Second International Conference “Modern Problems in Modeling Materials for Mechanical, Medical and Biological Applications” (MPMM&A-2022)

Theses of reports
(September 26 - 30, 2022, Rostov-on-Don)

Rostov-on-Don
2022

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The Proceedings contain theses of papers presented at the Second International Conference “Modern Problems in Modeling Materials for Mechanical, Medical and Biological Applications” (MPMM&A-2022).

The conference focused on the results of work in the following areas: modelling of hard biological tissues; modelling of soft biological tissues; modelling of composite materials; modelling of piezo-active materials; topical problems of computer engineering; didactic basis for the training of modern engineers.

Materials are published in the author's edition.

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Michael Vincent Swain

To the 75th birthday

Michael Vincent Swain, Emeritus Professor, Department of Biological and Biocompatible Materials, Faculty of Dentistry, The University of Sydney, Australia, is one of the world's leading experts in biomechanics and bioengineering.

Professor Swain has been collaborating with Don State Technical University since January 2014. He is currently the head of the laboratory of mechanics of biocompatible materials at DSTU.

Professor Swain's research interests include materials science, biomaterials, dental materials, and ceramics. He has contributed significantly to the development of modern ceramic and composite materials for implantation, developed a method for determining the mechanical properties of a wide range of materials with a spherical indenter (Field-Swain method), made a number of discoveries in the study of the properties of pathologically altered dental tissues and the human eye.

Professor Swain is a member of the American Ceramic Society, the Australian Ceramic Society, and the International Society of Ceramics. He is the author of 732 publications indexed in Scopus and the Web of Science Core Collection. His h-index is 84.

Professor Swain is currently the leader of the Russian Government grant 14.Z50.31.0046 "Biomechanics of Oral and Ocular Tissues and Optimized Biocompatible Implant Materials". He is a recipient of the Richard Brook Award of the European Ceramic Society and Thomson Scientific Publishers.

We wish Professor Swain good health, conquering new heights in life and science.

Conference Organizing Committee

Nonuniqueness in a Constrained Minimization Problem of Orthotropic Elasticity

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We consider the equilibrium problem, with no body force, of a cylindrically orthotropic circular disk subjected to a prescribed displacement along its boundary. In classical linear elasticity, the solution of this problem predicts material overlapping, which is not physically realistic. One way to prevent this anomalous behavior is to consider the minimization of the total potential energy of classical linear elasticity subjected to the local injectivity constraint. In this context, the problem becomes nonlinear and bifurcation occurs from a radially symmetric solution to a secondary solution. In this work we present analytical and computational results indicating that this secondary solution is rotationally symmetric. This solution presents a novel behavior that is not reported in the literature. The tangential displacement is linear near the center of the disk and the corresponding angle of rotation has the value π at this center and decreases as we move away from it.

In Fig. 1 we plot both tr **E**, which is the trace of the infinitesimal strain tensor **E**, and J-1, where J is the determinant of the deformation gradient, versus the radius R of the orthotropic disk. Here, we impose $J \geq 0.1$ everywhere in the disk. We see from this figure that, far from the center of the disk, the corresponding curves are very close to each other. As we approach the center of the disk, the curves become very different. This is expected since, far from the center of the disk, strains are small and the injectivity constraint is not active, $J > 0.1$, yielding tr **E** $\approx J - 1$, whereas, near the center of the disk, strains are large and the injectivity constraint is active, $J = 0.1$.

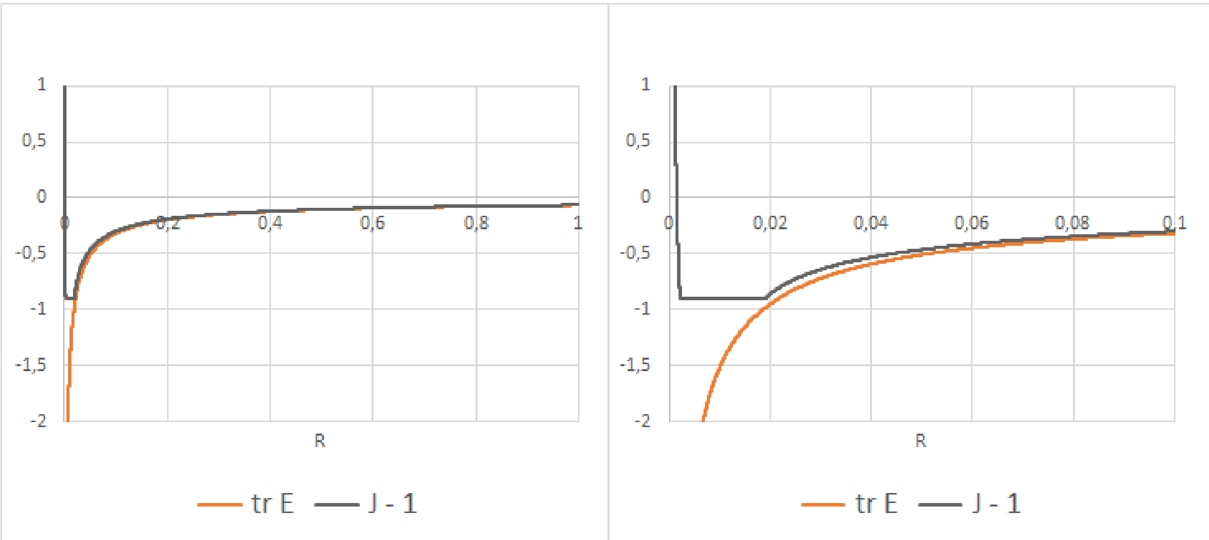

Fig. 1. tr **E** and J - 1 plotted against the radius R for $R \in (0,1)$ (left) and $R \in (0,0.1)$ (right)

Results of this research are published in [1] and are of interest in the investigation of solids having stiffer response in the radial direction than in the tangential direction, such as in the case of carbon fibers with radial microstructure and certain types of wood.

Acknowledgements: The work is supported by CNPq and CAPES - Finance Code 001.

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The Problem of Identification of the Parameters of Hyperelastic Materials by the Results of Three Types of Experiments

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Biological tissues, such as vessels, muscles, ligaments, should be modeled only taking into account their essentially nonlinear behavior. The most common forms of the function of the specific strain energy are already included into the widely used programs for numerical calculations of nonlinear elastic bodies. The properties of materials are determined by the values of model parameters (constants of materials), which are embedded in the form of "lists of materials" into the programs. These constants are determined based on the results of experiments under various stress-strain states. Mainly, these are experiments on uniaxial tension and less often on equibiaxial tension and pure shear at different levels of deformations.

In this paper, the analysis of the validity of constants for some common nonlinear elastic incompressible materials (models) obtained by identification according to one of the types of stress-strain states (uniaxial tension, equibiaxial tension and shear) and used for calculations of the other two mentioned above types is carried out. It is shown that the obtained material's constants cease to correlate with experimental data with an increase in deformation over 5...20% (the level also depends on the chosen form of specific energy). However, when deformations tend to be infinitesimal, the constants of materials converge to the same "linear" values.

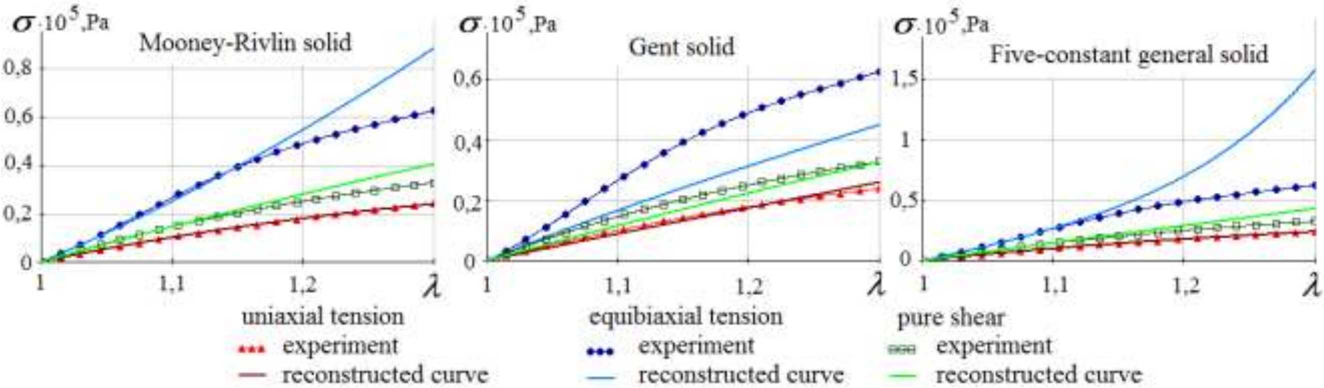

Fig.1 Divergence of experimental and reconstructed curves at the identification of material parameters based on the results of uniaxial stretching for three types of models

There are no problems for using the models if the material's constants are obtained from experimental data at the same stress-strain state for which the design is calculated.

But if it is not possible to use the constants of the material, according to experimental data with the same stress-strain state for which the identification is made, then when choosing a model, it is necessary to study its approximating capabilities for different types of stress-strain state beforehand. For example, the graphs in fig 1 show that the Gent model with constants from uniaxial stretching is not suitable for calculations under biaxial stretching loads, even within small deformations.

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Mathematical Simulation of MyoRing Treatment of Myopia

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Nowadays laser vision correction provides safe and effective correction of myopia. However, with high degrees of myopia, including thin corneas, laser correction is not feasible, since in addition to residual myopia there is a high risk of postoperative keratectasia [1]. Currently, the MyoRing intrastromal implantation method proposed by A. Daxer is often considered as an alternative method for correction of high degree myopia on thin cornea.

In present paper the mathematical model that describes the stress-strain state of the cornea after MyoRing implantation is presented. Two-dimensional axisymmetric modeling is performed in the engineering simulation software ANSYS. The corneoscleral shell of the eye is modeled by joined spherical segments of variable thickness with different radii and different elastic properties under normal intraocular pressure 15 mm Hg. According to the technique, the ring is implanted into a corneal pocket 9 mm in diameter, formed by femtosecond laser, to a depth of 80% of the initial corneal thickness. The ring implantation process is modeled by three surface-surface contact pairs. The first contact pair sets the contact between corneal layers as a result of corneal pocket formation. The other two pairs simulate the contact of the ring with the lower and upper surface of the corneal pocket, in which the ring is inserted.

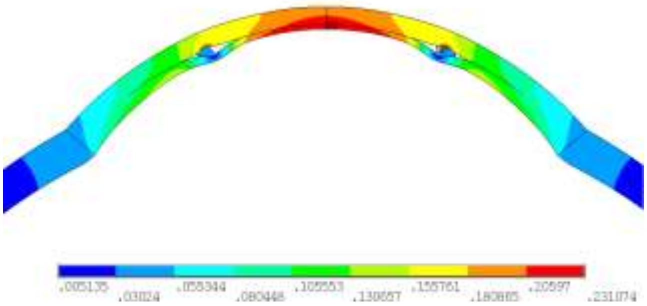

Fig. 1. Deformed cornea after MyoRing implantation

As a result of simulation, it is shown that ring implantation changes the corneal profile and enhances the biomechanical properties of the cornea by creating an additional framework with the ring. The effect of the diameter and thickness of the MyoRing implant on the stress-stain state of the eye and results of myopia correction is analyzed.

Acknowledgements: This research was supported by the Government of Russia grant no. 14.Z50.31.0046.

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Applied Theory of Oscillations of Electroelastic Plates with Gradient Porosity

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Based on the applied theory of plate vibrations, taking into account the nonlinear distribution of the electric potential in piezoelectric layers, a study of the stress-strain state and the electric field of a cantilever functional gradient bimorph is carried out. Such nonlinear dependences arise when solving problems of finding natural resonant frequencies and waveforms, or in the case of forced oscillations during their mechanical excitation, for some electrical boundary conditions, as well as for functionally gradient materials. On the basis of the developed theory, a plane problem of harmonic vibrations of a plate whose layers have electroelastic properties was investigated. It is assumed that the layers are made of porous ceramics [1], the volume fraction of the porosity of which varies so that its effective properties have a nonlinear dependence on the thickness of the plate. As the law of distribution of material properties over the thickness, we will consider a quadratic power law. To take into account such distribution, we introduce the shape function for the material constants of the following form

$$Y(a,\hat{a},x_3) = \frac{(\hat{a}-a)}{H^2} x_3^2 + a,$$

where a corresponds to the value of the material constant at the center of the plate and $\hat{a}$ corresponds to the constant near the surface.

In the problem, Kirchhoff's hypotheses for mechanical characteristics were accepted. Using the variational principle and the quadratic dependence of the electric potential on the thickness of the piezo layers, in which its distribution in the middle of the layer is an unknown function, a system of differential equations and boundary conditions was obtained. The results of the numerical experiment based on the obtained system of equations were compared with the data of finite element modeling in COMSOL Multiphysics software.

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

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On Modelling of Beam-Lattice Materials with Rigid Joints within the Cosserat Continuum

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We discuss the effective properties of beam-lattice materials made of flexible elastic fibers rigidly connected though massive joints. As an effective medium we use the nonlinear Cosserat continuum (micropolar medium). As a result of comparison of potential energy of semi-discrete structure and continuum we introduce the constitutive equations of Cosserat continuum. The latter inherit elastic properties of fibers. Similar approach was applied to derive the effective kinetic properties, which strongly depend not only on the elastic properties of fibers but also on mass distribution along fibers and shape and mass of joints. As a result, within the obtained effective medium one can observe coupling between translational and rotational waves.

Presenting results continued the investigations provided in [1, 2, 3].

Acknowledgements: The author acknowledges the support of the Government of the Russian Federation (Contract No. 14.Z50.31.0046).

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Integral Equations for Sliding Zone Detection on the Interfaces Between Layered Media

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A special incorrectly posed boundary value problem of fracture mechanics is considered in this study. The problem addresses the case of sliding zone (mode II crack) detection on the interface between or coating and substrates (or between layers in layered structures) that occurs as the result of rapid heating, migration of fluids or dynamic loading. Detection of sliding zone by the routine methods, such as x-ray, ultrasonic tomography, frequency analysis is limited. On the other hand the use of the strain/displacement monitoring on the free surface of the coating (layer) can have some advantages. In this study we consider a semi-inverse boundary value problem for elastic strip that models the coating in which tree boundary conditions are given on one side of the strip and one on another.

The Fourier transform is used to find analytical solutions of the problem. However the direct inverse transform is not applicable, which necessitates reduction to an integral equation of the Fredholm type of the first kind. Numerical approaches associated with non-stable solutions of the derived integral equation are discussed.

The Hierarchical Structure of Human Dentin

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Dentin of human teeth is a complex hierarchically organized structure; therefore, its deformation behavior significantly depends on the structure at different scales. It consists of 70% bioorganic compounds, 20% inorganic compounds and 10% water. Under mechanical loading, at least under tension, dentin exhibits a brittle deformation behavior, while cracks in it advance in a viscoelastic manner. The majority of the studies of fracture of dentin was carried out on the macro- and micro-scales, while there are only few studies on the structure and accommodation of stresses in dentine at the nano-scale in the literature. Largely, this state is due to difficulties in preparing samples for a transmission electron microscope (TEM). The aim of this paper is to overview the structure of human dentin at different scales.

A priori, the dentin of human teeth is a bioorganic matrix filled with an inorganic phase. Dentinoblasts, in comparison with other cells, contain an increased concentration of calcium and phosphorus, from which calcium hydroxyapatite is formed. TEM studies at x10^5 and higher magnifications show that the 13-14-year-old adolescent dentin matrix is in an amorphous state. It consists of layers with a thickness of 50-100nm, located perpendicular to the central axis of the tooth. Concentric cells 50–100 nm in size in the layers are observed, separated by dark boundaries 10–20 nm wide. With the age of 16-18 years, collagen fibers with a thickness of about 5 nm are formed in the dentin matrix, which plays the role of reinforcing elements. Calcium hydroxyapatite was not detected in teenage dentin foils, while many hydroxyapatite nanocrystals 20–40 nm in size were observed in foils from mature dentin. The solubility of calcium hydroxyapatite in concentrated phosphoric acid, which is used to prepare thin foils for TEM, decreases with the patient's age: it takes 40 minutes to prepare a sample from teenage dentin and several hours from mature dentin. Indeed, teenagers' teeth are more susceptible to caries than the teeth of adults.

At the microscopic level, the main morphological element of dentin is the dentinal canals. They are located between the pulp chamber and the border with enamel or cementum. The diameter of the channels varies from 5 μm near the pulp to 0.8 μm in the area of the dentin-enamel junction (DEJ) and dentin-cement junction. The density of channels near the enamel is less than that of the pulp chamber. There is an area between dentin and enamel in which both dentinal canals and enamel prisms are absent. When a crack in the enamel reaches the DEJ, it begins to grow not into the dentin but moves along the border. Such behavior can cause the enamel to break away from the tooth. At the macroscopic level, accessible to observation with the naked eye: dentin looks like a homogeneous structure of white color with a yellowish tinge. Hence, a dentist can notice the pathology of the tooth by changing the color and structure of the dentin.

Based on the study, it may be concluded that the dentin of human teeth is a biopolymer reinforced with collagen fibers and particles of calcium hydroxyapatite. Its viscoelastic properties are close to filled polymers, where bioorganic compounds including collagen fibers provide elasticity and plasticity, while calcium hydroxyapatite nanocrystals serve as a filler that strengthens the dentin. Knowledge of the features of the structure of dentin at different scale levels is helpful to a dentist in developing tactics for the treatment of diseases associated with changes in the morphology of dentin, for example, caries.

Laboratory Filtration Factor Determination Technique

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In the present work the experimental method for obtaining the filtration coefficient of filtering object is presented. Fine-grained sponge material was used as a filtering material.

Filtration is the movement (leakage) of liquids and gases through porous media under the influence of any factors. Historically, the filtration law was derived by Henry Darcy [1] where it establishes a linear relationship between the volumetric flow rate of a liquid or gas and the hydraulic gradient (slope, pressure drop) in porous media, for example, in fine-grained, sandy and clay soils.

The integrated form of the Darcy law is known:

$$Q = \frac{k_{п}A}{\eta L}\Delta p \quad (1)$$

where Q – flow velocity, $k_{п}$ – permeability coefficient of the porous medium, A – cross-sectional area, η – dynamic viscosity of the liquid, L – thickness of the porous medium, Δp – pressure drop.

Taking into account the results [2], it follows that the relationship between the filtration coefficient and the permeability coefficient of a porous medium:

$$k_{ф} = \frac{QL\rho_{ж}g}{A\Delta p} \quad (2)$$

To find the filtration coefficient, an installation was assembled according to the example of the Darcy scheme. As a sample, a sponge filter material is proposed that simulates soft poroelastic tissues, and distilled water is used as a liquid.

This approach makes it possible to simulate the behavior of biological tissues, namely, to consider the permeability of poroelastic liquid-saturated bodies with an elastic skeleton.

In the future, it is planned to use this method on biological tissues, such as the human cornea, to calculate dependencies under various loads, which will provide more information about the mechanical characteristics of eye tissues [3].

Acknowledgements: This work was supported by the Russian Science Foundation grant 22-19-00732. Experiments were made in Nanocenter of Research and Education Center "Materials", Don State Technical University (http://nano.donstu.ru).

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Lightly Loaded Hydrodynamic Contact of Two Bodies Considering Lubrication Modeled by a Non-Newtonian Fluid

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The use of lubricants in friction units (bearings, gears, moving elements of machine engines and gearboxes, etc.) leads to a decrease in friction and, as a result, an increase in the service life and a decrease in energy costs. To control the viscosity, thermal stability and other characteristics of the lubricant, various kinds of polymer additives are used. The content of polymers in the lubricant causes the lubricant to behave as a substantially non-Newtonian fluid. Complex rheological models are used to describe the behavior of non-Newtonian fluids.

In the present work, we consider a plane contact problem for a lightly loaded hydrodynamic thrust bearing lubricated by a non-Newtonian fluid described by the Giesekus rheology [1]. Fluids described by the Giesekus model make it possible to correctly describe the behavior of real lubricants at low and high shear stresses. Giesekus rheology takes into account the rheology of the base lubricating oil (solvent) and the polymeric additives dissolved in it. The case is considered when the viscosity of the polymer components, the solvent and the parameter characterizing the relaxation time are functions of pressure (exponential dependences are used). The gap between the rigid surfaces of the contacting bodies is described by the following formula:

$$h(x) = h_i + mx, \quad m = \frac{h_e - h_i}{L}, \quad m = m_0\varepsilon, \quad \varepsilon = \frac{h_i}{L}, \quad \varepsilon << 1,$$

where h_i and h_e – clearance at the entry and exit points, respectively; L – contact zone width.

To solve the problem stated, the perturbation method with respect to a small parameter was used. The decomposition of the main characteristics (pressure, stresses, lubrication rates, etc.) was carried out in terms of a small parameter α, which characterizes the mobility coefficient, which describes the degree of alignment of polymer molecules with the lubricant flow. When solving, two terms of the corresponding expansions were taken into account. The simplification of the basic equations describing the considered model and rheological relations was carried out under the assumption that the mobility coefficient α is much larger than the parameter describing the ratio of the characteristic dimensions of the contact along the z and x axes. A similar case for a constant viscosity of polymers and a solvent, and another form of bearing, was considered in [2]. To determine the zero and first terms of the pressure expansion, the corresponding Reynolds equations were obtained. In the general case, the solution of these differential equations was obtained numerically. The influence of the parameter m_0 characterizing the gap, the viscosity of the polymer additives and the solvent, the relaxation time on the contact pressure, the friction force, and the energy loss was analyzed numerically.

Acknowledgements: This work was supported by the Government of Russian Federation, grant no. 14.Z50.31.0046.

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Diffusion of Cryoprotectant Through the Membrane of Reproductive Cells

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The paper considers the development of a new technology for low-temperature preservation of fish reproductive cells. In particular, such a technology can be used for sturgeon fish.

For this purpose, mathematical modeling of acoustic influence on biological objects was performed.

The acoustic effect on reproductive cells comes down to two main steps.

At the first stage of cryopreservation, a special piezoactuator creates an acoustic field in the cryoprotector containing reproductive cells.

A mathematical model of such an effect is constructed within the framework of continuum mechanics. For this purpose, the equations of deformable solid mechanics in axisymmetric formulation (theory of elasticity and electroelasticity) and equations of motion of liquid and gaseous media (in acoustic approximation) [1, 2] are used. Such a model represents an initial boundary-edge problem and, in the general case, its solution can be constructed only numerically with the use of appropriate software complexes of finite element analysis.

As a result of the numerical analysis [3], the corresponding field of ambient velocities is found. It is shown that the acoustic field in the volume of the suspension is effectively excited in the first bending mode. However, this field is not homogeneous, as evidenced by the velocity distribution. Therefore, in the process of acoustic influence, it makes sense to use stirring of the solution. At the same time, the presence of areas with intense positive and negative vertical velocity components should probably automatically lead to the mixing process.

The second stage considers the diffusion of the cryoprotectant through the cell membrane. This process is generally described by a system of differential equations based on Fick's laws and the equation of state of the medium. Given the current variety of models of intracellular transport of substances, within the framework of the mechanical model considered in this paper, we assume that the corresponding diffusion coefficients are preliminarily determined from biological experiments.

The numerical experiment was performed using the FlexPDE program for scenario models of differential equation solutions using the finite element method.

As a result of numerical experiments it was found that the diffusion of the cryoprotectant inside the cell depends on the amplitude of velocity and time of exposure, but weakly depends on the frequency of oscillations. Thus, for effective protection of reproductive cells with the cryoprotectant, the suspension should be exposed to the piezoactuator near the resonance frequency.

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Experimental Testing and Finite Element Modelling of Ceramic Bricks for Compressive Strength

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Compressive strength is the main parameter determining the area of use of most building materials. Correct determination of strength values and reduction of systematic errors is the basis for reliable prediction of bearing capacity of any designed structure.

During laboratory tests on the compressive strength of ceramic brick specimens, the main type of the stress-strain state is non-uniform three-axial compression. The volumetric stress state is caused primarily by the presence of contact friction forces between the specimen and the die. This in turn leads to an overestimation of strength indicators [1]. The paper analyzes the change in the stress-strain state of specimens during tests depending on one of the varied parameters - the method of surface preparation for testing.

Varying the methods of specimen preparation for testing leads mainly to changes in the friction coefficient in the contact zone "specimen surface – test press platen" and, accordingly, to changes in the type and force of failure. The use of different specimen types also affects the magnitude of the failure load by changing the height and cross-sectional area of the specimens.

Based on the series of experiments, the following ways of adjusting the test methodology are proposed:

– reducing the friction coefficient by using a felt pad;

– changing the ratio of specimen height to diameter towards transition to "high" cylinders with natural constraints dictated by the absence of longitudinal bending;

– transition to "cylinder with flutes" specimens by analogy with the axial tension test.

In this work, we performed finite-element modeling of the stress-strain state of hand-formed bricks [2, 3]. Modeling was carried out using the software package of finite element analysis ANSYS. The results of the numerical experiment agree well with the results of the field experiment.

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A Mathematical Model for Describing the Indentation Process of the ZnO Coating

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An effective mathematical model for describing the experiment on indentation of samples with layered or functionally graded coatings was proposed. It is based on the solution for the contact problem of the theory of elasticity of the conical punch indentation into elastic half-space with a coating [1]. Results of mathematical modelling and experiments on indentation of a ZnO coating manufactured by the method of pulsed laser deposition on a silicon substrate were compared. The microgeometrical characteristics, as well as the chemical composition of the coating, were studied.

Elemental analysis of the coating demonstrated a good deposition quality and confirmed the good stoichiometric composition of the layer. Based on the Oliver-Pharr method, the Young's modulus of the substrate and the effective Young's modulus of the coating-substrate system were obtained (Fig. 1).

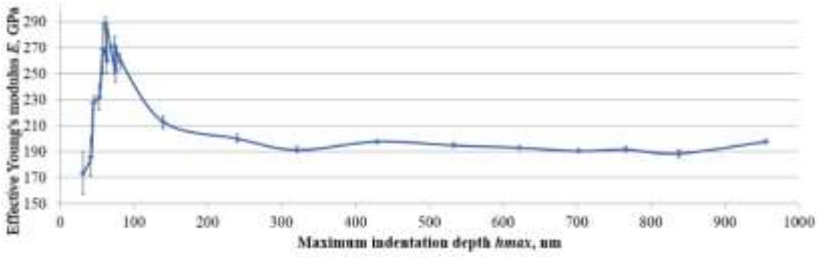

Fig. 1. Experimental results of the nanoindentation tests

The mathematical modeling of this process with high (up to tenths of a percent) accuracy was conducted. A good agreement was observed between the behavior of the theoretical and experimental results (Fig. 2), however, a partial increase in the theoretical values of the Young's modulus was found. The model may be used for research of a wide range of materials [2].

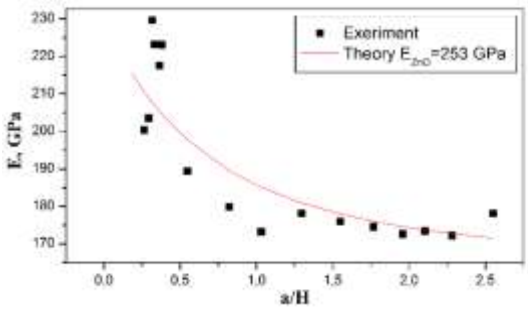

Fig. 2. Comparison of theoretical results and experimental data of the nanoindentation tests

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UV and IR Detecting Properties of ZnO Nanorod Arrays

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The structural, optical, and electrical properties of zinc oxide nanorod arrays grown by carbothermal synthesis on oxidized Si (001) substrates were studied. These rods served as the active element of the photodetector prototype.

The prototype was fabricated using pulsed laser deposition of a ZnO film [1], methods of direct and reverse photolithography [2], pulsed laser deposition of catalytic Au nanoparticles [3], and the method of carbothermal synthesis for growing arrays of nanorods [4]. The result was a structure with alternating ZnO bands width of 30 micrometers and a period of 30 micrometers, coated with ZnO nanorods. Contacts to the resulting structure were made using silver paste.

Studies using a scanning electron microscope showed that a dense network of misoriented nanorods grew in the space between the ZnO strips, while nanorods with a predominantly vertical orientation grew on the surface of the strips. The resulting nanorods had a relatively low concentration of point defects and had a high crystallinity. This was confirmed by studying X-ray spectra and photoluminescence spectra. The current-voltage characteristics of the prototype had a pronounced asymmetric diode nonlinearity.

The spectral sensitivity of the prototype was measured by exposure to a halogen lamp. Sections were cut out from the lamp spectrum and the response was recorded at each wavelength segment from 300 nm to 800 nm with a step of 20 nm. The obtained spectral intensity of the prototype showed predominantly ascending character from 300 nm to 800 nm with a pronounced peak in the interval from 340 nm to 380 nm.

Next, a study of the time-resolved photoresponse of the prototype was carried out using a nanosecond laser. The prototype showed high sensitivity to optical radiation and a very fast response to single nanosecond laser pulses.

Acknowledgements: The study was carried out at the Research and Education Center “Materials” of the Don State Technical University (https://nano.donstu.ru/) and was supported by the Russian Foundation for Basic Research, project 20-07-00637 A.

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Piezoelectric Generator Based on Shear Oscillations

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Shear oscillation of piezo devices can be utilized for energy harvesting [1]. In this study we developed a FEM model for evaluating the efficiency of porous piezo ceramics for piezo transducer working on shear oscillation. Material properties of porous ceramics were obtained using ACELAN-COMPOS package [2]. PZT-4 was used as full-bodied piezo material. The set of 9 porous materials was imported to COMSOL package [3] to build a parametric sweep model. Geometry and working shape are presented on Fig. 1.

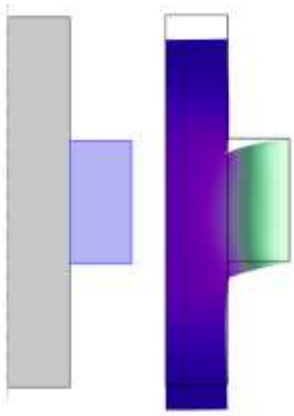

Fig. 1. Geometry of the transducer (left) with isotropic base and piezo element (blue), and eigen working shape (right)

Because e_{15}^{eff} coefficient reduces more than e_{33}^{eff} with larger porosity, the effectiveness of the porous ceramics for such device was not growing. Full bodied ceramics showed the best results in terms of electro-mechanical coupling coefficients (EMCC) that was measured by computing resonance and antiresonance frequencies. Results in forced oscillations mode near the first coupled eigen frequency also showed loss in output potential of the device.

Finite element model obtained in the study can be used for any set of effective material properties. The combination of ACELAN-COMPOS material properties identification and parametric sweep over material properties in COMSOL allows to perform series of numerical experiments fast and automated.

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ACELAN-COMPOS Package: New Features

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Majority of finite-element packages have client-server architecture or a similar design that allows to split computational modules from user interface. This approach was used for distributed computing to speed up the FEM analyses [1]. ACELAN-COMPOS package [2] has been developed in such modular manner. In this study we discuss the new distributed structure of the package.

New layer of interaction between the web UI and finite-element library is structured in two ways: modern web UI and command line interface. Previous approach with monolith application was dependent on the stability of webserver which was heavily affected by long computational tasks. New approach allows to use both local and cloud-based computational modules. Web-application manages the load between computational nodes available to each user and allows user to host own nodes on local machine.

Another important feature of new interface is advanced support of ACELAN scripting language. Limited support for scripting languages in modern FEM packages leads to usage of general-purpose programming languages like Python. But the description of finite element model and related numerical experiment can be described in declarative way using domain specific language. We developed custom interpreter with syntax highlighting and code completion for custom language that allows to setup model rapidly and to re-use them in series of experiments. The most important part of the project relies on the state management and caching on the server side for reducing computational time.

Since the main purpose of ACELAN-COMPOS package is to obtain effective moduli of piezo-composites, the DSL includes built-in features to describe the distribution of components and relative material properties. Output of the identification problems can be stored as new material to the material database for further usage as input for other problems. Visualization of results is implemented as text, tabular or graphical output, depending on the tasks. Graphical output for 2D problems is built on the vector graphics base, and for 3D polygonal models built with WebGL are used.

Technological stack of the package now consists of three main layers: monolith UI and scripting language app based on Ruby on Rails framework, CLI modules and class library with FEM algorithms and related data structure, both implemented in C# on the .NET platform. All modules are cross-platform and can be used both on Linux and Windows systems.

Future development of the client modules of package will be focused on the advanced job monitoring for time-consuming tasks and on the new methods of representing and describing the structure of composites representative volume.

Acknowledgements: The work was supported by the Russian Science Foundation (grant number No. 22-11-00302).

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Eggshell as a Candidate to Biomimetic Restorative Material for Dentistry

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Design of restorative materials for dentistry is the actual task for the biomedical materials science. Despite success in this direction, a clinical practice demands a new generation of restoratives, which exhibit service characteristics close to the tooth hard tissues. Few conditions need to be satisfy for these materials. The first, their biocompability should be similar to the human dentin and enamel. The second, their mechanical properties should be also close to the tooth hard tissue. The third, their workability and cost should be on the level of modern commercial restoratives. Searching for a prospective restorative material for dentistry that meets these hard conditions is the aim of this work.

According to chemical content, bird's eggshell is the calcium carbonate of the biological genesis, which a good biocompability with human body. It could be considered as the candidate, if its mechanical properties would be close to dentin and enamel. Tooth enamel is the biomineral, too. Therefore, deformation behavior of bird's eggshell are compared with tooth enamel and some rocks. It was shown that the behavior of all model materials depends on the geometry of applied loading. Under tension, their deformation behavior on the macroscopic scale is brittle, while it is viscoelastic under compression. Deformation behavior of the model materials on the microscopic scale was examined by the crack evolution that grows on the viscoelastic scenario.

The next condition is workability of the eggshell based material. Hen's eggshell was milled to a powder (the average size of particles is few micrometers). The samples for mechanical testing were compacted under pressure. Some part of samples having a tablet shape was compacted with the rubber glue (BF6). Uniaxial compression and diametral compression (Brazilian testing) were applied as deformation schemes for mechanical testing at room temperature. It was shown that the compacted powder exhibits deformation behavior close to a rock, while the compacted powder with rubber glue behaves like a rubber or dentin. Another word, the properties of eggshell based powder material depend on the characteristics of a glue or filler, which can vary in wide limits. It was shown that mechanical properties of eggshell of different birds are the similar; however, only hen's eggs could be supplied in the commercial parcels from hen's farms. Hence, the eggshell meets the conditions mention above that allows considering it the prospective biomimetic restorative material for dentistry.

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Mathematical and Computer Modeling of the Processes of Drying an Elastic Solid

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The problem of drying of a linearly elastic porous body is considered. According to two experimental facts: the first is reducing the size of the body with a decrease in humidity, a phenomenological theory of the dependence of mechanical stresses on relative humidity is constructed; second is with decreasing humidity, Young's modulus increases, is assumed the functional dependence of this module on relative humidity. The initial boundary value problem is formulated, in which, due to the low speed of the drying process, inertial terms are neglected.

Mathematical formulation of the problem. For the components u of an unknown displacement vector and relative humidity φ, the system of differential equations has the form:

$$\nabla \boldsymbol{\sigma} = 0 \tag{1}$$

$$\Delta\varphi = \frac{c\rho}{k}\frac{\partial\varphi}{\partial t} \tag{2}$$

In the reduced system (1) – equilibrium equations without taking into account mass forces, (2) – diffusion equation in which c – coefficient specific heat of the body, ρ – density, k – diffusion coefficient and in this formulation of the problem these parameters are considered constant. Cauchy's relations:

$$\boldsymbol{\varepsilon} = (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathrm{T}})/2$$

Defining equations taking into account the linear dependence on φ:

$$\boldsymbol{\sigma} = \lambda\, \mathrm{tr}\boldsymbol{\varepsilon}\, \boldsymbol{E} + 2\mu\boldsymbol{\varepsilon} + \varkappa(1-\varphi)\boldsymbol{E}$$

For the Young's modulus E, the following three-parameter dependence on relative humidity is selected φ:

$$\mathrm{E} = \gamma\left(\beta\frac{e^{-\alpha(\varphi-0.5)}}{1+e^{-\alpha(\varphi-0.5)}} + 1 - \beta\right),$$

where α, β, γ are parameters. Mechanical boundary conditions at the boundaries – absence of displacements and absence of stresses. Boundary conditions for relative humidity at the borders are constant humidity and drying conditions across the border are maintained.

The problem was solved by the finite element method in the FlexPDE package. In the numerical experiment, the entire boundary of the region is stress-free and the same drying conditions are set on it. At the same time, the shape of the region remains rectangular when entering the stationary mode, and the humidity becomes constant in all areas and is equal to the humidity of the environment.

Nonstationary model of drying of a solid deformable body relative to the components of the displacement vector and relative humidity is constructed in this work assuming a smooth dependence of Young's modulus on relative humidity, with the remaining physical coefficients constant. Numerical experiments were carried out for a rectangular area and a model material to determine the stress-strain state and relative humidity under various boundary conditions. The results of calculations qualitatively coincide with possible field experiments, which indicates the adequacy of the model.

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Training Bachelors in Engineering Using Active Problem-Situation Analysis Methods

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The urgent task facing higher education is the intensification of the learning process, in particular, in undergraduate education. In turn, this requires not only obtaining deep theoretical knowledge in the process of learning, but also acquiring relevant skills and abilities [1-3].

Preparing bachelors for future professional activities requires a teacher to actively use interactive forms of learning. This approach implies a slightly different logic of the educational process as compared to the traditional form of learning. I.e. the formation of new knowledge goes not from theory to practice, but from practice to its theoretical comprehension. Students have to acquire the necessary theoretical knowledge in order to successfully perform specific practical tasks. This increases their motivation to learn and contributes to more effective learning.

The use of case-method in the educational process seems to be the most appropriate for the purpose of training bachelors to solve professional research tasks. The method of case-study is a non-game imitation active training method, which aims to analyze the situation arising in a particular situation and develop a practical solution with the joint efforts of a group of participants. Application of this technology in the learning process allows effective implementation of all universal competencies, as well as a number of general professional and professional competencies.

Engineering case is a practical problem that occurred (or still occurs) in real engineering activity. Such a case is based on the use of a description of a real situation, its analysis, parsing the essence of the problem, finding possible solutions and choosing the best one. The main difference between engineering cases and business cases is that they are based on specific engineering problems with a well-defined set of input data. However, these problems, as a rule, have several possible correct solutions.

When using the case-method in the educational process there was a high interest of the participants, group cohesion, increased assimilation of theoretical information, development of research skills. Thus, the use of the case-method in conducting classes significantly increases students' motivation to learn new knowledge and contributes to increasing the productivity of the bachelor's learning process. In its turn, it provides even more effective training of future specialists.

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On the Question of Attenuation of Acoustic Waves in an Acoustic Waveguide

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The study of wave attenuation in acoustic waveguides is an urgent problem that includes various damping mechanisms. Among them, one can note the phenomenon of hysteresis in a piezoceramic emitter and receiver, energy removal through fasteners, the accounting of the viscosity of an acoustic fluid, and energy leakage through an elastic surface limiting the waveguide. Obviously, in quantitative terms, each of the listed mechanisms creates its own contribution to the damping process, but each of them can be estimated when considering a specific mathematical problem. In the presented work, the impedance attenuation on the side surface of the waveguide is considered when the elastic properties of the waveguide wall are taken into account.

The harmonic mode of vibrations generated by a piezoceramic element - a source of vibrations, and feelled by another piezoceramic element - a receiver of vibrations is considered. In the acoustic zone, we consider an axisymmetric problem for an acoustic fluid with conjugation conditions for solutions at the interfaces between the acoustic fluid and ceramic bodies in the integral sense. The use of impedance boundary conditions on the side surface of the waveguide generates a spectral problem in which complex roots are found. For numerical simulation, only the piston mode was taken into account. An additional equation for the flow of current through an external circuit makes it possible to close the system of equations and obtain an output signal at the wave receiver.

The results of the work can be used for medical purposes to study blood flow in vessels with elastic walls. They are also of interest when modeling a non-stationary solution to a problem.

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One Probabilistic Model of the Theory of Thin Shallow Shells

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The static boundary problem for a thin elastic spherical shell with a piecewise smooth boundary *(a spherical dome)* was first posed by Vlasov [1] and Goldenveiser [2] in the framework of the momentless technical theory of shells. The mathematical formulation of this problem and its complete solution are given in [3] using the method of generalized analytic functions. For some special classes of convex domes this problem is solved in [4]. In particular, for *canonical* domes the quasi-correctness of the main boundary value problem is established. In the present paper we introduce new concepts which allow us to give a complete picture of the solvability of the quasi-correct problem for canonical domes and to refine the results.

Such concepts as quasi-stability and the order of quasi-correctness are introduced. It is established that a thin flat shell, the middle surface of which contains n ($n \geq 2$) corner points with internal angles $\theta = \frac{\pi}{3}$, is not quasi-stable, and its order of quasi-correctness is a discrete random variable taking the values 2n-3, 2n-2,...,3n-3.

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Gradient Thermal Conductivity Model for an Inhomogeneous Pipe

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Problems of thermal conductivity and thermoelasticity of cylindrical bodies are well studied [1]. However, these models do not take into account the scale effects that arise during the deformation of microcylinders. To describe scale effects, the gradient theory of thermal conductivity is used [2, 3]. However, analytical solutions to the problem of gradient heat conduction were obtained only for the layer. The problem of gradient thermal conductivity for a pipe remains unexplored.

The report considers the distribution of heat in an inhomogeneous pipe, on the inner surface of which zero temperature is maintained, and on the outer surface there is a constant heat flux. On the basis of the variational principle of gradient heat conduction, an equation for the propagation of heat in terms of heat flow, as well as an extended range of boundary conditions, is obtained. The heat conduction equation in terms of heat flow is a 3rd order differential equation with variable coefficients containing a small parameter at the highest derivative. To find the gradient terms, a 2nd order differential equation is obtained, the solution of which is expressed in terms of the Whittaker functions. An approximate asymptotic expression for the heat flux is also obtained for a small value of the scale parameter. The formula for finding the temperature for arbitrary laws of the thermal conductivity is obtained by integrating the expression for the heat flux.

In the first series of calculations, the pipe was assumed to be made of a functionally graded material with power laws of change in the thermal conductivity coefficient. In the second series of calculations, a two-layer pipe was considered. The thermal conductivity coefficients of the pipe layers differ by a factor of 10. The results of calculating the distribution along the radial coordinate of the heat flux and temperature are considered. In the course of calculations, it was found that the heat flow at the conjugation boundary suffers a discontinuity, which is associated with the difference in the thermal conductivity coefficients of the layers and the continuity of the first temperature derivatives on the conjugation surface. A study was made of the influence of the inhomogeneity parameter in a power law simulating the thermal conductivity coefficient of an inhomogeneous pipe on the distribution of heat flux and temperature along the radial coordinate.

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Gradient Electroelasticity Models for Finite Bodies

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The problems of electroelastic deformation of finite bodies are well studied [1]. However, these models do not take into account the scale effects that arise during the deformation of microsized bodies. To correctly describe the experimental data for microsized bodies, the gradient theory of electroelasticity is used [2, 3]. However, the problems of obtaining analytical and numerical solutions for inhomogeneous electroelastic bodies, taking into account scale effects, remain unexplored.

As the first task in the report, the bending of a horizontally inhomogeneous piezoelectric beam is considered. The lower and upper surfaces of the beam are electroplated. Three types of loading are considered: 1) load uniformly distributed along the length; 2) transverse force at the other end of the beam; 3) supply of electric potential to the upper electrode. The beam bending is modeled based on the Euler-Bernoulli hypotheses and the quadratic distribution of the electric potential. Based on the application of the variational principle of gradient electroelasticity, a system of differential equations of bending and electrostatics is obtained, as well as an extended range of boundary conditions. To find the bending moment and deflection of the middle line of a homogeneous beam, exact analytical expressions are obtained. In the case of an inhomogeneous beam at large values of the scale parameter, the solution is based on the zeroing method. On specific examples, the calculations of moments and deflection were carried out, both in the case of a homogeneous and inhomogeneous beam. It was found that an increase in the value of scale parameters reduces the values of deflections, and an increase in the connectivity parameter increases deflections. The influence of the inhomogeneity parameter in the power law, which models the electromechanical characteristics of the beam, on the distribution of deflections along the horizontal coordinate is studied.

As the second problem, the deformation of radially polarized cylinder under the action of a normal mechanical load applied to the lateral surface of the cylinder is considered. There are no electrodes on the surface. After eliminating the electric potential from the relations for the stress components, the problem of the gradient theory of elasticity with stiffened elastic moduli is obtained. In the case of an inhomogeneous cylinder at large values of the scale parameter, the solution is based on the zeroing method. It was found that an increase in the scale parameter reduces the values of radial displacements and total stresses.

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Numerical Analysis of Bandgap in 2D Chiral Metamaterials

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Bandgaps in chiral metamaterials are of importance in the applications for noise reduction and vibration isolation. By using the finite element numerical analysis, two similar chiral structures are studied, as shown in Fig. 1 (a) and (d). Dispersion curves of Fig. 1 (a) is shown in (b) and (c) for rib thickness equal to 3 mm and 5 mm, respectively. Similarly, Fig. 1 (e) and (f) show the dispersion curves for rib thickness equal to 3 mm and 5 mm, respectively. As can be seen, the slight differences in the shape of the four chiral arms can strongly affect the bandgap patterns. Therefore, the rib thickness and the shape of chiral arms play a significant role in optimally designing chiral metamaterials.

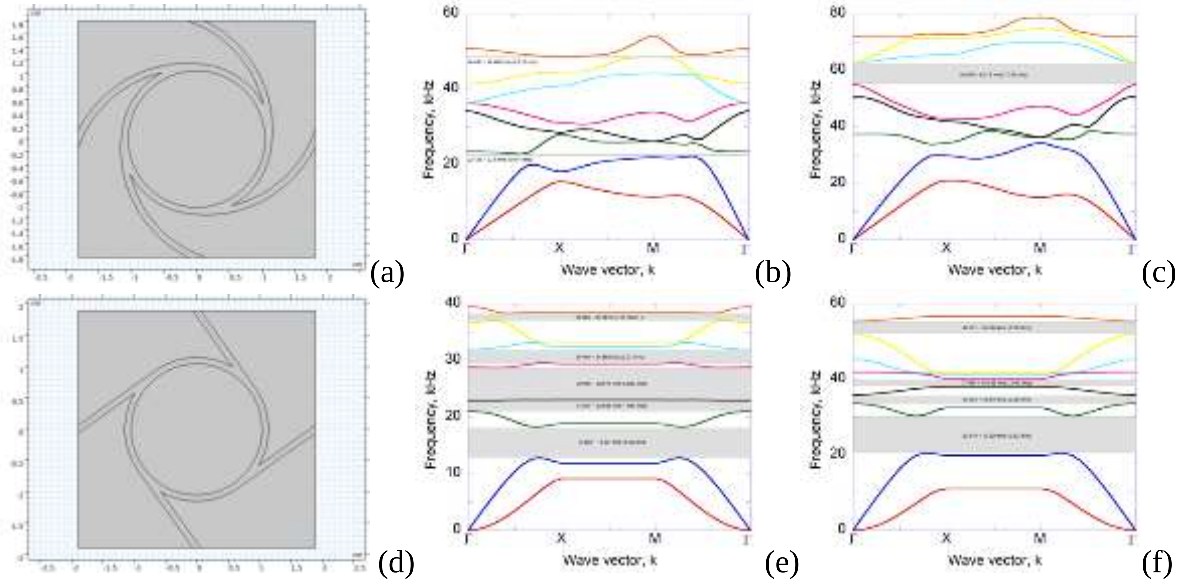

Fig. 1. Comparison of the bandgaps between the two chiral metamaterials

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Comparison of Numerical Methods in the Analysis of Wave Propagation in an Inhomogeneous Elastic Rod

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When constructing mathematical models, the question becomes about the reliability of the results obtained. This problem is especially critical when calculating bodies with functionally inhomogeneous properties, where it can be difficult to find an analytical solution for testing the numerical method.

In this paper, the longitudinal oscillations of an elastic rod in time domain are considered. Various analytical solutions of the problem with inhomogeneous Young's modulus are obtained on the basis of Legendre polynomials. These expressions are used to compare the effectiveness of the Finite difference method and the Finite element method, as well as time integration methods.

Also, when solving inverse problems and optimal control problems, it is required to obtain the dependence of the perturbation in solving the direct problem on the perturbation in coefficients, i.e. the Fréchet derivative. Effective methods of obtaining it, in the case of linear systems, take into account the absence of changes in material properties over time [1]. The presence of a representation of the Fréchet derivative obtained from the analytical solution made it possible to compare them. So, for the parameters of displacement, velocity and acceleration, approaches were compared where the Fréchet derivative is calculated as a time convolution from the solution of a direct and adjoint problem, where eigenvalues and eigenmodes are used for this, and where the Fréchet derivative matrix in the time domain is calculated from the Fréchet derivative in the frequency domain using a Discrete Fourier transform.

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Indentation of Poroelastic Materials

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Since the 1970s, much attention has been paid to the study of porous materials. Porous materials are of interest to the industrial sector. In addition, interest is growing in the study of the microstructure of poroelastic materials in order to create new biocompatible materials for the manufacture of implants.

The determination of the mechanical properties of inhomogeneous materials, including those with a microstructure, is usually carried out by means of indentation of a material sample. Mathematical modeling of the indentation process consists in setting the corresponding contact problem, as a result of which all the main characteristics of the contact between the indenter and the material sample are determined, and it allows making conclusions about the properties of the material based on the results of theoretical and experimental studies.

For porous bodies, the theory of microdilation is used. The concept of microdilation is associated with the redistribution of porosity in a medium under the action of a load. The relative volume of pores, which varies in stretched or compressed parts of the body, is taken as an independent kinematic variable.

In this work, within the framework of the theory of microdilatation, we consider the static contact problem of indentation of a poroelastic layer by a rigid strip indenter with a flat base, which settles into the layer material under the action of a load. The lower boundary of the layer is rigidly linked to the non-deformable base. The 3D-problem of indentation of a poroelastic layer is equivalent to the 2D-problem of indentation of a poroelastic strip. The solution of the 2D-problem of strip indentation is reduced to the solution of an integral equation of the first kind of the Fourier convolution type with a difference kernel with respect to unknown stresses on the contact. By selecting and inverting a singular integral operator, the integral equation is reduced to an integral equation of the second kind, the solution of which is carried out by the method of successive approximations. An effective solution of the integral equation of the problem made it possible to obtain formulas for all basic mechanical characteristics of the layer material, including the distribution function of the relative pore volume. The effect of nonclassical parameters of the poroelastic material of the layer (coupling coefficient and pore stiffness coefficient) on the distribution function of the relative pore volume over the layer thickness and on the main contact characteristics, such as the contact force on the indenter, contact stresses, horizontal and vertical displacements of the free surface outside the contact area, is analyzed. Comparison of the values of vertical and horizontal displacements showed that the horizontal displacements of the surface of the material of the poroelastic strip outside the contact area in absolute terms are 4–5 times less than the corresponding vertical displacements of the surface at the same points. It has been established that the distribution function of the relative pore volume reaches its maximum value at the contact under the midpoint of the indenter base, its minimum value - at the lower edge of the strip, and its values are proportional to the force acting on the indenter.

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Bite Force Estimation on the Tooth Fissure Using Mathematical Modelling and Micro-CT Results

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The occlusal surface of molars and premolars has a certain number of wedge-shaped (V-shaped) notches called fissures. Tips of fissures represent natural stress concentrators. In the present paper the X-ray microtomographic (micro-CT) research of the tooth enamel was conducted. The study revealed the area with a reduced mineral density in the vicinity of the fissure tip. Assuming that the enamel mineral density decrease occurs due to the mechanical load on the occlusal surface of the tooth during crushing of food, the degree of stress concentration at the fissure tip is determined by solving the problem of the stress-strain state of the tooth crown enamel with a wedge-shaped (V-shaped) notch. The study of stresses in the vicinity of the fissure tip made it possible to construct the boundaries of the enamel virtual fracture areas. Comparison of the sizes and locations of areas with a reduced enamel mineral density, obtained using micro-CT, with the sizes and locations of areas of virtual enamel fracture, obtained by theoretical means, made it possible to establish their approximate congruence. This circumstance made it possible to recreate by mathematical means the nature and magnitude of the force load on the lateral surface of the fissure, which contributes to the formation of areas of reduced enamel mineral density in the vicinity of its tip (Fig. 1). In the course of theoretical studies, the degree of influence of the main parameters of the fissure – the fissure opening angle, the bite force, the fissure depth, the distance of the load application that wedged the fissure, the imperfection of the lateral surface of the fissure – on the geometrical characteristics of the virtual fracture area, such as its area and diameters, was determined.

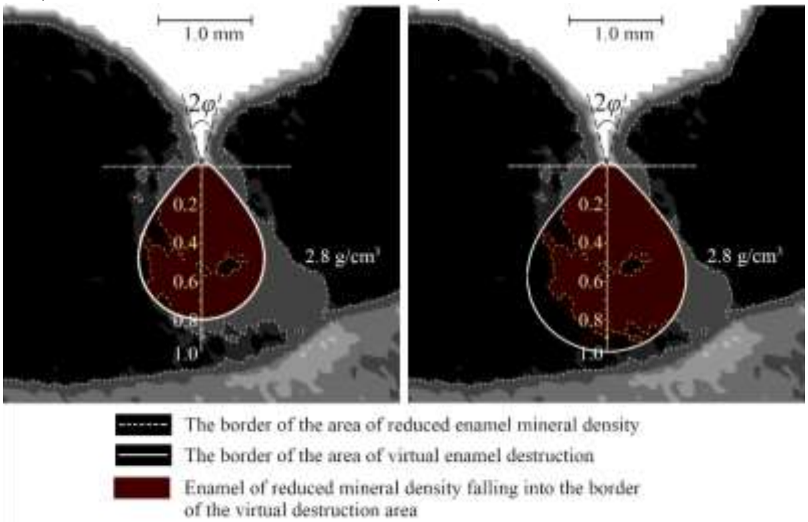

Fig. 1. Comparison of the imposition of a virtual fracture area and an area of reduced enamel mineral density on the micro-CT fissure image with the bite forces: 1350 N/mm (left) and 1700 N/mm (right)

Acknowledgements: This work was supported by the Government of Russian Federation, grant no. 14.Z50.31.0046. Experimental research was carried out at the Nanocenter of DSTU (https://nano.donstu.ru/).

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Статистический анализ изменения биомеханических свойств роговицы после операций по коррекции зрения

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Проводится сравнение биомеханических свойств роговицы у пациентов с миопией до и после проведения кераторефракционных вмешательств по методике ReLEx SMILE с помощью анализатора CORVIS ST. Группу составили 23 пациента (46 глаз) со сферической рефракцией -3,8±1,8 дптр.

Статистическому анализу были подвергнуты следующие показатели: ВГД и ВГД корректированное (IOP и IOP correct, мм рт. ст.), т.е. ВГД без учета и ВГД с учетом биомеханических свойств роговицы соответственно. Амплитуда деформации (Deformation Amplitude, DA в мм.), которая описывает амплитуду деформации роговицы по времени и позволяет косвенно оценить «мягкость» роговицы. Коэффициент деформации (DA ratio), который указывает на соотношение амплитуд смещения роговицы в центре и в 2-миллиметровой зоне от апекса, что позволяет судить о степени «жесткости» роговицы (чем меньше показатель, тем больше жесткость). Параметр жесткости SP-A1 описывается в виде формулы силы, деленной на смещение роговицы, и определяется конечным значением давления, разделенным на амплитуду прогиба в точке A1. Обратное значение интегрированного радиуса ICR, мм-1 (Inverse Concave Radius, ICR), т.е. обратное значение вписанного радиуса кривизны роговицы. Индекс модуля жесткости SSI, который описывает модуль жесткости роговицы. Толщина роговицы в центре (CCT), мкм, т.е. толщина роговицы в центральной зоне.

Выборка являлась достаточно малой, поэтому пропуски заполнялись средними значениями анализируемой переменной.

В результате проведенного статистического анализа показано, что по критерию Стьюдента среднее значение параметра IOP до операции значимо различается со средним значением параметра IOP после операции. Для сравнения средних значений параметра Deformation Amplitude до и после операции был применен критерий Вилконсона. В этом случае значимого различия по этому параметру не было обнаружено. Сравнение средних значений параметра Inverse Concave Radius с использованием критерия Стьюдента показало статистически значимое различие. Использование критерия Стьюдента для сравнения средних параметра индекса модуля жесткости (SSI) показало, что различия статистически не значимы. Для параметра толщина роговицы в центре (CCT) было показано статистически значимое различие в группах. Также значимое различие было показано для параметра жесткости SP-A1. По остальным параметрам не были получены значимые различия.

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Волны в волноводе с произвольным поперечным сечением

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Рассмотрен ряд смешанных задач о распространении бегущих волн в волноводе с произвольным поперечным сечением. Задача в безразмерной постановке сведена к операторному уравнению. Оператор представлен в виде квадратичного пучка операторов, содержащего два спектральных параметра: безразмерные волновое число и частоту колебаний.

Исследована структура дисперсионного множества – сочетания спектральных параметров, при которых существуют нетривиальные решения задачи. Методами теории возмущений изучена его структура для малых спектральных параметров. В области малого волнового числа изучены свойства получившейся последовательности задач. Показано разделение задачи нулевого приближения на плоскую и антиплоскую. Сформулированы условия, при которых операторы обладают свойством положительности и положительной определенности. Построены квадратичные представления ветвей дисперсионного множества. Показано, что ветви дисперсионного множества пересекают частотную ось под прямым углом, в случае, когда соответствующая точка не является кратным корнем дисперсионного уравнения. Для волноводов с поперечным сечением трех типов (круглое, квадратное, треугольное) численно на основе слабой постановки и МКЭ построены вещественные ветви дисперсионного множества. Также дисперсионные ветви построены приближенно на основе асимптотических формул. Проведено сравнение и определены области применимости квадратичного приближения для дисперсионных ветвей. При проведении вычислительных экспериментов выявлены близкие пары точек на частотной оси. Для ветвей, порожденных этими точками, наблюдается наибольшая разница с квадратичным приближением. Предложенный подход позволяет исследовать структуру дисперсионного множества для широкого класса анизотропии, неоднородности и граничных условий, в том числе и смешанного типа. Численные расчеты проведены для изотропного волновода с частично защемленной границей и для однородного ортотропного волновода. Представлены приложения для волноводов с клинообразным поперечным сечением.

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