order to perform the imaging under load, the investigated specimens were mounted in a special test tooling that was installed in the X-ray computed tomography scanner. The tooling allowed an axial compressive force to be applied. After each loading step, the specimen was imaged.

The studied samples were produced by laser stereolithography on the ANYCUBIC Photon Mono X photopolymer printer.

Numerical experiments determined the critical loads corresponding to the first form of buckling for lattice structures, and it was found that the values of critical loads calculated from the vectors of dimensionless parameters λ adopted from [1] were found to be maximum.

In-situ experiments on press showed that the median critical load for both types of structures is almost the same.

During the in-situ experiments within the CT in conjunction with loading of the specimens, in addition to the global buckling, local buckling was also found.

By comparing the results from all experiments, the similarity of the nature of the first form of buckling was revealed.

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REFINEMENT OF THE CALCULATED GEOMETRY OF SAMPLES BASED ON IMAGE DATA

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Currently, the construction of a grid of objects based on image data is relevant; this approach is used in the finite element method. One of the urgent problems in solving by the finite element method is the automation of grid construction for objects of arbitrary geometry. In this case, the approach to grid construction can be the construction of an orthogonal regular grid with subsequent filtering of the relative proportion of the material content. This work presents a method for refining an orthogonal grid [1] for an object based on image data. The solution to the problem is reduced to the use of the flood-fill method, which involves analyzing the boundaries of the object for each grid element and subsequent changing the coordinates of the element nodes. In the finite element method [2], smoothing the grid for the object is a necessary step to achieve high accuracy of results. In the work, an algorithm for redefining the coordinates of the nodes according to image data is implemented and a number of test calculations are carried out. The applicability of the method to samples of arbitrary geometry in a two-dimensional setting is assessed. The proportion of the relative material content in the transformed finite element serves as a parameter for assessing the final result.

The smoothing algorithm consists of several steps. We divide the image into finite elements by an orthogonal grid, then exclude the elements in which the sample does not lie. We calculate the sample boundary in each element using the flood-fill algorithm [3], and then pull the grid nodes to the nearest points on the calculated boundary. Now we adjust the position of the points that belong to several elements. As a result, we obtain an irregular grid. Calculations were performed on model samples of the following shape: a sample with an oval boundary, a sample with a trapezoidal boundary, a sample with an arbitrary curved boundary. The studies considered binary images with a resolution of 1920x1080 pixels. One finite element was constructed on each image, the nodes of which were pulled to the object boundaries in accordance with the presented method. The following results were obtained as a result of the calculations: after executing the algorithm on the first sample, increase of the coefficient of the relative material content was 15 %, on the second sample – 40 %, on the third sample – 26 %. These results demonstrate the high efficiency of the presented method for constructing meshes of objects of arbitrary geometry in finite element method problems. Further development of the presented method can be aimed at expanding its application in three-dimensional problems based on voxel models.

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SOLUTION OF THE STRESS-STRAIN STATE OF THE WEDGE PROBLEM USING FEM: THE HOT SPOT PROBLEM

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The aim of this study is to analyze the influence of geometric parameters of crack-like defects on the stress-strain state of a material under the application of an external load. The shape and angular characteristics of cracks play a key role in stress concentration, which determines the resistance of a material to fracture. Issues of stress singularity at the boundary of bodies at points with sharp angles, known as hot spots, remain a pressing problem in mechanics. Such problems are important not only in the context of classical elasticity theory, but also for the analysis of real materials, including biomaterials, where geometric factors are directly related to durability and strength. This paper is devoted to the study of V-shaped cracks with an emphasis on numerical analysis methods. The dependence of the stress level on the opening angles and load distribution at the crack boundaries is considered. Particular attention is paid to the methods for eliminating stress singularities, which are aimed at increasing the accuracy of calculations and minimizing errors. The object of the study is a model of a crack in a material with elastic properties. The ANSYS program was used to describe the stress-strain state using the finite element method (FEM). The crack geometry is described by two half-lines forming an opening angle ϕ, on which a parabolic load distribution is applied. The mechanical properties of the material are characterized by the elastic modulus E = 81 GPa [1] and Poisson's ratio ν = 0,33. The boundary conditions are determined by rigid fixation of the model base, blocking all degrees of freedom of the nodes. The external load simulates the normal occlusal force characteristic of tooth enamel, with a maximum value of P = 291 N. The following approaches were used to eliminate singularities:

– Saint-Venant's principle – ignoring the effect of stresses at a significant distance from the hot spot.

– Rounding of sharp corners - modeling smooth transitions in geometry.

– Plastic formulation – application of a bilinear material model to account for real mechanical properties.

Adaptive mesh refinement – use of small elements in areas with high stress concentration.

Automatic marking of maximum values with construction of distributions in the form of stress maps was used for the analysis of normal stresses. Numerical data were exported to text files for further processing and construction of dependencies. Numerical experiments were carried out on a model with a crack opening angle ϕ in the range from 40° to 70°. The results of the stress-strain state analysis showed that the level of maximum stresses (σ_{max}) decreases with increasing angle ϕ. Thus, for ϕ=40°: maximum stress σ_{max}=614 MPa; for ϕ =70°: maximum stress σ_{max}=319 MPa[2].

This pattern is explained by the redistribution of stresses at flatter angles, which reduces the concentration of forces in the fissure apex area [3]. The constructed stress maps demonstrated a clear decrease in the stress gradient with increasing opening angle. Modeling using corner rounding and plastic formulation made it possible to eliminate infinite stresses in hot spots, which is confirmed by the stability of calculations when refining the mesh.

The obtained results confirm that the crack opening angle is a critical parameter for assessing the stress-strain state of the material. An increase in the angle ϕ increases the stability of the material by reducing the stress concentration, which is consistent with previous experimental studies. Comparison with natural data showed a qualitative agreement between the numerical and experimental results. Steeper crack angles are less susceptible to failure under the same load conditions, which makes such structures more stable in real operation. These findings confirm the role of geometry adaptation in reducing the risk of failure. A gradual increase in crack angles can be considered as a natural protective mechanism that occurs under the influence of wear. The study analyzed the stress-strain state of crack-like defects with V-shaped geometry. The effect of crack angles on the level of maximum stresses was demonstrated, approaches to eliminating singularity and increasing the accuracy of numerical calculations were identified.

The proposed methods and results of the analysis can be used to develop new structural materials, as well as in dentistry to assess the strength of enamel under occlusal loads. In the future, it is planned to study the effect of inhomogeneous material properties and complex loads on crack behavior.

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MECHANICAL MODEL OF A HYPERELASTIC CORNEA WITH A CLOSED RING

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The article deals with deformation of a thin shell consisting of two spherical segments of variable thickness under the action of normal pressure, in which the thickness of the smaller segment changes due to the implantation of a ring insert inside the layer. This model is used to describe the stress-strain state of the outer eye shell during vision correction using a flexible, polymethylmetacrylate (PMMA) intracorneal implant Myoring (enclosed ring). This technology was first proposed by A. Daxer in 2007 and its goal is to correct high degree myopia in eyes with thin corneas and to create an additional corneal framework by implanting the MyoRing.

Installation of a rigid ring not only gives the cornea the correct shape, but also enhances its mechanical properties by creating an additional corneal framework.

In this paper, the 2-parameter Muni-Rivlin hyperelastic model is used to evaluate the effect of nonlinear corneal properties on the change in corneal profile as a result of surgery. Finite element modeling is made in ANSYS software package. The outer shell of the eye is represented by two spherical segments of variable thickness that define the geometry of the cornea and sclera of the eye. The composite shell is assumed to be filled with an incompressible fluid of pressure p. According to the MyoRing implantation technique, the cornea is split into two separate layers with a closed ring between them, which is rigid compared to soft cornea. Contacts are made between the corneal layers, the upper and lower surface of the ring with contact areas within the cornea. The nonlinear problem at large deformations is solved.

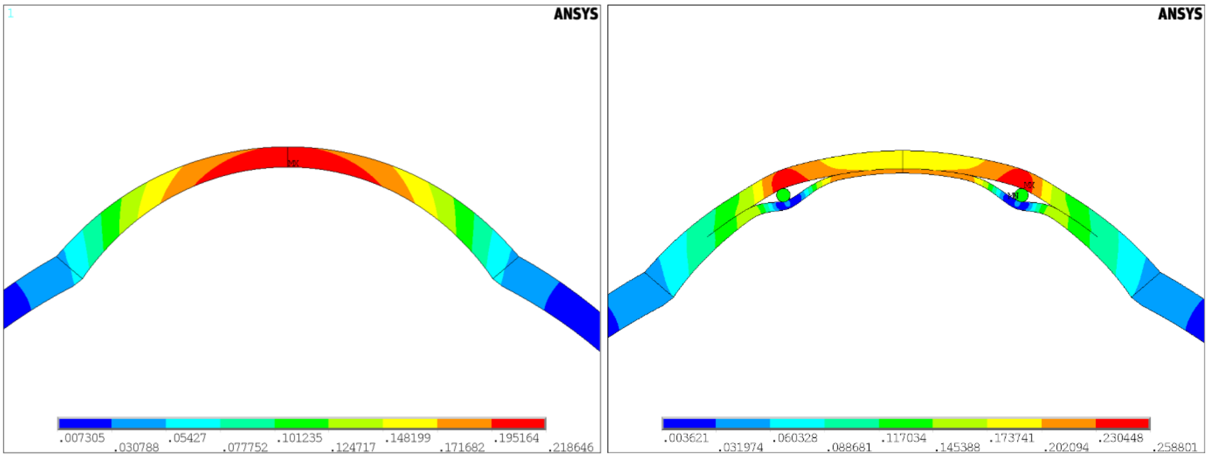

Fig. 1. Changes in corneal deformation before (left)
and after implantation of the Myoringa ring (right)

Calculations have shown that the correction results are affected not only by the height of the ring, but also by the elastic properties of the cornea itself. The stresses in corneal implants increase considerably. Thus, MyoRing can significantly strengthen the cornea by creating an additional framework with the ring. The use of the hyperelastic dual-constant material Muni-Rivlin allowed to obtain corneal deformations close to clinical data.

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ABOUT LATTICE STRUCTURES FOR FURTHER PRODUCTION OF IMPLANTS

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Currently, methods devoted to the structural design and topological optimization of lattice implants are widely used [1, 2]. The main task of these methods is to design such a heterogeneous structure that has not only the necessary strength, but is also able to stimulate the growth of bone tissue [3, 4]. Stimulation of bone tissue growth can be achieved by introducing bone cement into the heterogeneous structure [5, 6]. One of the ways to produce such implants is additive technologies.

The goal of the study is to determine the physical and mechanical properties of various types of lattice structures for further manufacturing of implants.

To determine the physical and mechanical properties of the structures, two series of four-point bending tests were carried out. In the first series, samples of the studied structures were loaded without using the cement. In the second series, cement was introduced into the irregular structures. Full-scale experiments were also carried out for solid samples.

The geometry of the structures was reconstructed and manufactured using additive technologies. The samples were printed on the Anycubic Photon Mono X photopolymer 3D printer. Anycubic Basic photopolymer resin was used for manufacturing. The tests were carried out on a UTS 110M-100 tensile testing machine. The loading diagram was used to analyze the obtained data during full-scale tests. The maximum forces of the samples were determined from the loading diagrams. The bending stiffnesses of the lattice structures were determined on the linear sections of the loading diagrams.

When cement is added to the pores of lattice structures, the values of flexural stiffness of the studied structures do not have a significant difference, which means that the geometry of the lattice structure has little influence on the rigidity characteristics. The small influence of geometry on the stiffness characteristics is explained by the material used to manufacture the structures.

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OPTIMIZATION OF LONGITUDINAL DISTRIBUTION OF POROSITY OF PIEZOELECTRIC STRUCTURES

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Modern technologies for harvesting and storing environmentally friendly energy are increasingly utilized as autonomous power sources across various industries. Such systems efficiently convert wind, solar, wave, and mechanical vibrations into usable energy. A notable class of devices within this framework is piezoelectric generators (PEGs), which leverage mechanical energy, often in the form of vibrations. In particular, multilayer structures incorporating piezoelectric elements have demonstrated significant effectiveness in enhancing energy conversion

In our previous work [1], we developed an applied model to describe the bending vibrations of bimorph plates with functionally graded (FG) characteristics. Functionally graded piezoelectric materials (FGPMs) are advanced composites designed to exhibit a continuous spatial variation of material properties, which allows for improved mechanical, thermal, and electrical performance. This gradual variation is particularly advantageous for piezoelectric devices, as it enables the fine-tuning of material properties to maximize energy harvesting efficiency. In this paper, we focus on optimizing the performance of functionally graded bimorphs with fixed geometric parameters by adjusting the material properties, particularly in the context of piezoelectric energy harvesting.

Our study presents two combined optimization approaches aimed at improving the performance of FG bimorph piezoelectric structures: global optimization approach and finite-dimensional optimization using evolutionary algorithms

The first method involves identifying a global optimum by introducing state functions, control variables, and additional optimization criteria. In this context, we explored the distribution of material properties–specifically, the elastic modulus–along the longitudinal axis of the bimorph. By applying optimization theory and defining the control variables, we achieved an optimal distribution of the elastic modulus, expressed as a fourth-order polynomial, which maximized the first resonant frequency.

The second approach employs evolutionary algorithms to optimize the system within a finite-dimensional parameter space. This method addresses the challenge of determining optimal material properties, which vary as continuous functions of the longitudinal coordinate. To constrain these variations, we introduced a porosity distribution function-a fourth-order polynomial form from the first approach–that reflects the gradation of material properties. By fixing the porosity at the ends of the bimorph and introducing a third control point, where both the position and porosity value were free parameters, we applied genetic algorithms to search for an optimal solution. This approach led to a significant improvement, increasing the first resonant frequency by 50%.

This study demonstrates the potential of functionally graded piezoelectric materials in the design of advanced energy harvesting systems. By carefully optimizing the material properties of FG bimorph structures, either through global optimization methods or evolutionary algorithms, we can significantly enhance the efficiency of piezoelectric generators.

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MECHANICAL PROPERTIES OF ARTERIES AND ATHEROSCLEROTIC PLAQUES

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The article describes the creation and application of a mobile test bench for studying the mechanical properties of soft tissues, and also considers the issue of choosing a material model for numerical modeling of atherosclerotic plaques and arterial walls.

To study the mechanical properties of plaques and arterial walls in the clinic immediately after surgical treatment, the mobile test bench (Fig. 1) was developed, allowing for tensile and compression tests to be carried out.

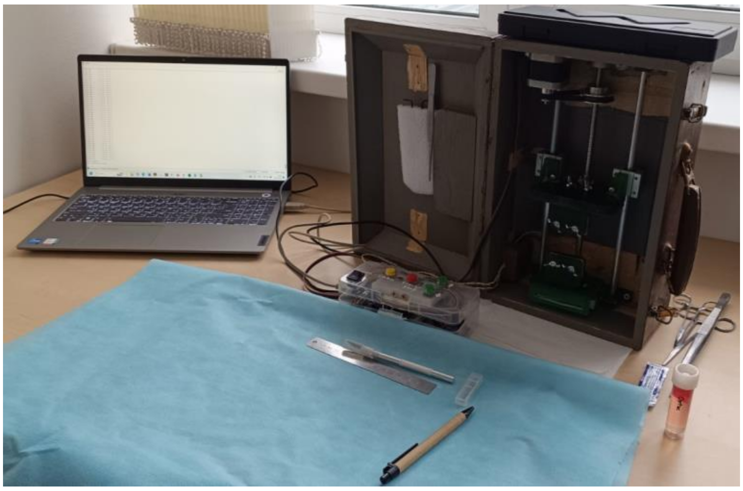

Fig. 1. Mobile test bench

As a result of the test, a file in .txt format is written to the SD card, containing data on the crosshead movements and the stress occurring at this moment, read by the strain gauge. Thus, knowing the dimensions of the sample before the start of deformation, a stress-strain curve can be constructed from such a set of points, and the elastic modulus of the material can be determined from the linear section of the chart.

In the case of modelling of atherosclerotic plaques in 3D, most researchers agree that a linearly elastic isotropic material model can be used [1]. When modelling the plaque in 2D to obtain better results, especially for the accurate calculation of the normal stresses in the plaque, it is noted that there is a need to use hyperelastic material models for the vascular wall.

A comparative numerical analysis was performed for models calculated using the mean Young's modulus (linearly elastic material model) for plaques and arterial walls obtained during experiments on the mobile test bench directly in the clinic, as well as using the hyperelastic material model (5-component Mooney-Rivlin model), the coefficients for which were also calculated on the basis of charts obtained on the mobile test bench.

As a result, it was shown that, as noted in some papers [2], for Young's moduli of material with values below 0.9 MPa, a linear-elastic material model can be used for wall modelling without loss of accuracy. For a refined calculation in 2D, the hyperelastic material model should be used when modelling the arterial wall.

The study was carried out within the framework of the State task FSRR-2023-0009.

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FUNCTIONALLY GRADED MATERIAL: OPTIMAL CHOICE OF YOUNG'S MODULUS DISTRIBUTION

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In the paper, the problem of free vibrations is presented within the framework of the isotropic elastic body model in tensor form. The object is made of a functionally graded material (FGM) [1, 2], the variable properties of which are described by Young's modulus and Poisson's ratio. In the general case of inhomogeneity, the solution to problem can only be constructed numerically. As an example, a two-dimensional problem of free axisymmetric vibrations of an inhomogeneous cylinder is considered. The numerical solution for the variation laws of Young's modulus E and Poisson's ratio ν is obtained using FEM in the

FlexPDE package [3, 4]. The calculation results showed that the effect of Young's modulus on the values of natural frequencies is more significant than the effect of Poisson's ratio.

The problem of maximizing the value of the first natural frequency with a variable Young's modulus is formulated in general form. It is assumed that a constraint on its average integral value is specified. An optimality condition is obtained using the extended Lagrange functional and the methods of variational calculus, which is a quadratic form with respect to the components of the strain tensor $\boldsymbol{\varepsilon}$:

$$M\theta^2 + N\varepsilon \odot \varepsilon = const,$$

where $M = \nu((1+\nu)(1-2\nu))^{-1}$, $N = (1+\nu)^{-1}$, $\theta = \mathrm{tr}\,\boldsymbol{\varepsilon}$, $\odot$ is the full tensor multiplication. It is noted that in the general case the formulated optimality problem is essentially nonlinear and special methods must be used to solve it. Analytical solutions for three one-dimensional problems are obtained. For the problem of free longitudinal vibrations of a rod the optimal variation law of Young's modulus is described by a quadratic function, and the displacement function is specified as a linear law. For the problem of free bending vibrations of a thin circular plate the optimal variation law of Young's modulus is described as a power law of the fourth degree with respect to the radial coordinate. For the problem of free radial vibrations of a solid thin disk the solution is constructed in the class of quadratic laws. To assess the accuracy and reliability of the obtained theoretical results, numerical modeling was performed in the FlexPDE package. Several functions satisfying a given constraint on the average integral value were selected. The problem of free vibrations was solved numerically for each of them. It is shown that with the found optimal variation law of Young's modulus the first frequency reaches its maximum value. Graphs of stress tensor components and the displacement function were also constructed.

The study was supported by the grant of the Russian Science Foundation № 22-11-00265, https://rscf.ru/en/project/22-11-00265/ in the Southern Federal University.

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EFFECT OF TYPE AND DIRECTION OF FUNCTIONAL GRADIENT ON THE MECHANICAL RESPONSE AND MORPHOMETRIC CHARACTERISTICS OF BONE SCAFFOLDS

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Surgery to restore the integrity of bone tissue is the second most common endoprosthetic procedure. This demand is driven by various traumas, treatment of oncological diseases or severe osteoarthritis of the joints. Tissue engineering approaches propose the use of scaffolds - lattice structures that provide structural support for the damaged bone fragment and stimulate the formation of living tissue [1]. For effective replacement, scaffolds should have physical and mechanical properties similar to those of bone tissue, and their structure should also be close to the structure of the bone fragment to be replaced.

There are several approaches to design of such biomedical structures. One of them proposes the use of cells based on triple periodic minimal surfaces. In this case, since the architecture of bone tissue is heterogeneous, structures are modelled with a functional gradient to obtain a structure with close properties [2, 3]. For TPMS-based structures, it is possible to change the porosity of the structure, the size of the unit cell, or to combine different types of unit cells within the same structure. It is important to understand how the functional gradient and its direction affect the properties of the final structure. This work considers structures based on gyroid surfaces with different cases of gradient type and direction. The influence of the gradient on both the mechanical response and the morphometric properties of the structures is evaluated.

The morphometric analysis showed a significant influence of the type of functional gradient on the architectural characteristics of the structures. At the same time, the direction of the gradient does not affect these characteristics. Mechanical analysis of functional gradient structures has shown an increase in stiffness characteristics when the gradient is oriented perpendicular to the compressive load. Such structures are subject to much less plastic deformation due to stress redistribution that occurs in them, and the overall stress state of the structure is also reduced. At the same time, the proportion of elements in which plastic deformations occur in models with a gradient of morphological structure is rather small, and the main part of these elements falls on the transition zone between geometries.

The results were obtained within the framework of research project No. FSNM-2024-0013.

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SELF-PROPELLED VORONOI MODEL OF CELL MONOLAYERS WITH PROLIFERATION AND APOPTOSIS.

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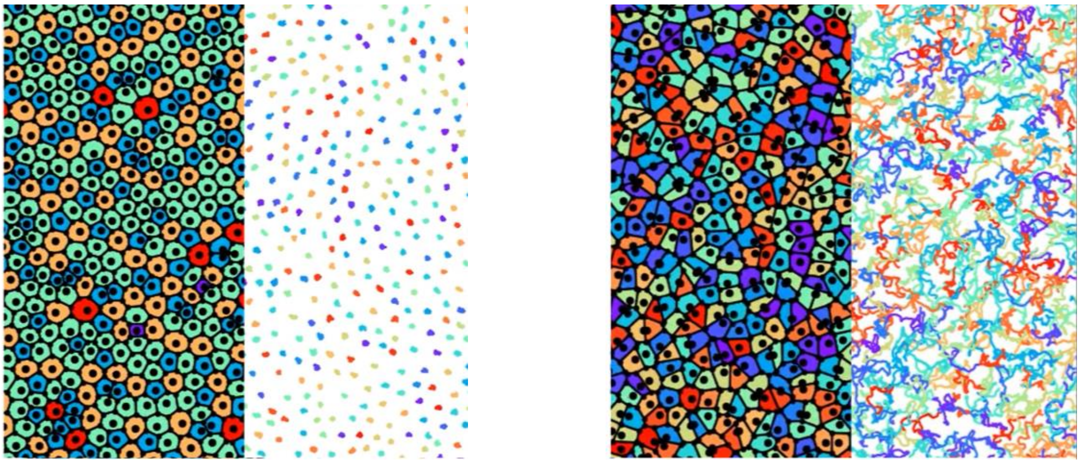
Epithelial monolayers perform a variety of essential functions in metazoans, ranging from transcellular transport and hormone secretion to wound healing. Despite their variety, all epithelia share several key features: they contain practically zero intercellular substance, and their cells are tightly packed, forming a continuous sheet. From geometrical point of view these cellular sheets can be viewed as packings of polygons (each cell being a polygon), which reveals another striking feature unifying epithelial monolayers, distributions of polygon types (DOPTs). In particular, healthy monolayers in many species have very similar distributions of cells by the number of their neighbors (polygon edges).

The topology of cell borders in cell layers has been studied since the beginning of the 20th century. Nonetheless, only during the last two decades substantial progress has been made in modelling of the epithelium on a scale of individual cells and understanding mechanisms governing its development and functioning. On the frontier of these studies are mathematical models that consider cells as polygons whose energy depends on their area and perimeter. The so-called self-propelled Voronoi model [1] was able to explain transition between soft liquid-like and solid-like states occurring in epithelia (see Fig.1) but failed to reproduce topology of the cell borders [2]. In this work we propose a model that introduces cell division and apoptosis processes in an attempt to provide a more adequate description of epithelial monolayers.



a) *b*)

Fig. 1. Comparison of topology of cellular borders and cellular movement trajectories in solid-like (*a*) and liquid-like (*b*) monolayer states

Importantly, by monitoring topology of cell borders and shapes of the cells it is possible to distinguish between healthy and pathological epithelia. Another possible area of application of our results is the development of biomimetic materials and bio-inspired architecture.

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FINITE ELEMENT ANALYSIS OF BONE TISSUE REMODELING IN SCAFFOLDS BASED ON THE EFFECTIVE POROELASTIC MODEL

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The analysis of bone tissue regeneration in this study is carried out in the area of its structural reorganization. When the scaffold is implanted into the solid substance of bone tissue, the process of reparative bone regeneration is launched in the area of contact with the surface of a foreign object. In the area under consideration, the process of restoring the integrity of the bone after a fracture is carried out with the help of structural reorganization of the undeveloped soft substance into dense bone tissue, which occurs as a result of differentiation of bone cells.

An effective finite element model of the bone-scaffold system in a three-dimensional formulation was previously introduced [1]. The main area of study in this model includes: the cortical layer of bone tissue; the spongy layer containing hematopoietic bone marrow; bone callus; a porous scaffold made of hydroxyapatite, which is common in medicine. An isotropic model of distribution of pore channels with different porosity φ is adopted in the scaffold volume.

The concept of mathematical modeling of bone tissue regeneration in the volume of a porous scaffold is based on the use of a single computer model of the studied biomechanical system and is explained in detail in the article [1]. The basis of the mathematical part of this algorithm is the equations of dynamic poroelasticity. They are designed to calculate elastic displacements and deformations, pore pressure and interstitial fluid flows in the regeneration zone and in areas of continuous media not associated with structural reorganization. At the initial moment of time, the physical and mechanical properties of the regenerating tissue correspond to granular tissue with low elastic-strength characteristics. The basis of the biological part of this algorithm is a model for describing the migration of active progenitor cells capable of differentiation and production of other cell types. Delivery of active cells to the regeneration area is carried out continuously for a specified time according to the diffusion law in accordance with the formulation of the initial-boundary value problem, which includes the tensor of diffusion coefficients and the concentration of cells at an arbitrary moment of time at the considered point of the area. This law, using Dirichlet boundary conditions, allows one to determine the concentration of cells at an arbitrary point in the regeneration zone at any given time.

Using the finite element calculation program [2], an analysis of bone tissue regeneration in a porous volume was performed at different values of active cell concentration in the bone callus and scaffold area. The bone tissue density distribution patterns in the studied volume were obtained, as well as graphs of its dependence on the concentration coefficient at a loading force of 500 N, a frequency of 200 Hz, a dynamic component coefficient of 0.005, a scaffold porosity of 50 and 90 % and a transition time to the maximum static force of 15 days. The presented data allow us to evaluate the effectiveness of the poroelastic model and select the parameters describing it that are necessary for the fastest fracture healing, which will subsequently be used in an improved finite element model of the metamaterial.

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DESIGN OPTIMIZATION BASED ON GENETIC ALGORITHM

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A current problem in the mechanics of solid deformable bodies is the optimization of structures [1]. The primary goal of this optimization is to preserve stiffness and strength characteristics while minimizing weight. The work explores the application of a genetic algorithm to optimize the cross-section of a beam under cantilever bending, based on data from a digital twin. Genetic algorithms are intended for solving optimization and modeling problems through the sequential selection, combination, and variation of the desired parameters, using mechanisms reminiscent of biological evolution.

The computational domain is defined by the object geometry, and kinematic and static conditions (see Fig. 1) were applied. A homogeneous isotropic material was used in the computations. The beam is rigidly fixed at both ends. A distributed load is applied to the upper surface.

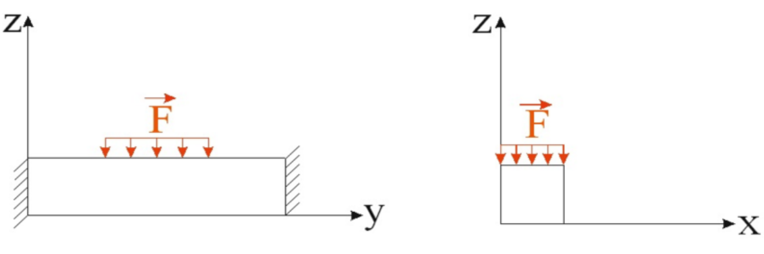

Fig. 1. Loading scheme of the beam:
longitudinal section (left), cross-section (right)

The genetic algorithm was based on the minimization of the objective function. The necessary parameters of the objective function were calculated based on the computed tomography data using the finite element method [2, 3]. A three-dimensional 8-node isoparametric finite element with trilinear approximation was utilized.

The first approach to solving this problem involved minimizing the sum of von Mises stresses. The optimized beam turned out to be 15% lighter than a solid beam of the same dimensions with practically the same value of the objective function. After a physical experiment, it was found that stiffness was lost. This is explained by a decrease in the reduced Young's modulus. The second approach was to minimize the sum of node displacements along the Oz-axis, since the load was applied in the Oz-direction. On an intermediate sample, beam turned out to be 9 % lighter, the displacements increased on average by 9.5%.

The research was funded by the subsidy allocated to Kazan Federal University for the state assignment in the sphere of scientific activities, project No. FZSM-2023-0009.

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MATHEMATICAL MODELING OF RISKS BASED ON THE RELATIONSHIP BETWEEN URIC ACID AND THE SEVERITY OF ATHEROSCLEROTIC LESIONS OF THE CORONARY ARTERIES ACCORDING TO COMPUTED TOMOGRAPHY DATA

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According to WHO, cardiovascular diseases account for 32 % of all deaths worldwide, 85% of which are myocardial infarction and stroke [1]. In view of this, the search for and further study of potential biomarkers of atherosclerotic lesions of the coronary arteries is one of the most priority tasks in cardiology to ensure more accurate and early diagnosis of cardiovascular diseases, as well as correct risk assessment and selection of the most effective preventive measures.

The aim of the study is to analyze the possibility of using uric acid in the clinic as a marker or risk factor for atherosclerotic lesions of the coronary arteries, using mathematical modeling methods .

Similar studies using various methods of mathematical modeling and statistical processing indicate a correlation between the level of uric acid and the risk of developing cardiovascular diseases. For example, in the article *by Wei Li et al. 2022* Continuous variables were tested for normal distribution using the Kolmogorov–Smirnov statistic. Normally distributed data were expressed as mean values, while variables with non-normal distribution were reported as median. Categorical variables were presented as frequency and percentage. The Kruskal – Wallis test was used to analyze group differences for continuous variables, and the chi-square test was used for categorical variables [2].

In Hu's study et al. demonstrated a nonlinear relationship between serum uric acid and cardiovascular mortality (Fig. 1) Thus, it was found that both low and high SUA levels were associated with increased all-cause and cause-specific mortality [3].

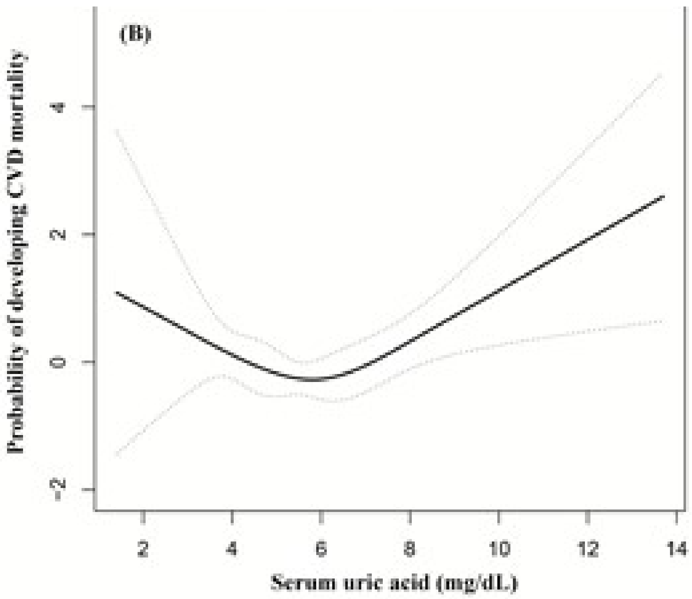

Fig. 1. Relationship between plasma uric acid concentration and risk of death [3]

The results of the study indicate the important role of uric acid in the pathogenesis of atherosclerosis and indicate the need for regular monitoring of its level for effective stratification of cardiovascular risk. This approach can contribute to the early diagnosis of atherosclerosis and optimization of preventive and therapeutic measures. mathematical modeling indicate the important role of uric acid in the pathogenesis of atherosclerosis and indicate the need for regular monitoring of its level for effective stratification of cardiovascular risk. This approach can contribute to the early diagnosis of atherosclerosis and optimization of preventive and therapeutic measures.

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DETERMINATIONS OF MECHANICAL PROPERTIES OF A HIGHLY ELASTIC MATERIAL BY INDENTING A CIRCULAR MEMBRANE WITH A HOLE

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Usually, the indentation method for determining the mechanical properties of materials is applied to continuous circular membranes, in which the parameters of a given model of a highly elastic material are calculated based on the experimental «indentation force - indenter displacement». In [1, 4], a circular membrane with a hole is proposed to be used, and the maximum indentation force is fixed as experimental data. In [1], the mathematical model of indentation did not consider friction. However, in a number of studies, such as [2, 3], it has been shown that friction plays a significant role in indentation. In [4], the method of the work [1] is developed for cases where the coefficient of friction is less than 0,5.

This paper develops an approach to determine the mechanical behaviour of thin highly elastic films by indentation. An original approach for determining the material parameter from the maximum indentation force data is proposed for the neo-Hookean model of incompressible material. Based on this approach, the material parameter is calculated using experimental data from [4]. The calculated material parameter are given in Table 1, which compares the values of the proposed approach with the approach presented in [4] and the uniaxial tensile experiment data. The results are good.

Table 1

Comparison of calculated material parameter (MPa)

hole radius (mm)		Silicone rubber			Polydimethysiloxane (PDMS)		
		silicone oil	talcum powder	silicone grease	silicone oil	talcum powder	silicone grease
1,5	current	1,227	1,328	1,198	1,788	1,679	1,965
	[4]	1,264	1,352	1,224	1,831	1,733	2,054
1,75	current	1,184	1,257	1,161	1,813	1,701	1,916
	[4]	1,238	1,299	1,205	1,885	1,777	2,019
2	current	1,203	1,268	1,200	1,849	1,805	2,004
	[4]	1,247	1,301	1,236	1,908	1,864	2,090
	uniaxial	1,214 ± 0,022			1,727 ± 0,040		

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APPLIED MECHANICS IN THE PROJECT ACTIVITIES OF THE ADVANCED ENGINEERING SCHOOL "ROSTSELMASH"

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The Rostselmash Institute of Advanced Mechanical Engineering is participating in the implementation of the Priority 2030 development program of the Don State Technical University, within the framework of which the Multi-Purpose Machine Platforms and Test Equipment project is being implemented [1].

One of the key disciplines in the advanced engineering school is project activity. At the first stage, teams were formed and project activity topics were assigned. All topics were approved by the heads of the design bureaus and the testing department of the Rostselmash combine plant.

Each team included: "calculator", "designer", "hydraulicist", "automatic", "electronics engineer" and "technologist" (a sixth team member was added from the 2024-25 academic year). At the initial stage, initial data were collected for drawing up the technical specifications, the purpose and objectives of the research were substantiated [2].

After the first year of training, when all the necessary initial data had been collected, the technical assignment had been signed, the testing methodology had been developed, analytical calculations had been performed, etc., the students created a 3-D model of the proposed stand.

They designed 3-D models of the main parts and assemblies of the stand, then performed strength and thermal calculations, which confirmed the previously obtained analytical dependencies and conclusions (Fig. 1).

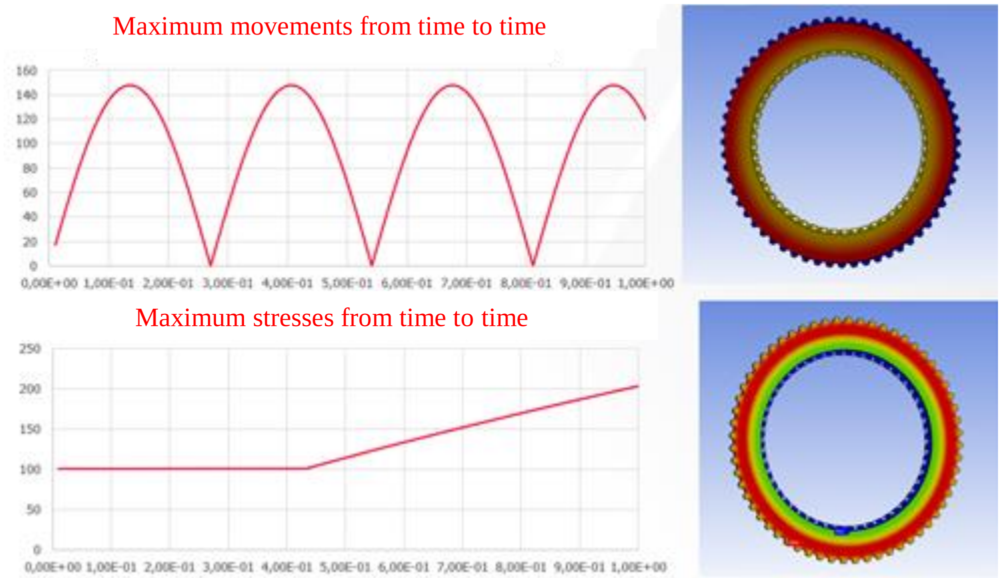

Fig. 1. Thermal calculation

During the second year, students will have to complete all technical documentation, draw up an estimate and coordinate the implementation of equipment with the testing center.

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POSSIBILITIES OF C/C++ PROGRAMMING LANGUAGE IN MODELING OUTCOMES IN CARDIAC PATIENTS

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The history of the application of mathematics in biomedical sciences goes back to 1798, when Thomas Malthus published his famous law of human population growth [1]. His work, based on simple mathematical models, predicted exponential population growth, which raised serious concerns about the future of humanity. However, the reality turned out to be more complex. In 1838, Pierre-François Verhulst modified Malthus' model by taking into account the limited resources [2]. His logistic population model was the first step towards a more realistic understanding of population growth and, more broadly, towards the application of mathematics to the study of biological systems. Many years have passed and mathematics has become an integral part of modern medicine [3]. In cardiology, for example, mathematical models are used to: 1) optimization of diagnostic and treatment processes: models allow to detect and diagnose diseases as efficiently as possible, as well as to determine optimal treatment strategies for each patient, taking into account their individual characteristics and risks; 2) prediction of disease development: mathematical models help to predict the course of the disease, which allows timely taking measures for its treatment and prevention of complications; development of new treatment methods: mathematical modeling is used to study the mechanisms of disease development The development of computing technologies, including high-performance computing and artificial intelligence, makes it possible to develop more accurate and complex models capable of analyzing huge amounts of data and predicting the results of disease and treatment. The C/C++ programming language is traditionally associated with high performance, flexibility, and the ability to work with low-level computer resources. These qualities make it an attractive tool for developing complex and resource-intensive mathematical models that require high accuracy and speed of computation. In cardiology, where modeling often involves processing large amounts of data, complex calculations, and integration with other software tools, C/C++ can provide significant advantages.

Objective. To evaluate the possibilities of C/C++ programming language for the development of mathematical models predicting the outcomes in cardiologic patients and to reveal the advantages and limitations of this approach.

Materials and methods of the study. The 1st study included data on female and male patients diagnosed with coronary heart disease (CHD) and atrial fibrillation (AF) (n = 100) and a comparison group of 100 people with CHD without AF, in whom the genotype frequencies of polymorphic variants rs10824026 of SYNPO2L gene, rs11556924, rs2200733, rs6795970 (Scn10A) were studied; the risk of AF was estimated. 2nd – risk assessment of postinfarction chronic heart failure development; 186 patients (mean age 63.5 years) who underwent MI were included; the main group included 86 people with signs of CHF above the 2nd functional class (FC) (NYHA), the comparison group included 100 people without signs of CHF or with CHF of the 1st FC (NYHA). 3rd – risk assessment of type 2 diabetes mellitus in combination with coronary heart disease; 100 patients with confirmed coronary heart disease (CHD) and type 2 diabetes mellitus (DM) (main group) were included, and in the comparison group – 100 people with CHD without DM. The capabilities of C/C++ language as an implementation tool for processing large amounts of data, performing complex calculations, integrating with Excel and creating a user interface were analyzed.

Results. Mathematical forecast models were built using regression module in Excel, converted the equation into C/C++ programming language. To estimate the risk FP it is necessary to enter the value of genotypes of polymorphic variants rs10824026 of SYNPO2L gene, rs11556924, rs2200733, rs6795970 (Scn10A), and the result of risk assessment is displayed on the computer monitor screen and is defined as “increased” or “low”. To assess the probability of CVD after myocardial infarction, it is necessary to enter the values of the indicators into the program environment: if the patient suffers from atrial fibrillation (except when it is first detected during infarction), we set the value of X4 as 1, otherwise we enter 0; if acute heart failure is detected according to Killip classification above II degree, we set the value of X6 as 1, when Killip 0-I we enter 0; indicate the level of triglycerides in blood before discharge as X9, setting a specific number; if ST-segment elevation is detected on ECG, the value of X16 is 1, otherwise - 0; in the presence of reduced left ventricular ejection fraction (X21 is 1), or its absence (X21 is 0). The result of the risk assessment will be shown on the computer monitor and is indicated as “high” or “low” [5]. To determine the risk of type 2 DM it is necessary to enter the value of genotype variant rs2464196 of HNF1A gene, and the result of risk assessment will be displayed on the computer monitor and is indicated as “increased” or “low” [6].

Thus, the programming language has significant potential for developing high-performance mathematical models in cardiology. Its advantages include high performance, flexibility, ability to handle large amounts of data and integration with other software tools. However, successful application of C/C++ in this field requires high qualification of developers and deep understanding of medical aspects of the problem.

Conclusion. Using C/C++ language in modeling outcomes in cardiological patients is a promising direction which allows to increase the accuracy of prognosis, to optimize the processes of diagnostics and treatment, and also to individualize the approach to each patient. Further research in this area may lead to the development of new tools that significantly improve the quality of medical care.

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PCSK9 TARGETED THERAPY IN HIGH, VERY HIGH AND EXTREME RISK PATIENTS: A CONCEPT OF THE COURSE AND PROGNOSIS MODELING OF CARDIOVASCULAR DISEASES

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Dyslipidemia with prevalence of very low density lipoproteins (VLDL), triglycerides (TG) and cholesterol (CH) in blood plasma contributes to development of diseases of atherosclerotic genesis, which today remain the main cause of mortality among the population, ranking first among all causes of death in the world and annually taking lives of 4 million inhabitants of the Earth. In this regard, there is a need to search for drugs that reduce the level of CH, TG and VLDL in blood plasma. Such a group of drugs are PCSK9 inhibitors [1].

The aim of the study is to analyze the formed concept of the course of cardiovascular diseases in patients with high, extremely high and extreme risks receiving PCSK9 targeted therapy, to evaluate the effectiveness of the treatment with a comparison group with further mathematical modeling of the prognosis for such patients.

At the moment, when accessing PubMed using the keywords “PCSK9 inhibitors” and “mathematical modeling”, no more than 7 results of in vitro studies and studies of real electronic patient records are available, which confirms the need to conduct research and build a working mathematical model of prognosis for such categories of patients.

Since the middle of the last century, mathematical methods of modeling have been widely used in a wide variety of areas of human activity, thanks to which new disciplines have emerged that study mathematical models of corresponding objects and phenomena, as well as methods for studying these models.

It is well known that mathematical modeling is a system of mathematical expressions describing the properties, relationships, structural and functional parameters of the modeling object. Elements of mathematical models are features that describe the objects of observation. In this case, the entire set of them is divided into controlled features that affect the system, and response features that characterize the state of the system being studied. Between the model and the object of interest to the researcher, there must be a certain similarity, which can consist either in the similarity of the physical characteristics of the model, or in the similarity of the functions performed by the object and the model, or in the identity of the mathematical description of the "behavior" of the object and its model.

Existing forecasting methods in medicine are, as a rule, linear regression models. The forecast is obtained by extrapolating the dynamics of the analyzed linear trend indicator. The widespread use of such models for solving such problems is due to their simplicity, as well as the degree of development of the mathematical apparatus for analyzing the model coefficients [2].

In foreign studies, a small number of scientific publications were found reflecting the results of mathematical modeling of the effectiveness of PCSK9-targeted therapy processes for dyslipidemia, but no prognostic model as such was presented.

Thus, mathematical modeling is a necessary tool in medical and biological practice, where significant volumes of experimental data have currently been accumulated, the storage, processing and analysis of which is impossible without the use of modern information technologies and effective mathematical methods for analyzing and modeling systems and the processes occurring in them.

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TRAINING OF A DYNAMIC SYSTEM BASED ON MACHINE LEARNING

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The difficulty of training dynamic systems using machine learning is that one has to predetermine all the states of the system before training. Optimization of the computation is currently an urgent task. In this research, a new approach is proposed based on the proposed state metric and adaptive state grid of the system.

In this research work the problem of stabilisation of the Kapitsa pendulum was posed:

$$\begin{cases} \dot{\varphi} = k\omega \\ \dot{\omega} = -sin\varphi \cdot (u(\varphi, \omega) \cdot cost + 1); \end{cases} \quad (1)$$

$$k = \frac{g}{lw^2} \quad (2)$$

where φ is the unmeasured deflection angle, ω is the unmeasured angular velocity, g is the free fall acceleration, l is the length of the light stick, t is the unmeasured time, u(φ, ω) is the control function.

The problem was solved using reinforcement learning algorithms: Q-Learning and SARSA. A metric, which is a modification of the Lyapunov function, was proposed to reduce the system states. This metric allows to determine the state of the system during training. In the same way, an initial grid of states was introduced. During training, the grid was modified using the adaptive state grid algorithm.

For each method, 100 training sessions were performed. For each training, 50 tests with different initial data were performed. The Lyapunov exponent and correlation dimension values were used to analyse the obtained training results. The non-positive values of the Lyapunov exponent for the Q-Learning algorithm were 84% of the total number of tests. For the SARSA algorithm, it was 79%. For cases of non-positive Lyapunov exponents for the Q-Learning method, the median value of the correlation dimension was 1.96 with lower and upper quartiles of 1.74 and 2.27, respectively, while for positive ones it was 2.4 (1.95, 2.82). For cases of non-positive SARSA Lyapunov scores, the median value of the correlation dimension was 1.86 with lower and upper quartiles of 1.6 and 2.17, respectively, and 2.23 (1.82, 2.68) for positive ones.

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COMPUTER ANALYSIS OF EFFECTIVE PROPERTIES OF PIEZOELECTRIC METAMATERIALS USING FACE-CENTERED CUBE AS AN EXAMPLE

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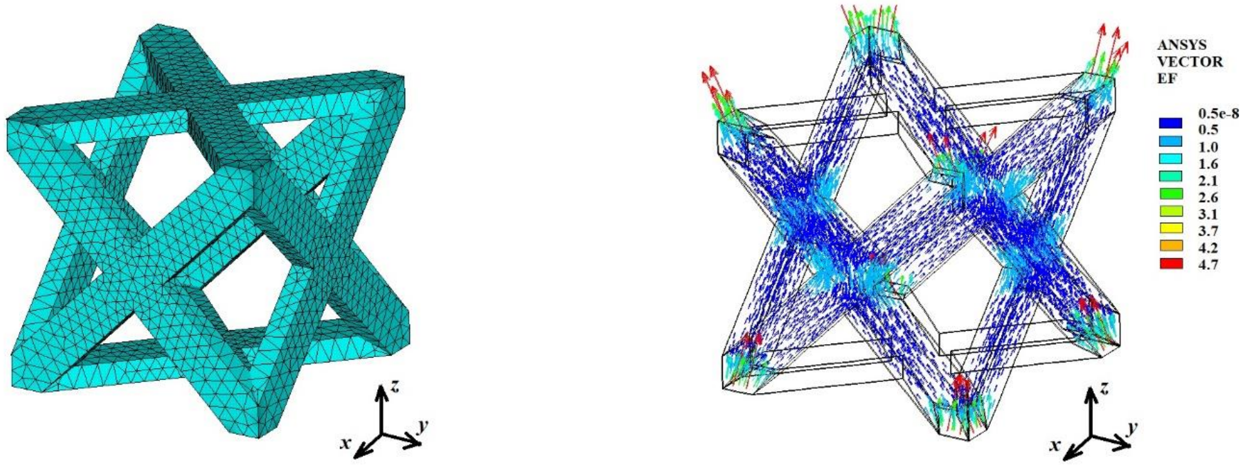
Piezoelectric metamaterials have been actively studied recently, which is due to the large-scale development of 3D printing technologies and the development of new polarization methods. This report considers theoretical problems of solving homogenization problems, finite element methods for modeling piezoelectric metamaterials and the influence of non-uniform polarization models on their effective properties.

Computational experiments were performed for a face-centered cube, which has both edges parallel to the coordinate axes and diagonal edges. Figure 1(a) shows an example of such a metamaterial with a coarse finite element mesh at a volume fraction of voids in the described cube of approximately 80%.

A feature of such a structure is its 3-3 connectivity, i.e. connectivity in three directions of the Cartesian coordinate system of both the cell material and the voids. In addition, depending on the polarization method, situations are possible when the cube edges will be polarized in different directions, and some edges may be unpolarized. Thus, from the result of the finite element solution of the cell polarization problem in the direction of the Oz axis in the simplified formulation from Fig. 1 (b), it is evident that the polarization field in this case has different values in magnitude and different directions.



a) *b*)

Fig. 1. Face-centered cube cell: finite element mesh (*a*)
and vector field of possible polarization (*b*)

The calculation results allowed us to establish the type of anisotropy of the equivalent homogeneous medium (4 mm) and to analyze the dependences of effective moduli on porosity for different polarization models. The results were compared with similar ones obtained for the complete symmetric Gibson-Eshba cell. It was noted that considering non-uniform polarization can have a significant effect on the values of effective piezomoduli, especially transverse piezomoduli.

Similar calculations were also carried out and their analysis was given for regular lattices composed of piezoelectric cells of a face-centered cube.

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MODELLING OF ULTRASONIC SPHERICAL TRANSDUCER FROM POROUS PIEZOCERAMICS WITH SPLIT ELECTRODES

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In this paper, we study a spherical transducer made of porous thickness-polarized piezoceramics that emits ultrasonic acoustic waves into the surrounding liquid medium. One of the spherical faces of the emitter is covered with a solid electrode, and the other electroded face has cuts. In the steady-state oscillation mode at a fixed frequency, as shown in [1], it is possible to control the focus position by applying electrical potential to the split electrodes with a certain phase shift. Naturally, a controlled change in focus increases the capabilities of the transducer, for example, for stopping bleeding in the field. It is also known that an increase in the efficiency of a spherical emitter of medical ultrasound can be achieved by using porous piezoceramics instead of dense ones [2,3]. Here, we analyze the possibilities of a controlled focus shift and an increase in the intensity of acoustic pressure in the focal spot due to the use of cuts and porosity of the piezoceramic material in the transducer.

The transducer was modeled in an axisymmetric formulation in the ANSYS APDL finite element package. The developed programs made it possible to construct regular finite element grids with a given number of split electrodes and take into account thickness polarization using element coordinate systems rotated in radial directions. Porous piezoceramics was specified as a solid piezoelectric material with effective properties determined from separate studies conducted earlier.

As a result of finite element calculations in ANSYS, the capabilities of this transducer for controlled change of focus depending on the number of split electrodes and the porosity of the piezoelectric ceramics were determined.

The analysis of the results allowed us to conclude that for the studied focusing emitter made of porous piezoceramics, the number of split electrodes and porosity significantly affect the possibilities of shifting the focus and the intensity of the sound pressure in the shifted focal zone. Thus, the multi-electrode coating and phasing allow us to control the type of focal region in the working acoustic medium and, as a result, increase the efficiency of the ultrasonic transducer under consideration.

The study was financially supported by the Russian Science Foundation (grant No. 22-11-00302) at the Southern Federal University.

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ON OPTIMIZATION OF VARIABLE STIFFNESS IN PRESTRESSED PLATES

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The problem of steady-state oscillations of the prestressed inhomogeneous elastic plate in an axisymmetric statement is considered (Fig. 1). The variational and weak formulations of the problem are presented. The case of free vibrations of simply supported plate is investigated. The problem of finding the optimal distribution of the plate's elastic modulus and the corresponding oscillation shape in order to maximize the first natural frequency is studied. An isoperimetric condition for the variable stiffness function is proposed. Based on the Rayleigh energy ratio, the minimum principle for the first eigenvalue and the corresponding eigenfunction is formulated. The optimality condition is formulated on the basis of the variational principle using the proposed elastic energy relation.

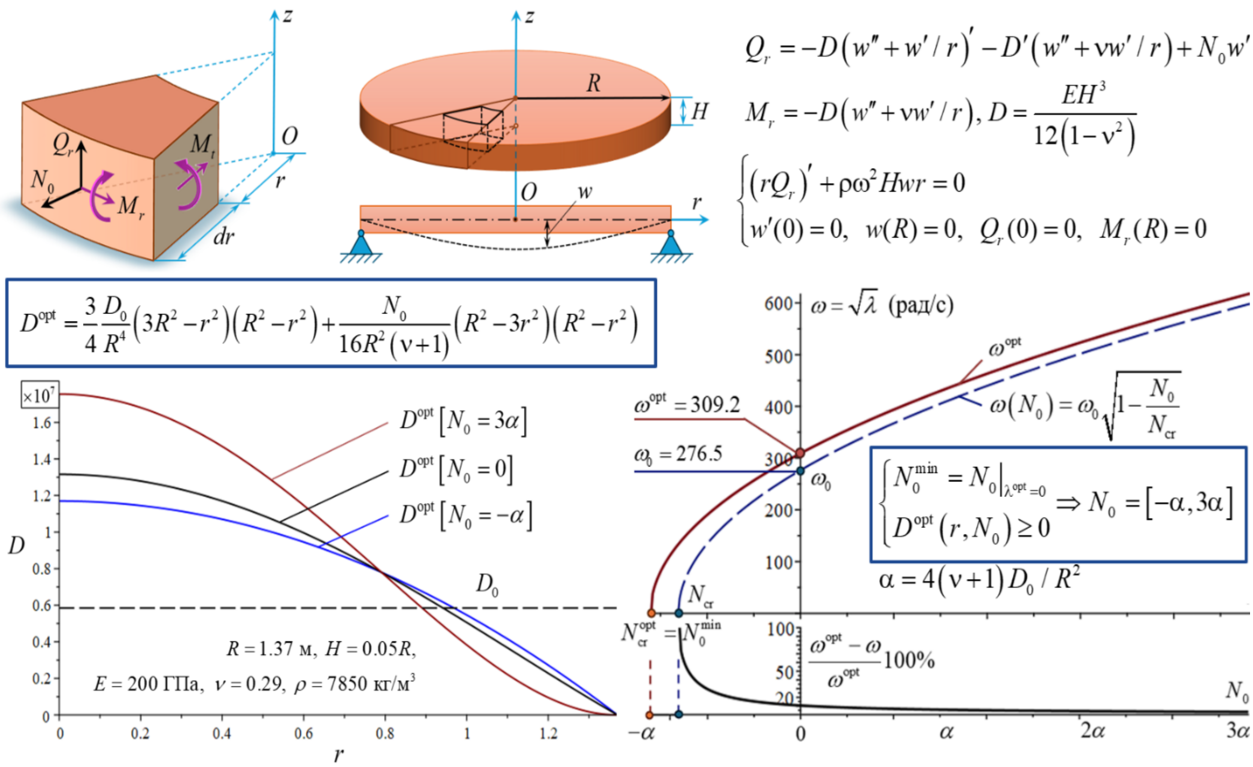

Fig. 1. Top: vibrations of a prestressed inhomogeneous plate; N_0 – radial prestress component; Q_r – shear force; M_r – bending moment. Bottom: optimal stiffness distribution D^{opt} for various prestress levels; dependence of the 1st bending resonance on prestress for homogeneous and inhomogeneous (for $D = D^{opt}$) plates

An explicit representation is obtained for the functions of the optimal oscillation shape and optimal stiffness, taking into account the initial radial stretching or compression of the plate. The range of possible prestressed values has been determined; the stability criteria is presented. The results of solving the problem in the form of building optimal laws for the stiffness inhomogeneity in the class of smooth functions in the revealed prestress range variation are obtained and analyzed.

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DEVELOPMENT AND ANALYSIS OF THE MATHEMATICAL MODEL OF BIOLOGICAL PURIFICATION OF ARTIFICIAL AQUATIC ECOSYSTEMS

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The article considers a method of biological purification of artificial aquatic ecosystems using the computational fluid dynamics and deep learning in purification of artificial biosystems. The processes involving microorganisms and conditions optimizing their activity for better water quality are described. Presented approach combines machine learning and modelling of water fluxes for purification efficiency improvement and prediction of contamination parameters.

Water quality assessment is necessary for making informed decisions, environment preservation and sustainable management of water resources, especially under condition of increasing anthropogenic contamination. Traditional approaches often face with challenges and inaccuracies in prediction which requires improvement of modelling methods. The objective of present research is to determine a way to eliminate limitations of existing methods via synergy between deep learning and modelling of fluid dynamics which improves efficiency and accuracy of prediction.

The major role in controlling purification processes plays data describing content and physiological features of microorganisms performing process of biological purification. Information on conditions in which mineralizers will feel most comfortable, quickly process organic substances in drains is necessary. Having this information, the biological purification process can be made faster and cheaper.

Biological purification is performed using biochemical method based on the ability of microorganisms to utilize various dissolved organic and non-oxidized mineral compounds such as hydrogen sulfide, ammonia, nitrite in the process of their vital activity. Microbes are highly diverse in their physiological properties, both in terms of their need in nutrients and changes made by them in the environment. Conditions, in which they can live and develop, also vary which allows to eliminate various compounds, including toxic ones, from wastewater using biochemical method [1]. There are several stages in the process of biological purification of wastewater. The most important one is a physico-chemical stage. It is intended for purification from dissolved admixtures and, in some cases, from suspended matters. Many physico-chemical purification methods require preliminary deep extraction of suspended matters. For this purpode the coagulation process is widely used. After conduction of all purification stages, including biological and physico-chemical, for the final wastewater disinfection meant for discharge to a terrain or reservoir, UV-radiation units are used. In big cities, chlorine treatment is used along with UV-radiation meyhod. The chlorine treatment lasts 30 minutes and completes purification process at treatment plants [2].

CFD (Computational Fluid Dynamics) modeling is one of the subsections of continuum mechanics. Subsection is meant to calculate characteristics of stream processes via computational and physico-mathematical methods. CFD-modelling allows to estimate temperature and make a model of airstreams in an active or projectable data center. While using CFD-modelling method, it is necessary to go through the following stages: preparative stage (creation of model's geometry, necessary physical conditions, etc.); calculation (numerical calculation of main equations on basic physical parameters); analysis (presentation of results in the form of diagrams, tables, etc.)

For every research on fluid dynamics, it is necessary to use system from the following major equations of fluid and gas dynamic streams (continuity equation, momentum conservation equation, etc.) and select one of the methods for system's solution (finite-difference method, finite-volumes method, etc.) Computational fluid dynamics (CFD), also known as 3D hydraulic modelling, represents practical way of prediction and visualization of water streams under real-life conditions: in rivers, storm drains and floor drain systems. CFD solves fundamental flow equations which describe how physics laws manage fluid' movement. It also provides degree of detail and understanding that 1D and 2D hydraulic models cannot be obtained via separation of a stream into 3 directions.

Machine learning methods, especially deep learning, offer promising opportunities for accurate water quality assessment, albeit with some challenges. The investigation is aimed at the improvement of water quality prediction by means of its integration, particularly of bidirectional long short-term memory (Bi-LSTM) nets with computational fluid dynamics (CFD). While presenting new structure which combines Bi-LSTM nets with computational fluid mechanics, this investigation offers an innovative approach to the water quality assessment. Integration of these two methods presents a comprehensive solution for overcoming challenges typical for traditional methods. It promises high reliability and efficiency in water quality parameters prediction. Bi-LSTM net can be used along with CFD-modelling for simulation of contaminants' movement and diffusion in water bodies. Using empirical data on chemical oxygen demand (COD) and biological oxygen demand (BOD), this system aims to predict key factors affecting water quality. ANSYS software, working in Windows environment, facilitates the implementation of the proposed methodology. The assessment of the proposed model demonstrates superior performance compared to traditional methods, showing higher predictive reliability and lower error. Through a comprehensive comparative study, the Bi-LSTM and CFD-based approach outperforms existing methods in accurately predicting water quality parameters, thus emphasizing its effectiveness and potential for practical applications. Integration of Bi-LSTM nets with computational fluid dynamics represents a perspective way which will improve water quality assessment. The study emphasizes the importance of using advanced computational methods to solve problems related to water quality prediction, which ultimately contributes to informed decision-making and sustainable management of water resources [1].

Biological wastewater purification systems require not only consideration of natural processes, but also accurate mathematical modeling, which is necessary to improve purification efficiency. In 1987, a group of researchers led by Mogens Henze proposed the ASM1 model, which became the basis for the development of many other models and their modifications. The ASM1 model is based on the classical Herbert and Mono models and describes the growth and decay processes of nitrifying and denitrifying bacteria. These processes are of key importance for wastewater treatment because nitrification, provided by autotrophic bacteria, converts ammonium nitrogen to nitrate nitrogen in the presence of oxygen. In contrast, denitrification provided by heterotrophic bacteria under oxygen-free conditions removes nitrate nitrogen by converting it to gaseous nitrogen. In addition, ASM1 includes descriptions of important processes such as oxidation, alkalinity change, hydrolysis of organic matter, and ammonification.

The use of computational fluid dynamics (CFD) in combination with deep learning methods such as Bi-LSTM provides a significant advantage for predicting water quality parameters and improving the efficiency of biological purification of artificial ecosystems. The combination of these methods allows not only a more accurate simulation of the processes of movement and diffusion of pollutants in water bodies, but also takes into account the dynamics of growth and death of microorganisms, which is important for optimizing the conditions of their activity. Application of such a model can significantly improve wastewater purification processes, making them more accurate and reliable.

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STUDY OF THE MAGNITUDE OF THE SUPPORTING PRESSURE IN TRAIN CABINS

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In view of the active electrification and automation of motor vehicles, more attention has recently been paid to optimizing the operation of climate control systems, which allows not only to achieve comfortable microclimate indicators, but also reduces the energy consumption of the climate control system.

The standard HVAC (heating, ventilation and air conditioning) parameters include temperature, speed, air humidity, oxygen and carbon dioxide concentration. However, in the cited works, insufficient attention is paid to studying the issue of excess internal pressure, which ensures the operation of the climate control system in different operating modes.

Below in this work, all designations and pressure values are given as excess pressure relative to the standard atmospheric pressure.

The following factors can be distinguished as criteria for the range of excess internal pressure:

– the maximum pressure value should be regulated by the technological strength features of the cabin body. For example, there are cases when the cabin windows were "squeezed out" by excess pressure due to malfunctions of the outlet valves - P_1;

– the maximum pressure should be limited by sanitary requirements for the criterion of impact on human health P_2. An increase in atmospheric pressure of no more than 10 mm Hg or 1333 Pa is considered harmless;

– the lower range of values is determined by the technological features of the cabin, consisting of the presence of leaks. In order to prevent gas exchange and the penetration of contaminants through leaks, increased pressure is created in the cabin, which is pumped up by the fans of the air conditioning system. Moreover, the external pressure should be estimated not relative to the atmospheric pressure, but relative to the excess external pressure on the cabin body, which is formed due to the resistance to the movement of transport.

Thus, the range of the desired value of increased pressure in the cabin P_{int} can be represented as follows:

$$P_{norm} < P_{ext} < P_{int} < P_2 < P_1.$$

In this paper, research is carried out using the example of a train cabin [1]. To find the external air pressure P_{ext} , the problem of combine movement in a wind tunnel is numerically considered, based on the Navier-Stokes equations [2-3], the air pressure on the cabin skin is found depending on the speed of movement.

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AN AVIAN EGGSHELL AS THE NOVEL MODEL SUBSTANCE FOR DENTAL MATERIALS SCIENCE

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Biominerals or minerals of biological genesis play an important role in biological systems and organisms. For example, their mechanical properties govern by deformation behavior of hard tissues of human body. However, their small volume in human organs and connecting etic problems demand a searching for a substitution of tooth enamel and bone tissues for laboratorical studies of mechanical properties of human body biominerals. An avian eggshell is the prospective substitution [1], which can be used for the solving of some task of dental materials science [2].

Bird eggshell is mineral consisted of 90% of calcium carbonate of the biological genesis. This paper devotes to discussion of deformation behavior of eggshell of some domestic and wild bird, including hen, goose, gray heron, black-headed gull, buzzard, and capercaillie. 3pts bending was chosen as the deformation scheme. Working surfaces of specimens were documented with a help of optical microscope, while their fracture surfaces was examined on scanning electron microscope. Two kits of specimens were cut from each bird eggshell. Bending was carried out on dry and wet samples on air. Cracks in eggshell under bending was also studied during in situ test on a light microscope.

It was confirmed that specimens of bird eggshell exhibit brittle behavior on the macroscopic scale in both dry and wet states. However, crack width could be grown by the increasing of the arrow of bending as in plastic metals under tension. Water environment stimulates small decreasing of strength of an eggshell under bending, but does not change the brittle type of deformation behavior. Crack morphology in a bird eggshell is close to dangerous crack in neck region of a plane aluminum sample. It means that biomineral having covalent chemical bonding exhibits some features of fracture behavior, which are inherent to a metal, on the microscopic scale. The cause of this effect is discussed.

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INVESTIGATION OF STATIC STABILITY LOSS IN A MICROPOLAR FLEXIBLE SPHERICAL SHELL WITH CIRCULAR PLANFORM

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Flexible axially symmetric spherical shells, both standalone elements and components of complex structures, are widely used in aerospace and aviation technology, shipbuilding, automotive engineering, power and chemical engineering, instrument making, and in medicine. This study investigates the static stability loss in flexible spherical shells with a circular planform and micropolar structure [1, 2]. The shell material is homogeneous, isotropic, and elastic.

In deriving the equations of motion for the shell element, the Kirchhoff-Love hypothesis is applied. The shell is assumed to have hinged and movable boundary conditions. To reduce the system of nonlinear partial differential equations to a Cauchy problem, the finite difference method with second-order accuracy is employed. The Cauchy problem is solved using the fourth-order Runge-Kutta method [3, 4]. The load-deflection ratio is obtained using the stabilization method (see Fig. 1).

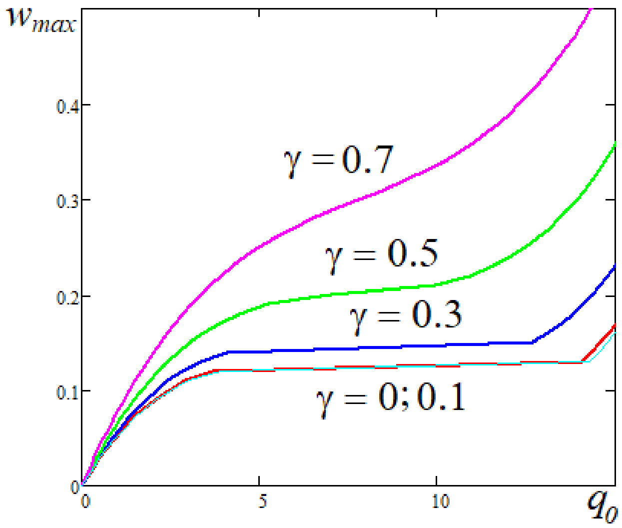

Fig. 1. Load-Deflection ratio

The study analyzes the influence of the scale-dependent length parameter on the static stability of the shell. For a $\gamma = 0;\ 0.1$ the critical loads are identical. As the parameter $\gamma = 0.3$ increases, the critical load also increases. When the parameter γ reaches $\gamma = 0.5;\ 0.7$ a certain threshold, static stability loss is absent, though an inflection point appears, resembling the behavior of shells with low curvature. Thus, increasing the scale-dependent parameter γ enhances static stability.

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INTERLABORATORY STUDY OF THE RELATIONSHIP BETWEEN ELASTIC PROPERTIES AND BONE MINERAL DENSITY

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The purpose of this study was to analyze the elastic characteristics of the spongy bone of bovine vertebrae during compression with an assessment of the degree of anisotropy and their dependence on the volumetric bone mineral density (vBMD), as well as an analysis of interlaboratory reliability during such experiments.

To achieve this goal, the following tasks were solved:

– Experimental study of the mechanical behavior of spongy tissue of cow vertebrae under uniaxial compression in two different biomechanical laboratories.

– The vBMD calculation is based on firing a bone sample in a muffle furnace.

– Analysis of the dependences of the modulus of elasticity on vBMD.

– Interlaboratory comparison of the modulus of elasticity and the obtained dependence between the modulus of elasticity and vBMD.

The samples were cut in three directions: along (the Z axis) and across (the X and Y axes) of the vertebra. The height of the samples varied from 25 to 45 mm, width (length) - from 5 to 9 mm.

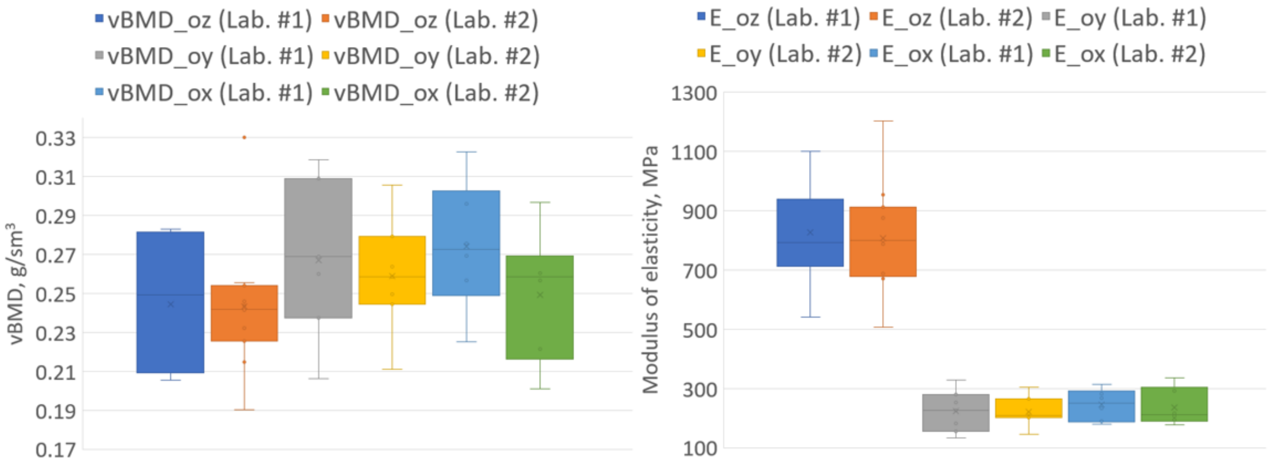

Fig. 1. Statistical distribution of the measured values of vBMD (left) and elastic modulus (right)

The axial modulus of elasticity was about 3.5 times higher than the transverse one. It has been shown that vBMD with a high coefficient of determination (more than 0.72) determines the modulus of elasticity. The high similarity of the results of experiments conducted in two different laboratories at different test facilities was demonstrated.

The study was carried out within the framework of the State task FSRR-2023-0009.

NUMERICAL ANALYSIS OF MECHANICAL PROPERTIES OF SHORT FIBER-REINFORCED POLYMER ABS COMPOSITES WITH VARIATION OF MORPHOLOGICAL CHARACTERISTICS

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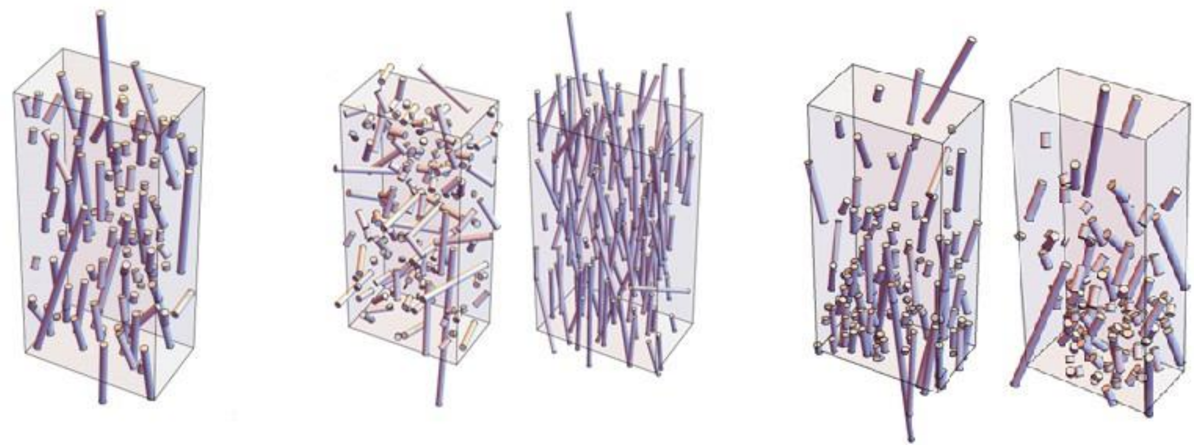
Additively manufactured composites represent a new class of materials with unique tunable properties. Compared to traditional materials, composites offer unprecedented physical and mechanical properties through the capabilities of pre-design, which can be tailored for a wide range of applications. In this work, composite material models with different properties of short fiber morphometry (Fig. 1): length, fiber angle orientation and its distribution gradient in the structure were studied. The combination of distribution gradient and change in fiber angle orientation distribution were examined. The effects of the above parameters are investigated in terms of mechanical response, with analysis of anisotropy of the effective elastic modulus and statistical analysis of minimum principal stresses distribution.



Model based on microtomography data | Models with variation of orientation angle and fiber length distribution | Models with short fibers gradient

Fig. 1. Models of reinforced structures with different morphological parameters

The matrix used is acrylonitrile-butadiene-styrene (ABS), with short carbon (CF), glass (GF), and basalt (BF) fibers as reinforcing particles. Geometrical parameters were determined using microscopic tomography and images obtained from optical and scanning electron microscopes [1, 2].

The analysis of the results showed that fiber length variation has the greatest impact on mechanical properties. As the range of orientation angle distribution increases, the properties of two-phase structures become close to isotropic. At the same time, the presence of a gradient in the distribution of short fibers within the structure altered the effective properties by no more than 1%, while the degree of anisotropy did not increase.

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ON A METHOD FOR ASSESSING EFFICACY OF TOOTH ROOT CANAL INSTRUMENTATION PROCEDURE

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In the paper a novel method for assessing the efficacy of root canal treatment using rotary dental instruments (files) in *ex vivo* conditions, which is based on the experimental technique of the computed X-ray microtomography is presented. The idea of the method is to accurately compare three-dimensional models of teeth before and after canal instrumentation with subsequent analysis of the effect of this intervention on the width of the canals at some key points from the point of view of the dental clinician (1 mm from the apical foramen; 3 mm from the apical foramen; convergence of canals; the mouth of the canals). Thus, the obtained data in the form of a number of virtual tooth slices is segmented, and the root canal volume is calculated using specialized software developed in accordance with a specific protocol. Additionally, the method includes analysis of the microgeometry of the root canals, allowing for a deeper understanding of the structural characteristics of the teeth treated. As an illustration of the application of the proposed method, the study considers the features of root canal instrumentation in human two- and three-root molars, which emphasizes the importance and relevance of this approach in the field of clinical practice. Procedure was performed by a practicing dental clinician using the ProTaper Next file system (Maillefer, Ecublanc, Switzerland) in accordance with the manufacturer's recommended protocol. Microtomography of both samples was carried out using an Xradia Versa 520 unit (Carl Zeiss Xray Microscopy, Inc., Pleasanton, USA) in cylindrical polymer holders with distilled water with the same parameters: X-ray tube voltage 110 kV, power 9.5 V, pixel size 14.7 µm, rotation sample at 360°, exposure time 1 s, filter on X-ray tube HE6. The human molars were removed from patients for orthodontic indications at the State budgetary institution of the Rostov region “Dental clinic” in Rostov-on-Don. The local independent ethical committee of Don State Technical University approved the study (conclusion No. 1 of January 15, 2024), patients provided informed consent.

The work was carried out with the financial support of the Russian Science Foundation, grant No. 22-19-00732. The results were obtained using the resources of the Resource Center of Collective Usage “Materials” of Don State Technical University.

MODELING OF SURFACE DAMAGE OF A BUILDING STRUCTURE ELEMENT AND ITS DYNAMIC PROPERTIES

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The main power elements of building structures are concrete or reinforced concrete structures. Over time, due to the action of aggressive environments (humidity, temperature differences, etc.), microcracks appear on the outer surfaces of these elements, leading to the appearance of damaged layers. Timely monitoring of the damaged state of these elements can prevent their destruction and possible consequences associated with this.

In this paper, a damaged extended structural element is modeled by a two-layer elastic strip, the upper layer of which is relatively thin and has different material properties and models damage. It is assumed that the damaged layer is a porous material and its effective properties, depending on the percentage of porosity, are calculated in the ACELAN-COMPOS package [1]. Thus, the thickness of the upper layer and porosity characterize the degree of surface damage, and the problem of monitoring the damaged state is reduced to identifying these two parameters. As additional information for solving this inverse geometric and coefficient problem, data that can be measured in a full-scale experiment are considered, namely, the spectrum of natural frequencies and the maximum amplitude of displacements during steady-state oscillations under the action of force excitation.

The finite element method implemented in the ACELAN package [2] is selected as a method for solving direct problems of model and harmonic analysis. The dependencies (surfaces) of the first resonant frequency and maximum deflection of the strip on the thickness of the damaged layer and the percentage of porosity are constructed. A joint analysis of these surfaces and their level lines indicate the possibility of restoring the parameters characterizing the damaged state of the structure.

Thus, the possibility of solving the indicated inverse problems is shown, and therefore the answer to the question about the state of the structure. The next step of the study in this direction is to model implanted piezoelectric sensors and sensors and read additional information from their readings.

The work was supported by the Ministry of Science and Higher Education of the Russian Federation, agreement: № 075-02-2024-1431.

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IDENTIFICATION OF DAMAGE TO AN EXTENDED ELEMENT OF A BUILDING STRUCTURE BASED ON CHANGES IN THE WAVE NUMBERS OF PROPAGATING WAVES

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Many building structures are extended concrete or reinforced concrete structures (pillars, supports, bridge spans, etc.). Over time, damage accumulates on the surface of these elements, the monitoring and identification of which is an important task to ensure the safety of the operation of these structures. The paper presents mathematical modeling of such damaged elements within the framework of the anisotropic linear theory of elasticity and solves the inverse problem of identifying the damage parameters.

The damaged element model is an extended structural element (layer, strip, endless beam of a certain section); the damaged layer is located on the surface that comes into contact with the aggressive environment. This layer is characterized by "weakened" mechanical properties compared to the main material of the structure. In the work, it is modeled by a porous material, the effective properties of which are in the ACELAN-COMPOS package [1]. Thus, in these models, the damage parameters are the thickness and percentage of porosity of this surface layer.

Identification of these damage parameters is based on the analysis of changes in the characteristics of elastic waves propagating in them. For this purpose, in the work in the FlexPDE package, programs for calculating dispersion curves for various cross-sections of the considered waveguides and anisotropic materials were developed. Their dependencies on the thickness of the damaged layer and its percentage of porosity were constructed. Analysis of these dependencies for various branches of dispersion curves shows the possibility of identifying damage parameters. Further development of this direction will be associated with the use of information obtained from the characteristics of waves excited by real sources.

The work was supported by the Ministry of Science and Higher Education of the Russian Federation, agreement: No. 075-02-2024-1431.

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IDENTIFICATION OF SCALE IN STEAM BOILER TUBES BASED ON THE SOLUTION OF A NON-STATIONARY HEAT CONDUCTION PROBLEM

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The formation of scale in steam boiler tubes has a negative effect on their performance, so the problem of monitoring their condition is of great importance. The main feature of such a process is the possibility of non-destructive testing, for which two types of data can serve as information: acoustic measurements and thermal ones. This paper considers the solution of the inverse geometric problem of determining the scale thickness on the inner surface of the tube based on the solution of direct non-stationary problems of heat conductivity.

Due to the periodicity of the boiler wall structure, a flat formulation of the problem is considered for half of the cross-section of the periodicity element in the form of a two-layer semi-ring and half of a flat panel between the tubes. The tube is filled with water or steam or both components. The problem is solved within the framework of the theory of heat conduction for a composite body. On the left (inner) surface of the element, the heat flux from the combustion of gas or coal is specified, on the right (outer) surface, heat exchange with the environment. In the case when water and steam are considered simultaneously, the boundary between them is not constructed, but is determined from the value of the vaporization temperature, while a surface heat source (negative) corresponding to the energy of vaporization is specified on this boundary. In addition, a volumetric heat source (negative) is specified in the liquid phase, which models the flow of water through a section with a lower temperature.

To solve the described nonlinear (coefficients and source position depend on the temperature of the environment) non-stationary problem of heat conduction, the finite element method (FEM) implemented in the FlexPDE package is used. In the finite element approximation, the source of vaporization is modeled by a narrow Gaussian curve similar to [1]. Based on the developed program, the non-stationary problem of heat conduction is solved and the temperature inside the region and on the right (external) surface is calculated. The temperature dependencies at the points of this surface are constructed. The temperature monotonically depends on the thickness of the formed scale. Thus, the analysis of these dependencies allows us to uniquely solve the posed inverse geometric problem.

In further development of this topic, it is proposed to use the constitutive relation for liquid and gaseous media, i.e. the relationship between temperature, pressure and volume.

The work was supported by the Ministry of Science and Higher Education of the Russian Federation, agreement: No. 075-02-2024-1431.

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USING POROUS PIEZOCERAMICS IN A STACKED PIEZOELECTRIC ELEMENT

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Piezoelectric transducers are widely used in all areas of human activity, including medicine and health care. This causes scientists to be very interested in the topic of modeling, creating new designs and optimizing devices with piezoelectric elements. One way to increase the efficiency of such devices is to use piezoactive composite materials, including porous piezoceramics.

The work is devoted to the numerical study of the efficiency of using porous piezoceramics in a stack piezoelectric element, which can be used as a power element of a drive, a piezoelectric generator, an ultrasonic emitter. The use of porous piezoceramics in stack piezoelements has not received enough attention in the literature.

The paper presents a finite element model of a stack piezoelectric element consisting of eight counter-polarized cylinders. The finite element method implemented in the ACELAN package [1] is used as a solution method. The effective properties of porous piezoelectric ceramics are calculated in the ACELAN-COMPOS package [2]. An analysis of its output characteristics is carried out depending on the percentage of piezoelectric ceramics porosity, which varies from 0% to 80%. Models of different operating modes of this device are considered, namely, as a force element (actuator), an energy harvesting device (piezoelectric generator) and an acoustic wave emitter. In the low-frequency region (the natural frequency of the first axial resonance and below), the dependences of the natural frequencies of resonance, antiresonance and KEMS, force and energy characteristics, output electric potential and oscillation amplitude of the free end are constructed.

Analysis of the obtained dependencies showed that with increasing porosity, the output potential and the amplitude of free end oscillations increase significantly, i.e. porous piezoceramics are appropriate to use in PEG devices and acoustic wave emitters. In addition, the task of developing a two-phase PEG when operating on the second longitudinal axial mode has been set.

The study was carried out at the expense of the Russian Science Foundation grant No. 22-11-00302), https://rscf.ru/project/22-11-00302/ at the Southern Federal University

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MODELING OF THE POLARIZATION OF A HIGHLY POROUS PIEZOCOMPOSITE OPEN CELL AND ITS MECHANICAL PROPERTIES

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The problem of deformation of a flat cell of a highly porous piezoactive composite with inclined ribs is considered. Highly porous composites, such as metal foams, are widely used due to their mechanical properties. Various methods of their mathematical modeling, including those based on periodic Gibson-Ashby cells, are presented in the literature. Piezoactive composites also have a number of properties, such as high sensitivity of sensors, a wide bandwidth, which is the reason for the interest in their modeling. However, when constructing such models from piezoceramics, a certain difficulty arises associated with the choice of the distribution of preliminary polarization. It should be noted that this issue, especially for highly porous piezoceramics, has not been sufficiently studied in the literature. Therefore, in this paper, the issue of the influence of the polarization model on the characteristics of the piezoactive composite is investigated.

The design material is PZT-4 piezoceramics, the polarization of which significantly depends on the conditions of its induction (model geometry, electrode arrangement). For a highly porous composite, which is considered in this paper, this issue is of particular importance, since non-uniform polarization can occur in the composite elements, and some elements remain practically unpolarized. In this regard, the study is divided into two steps: in the first, residual polarization is induced based on the theory known in the literature, the implementation of which is carried out in the ACELAN package [1]; in the second, a number of problems are solved for a composite cell and the dependence of its properties on the polarization model is found. The finite element method implemented in the ACELAN package [1] is used as a method for solving the corresponding boundary value problems of electroelasticity for piecewise inhomogeneous bodies.

The problem of determining the non-uniform polarization for two types of flat cell designs with highly porous piezoceramics is solved. Some features of the obtained polarization distribution are noted, in particular, its non-uniformity and the presence of opposite polarization in some edges. The problems of determining the natural frequencies and oscillation modes "inside the cell" and their dependence on the polarization model (uniform and non-uniform) are solved. It is noted that some frequencies differ by 10%, and the oscillation modes qualitatively coincide. The work also analyzes the dependence of the stress-strain state and output characteristics on polarization, and the difference in some values reaches 15%.

The study was carried out at the expense of the Russian Science Foundation grant No. 22-11-00302), https://rscf.ru/project/22-11-00302/ at the Southern Federal University.

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THE SIMPLIFIED MODEL OF THE INTERACTION OF THE ARTIFICIAL LENS WITH THE INTRAOCULAR BAG

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The problem of replacing the human eye lens, despite the widespread use of these operations, continues to interest the scientific community. Several tasks of its optimization should be noted, among which the following can be highlighted: development of new models of lens implants; development of new tools. In this paper, the first task is considered, in which the lens model presented in [1] is investigated. A notable feature of this model is that the artificial lens is two lenses (optics) to the outer round edge of which elastic curvilinear rod elements (haptics) are attached, which rest on the inner part of the intraocular sac. Under the action of the ciliary muscles, the outer edges of the haptic elements are deformed in the radial direction, while the lenses perform axial movements. This design of the artificial lens allows the accommodation process, which significantly expands the capabilities of the implant compared to single- or dual-focal lenses.

The main problem of developing such an implant is the choice of the dimensions and rigidity of the haptic elements. In [1], three-dimensional finite element models of such devices and their interaction with the intraocular sac are constructed. However, the calculation of this interaction is associated with certain difficulties, namely, the description of the contact interaction, a large number of finite elements. In this paper, a simplified model of the structure and its interaction with the intraocular sac is constructed. Due to the fact that the main elements have axial symmetry, the problem is considered in an axisymmetric formulation. The finite element package ANSYS is used for the solution. Two models are constructed: in the first, the walls of the sac are modeled by two-dimensional axisymmetric elements of the PLANE type; in the second, by elements of the SHELL type.

At the first stage, the direct problem of interaction of haptics of a given geometry with the internal walls of the intraocular sac was solved, i.e. the dependence of the axial displacement of the upper lens on the efforts of the ciliary muscles was constructed. The next problem to be solved is the problem of optimizing haptics.

The work was supported by the Ministry of Science and Higher Education of the Russian Federation, agreement: No. 075-02-2024-1431.

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MODELS OF LENS TISSUE DESTRUCTION DURING LENS REPLACEMENT SURGERY

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The problem of replacing the human eye lens, despite the widespread use of these operations, continues to interest the scientific community. Several tasks of its optimization should be noted, among which the following can be highlighted: development of new models of lens implants; development of new tools. In this paper, the second task is considered, in which the Finite Element Modeling of a Lensotome Tip with Piezoelectric Drive presented in [1] is investigated.

The work does not take into account the interaction of the lensotom needle with the lens tissue; this work discusses models of this interaction, which results in the destruction of the lens. Since the modulus of elasticity of the lensotom needle is two orders of magnitude greater than the modulus of the lens, it can be approximately considered an absolutely rigid body and only the lens tissue can be modeled. In the first problem, the kinematics of the needle is set and the stress-strain state of the lens is studied within the framework of the linear theory of a viscoelastic body. Mechanical stresses in the contact area are calculated and von Mises stresses are considered as a criterion. The second model is the force action on the tool that interacts with the lens.

Different modes of instrument movement are considered: axial, rotational, transverse and different geometry of its front end. In addition to the destruction process, the lens movements are monitored, since with its large amplitude, damage to the ciliary muscles is possible. In this matter, the fact that a vacuum is created in the needle tube, which acts on the lens tissue in the opposite direction, is important.

The first stage of the work consists of constructing models of interaction of the tool with tissues in the finite element package ANSYS, and selecting a destruction model. Future stages will be the analysis of various movements of the tool, including frequencies and amplitudes of oscillations. Based on this analysis, the optimal destruction mode will be selected.

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DESIGNING SCREW PRESS FOR TESTS COMBINED WITH OPTICAL MEASUREMENTS

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The modern development of technologies in the field of additive manufacturing allows to create structures with irregular internal structure. But internal defects may occur during the production of such products. To date, the most popular method of studying the internal structure is computed tomography, which allows you to get the necessary information without having to destroy the specimen [1]. Existing analogs have a limited shooting area and the maximum load reaches up to 2kN. Therefore, the aim of this work is to create an automated tooling to perform compression tests inside a CT scanner [2].

The advantages of using automatic loading are: providing uniform pressure on the sample under study, allows you to monitor the failure of the sample in real time, eliminates the possibility of operator error.

To achieve the goal, the following tasks were solved: production of automation of the loading process, development of the control system [3], creation of a graphical user interface, and conducting experiments.

As a test of the device performance. Test tests were conducted, in which a sample in the form of a 3D-printed cube with dimensions 20x20x20 was loaded. The data recorded during the loading in a text file was checked against the readings of the stationary testing device UTS 110M-100. The coefficient of determination is 0.997.

Thus, as a result of the work performed, the mechanical uniaxial loading device has been improved by replacing the mechanical part of the existing tooling with an automatic one.

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ELASTIC WAVES EXCITATION AND FOCUSING BY A PIEZOELECTRIC TRANSDUCER WITH INTERMEDIATE LAYERED ELASTIC METAMATERIALS WITH PERIODIC ARRAYS OF INTERFACIAL VOIDS

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For nondestructive inspection of metallic and composite structures, ultrasonic methods relying on elastic waves as a physical basis are widely adopted [1]. A common way for the excitation of wave motion in the examined construction is to use piezoelectric transducers of different types.

Elastic metamaterials (EMM) are composite elastic materials with artificial microstructures made to exhibit unusual mechanical wave characteristics such as waveguiding, wave focusing and lensing, energy conversion etc. Since EMM can be used to manipulate elastic wave propagation, EMM employment as elements of transducers and sensors has a significant potential [2].

The aim of this study is to consider the employment of EMM for providing advanced characteristics of wedge transducers. A schematic design of the considered transducers with EMM is depicted in Fig. 1.

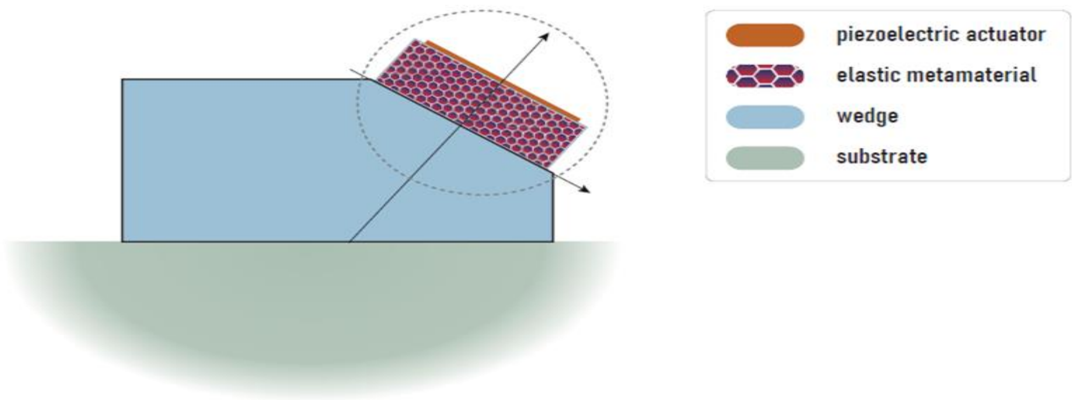

Fig. 1. An example of possible design of the proposed configuration of the ultrasonic transducer with the piezoelectric actuator and EMM intermediate

An elastic metamaterial consists of a given number of cells, each of which consists of two elastic layers. There is an array of crack-like voids of a given width with a given distance from each other in each cell at the interface of the layers. Elastic waves are excited by a piezoactuator located on the upper surface of an intermediate block made of elastic metamaterial. Numerical experiments have shown that the proposed configurations with EMM insertion can sufficiently change wave energy transmission from a piezoelectric active element into media for various frequency ranges (relatively low frequencies as well as higher ones) [3].

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INVESTIGATION OF A DYNAMIC SYSTEM WITH A BIONIC CONTROL SYSTEM

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Artificial intelligence methods and neural networks have found great application in classification, clustering and management tasks. Despite the existence of classical approaches to solving optimal control problems, such as the Pontryagin maximum principle and Bellman dynamic programming [1, 2], machine learning methods and genetic algorithms reduce the smoothness requirement for defined functions, but at the same time, most research in this field has a number of fundamental limitations.

This paper presents a method for implementing dynamic system control using a neural network model [3]. The work was performed in a package of application programs for modeling dynamic systems – MATLAB SIMULINK. The task of stabilizing a dynamic system using a bionic control system was considered. An example of a dynamic system was a two-dimensional model with two pairs of antagonist muscles, the biomechanical Millard model was used as a muscle model [4]. A bionic control system was used to control muscle activation, the architecture of which is described in Rybak's work [5, 6].

The purpose of this work is to create a dynamic system management system based on a neural network model with feedback.

As a result of the work carried out, a reliable dynamic system was built and the connection between the programs controlling and modeling the dynamic system was implemented. Functional blocks were identified and a control system for muscle regulation based on a neural network was built, a bionic control system was created, and a stable position was achieved for a certain time.

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ANALYSIS OF LONGITUDINAL VIBRATIONS OF A ROD BASED ON THE GRADIENT THEORY OF ELASTICITY

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The analysis of vibrations of micro-sized rods is of great interest due to the need for mechanical calculations of elements of micro-electromechanical systems [1]. However, the classical theory of elasticity cannot describe scale effects that are manifested by the dependence of the frequency spectrum of free vibrations of a body on its dimensions and microstructure features [2]. Description of scale effects is possible from the standpoint of the gradient theory of elasticity (GTE), in which the scale parameters of the dimension of length are included in the constitutive relations as factors.

The problems of finding the spectrum of eigenvalues and eigenmodes of longitudinal vibrations of an elastic rod are studied, taking into account scale effects for three types of boundary conditions: 1) one end is rigidly fixed, and the other is free; 2) both ends are rigidly fixed; 3) both ends are free. GTE problems are singularly perturbed, since they contain differential equations with a small parameter at the highest derivative. Such problems can be solved using the Vishik-Lyusternik asymptotic method [3]. The expression for the amplitude of the rod displacement is represented as a sum of three functions, where the first term of the sum describes the change in the amplitude of oscillations far from the rod boundaries (classical solution), and the second and third terms are boundary layer functions. Each of the functions in the expression for the displacement is represented as an expansion in a small parameter. Restricting ourselves to two approximations in the Vishik-Lyusternik method, we obtain asymptotic corrections to the natural frequencies and modes of oscillations of the rod for a small value of the scale parameter. Accurate values of the spectrum of eigenvalues in the gradient formulation are obtained by solving frequency equations, which are obtained from the equality to zero of the determinant of the system of algebraic equations under satisfying the boundary conditions.

To check the accuracy of the asymptotic formulas, a comparison of the eigenvalues obtained by solving the frequency equation and by the asymptotic formulas for different values of the scale parameter is performed. Calculations have shown that: 1) if both ends of the rod are free, no scale effects occur; 2) as the rod length decreases (the scale parameter increases), the eigenvalues increase; 3) an increase in the scale parameter leads to a decrease in the displacement amplitude, with the gradient effect being most pronounced in the vicinity of the clamped ends; 4) approximate asymptotic formulas for finding the eigenvalues give a relative error of less than 1% when the scale parameter does not exceed 0.06.

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ON THE IDENTIFICATION OF TWO-DIMENSIONAL LAWS OF CHANGE OF VARIABLE THERMOPHYSICAL CHARACTERISTICS

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In recent years, functionally graded materials (FGM) have been increasingly introduced into various fields of technology. These are composite materials whose thermophysical properties change uniformly along a developed profile [1]. Due to the multi-stage technology of FGM production, the laws of change in thermophysical characteristics in the finished product may differ significantly from the specified ones. To solve this problem, it is necessary to use the apparatus of coefficient inverse problems of heat conductivity (CIHP) [2, 3]. In most cases, to solve one-dimensional CIHP, the minimization of the residual functional [3] or the iterative algorithm of the Newtonian type [2] is used, at each stage of which the integral Fredholm equation of the first kind with smooth kernels is solved. Despite the relevance of the problem, in domestic and foreign literature there is a shortage of studies devoted to the identification of two-dimensional inhomogeneous laws of change in thermophysical characteristics in solids. The direct and inverse problems of heat conduction for a functionally graded rectangle are investigated. Its lateral faces are thermally insulated, the lower boundary is maintained at zero temperature, and the following are specified on the upper boundary: 1) temperature; 2) heat flux.

The direct problem in a weak formulation is solved using the finite element method in the FreeFEM++ package. The accuracy of the solution of the direct problem for a homogeneous rectangle in the FreeFEM++ package is estimated by comparing it with the analytical solution. The analysis demonstrated the high accuracy of the FEM solution.

Using the projection method and the finite element method, an iterative-regularization scheme is constructed for solving the inverse problem of identifying two-dimensional laws of heterogeneity of thermophysical characteristics based on temperature or heat flux measurements on the upper section of the boundary in a given time interval. At each iteration, it is necessary to solve an ill-conditioned system of linear algebraic equations with respect to corrections to the expansion parameters of the desired functions. The initial approximation is also chosen in the form of constants by minimizing the residual functional on the grid, using information about the limited thermophysical characteristics. Numerical results of the reconstruction of some two-dimensional laws of non-uniformity of the thermal conductivity coefficient and specific heat capacity of a rectangle are discussed.

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ON INCREASING THE FREQUENCY OF NATURAL BENDING VIBRATIONS

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The optimization problem of increasing the minimum frequency of natural bending vibrations of a non-uniform beam is considered. Young's modulus variable along the axial coordinate is taken as the control function. Two types of problems are considered: in the problem of the first type, only the isoperimetric condition is imposed on the Young's modulus [1]. In problems of the second type, additional restrictions [2] are imposed on the minimum value of the elastic modulus. For problems of both types, an optimality condition is obtained based on the variational approach.

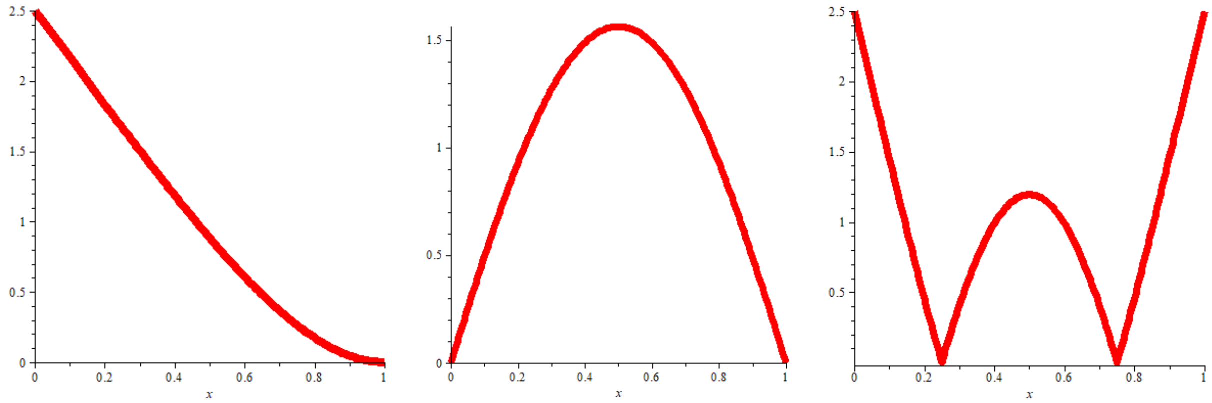

Fig. 1. Dimensionless Young's modulus along the axial coordinate: console (*a*), hinged support (*b*), both ends fixed (*c*)

Optimal solutions are constructed in analytical form. Various boundary conditions are considered: cantilever fastening, hinged support, rigid fastening of both ends [1], and spring-type boundary conditions. For the latter, asymptotic expansions of the function describing the dependence of the natural frequency of oscillations on the parameters included in the boundary conditions are constructed. The problem of the second type shows the existence of regions where Young's modulus reaches a minimum value. In these regions, the deflection function is found in the same way as when solving the problem for a homogeneous beam. In the remaining region, the solution is described by polynomials arising from the integration of the optimality condition. When describing the solution many parameters are introduced. Some of them are determined analytically from the solution of a system of linear algebraic equations. The frequency of natural oscillations and special points (coordinates of the boundaries of the homogeneous and inhomogeneous regions) are found numerically from the nonlinear system.

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MATHEMATICAL MODELING OF OUTCOMES IN PATIENTS WITH ATRIAL FIBRILLATION AFTER RADIOFREQUENCY ABLATION

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Atrial fibrillation (AF) is the most common sustained cardiac tachyarrhythmia and is associated with decreased quality of life and increased mortality and morbidity from other cardiovascular diseases. Radiofrequency catheter ablation has become the treatment of choice for AF since the beginning of the 21st century. The primary goal of this method is to eliminate symptoms and improve quality of life. The secondary goal is to improve outcomes and prognosis in patients with AF [1]. Catheter ablation of atrial fibrillation (AF) has become an important rhythm control strategy and is currently the most common cardiac ablation procedure performed worldwide. The principle of catheter ablation is to achieve electrical isolation by linear destruction of cardiac tissue, making AF a curable disease [2]. Current guidelines recommend the procedure for patients with symptomatic paroxysmal or persistent AF who are refractory or intolerant to antiarrhythmic drugs. This procedure can also be considered as a first-line method in selected asymptomatic patients. Data from large registries indicate that AF ablation can reduce mortality and the risk of heart failure and stroke, but data from randomized controlled trials are inconclusive [3]. Another pressing issue is the fact that a high proportion of patients who have undergone this procedure experience recurrent arrhythmia [4]. All of the above dictates the need to create a software calculator based on mathematical modeling of outcomes in patients with atrial fibrillation after radiofrequency ablation, in whom biological markers were assessed before the procedure. It is also necessary to select the most appropriate combination of markers based on mathematical methods, which will be assessed in this group of patients. The constructed model can subsequently be corrected and improved using artificial intelligence (AI) through machine learning, including the use of neural networks, in order to create the most optimal system for predicting outcomes in patients with AF before the RFA procedure [7].

The aim of the study is to analyze the course and prognosis of atrial fibrillation in patients after radiofrequency ablation using biological markers and to evaluate the possibility of mathematical modeling of outcomes in these patients.

Currently, when accessing PubMed using the keywords “atrial fibrillation” and “radiofrequency ablation”, more than 116,800 and 53,600 results of studies are available, respectively, with about a third of them published in the last 5 years, which confirms the relevance and demand for solving this problem.

On the one hand, it is possible to control the rhythm in atrial fibrillation without using invasive methods such as radiofrequency ablation, but a long-term cost-effectiveness analysis comparing RFA with antiarrhythmic drugs showed that, compared with antiarrhythmic drugs, radiofrequency ablation significantly improves clinical parameters and quality of life in patients with paroxysmal or permanent AF. The analysis also showed that from an economic point of view, radiofrequency catheter ablation is a cost-effective therapy in the long term [5]. On the other hand, rhythm control can be achieved by surgical ablation, which, even when using a thoracoscopic approach, is more invasive than RFA. A 2021 review found no evidence that the results of independent thoracoscopic surgical ablation were superior to those of catheter ablation in achieving freedom from AF after a single procedure without antiarrhythmic drugs. Moreover, surgical ablation is associated with a longer hospital stay, less improvement in quality of life, and higher costs than catheter ablation [6]. However, to date, the problem of AF recurrence after RFA remains, worsening the quality of life and outcomes in such patients and creating additional economic costs and a burden on healthcare in general. The solution to this problem may be in the use of mathematical modeling and artificial intelligence.

AI is a broad term that encompasses initiatives that use computers to perform tasks that would normally require human intervention. Artificial intelligence techniques are well suited to predicting clinical outcomes. In practice, AI techniques can be thought of as functions that learn the outputs that accompany standardized inputs in order to make accurate predictions when new data is used. Current methods for cleaning, creating, accessing, extracting, enriching, and presenting data to train AI clinical prediction models are well understood. The use of artificial intelligence to predict clinical outcomes is a dynamic and rapidly evolving field with emerging methods and applications. Machine learning approaches, including Random Forest and XGBoost decision methods, and deep learning methods, including deep multilayer and recurrent neural networks, provide unique opportunities for accurate prediction based on high-dimensional multimodal data. In addition, AI methods improve our ability to accurately predict clinical outcomes that were previously difficult to model, including time-dependent and multi-class outcomes [7]. All of the above dictates the need to use mathematical methods to model outcomes in patients with AF after RFA, search for potential biological markers, and then select those whose predictive role in relation to AF recurrence will be statistically significant. Once created, this model should be designed as a convenient clinical calculator, the correction and improvement of which with the addition of new data can be carried out using AI.

A literature review has shown the benefit of using many markers that were typically collected before RFA, which determines their potential predictive role in the further course and prognosis of AF. A 2022 meta-analysis found a close association with AF recurrence after RFA in high levels of pro-B-type N-terminal natriuretic peptide, high-sensitivity C-reactive protein, carboxyl-terminal telopeptide of type I collagen, and interleukin-6 collected before RFA. Elevated serum C-reactive protein levels are indeed positively associated with atrial fibrillation, but Mendelian randomization studies do not confirm this result [8]. A 2024 study used a combination of markers: thyroid stimulating hormone (TSH), free thyroxine (FT4), and brain natriuretic peptide (BNP). It was found that patients with three "abnormal" biomarkers had a three-fold higher risk of AF recurrence than patients without "abnormal" biomarkers, confirming the importance of studying a combination of markers rather than each in isolation [9]. The 2024 review mentions most of the markers already listed, as well as the NLRP3 inflammasome, some microRNAs and circRNAs, the increased or decreased level of which is closely associated with AF recurrence after RFA, transforming growth factor-β1 (TGF-β1), platelet-to-lymphocyte ratio (PLR), N-terminal propeptide of type I and type III procollagen (PINP), interleukin-2 (IL-2) and interleukin-18 (IL-18), tumor necrosis factor-α (TNF-α) were especially prominent in terms of prognosis – fibroblast growth factor-23 (FGF-23), matrix metalloproteinases (MMPS) – MMP-1, MMP-2, MMP-3 and MMP-9, neutrophil-to-lymphocyte ratio (NLR), systemic immune inflammatory index (SII), also various scales were used in this study and imaging methods for predicting AF recurrence [10].

Thus, it is necessary to emphasize once again the importance of the AF problem by the fact that the number of patients with this disease is growing every year, and the RFA procedure has become a standard method of treatment. It is necessary to create a convenient clinical tool or calculator using biological markers as indicators, which would be convenient and easy to use, interpret and would be able to help select a contingent of patients for RFA by assessing the risk of relapse after this procedure, which would increase the number of successful RFA in terms of AF relapses in low-risk patients, and in high-risk patients, a different management tactic would initially be chosen, namely, ventricular rate control, which does not imply further rhythm restoration. In order for this system to be more promising, it is necessary to use mathematical modeling methods for its formation, and machine learning using neural networks for subsequent improvement.

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ANALYSIS OF EXPERIMENTAL DATA ON INDENTATION OF TIN-BASED COATINGS

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An analysis of experimental data on indentation of TiN-based coatings with different stoichiometric composition was conducted. An original mathematical model [1], based on the solution of the contact problem of elasticity theory for bodies with homogeneous, multilayer and non-homogeneous coatings, was used to analyze the experimental data. The relationship between the force P applied to the indenter and its sinking depends on the shape of the indenter and for a spherical indenter is expressed as:

$$P = \frac{4a^3 E_s^{(\mathrm{ef})}}{3R}\left[1 + 3\sum_{i=1}^{N} C_i \left(\mathrm{ch}(A_i\lambda^{-1}) - A_i^{-1}\lambda \mathrm{sh}(A_i\lambda^{-1})\right)\right]. \qquad (1)$$

For a spherical indenter, the relationship between the sinking δ and the stamp radius R is expressed as:

$$\delta = \frac{a^2}{R}\left[1 + 2\sum_{i=1}^{N} C_i\, \mathrm{ch}(A_i\lambda^{-1}) + 2\lambda^2 \sum_{i=1}^{N}\left(A_i^{-2} - B_i^{-2}\right)\right], \qquad (2)$$

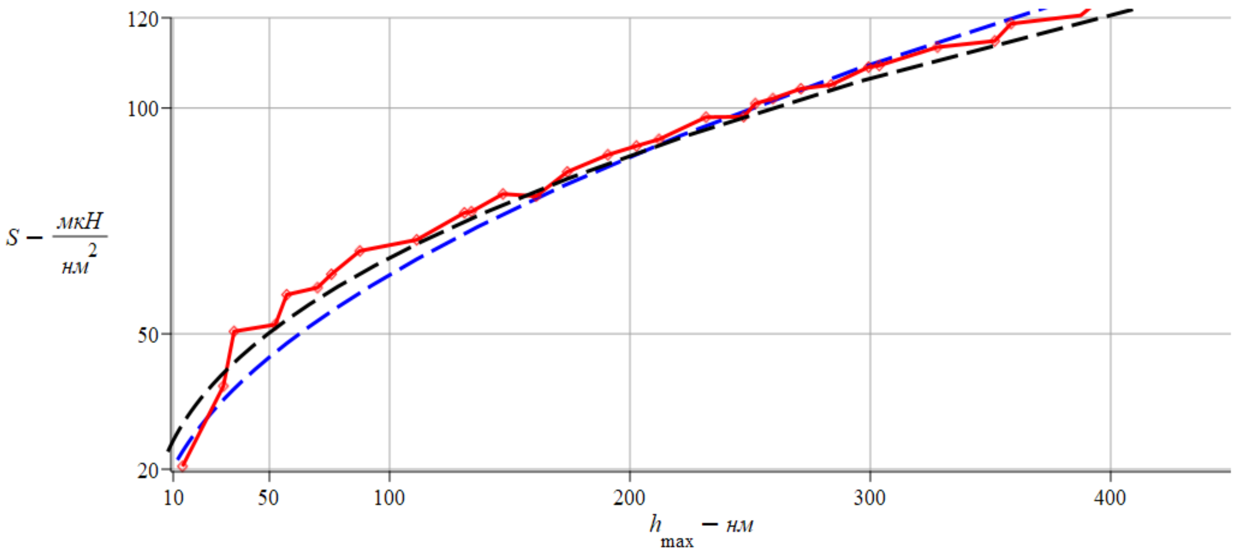

Fig. 1. Comparison of the stiffness (dP/dδ) – indentation depth curves obtained experimentally (red curve), using a mathematical model of the layered structure (black curve) of the sample and without taking into account the layered structure (homogeneous half-space model) (blue curve)

Where (1)-(2) C_i and D_i are constants determined from solutions of the system of corresponding linear algebraic equations; $E_s^{(ef)} = E_s/\left(1-\nu_s^2\right)$, E_s and ν_s Young's modulus and Poisson's ratio of the substrate; $\lambda = H/a$; H - coating thickness; A_i and B_i constants that depend on the elastic properties of the coating and the substrate.

A comparison was made between theoretical data and experimental data obtained by indentation.

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ONE APPROACH TO CRACK THEORY PROBLEMS RESEARCH FOR INHOMOGENEOUS PLANAR WAVEGUIDES

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Crack theory problems in planar and cylindrical waveguides of homogeneous structure have been investigated in detail. The problems are investigated both with using models of elastic media and taking into account rheological properties, and within the framework of models of the non-classical gradient theory of elasticity [1]. Different variants of single-layer and multilayer structures in the framework of both isotropic and anisotropic models.

At the same time it should be noted that in problems of the crack theory in inhomogeneous functionally gradient (FG) structures have been investigated to a much lesser extent. This is due to the fact that in this case the solution of the direct problem is related to the solution of the boundary value problem with variable coefficients, which is possible only numerically with the use of appropriate numerical methods. Impossibility to obtain the solution of the direct problem in analytical form makes it difficult to carry out the following analyses and separation of asymptotic estimates and solutions. However, some results and schemes, tested in the case of homogeneous waveguides [2], can be transferred in the case of FG waveguides.

The problem of steady-state oscillations of an elastic inhomogeneous in thickness in a plane waveguide with delamination at the lower boundary is investigated. The solution of the direct problem is obtained by reducing the initial boundary value problem to an integral equation (IE) with respect to the crack opening function: dispersion curves for different laws of change in the mechanical characteristics of the medium are constructed, the IE is analysed and its discrete analogue is constructed on the basis of the collocation method, the wave field at the upper boundary of the waveguide is constructed. The displacement field at the upper boundary is analysed as a function of the size and position of the stratification and for different laws of change of mechanical properties.

The asymptotic solution of the direct problem for defects of small relative size is obtained. Numerical results of exact and asymptotic solutions are compared, and the ranges of performance of the asymptotic approach are determined. The inverse geometrical problem on determination of geometrical parameters of the delamination on the basis of the obtained asymptotic formulas is solved. The proposed scheme for solving the inverse problem is based on the sequential determination of the geometrical parameters of the defect from one-dimensional ptimization problems and simple formulas.

Numerical calculations of the solution of the direct and inverse problems are carried out.

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