

## ORGANIZATIONAL DETAILS

All the details concerning participation in the work of the conference and other organizational details you can find at our website

RUSSIAN ACADEMY OF SCIENCES



Institute for Problems in Mechanical Engineering



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XLV International Summer School - Conference

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BOOK  
OF ABSTRACTS

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St. Petersburg, Russia, 2017

# XLV International Conference “Advanced Problems in Mechanics”

June 22-27, 2017,  
St. Petersburg, Russia

## APM 2017 BOOK OF ABSTRACTS



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## General Information

The International Conference “Advanced Problems in Mechanics – 2017” is the forty fifth in a series of annual summer schools held by Russian Academy of Sciences. The Conference is organized in commemoration of its founder, Ya.G. Panovko, by the Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences (IPME RAS), Peter the Great St.Petersburg Polytechnic University (Institute of Applied Mathematics and Mechanics), Scientific Council on Solid Mechanics (RAS) (chairman N.F. Morozov), Russian National Committee on Theoretical and Applied Mechanics (chairman I.G. Goryacheva) under the patronage of the Russian Academy of Sciences (RAS) and the University of Seville (Universidad de Sevilla). The Conference is partially supported by Russian Foundation for Basic Research. The main purpose of the meeting is to gather specialists from different branches of mechanics to provide a platform for crossfertilisation of ideas.

The list of problems under investigation is not limited to questions of mechanical engineering, but includes practically all advanced problems in mechanics, which is reflected in the name of the conference. The main attention is given to problems on the boundary between mechanics and other research areas, which stimulates the investigation in such domains as micro- and nanomechanics, material science, physics of solid states, molecular physics, astrophysics and many others. The conference “Advanced Problems in Mechanics” helps us to maintain the existing contacts and to establish new ones between foreign and Russian scientists.

Young scientists’ school-conference “Modern Ways in Mechanics” (MWM), which is held within the annual international conference “Advanced Problems in Mechanics” (APM), is meant for broadening scientific outlook of young researchers in the field of mechanics and also for organizing their scientific dialogue. It is supposed that students, Ph. D. students and young Ph. D.’s under 30 (date of birth is later than 12/31/1986) from different all over the world, specializing in the sphere of theoretical and applied mechanics become the main participants of the conference. In order to attract the largest possible number of various scientific areas and schools, organizing committee suggests a partial compensation for the costs connected with participation in conference, as well as extensive cultural program. One of the major purposes of conference is transfer of scientific experience from well-known scientists to their young colleagues.

## History of the School

The first Summer School was organized by Ya.G. Panovko and his colleagues in 1971. In the early years the main focus of the School was on nonlinear oscillations of mechanical systems with a finite number of degrees of freedom. The School specialized in this way because at that time in Russia (USSR) there were held regular National Meetings on Theoretical and Applied Mechanics, and also there were many conferences on mechanics with a more particular specialization. After 1985 many conferences and schools on mechanics in Russia were terminated due to financial problems. In 1994 the Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences restarted the Summer School. The traditional name of “Summer School” has been kept, but the topics covered by the School have been much widened, and the School has been transformed into an international conference. The topics of the conference cover now all fields of mechanics and associated into interdisciplinary problems.

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The conference is organized with help of our service agency “Monomax PCO”: [www.monomax.ru](http://www.monomax.ru)

## Scientific Program

Presentations devoted to fundamental aspects of mechanics, or spreading the field of applications of mechanics, are invited. We are particularly keen to receive contributions that show new effects and phenomena or develop new mathematical models. The topics of the conference cover all fields of mechanics, including, but not restricted, to

- mechanics of media with microstructure
- nano- and micromechanics
- computational mechanics
- wave motion
- nonlinear dynamics, chaos and vibration
- solids and structures
- fluid and gas
- mechanical and civil engineering applications
- molecular and particle dynamics
- biomechanics and mechanobiology
- phase transitions
- dynamics of rigid bodies and multibody dynamics
- aerospace mechanics

## Accompanying Events

[MS1] Minisymposium in memoriam of Antonio Castellanos Mata (Contact person: Elena Grekova)

[MS2] Minisymposium "Nonlinear wave dynamics of generalized continua" (in memory of E. Aero and G. Maugin) (Organizers: Alexey V. Porubov and Vladimir I. Erofeyev)

[MS3] Minisymposium "Finite Element and Isogeometric Analysis of Advanced Problems in Mechanics" (Organizers: Jarkko Niiranen and Antti Niemi)

Four different forms of presentations are offered, namely, plenary lectures (35 minutes), presentations at minisymposia (25 minutes) and short communications (20 minutes), and posters.

The working language for oral and poster presentations are English and Russian. Attention: each participant may only give one oral presentation. The number of posters for each participant is not limited. The Summer School – Conference has two main purposes: to gather specialists from different branches of mechanics to provide a platform for cross-fertilization of ideas, and to give the young scientists a possibility to learn from their colleagues and to present their work. Thus the Scientific Committee encouraged the participation of young researchers, and did its best to gather at the conference leading scientists belonging to various scientific schools of the world.

We believe that the significance of Mechanics as of fundamental and applied science should much increase in the eyes of the world scientific community, and we hope that APM conference makes its contribution into this process.

We are happy to express our sincere gratitude for the help in organization to Russian Foundation for Basic Research, Russian Academy of Sciences (RAS), the Ministry of education and science of the Russian Federation, St. Petersburg Scientific Center RAS, Federal Agency for Scientific Organizations, the University of Seville (Universidad de Sevilla) and Vicerrectorado de Investigación de la Universidad de Sevilla. This support has helped substantially to organize the conference and to increase the participation of young researchers.



*Russian Academy of Sciences*



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# ABSTRACTS

## ANALYTICAL AND NUMERICAL METHODS IN THE MASS-POSITION DETERMINATION MEMS PROBLEM

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In this work we consider the problem of mass and position determination of an entity attached to the surface of an electrically actuated microbeam or carbon nanotube. As the effective method to detect this entity's characteristics is to track the frequency shifts in microbeam's modes of vibrations, we investigate the analytical expressions for the shifts and mass-position relation to be able to determine entity's mass-position using experimental data of the microbeam's spectrum. Statical and dynamical analysis of the presented nonlinear problem of electroelasticity is performed, where the microbeams are modeled as Euler–Bernoulli beams, including the nonlinear electric forces and the added entities, which are modeled as discrete point masses. Acquired results then compared to finite-element solution of corresponding coupled-field electromechanic problem from ANSYS.

## DYNAMICS OF GRAVITATING SYSTEM OF GAS AND DUST CLOUD

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Due to the gravitational force, cloud of dust and gas can contract and form planet. Here we present a simple model for the dynamics of one dimensional of self-gravitating spherical symmetrical gas and dust cloud.

We applied analytical and similarity solution methods to the equations of one dimensional of self-gravitating spherical symmetrical gas and dust cloud.

We used a Cole-Hopf transformation to simplify the equations of dynamics and thereafter we applied method of characteristics to reduce partial differential equation to a system of completely solvable ordinary differential equations.

We applied to the problem too, similarity solution method which reduce the partial differential equations to a system of ordinary differential equations. The Runga-Kutta method has been used for numerical calculation of the problem.

## TOWARDS INTERNAL LENGTH GRADIENT CHEMOMECHANICS

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This lecture outlines a number of key concepts and ideas that have not been explored in the area of chemomechanics or mechanochemistry, i.e. the meeting point of mechanics and chemistry. The aim is to cast these ideas into an initial mathematical framework for describing a variety of coupled chemomechanical phenomena occurring in material engineering and earth systems, as well as in the human body. Emphasis is placed on novel nanomaterials and modern technological processes such as those employing nanofilters and nanocatalysts, as well as on brain functioning. The new viewpoint advanced here is that in order to capture and control chemomechanical instabilities at the nanoscale we need to resort to internal length and time scales associated with the evolution of the underlying local mechanical stress and chemical agent. One convenient way to account for this is through the introduction of second spatial (Laplacian) and time (inertia) derivatives of the pertinent mechanical and chemistry variables in the constitutive equations describing the evolution of the chemomechanical system at hand.

*The support of the Ministry of Education and Science of Russian Federation under Mega Grant Project "Fabrication and Study of Advanced Multi-Functional Metallic Materials with Extremely High Density of Defects" (No. 14.Z50.31.0039) to Togliatti State University is gratefully acknowledged.*

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[2] Aifantis, E. C. "Towards Internal Length Gradient Chemomechanics." *Rev. Adv. MaterSci.*48(2017), *In press*.

## **CONTACT PROBLEM ON INDENTATION OF A CONDUCTIVE PUNCH INTO AN ELECTRO-ELASTIC PIEZOELECTRIC FUNCTIONALLY-GRADED HALF-SPACE**

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Indentation of a rigid punch into an electro-elastic piezoelectric half-space with functionally graded piezoelectric coating is considered. Electromechanical properties of the coating vary with depth according to arbitrary independent differentiable positive functions. Electromechanical properties of the substrate are constant. The punch is assumed to be an ideal electric conductor. Constant electric charge and normal centrally applied indentation force are applied to the punch. The problem is reduced to the solution of a system of two dual integral equations over Hankel images of contact pressure and electric induction. Kernel transforms of the integral equations are constructed numerically. Using specially design approximations of the kernel transforms the approximated solution of the problem is constructed in analytical form. The solution is asymptotically exact for small and large values of relative coating thickness. Numerical results illustrating some features of the electro-elastic deformation of the piezoelectric materials with homogeneous or functionally-graded coatings are provided.

*This research was financially supported by Russian Science Foundation grant no. 15-19-10056.*

## **FORMATION OF THE TRANSITION ZONE BETWEEN THE MATRIX AND THE INCLUSION DURING THE SYNTHESIS OF COMPOSITE**

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During the synthesis of composite, an interface zone between the matrix and inclusion with a new chemical composition is formed. The processes near the phase boundary defining the physical and mechanical properties and performance characteristics of the product are of particular interest. The thickness of this layer and its chemical composition significantly affect the properties of the composite. They depend on the technological parameters of the process of composite synthesis. To solve this problem numerically, it is necessary to know the thermal and kinetic parameters.

In this work, we evaluate the parameters necessary for the numerical analysis of the spherically symmetric problem and investigate influence technological parameters on the composition and thickness of the interface zone between a coated particle and the matrix. The model takes into account diffusion and the stages of phase formation in the transition zone.

## **REACTION OF LIVING CELLS TO PHARMACOLOGICAL AGENTS: IDENTIFICATION BY AFM**

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Atomic force microscopy (AFM) studies of living cells have become more attractive due to the new possibilities of increasing substantially the quantitative data output and improving the obtained data interpretation. Recently, the leading manufacturers of AFM equipment elaborated quasistatic modes, such as PeakForce Quantitative Nanomechanical Property Mapping (Bruker), HybriD (NT-MDT), Quantitative Imaging (JPK Instruments), that allow probing the sample relief and simultaneously its local mechanical properties with high speed and nanometer resolution. In particular, Young's modulus is a practical parameter for physiology and pathology of living eukaryotic cells characterization as well as their reaction to drugs. It is important that analytical models of indentation are developed [1], which substantially correct the value of the Young's modulus in the case, which is relevant for many experiments, when

the indentation depth is comparable to the thickness of a soft sample on a solid substrate. It is also noteworthy that the studies can be carried out under physiologically relevant conditions, i.e. in liquid and at 37° C, and the cell damage is minimized in the course of measurements, since the destructive lateral forces in the quasistatic modes are significantly suppressed.

These opportunities were used in our AFM experiments, aimed, ultimately, to identify the response of living cells to pharmacological agents. We studied the heart fibroblasts and dorsal root ganglia sensory neurons of chick embryos, rat erythrocytes, blood vessel endothelial cells of mice. The results were partially published in [2-6].

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### SELF-SIMILARITY IN NEGATIVE IONIZATION FRONTS AND GEOMETRICAL DIFFUSION

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We will present a study of the properties and structure of anode-directed ionization fronts without diffusion, based on a minimal streamer model for non-attaching gases. The model includes impact ionization processes as source terms. When magnetic effects can be neglected has been discussed, an electric shielding factor can be defined, and the physical quantities can be expressed as a function of it.

A Burgers type equation is obtained for the evolution of the electric shielding factor. Thus, the analytical and numerical study of the ionization fronts can be performed by using a Lagrangian formulation. The power of this formulation makes it easier to treat the cases of non-homogeneous initial electric field in electric discharges with curved symmetries. We will apply this formulation to a discharge between planar and curved electrodes (with cylindrical and spherical symmetries). When an initial seed of ionization is placed near the cathode, a travelling wave develops towards the anode. The shape and the velocity of this wave depends on the asymptotic behaviour of the initial charged particle densities.

If the initial density is compactly supported, then the travelling wave is a shock front, whose velocity is equal to the drift velocity of electrons. This behaviour was predicted for the planar case but we have found that a similar situation takes place in the cases of cylindrical or spherical symmetries. We will derive power laws for the velocity and the amplitude of the shock fronts in the cases of curved symmetry.

When the initial particle density is not compactly supported, but decays exponentially with the distance from the cathode, a shock front does not appear.

In the planar case, we will see that the velocity of the front is then constant and is larger than the drift velocity of the electrons. However, if the initial particle density decays more slowly than exponential with the distance from the cathode, accelerated fronts appear.

In the cases in which the physical situation has cylindrical or spherical symmetries and the initial ionization seed decays exponentially fast to infinity, we will see that the velocity follows the same power laws as the compactly supported case. However, the structure of the travelling wave is rather different. We will prove that the asymptotic behaviour of the charged particle densities is self-similar. Even if diffusion has not been considered, the front spreads out linearly in time. This is a remarkable feature: it is a diffusive behaviour of the solutions of the minimal streamer model caused by the geometry of the electric field, and we can call it geometrical diffusion. Our analysis opens the way to consider geometrical effects in the stability of ionization fronts.

### ON THE CONDITIONS OF TRANSITION TO THE UNSTABLE STATE OF THE COMPRESSIBLE PLASTIC AND ELASTIC-VISCOUS MATERIALS

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On the stress-strain curves, obtained in simple tension for the metallic specimens, a region of instability due to the formation of a neck is observed. In the theory of plasticity the conditions of transition to the unstable state and the appearance of the maximum point on the stress-strain curve are defined. In the formulation of this condition the assumption of incompressibility of the material is accepted. However, this assumption cannot be justified, because in

the neck region the numerous damages appear, i.e. the material becomes compressible. In the paper the condition of transition to unstable state for a compressible plastic material is formulated. For an incompressible material this condition was first considered by Hill. The effect of compressibility is determined using the current value of the lateral deformation coefficient. Taking into account this coefficient the rheological equations for compressible media, generalizing the relations for incompressible plastic and elastic-viscous materials, are proposed. The analytical solutions of these equations are obtained and the corresponding theoretical stress-strain curves, depending on the current value of the lateral deformation coefficient, are plotted. In particular, it is shown that for a compressible material in the region of instability the maximum point is shifted. In the case of the Hill's condition there is a fixed maximum point on the stress-strain diagram.

*Financial support of the Russian Foundation for Basic Research is gratefully acknowledged (Grant N 15-01-03159).*

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### **FORMULATION AND EXPERIMENTAL JUSTIFICATION OF HIGH-TEMPERATURE CREEP FRACTURE CRITERION**

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The new results on the effect of thermal embrittlement (embrittlement of structural metallic materials under prolonged action of relatively low stresses and high temperatures) are obtained. The main attention is focused on the formulation of the relations for the damage parameter and the development of the long-term strength criterion. For comparison of the obtained relations with the experimental results observational studies were performed on the determination of damage accumulation under high temperature creep conditions for various metals and alloys: copper, aluminum, Magnox AL80, Nickel and 0.1% palladium alloy, various heat resistant alloys. The experiments were carried out at different temperatures and levels of tensile stresses. Dwell times under load to failure were within 30-500 hours. Theoretical curves of density change were compared with the experimental results for some of these metals and alloys. At this time interval the damage function is expressed as a straight line. It is shown, that the experimental points are consistent with the theoretical curves. In this case they have the general character irrespective of the material and the temperature-power effects, which indicates the existence of a single law of damage processes and indirectly confirms the selection of a physical damage parameter as the ratio of the current density of the material to the initial density. Financial support of the Russian Foundation for Basic Research is gratefully acknowledged (Grant N 15-01-03159).

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### **EFFECT OF THE AERO-THERMO-ACOUSTIC TREATMENT ON THE PROPERTIES OF RAPID STEELS**

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The work is devoted to improvement of characteristics of rapid steels. The subject of this study is microstructure changing during aero-thermo-acoustic treatment in comparison with conventional kinds of heat treatment and characteristic changing of rapid steels under aforementioned treatment. Materials for the study were as follows: rapid steel R6M5 and American brand high speed steel HCV and HS grades. These materials were investigated metallographically after aero-thermo-acoustic treatment and compared after standard

heat treatment. Aero-thermo-acoustic processing (ATAP) [1-2] is one of the combined tools, which effects on materials. During this treatment temperature and acoustic fields effect to form the desired material properties throughout the volume of a material and a surface layer. This paper deals with the experimental study of the microstructure of rapid steels after aero-thermo-acoustic treatment in combination with standard heat treatment (SHT) in different variations and clarify the physical mechanisms that cause changes in the mechanical and structural characteristics that determine the durability and strength indicators.

The main result of this work is determination of dependence of aero-thermo-acoustic treatment regimes influence on rapid steels behavior. It was revealed that application of aero-thermo-acoustic treatment technology can be used for strength characteristics increasing of rapid steels.

1. The effect of aero-thermo-acoustic treatment on the structure of the materials: a processing structure homogenization occurs and the grain refinement and reduction in size of carbides
2. Rapid steel drills after ATAP 6.8 times stronger and more productive than similar drills after SHT.
3. In almost all cases, these steels after ATAP increase in microhardness is observed in 10-33 percent compared to SHT.
4. Application ATAP improves the durability of the cutting tool. Consequently, it can be used in tool production to increase the characteristics of high-speed steels

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## HEAT PROPAGATION IN AN IDEAL ONE-DIMENSIONAL CRYSTAL HEATED BY A SHORT THERMAL PULSE

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The equations for the heat flux and kinetic temperature are analytically derived for one-dimensional defect-free harmonic crystals based on the correlation analysis and the long-wave approximation in [1]. Unlike the other equations of the hyperbolic heat conduction [2, 3], the equation [1] is time-reversible and has only one independent parameter, the speed of sound. This equation also holds true for the one-dimensional harmonic crystal on an elastic foundation [4].

The analytical solutions of this differential equation are obtained for various initial and boundary conditions, namely: a thermally insulated half space heated by an instantaneous point source located at its edge, the cooling of an evenly heated half space under the boundary conditions of the first kind, heating of a half-space and a layer with a short laser pulse distributed in the media according to the Beer–Lambert–Bouguer law. The solutions are obtained both in the closed form and in a form of a series. The detailed analysis of the obtained solutions is conducted: we have built the envelope curves for the solution profiles, studied the asymptotic behavior of the solutions and plotted the temperature with respect to time at the both ends of the heated layer. All the obtained results are compared with the analogous solutions within the classical Fourier and hyperbolic heat transfer models. The analytical results are confirmed by computer simulations.

The main emphasis in this work is on the studying of the possibility to measure the described effects experimentally. The work tries to predict the complications that can possibly occur and give the estimated values of time and space resolution required to fix experimentally the difference between the temperature values predicted by classical Fourier's law, the hyperbolic heat transfer model and model [1].

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The connection between the behavior of materials with defects such as cracks perpendicular to the boundaries of elastic bodies and lithospheric plates with faults in case of various external influences in layered bodies is explained. Such behavior of these mechanical structures is seen during different types of external influences. The block element method is applied, which allows to investigate arising boundary problems difficult to study with other approaches. The stress-strain state of block structures generated by the studied mechanical problems was investigated, and the conditions of stress concentration build-up in hazardous areas were found. It was established that there are parameters, the role of which is paramount in assessing the possibility of destruction of the structures under consideration. The conditions allowing to exclude the occurrence of damage because of defects and faults, or to reduce the level of destruction were formulated for a number of problems.

*This work was supported by the Russian Foundation for Basic Research, projects nos. (14-08-00404), (15-01-01379), (15-08-01377), (16-41-230214), (16-41-230218), (16-48-230216), (17-08-00323), by the Program no 1-33P of the Presidium of the Russian Academy of Sciences, projects (0256-2014-0006), and from (0256-2015-0088) till (0256-2015-0093).*

## **SHELL MODELS IN STRAIN GRADIENT ELASTICITY: VARIATIONAL FORMULATIONS AND ISOGEOMETRIC IMPLEMENTATION**

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The goal of the present work can be divided into two main parts. The first one is development of a physico-mathematical model for shells in the framework of strain gradient elasticity theory by following the previous works in the field (e.g. [1-3]) with appropriate variational formulations. The second part is the implementation of a reliable and efficient numerical method as an isogeometric [4] open-source user subroutine into a commercial finite element software with the aid of experience of existing implementations for shells in the classic elasticity theory [5].

Such an approach allows one to use the advantages suggested by strain gradient elasticity theories for modelling materials with microstructure on different scales or macro-objects with substructures. The multi-scale models and numerical methods finally target at solving complex engineering problems of different fields.

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## **MECHANICS OF PENETRATION AND STRUCTURAL PROTECTION IN THE FRAME OF OPTIMIZATION GAME THEORY**

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The questions of the shape optimization of an axisymmetric rigid impactor and structure optimization of layered perforated plates are studied on the base of the Nash game approach [1], [2] for layered plates made on the given set of materials. As a criterion of the multipurpose optimization problem it is chosen the ballistic limit velocity under additional constraints on the impactor mass and the layered shield mass. The process of penetration of the rigid body into an elastic-plastic medium is modelled by the application of the two parts representation for the resistance force [3].

It is proposed and realized the solution algorithm of the conflict game problem: the optimal shape impactor against the optimal structure layered shield. It is considered the case when the impactor mass is given and does not depend on its volume and also the case with the constraint on the impactor mass (volume). With the application of an evolution numerical method (genetic algorithm) the optimal shapes of penetrating bodies and corresponding optimal shield structures are found and analyzed for all cases.

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### EXPERIMENTAL INVESTIGATION AND NUMERICAL ESTIMATE OF INTERFACE FRICTION IN ARAMID WOVEN FABRICS

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The processes of energy dissipation in woven barriers at a low-rate penetration are strongly influenced by friction [1]. As a result, the successful optimization of the ballistic efficiency of the woven protective layers should include the investigation of friction under the suitable loading conditions.

A common approach to the determination of the friction parameters is based on the results of experiments of the yarn pullout from a fabric layer [2-3]. More realistic method involves the use of the experimental data of the woven layer pullout under the conditions of transversal compression [4]. We propose a further development of this approach. The new experimental equipment is designed for pulling out the fabric layer of the multilayer woven package under the transversal compression. The proposed device allows us to specify the compressive loads in a wide practice range. The integral characteristics of friction obtained as a result of experiment can be implemented in the numerical models of fracture.

The geometrical parameters both of yarns (up to filaments) and of woven architecture were defined for several specimens of fabrics. Elastic moduli and strength limits of aramid yarns were determined. The required range of the transverse compression is estimated by the use of FE-modelling of impact loading of one- and four-layer protective plain-woven barriers. According to obtained estimations, the values of transversal compressive load in our tests vary from 200 N to 2000 N. On the base of the numerical modelling of the proposed experimental equipment the stress distribution uniformity in the middle fabric layer was investigated. The static and dynamic friction coefficients for plain weave aramid fabric were defined for the cases of textile-textile and textile-duralumin interfaces.

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### EXPERIMENTAL STUDY OF ALUMINUM ALLOY DURABILITY UNDER MULTIAXIAL FATIGUE LOADING

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The study is considered the fatigue life of metals under multiaxial loading. The relevance of this study is concerned with optimization of structures operating under complex stress-strain loading conditions. It can be used for structures designing in aircraft or machine-building industry. The aim of this work is estimating of reducing lifetime aluminum

alloy specimens under multiaxial cyclic and combined static-cyclic loading.

The mechanical tests on the corset-type specimens made of aluminum alloy are carried out by using the electrodynamic system Instron ElectroPuls E10000. Three types of experiments were carried out in this work: biaxial static torsion and cyclic tension, biaxial static tension and cyclic torsion, proportional biaxial cyclic tension-torsion loading. In the first and second case specimens were tested with two amplitude of cyclic loading. The static loading was gradually grown from specimen to specimen. In the third case specimens were tested with constant amplitude of stress intensity and different relation between tension and torsion modes. During the tests number of cycles was recorded. The experiment was carried out until failure or macrocrack appearance on samples surface.

As result, the fatigue life versus static components of loading diagrams and the life time versus relation between tension and torsion modes curves are constructed and analyzed. These curves were compared with curves constructed with the use of different multiaxial fatigue fracture models.

*The work was carried out in the Perm National Research Polytechnic University with support of the Russian Foundation for Basic Research, the grant №16-01-00239.*

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## STABILITY ASSESSMENT OF A TIBIA FRACTURE FIXATION IN THE CASE OF THERMAL STRESSES

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Fractures of a tibial diaphysis constitute the largest percentage among all cases of fractures of long bones, namely 32-37%. Internal osteosynthesis is one of the modern operational treatment methods of these fracture types. Problems of determining thermal stresses and their further consideration when choosing a treatment method of a patient are resolved with regard to such the medicine section as the traumatology. However, temperature drop at a bone surface in an installation place of a plate and screws during surgery and temperature change of fixators after sealing of a wound are not taken in conducting similar studies for biotechnological systems (BTS) "bone-plate-screws". The aim of this study is determination of maximum values of thermal stresses in components of a BTS "tibia bone-plate TRKh-screws".

3-D computer models of a tibia bone and a segmental fracture of this bone are created in the CAD SolidWorks. Fragment is localized to a middle third of a diaphysis, its size – 50 mm. Height of a diastase is 0.5 mm. Modelling of an internal osteosynthesis of the segmental tibia fracture are performed by a plate TRKh (named after the plate authors – Dr. S.Tkachenko, Dr. V.Rutsky and Dr. V.Khomutov) and 9 screws. An area, which is a contour projection of the plate TRKh, is built on the tibia bone surface.

3-D computer finite element model of the BTS "tibia bone-plate TRKh-screws" is created in SolidWorks Simulation module. Diaphysis consists of cortical bone tissue, epiphyses and metaphyses – of cancellous tissue, fixators – of titanium alloy VT6. Temperature of the tibia bone is 37 °C, temperature of the area – 34.5 °C. Air temperature in an operating room is 21 °C.

Maximum values of thermal stresses occurring in components of the BTS "tibia-plate TRKh-screws", do not exceed values of dangerous stresses for materials of these components according to the results of this study. Stability fixation of the segmental fracture is not violated. Heating the area on the tibia surface and fixators to 37 °C occurs for 30 minutes.

## HOW A DISSIMILAR-CHAIN SYSTEM IS SPLITTING

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In 1971 Thomson published a solution of a splitting problem in the elastic double-chain system (Thomson, R. et al., J. App. Phys. 42(8), 1971). We consider a generalization of the Thomson's model for different chains in both the quasi-static and dynamic regimes. This system represents a more complex waveguide characterized by three wave speeds, two for the separate chains and one for the connected system. Accordingly, there exist three wave ranges where the splitting could propagate. Based on this model we reveal the conditions of the transition modes realizations and determine to what extent a particular formulation, quasi-static, dynamic, discrete or continuum, is adequate. The analysis allows to

define characteristics of such processes and to demonstrate strength and weakness of different formulations. Analytical solutions for steady-state regimes are presented and analyzed in detail. It is shown, in particular, that the splitting can propagate steadily in the subsonic speed range and also in a part of the intersonic one. At the same time, the other part of the intersonic regime represents a band gap. The force - speed relations are presented, and the difference between the static and dynamic thresholds is demonstrated. We find that in the case of a considerable difference in the chain stiffness, the dynamic threshold is below the quasi-static one in both the subsonic and intersonic regimes. Surprisingly, the lowest threshold corresponds to the latter. Also, the energy and parameters of waves radiated by the front of the splitting are found. The admissibility of the steady-state solutions is checked analytically by the use of a 'first filter'.

### **EXPERIMENTAL STUDY OF STOCHASTIC EFFECTS IN ADAPTIVE TIP-TILT CORRECTION FOR HORIZONTAL-PROPAGATING SIGNAL BEAM IN ATMOSPHERE**

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An experimental study of the dynamics of of adaptive correction of tilt collimated energy beam at the output of 1350-meter trace are presented. In the processing of experimental data used the method of phase portraits and chaotic maps, allowing visualization of the unstable processes and bi-stable states of the system. Feature corrective procedures to near ground of tilt communication track with dynamical and statistical spatial inhomogeneity and non-stationarity refractive processes, affected the beam. Usually, available to the actuator range of frequency correction on long trace, crossed only the low-frequency part of the refractive modulation frequency band for the displacement vector for beam center. In this mode, the efficiency of the impact should be increased by connecting the feedback loop from the output. Proposed the statistical model and the criteria of efficiency correction algorithms in conditions of weakly and strongly developed turbulence. In the representation of the spectral filters are considered canonical adaptation algorithms - proportional, integral and differential - for regime quasi-regular atmospheric currents and turbulence coherent mode, the equivalent of the development process of self-organization under conditions of high temperature gradients near the surface layer. Ambiguity of observed for positional values dispersion parameters of the first space moments of a signal beam for the given meteo regimes on a trace in absence of correcting influence, and at inclusion of process of adaptive correction is under discussion.

### **PLASTIC DEFORMATION THROUGH STRESS-INDUCED MIGRATION OF HIGH-ANGLE GRAIN BOUNDARIES IN METAL-GRAPHENE NANOCOMPOSITES**

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A theoretical model is suggested which describes plastic flow through stress-driven migration of high-angle grain boundaries in metal-graphene nanocomposites. In the framework of the suggested model, stress-driven GB migration gives rise to the formation of wedge disclinations at GB junctions and edges of graphene inclusions. Energy and stress characteristics of stress-driven GB migration are calculated in several metals (aluminium, nickel and Gum metal). It is found that graphene inclusions strengthen metal-graphene nanocomposites. This is well consistent with experimental data reported in literature [1]. Also, it is revealed that graphene inclusions in metal-graphene nanocomposites either hamper or enhance unstable GB migration and thereby grain growth driven by stress, depending on inclusions length.

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## WAVE MECHANICS

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The equations of nonlinear wave mechanics of deformable systems have a complex analytical structure and often contain a gradient, non-gradient and nonlinear terms of high order. Exact solutions of such non-integrable equations exist for some non-trivial conditions on the equations coefficients. Finding the conditions and building the corresponding exact solutions plays an important role in the verification of numerical methods for solving equations and in problems of acoustic diagnostics and nondestructive testing of materials. In this paper, we propose a method of constructing exact solutions to integrable and non-integrable equations of wave mechanics based on the determination of the exact sum of perturbation series. For summing series, we use a criteria of equality of sequential diagonal Pade approximants, the minimum order of which is determined by the pole order of the equation's solution. When the criteria are met, there are conditions on the coefficients of the equation, in which the Pade approximants are desired exact solutions. The analysis shows that the proposed method can be effective for nonlinear evolutionary equations having no arbitrary functions of independent variables and special functions of the dependent variable as their coefficients.

## 2D GRANULAR DYNAMICS SIMULATIONS OF UNIAXIAL AND UNIFORM COMPACTION OF POLYDISPERSE NANOPOWDERS

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Two granular systems (I and II) corresponding to oxide nanopowders having different agglomeration tendency have been simulated by the granular dynamics method. The interaction of particles involves [1, 2]: the elastic forces of repulsion (modified Hertz law), the tangential forces of "friction" (Cattaneo – Mindlin, Reissner – Sagoci, Lurie, Jäger laws), the dispersion forces of attraction (modified Hamaker's formula), and in the case of II type system the opportunity of creation/destruction of hard bonds of chemical nature [3]. The processes of the uniaxial compaction and the isotropic compaction of model systems with different particle size distributions have been studied. The model systems are: monosized systems with particle diameter  $d$  equal to 10, 20, or 30 nm; bidisperse systems with different content of large ( $d = 30$  nm) and small ( $d = 10$  nm) particles; polydisperse systems described by log-normal distribution function with different width. Non-monotone dependence of compact density on content of bidisperse system has been revealed: in the vicinity of percentage of small particles about 80 – 90 % the bidisperse compact density exceeds by 1-2% of maximum density of corresponded monosystems. The width of distribution function of polydisperse systems has been varied from zero (monosystems) up to 0.47, which is typical value for experimental nanopowders [4]. It is revealed that polydisperse compact densities differ weakly, less than 1%, from the monosystem density.

*The work has been fulfilled in the frame of state task project No. 0389-2014-0002 and supported by RFBR (project Nos. 16-08-00277, 16-33-00826 mol\_a).*

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## COMPACTION RATE INFLUENCE ON NANOPOWDER YIELD STRESS: 2D SIMULATION BY GRANULAR DYNAMICS METHOD

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The granular dynamics method is widely used for simulations of quasistatic compaction processes of micro- and nanopowders [1-3]. However the development of effective methods of magnetic pulsed compaction [4], when the strain rate is about  $10^4$ - $10^5$  s<sup>-1</sup>, necessitates simulating dynamical processes. In particular, the dynamical yield stresses, as a rule, do not equal to the static ones. To perform the qualitative analysis 2D simulations have been carried out. The uniform compaction of alumina nanopowder (particles diameter is 10 nm) at relative rates  $\nu = (1/\rho)(d\rho/dt) = 6.8 \times 10^8, \times 10^7, \times 10^6, \times 10^5, \times 10^4$  s<sup>-1</sup> has been simulated. The results of the simulations include follows: 1) the relative location of compaction curves, from initial density  $\rho_0 = 0.5$  up to the value  $\rho = 0.95$  that corresponds with pressure of about 3 GPa; 2) the magnitude and the duration of stress relaxation after compaction process. The positional relationship of uniform compaction curves is well described by the relation:  $p(\rho, \nu) = p_{stat}(\rho) + k_\nu \nu^{1/4} (\rho - \rho_0)^3$ , where  $p_{stat}(\rho)$  is the curve of quasistatic process ( $\nu \rightarrow 0$ ), and the coefficient  $k_\nu = 21.5$  MPa s<sup>1/4</sup>. For example, to reach maximal density ( $\rho = 0.95$ ) at compaction rate  $\nu = 10^8$  s<sup>-1</sup> the pressure by 200 MPa higher than that of quasistatic process is required.

*The work has been fulfilled in the frame of state task project No. 0389-2014-0002 and supported by RFBR (project Nos. 16-08-00277).*

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## DISLOCATION KINETICS BASED APPROACH TO PREDICTION OF MICROSTRUCTURE EVOLUTION OF ULTRAFINE-GRAINED COPPER ALLOY UNDERGOING MULTIDIRECTIONAL FORGING

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Existing models of plasticity and dynamic recrystallization [1] do not provide a possibility to predict the whole variety of different processes of defect structure evolution in metals in the course of severe plastic deformation (SPD). Besides that, most of them do not take into account non-equilibrium dynamical nature of these processes and relationships between different defect structures. All of this makes it impossible to predict changes in the strength properties of metallic samples subjected to deformation and to developed theoretical methods for determination of optimal regimes of SPD [2]. This paper presents an attempt of self-consistent description of evolution of several structural material variables. These variables include dislocation/cell size, mobile/immobile dislocation density, fractions of high angle grain boundaries (HAGBs) and triple junctions and so on. Introduction of explicit interconnection between different kinetic models (for dislocations, triple junctions, HAGBs, etc.) substantially reduces the number of “tuning” parameters and results in a self-consistent description of the involved processes. The developed theoretical model was embedded into FEM numerical code and used to simulate deformation of copper sample undergoing multidirectional forging. The received modeling results include both the evolution of metal defect structure and the spatial distribution of defect structure within the sample volume. Different properties of microstructure have a corresponding (and in many cases considerable) mechanical effect. In that connection the development of numerical approaches that can reliably predict microstructure evolution for SPD processed metals is of a great importance for micromechanical engineering of metals.

*The study was supported by the grants from the Russian Foundation for Basic Research (project 16-31-60051) and the President of the Russian Federation (projects No. MK-4649.2016.1 and MD-7481.2016.1).*

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## MECHANISMS OF PLASTICITY AND PLASTIC ZONE AT THE I-MODE CRACK TIP IN DENTINE

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Dentin is a natural hierarchical composite – one of the main materials composing human and animal teeth [1,2]. The basic component of dentin structure is a mesh of intertwined organic collagen fibers (CFs) [3,4] which are connected to each other by a plurality of nodes. This mesh fills the space between dentin channels (cylindrical voids of ~3–5 μm in diameter), forming the mesoscopic scale level of dentin structure. The nanoscopic level of the structure is formed by an inorganic phase – the calcium hydroxyapatite nanocrystals, the most of which are located between CFs [5]. The CFs, which are the bundles of fibrils having semi-crystalline structure, form the basic microscopic structural unit of collagen. Individual fibrils are thin elongated nanostructures with diameters ~20–90 nm, up to several micrometers in length.

We have studied theoretically the following three possible mechanisms of inelastic deformation in dentin: (i) the plastic shear in the node of two CFs, (ii) the separation of CFs from one another in that node and (iii) the inelastic stretching of an individual CF due to local ruptures and relative shifts of tropocollagen molecules. Our theoretical estimates show that plastic shear in the node of CFs requires relatively small local shear stresses less than 150 MPa. Even less tensile stress is required for the separation of CFs from one another in the node and a slightly higher tensile stress is needed for partial longitudinal break of individual CFs [6].

For each of these mechanisms, we have estimated the size of plastic zone near the I-mode crack tip and shown that the detachment of CFs is the easiest mechanism of inelastic deformation. At very small external stresses less than 10 MPa, the break of CFs can be observed only in the close vicinity of the crack tip, and the plastic zone size should not exceed some hundreds of nanometers. The plastic zone size increases monotonically with increasing external stress and at the stress values higher than 50–100 MPa, it can reach tens of micrometers. These estimates qualitatively correspond to the plastic zone size observed by TEM in dentin samples with cracks [2].

*This work was supported by the Russian Science Foundation (grant No. 15-19-10007).*

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## NUMERICAL SIMULATION OF MICRO-LOCALIZATION BEHIND THE SHOCK WAVE FRONT AND PHYSICAL INTERPRETATION OF THE PARAMETERS OF STRAIN RATE SENSITIVITY OF ALUMINUM AND COPPER

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Strain rate sensitivity parameter is traditionally used to describe the changes in the yield strength of materials with increasing strain rate. At the same time, at high strain rates, there are additional effects of the material strain softening associated with an increasing in the density of mobile dislocations and reducing the dynamic yield stress [1]. The nature of this effect remains a scantily explored issue. We consider the phenomenon of micro-localization at the shock front in aluminum and copper by three independent positions: using dislocation plasticity based numerical simulation [1, 2], the integral criterion of plasticity [1,3] and comparison with the experimental measurements of the particle velocity dispersion [4]. It allows us to relate the amount of deformation intensity deviation with the mechanical parameter of the strain rate sensitivity and, thus, determine the class of materials to which these instabilities are mechanically significant.

*The study was supported by the grants from the President of the Russian Federation (MK-4649.2016.1 and MD-7481.2016.1) and the Russian Foundation for Basic Research (project No. 16-31-60051).*

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## FLOW OF VISCOPLASTIC SUSPENSIONS IN A HYDRAULIC FRACTURE

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Existing hydraulic fracturing simulators describe the flow of particle-laden suspension inside a hydraulic fracturing in the framework of power-law rheological model. According to rheological experiments, large concentration of solids provokes finite yield stress of hydraulic fracturing fluids, which has to be considered to provide accurate prediction of proppant placement and consequent fracture conductivity.

We continue to study flows of immiscible incompressible Bingham fluids in a narrow rectangular channel approximating a hydraulic fracture started in [1]. Using the lubrication approximation, three-dimensional Navier-Stokes equations are reduced to the system of advection equations for the fluid tracers and quasi-linear elliptic equation describing the pressure field. The system is solved numerically using the finite-difference approach and staggered rectangular grid. Advection equations are solved explicitly using the flux-limiting TVD scheme, while the pressure equation is solved implicitly using Picard iterations and multigrid linear solver with matrix-dependent restrictions and prolongations [2].

The model is validated against a number of experiments made in Hele-Shaw cells, namely, slumping of heavy oil in a slot; particle transport and bed formation in water; channeling of power-law fluids through the yield-stress fluid [1].

Parametric study of the displacement of Bingham fluids in a Hele-Shaw cell is carried out. It is found that the pillar of yield-stress fluid behaves similar to that of Newtonian one in the absence of Saffman-Taylor instability. Fingers developed through the pillar of yield-stress fluid trigger the development of unyielded zones. It is found that increase in Bingham number (which is the ratio of the yield stress to the typical viscous shear stress) leads to increase in finger shielding effect and increase in overall finger penetration zone.

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## EFFECT OF THE MICRO-DEFORMATION ON THE INTERNAL FRICTION BEHAVIOR OF AL-MG ALLOYS

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In this work, effect of preliminary micro deformation on the micro plastic behavior of non-porous and porous Al-Mg solid solutions was studied by the internal friction method using the Direct Torsion Pendulum Technique. The internal friction value of non-porous solid solutions increases gradually with the increase of preliminary micro deformation amplitude. The increase in internal friction is very considerable for the porous solid solution. This may be associated with the presence of intergranular pores. The parameters of the non-porous solid solutions, characterizing the dislocation mobility, increase slightly with the growth of the prior micro deformation amplitude. However, it has been noted that its increase is significant in the case of the porous solid solution. These variations can be attributed both to the interaction of the dislocations with the different obstacles present in the solid solutions, and to the phenomenon of diffusion of the atoms of solute element from the dislocation core to the volume of the polycrystal.

## DEFORMATIONS OF A PRE-STRETCHED AND LUBRICATED FINITE ELASTIC MEMBRANE DRIVEN BY NON-UNIFORM ELECTRO-OSMOTIC FLOW

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The microstructures in current common use are primarily rigid structures characterized by fixed boundaries. Microstructures which can be dynamically deformed into desired patterns may hold promise for new applications in various fields such as adaptable optics, soft robotics, and reconfigurable microfluidics. We suggest the achievement of such dynamic deformations by the use of non-uniform electro-osmotic flows in a narrow gap between a rigid plate and elastic membrane, where the induced pressure in the fluid is used to exert forces on the membrane. In practice, implementation of such configuration necessarily takes place on finite domain (e.g. a frame holding the membrane), and the placement in the case of thin elastic membrane requires its pre-stretching to obtain smooth and flat surface. Taking into account these considerations, in this work we analyze the viscous-elastic interaction between a viscous fluid and a pre-stretched and finite-size elastic membrane. Under the assumptions of strong pre-stretching and small deformations of the elastic sheet, and by applying the lubrication approximation for the flow, we obtain a linearized 6th order diffusion equation governing the deformation accounting for both bending and stretching. We derive the Green's function describing the solution in a rectangular domain, and use it to obtain several basic solutions for constant and time-varying square-shaped actuations, and explore the effect of pre-stretching on the resulting deformation. We further study the dependence of the deformation magnitude on the spatial wavenumber, revealing its effect on the transition between stretching and bending dominant regimes. Finally, we discretize the zeta potential distribution into individual squares (better representing finite gate electrodes) and study the effect of such discretization on the achievable resolution.

## THE SOLUTIONS OF NONLINEAR EQUATIONS OF FLAT DEFORMATION OF THE CRYSTAL MEDIA ALLOWING MARTENSITIC TRANSFORMATIONS

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Analytical models of crystal media are necessary for development of scientific bases of modern technologies of receiving materials with the necessary special mechanical properties. The nonlinear theory of deformation of crystal

media with a complex lattice has been constructed in the works [1,2]. Deformation of the media in this theory is described by vectors of acoustic  $\mathbf{U}(t, x, y, z)$  and optical  $\mathbf{u}(t, x, y, z)$  modes. For a case of flat static deformation the vectors  $\mathbf{U}(x, y)$  and  $\mathbf{u}(x, y)$  can be found from system of four connected nonlinear equations. The vector of macroshift  $\mathbf{U}(x, y)$  can be found in Papkovish-Neuber form. The system of the connected equations is reduced to a set of the separate equations. For the vector of microshift  $\mathbf{u}(x, y)$  one has found the sine-Gordon equation with variable coefficient (amplitude) before a sine. New solutions of this equation for amplitudes of the special forms are given in paper [3]. Other equations of system are the Poisson equations with sources in the right hand part which are defined by microshifts. For a case of constant amplitude the class of doubly periodic solutions is found for the sine-Gordon equation which are expressed through Jacobi elliptic functions. The analysis of the found solutions has shown that the nonlinear model describes specific topological features of deformation of crystal media which are implemented in the field of intensive external tension.

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### LOCALIZED LUMP-SOLITON-LIKE EXCITATIONS IN QUADRATIC AND TRIANGULAR MORSE LATTICE

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Localized supersonic long-living nonlinear modes excited in both quadratic and triangular lattices of point particles interacting via potential Morse bonds are studied in a frame of models of two kinds. First, numerical simulations on a base of Newtonian, for zero temperature, and Langevin, for non-zero temperature, equations are performed to define configurations (coordinates and velocities of all particles) of stationary (meta-stable) modes and their characteristics. Second, the partial differential equations are derived on a base of corresponding dispersion relations to analyze excitations of a lump-soliton kind. The equation is of the Kadomtsev-Petviashvili equation for a quadratic lattice but a differential operator includes additional terms in the equation for a triangular lattice. Equations of that type for a hexagonal lattice are discussed as well.

### THE ASSESSMENT OF THE ROLE OF THE WIEN EFFECT IN THE ELECTROHYDRODYNAMIC FLOW FORMATION IN A CLASSICAL ELECTRODE CONFIGURATION

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Generally, all electrohydrodynamic (EHD) flows emerging from sharp high-voltage electrode are believed to be caused by the injection charge formation whereas the field-enhanced dissociation (or the so-called Wien effect) is disregarded. Though the latter was theoretically predicted yet in 1934 [1] and later described in one of the most important book on EHD [2], the experimental evidence of that the Wien effect leads to the emergence of intensive EHD flows was made very recently [3]; moreover, it was made using a quite particular electrode arrangement.

In view of the above, the goal of the present work is the ascertaining the predominant mechanism of charge formation in a classical electrode configuration like blade-plane one. The configuration was chosen for the investigation as it features highly non-uniform electric field distribution, can be simulated in 2D approach, and allows observing velocity distributions in a convenient way. The study seeks to assess the role of the field-enhanced dissociation in the EHD flow formation by comparing experimental data and the simulation where only one charge formation mechanism—the Wien effect—is taken into account. Computer simulation involves the complete set of EHD equations: those of Poisson, Navier–Stokes, and Nernst–Planck. The experiment uses particle image velocimetry and dynamical current-voltage characteristic techniques to observe velocity distributions and electric currents.

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## TWO-SCALE MODEL OF HYDROTHERMAL SYNTHESIS OF NANOSCROLLS

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Two-scale model of hydrothermal synthesis of nanotubes is proposed. Macroscopic level of model includes two-phase hydrodynamics of liquid with nanotubes, heat transport and multicomponent convective diffusion in the liquid.

On the microscopic level of the model the scrolling of nanotubes [1] and evolution of nanotubes ensemble due to diffusion [2] is described.

As result of calculating the distribution of diameter and length of nanotubes is obtained. According with experimental data, the diameter of the nanotubes is asymptotically approaching the equilibrium value. This equilibrium diameter is determined by the chemical composition of nanotubes.

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## TRAVELING WAVES IN FLUIDS: KINK SOLUTIONS AND BIFURCATIONS WITH RESPECT TO THE WAVE SPEED

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In this talk, I will present some new results on traveling waves in fluids.

Two examples will be featured prominently: electromigration dispersion waves in a capillary and acoustic waves in thermoviscous perfect gases. In the former case, a reduction to Darboux's equation is obtained. In the latter case, a special case of Abel's equation is derived for inviscid but thermally conducting gases. (The case of viscous but non-thermally conducting gases leads to a more complicated nonlinear ODE.) A third example that I will discuss is a one-dimensional weakly-nonlinear model equation based on a Lagrangian-averaged Euler- $\alpha$  model (a nonlinearly dispersive regularization) of compressible flow in lossless fluids.

In all three contexts, exact (both implicit and explicit) solutions are constructed for traveling waves (specifically, topological solitons also known as "kinks") connecting distinct equilibria of their respective ODEs. For electromigration dispersion waves and acoustic waves in viscous but non-thermally conducting gases, the governing ODE is shown to exhibit a transcritical bifurcation with respect to the dimensionless wave speed at the value of unity. For the Euler- $\alpha$  model, no bifurcations arise, however, a kink solution with an oscillatory tail is found to emerge as the exact solution of a signaling-type initial-boundary-value problem for the linearized equation of motion, which connects to the work of Porubov and Maugin on dispersive kinks.

I will conclude the talk by highlighting the generic nature of kink-type traveling wave solutions across fluid mechanics.

## TIME-DEPENDENT BEHAVIOR OF GRANULAR MEDIA

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The granular media in a jammed state behaves like a solid, whereas under other conditions it may behave as a liquid or gas. However, in spite of resemblances it is a very unusual solid, liquid or gas. Of particular interest are the time-dependent deformation in a jammed (solid-like) state as well as conditions of the transition from a solid-like to a liquid-like states. Such transition has been observed when the jammed state breaks down and a "fluidization" takes place. Modeling of mechanical behaviour of granular media are commonly addressed by phenomenological methods of

continuum mechanics and macro scale experiments on one side and by statistical mechanics methods and numerical simulation combined with micro scale experiments on the other. There are numerous observations of a time-dependent deformation of granular media in a solid state that is deeply linked to its granular structure. The root causes of time-dependent deformation are micro fracturing along the grain contacts leading to sliding and rotation of individual grains, local rearrangement of grain clusters, grain crushing, chemical degradation, physical aging etc. Such micromechanisms of deformation are noticeably different from that in conventional materials like metals and polymers. A typical representative of the granular media is an unconsolidated sand. In this work we use a cohesionless sand to study the time-dependent deformation of granular material. Experimental observations and modeling effort in studies of sand deformation under step-wise loading with variable stress steps and hold time of constant load are reported. Analysis of a large body of experimental results and modeling efforts suggest that there is a very strong dependency of the sand deformation on the loading history. This paper presents a predictive modeling of granular media (sand) creep. The model employs an iterative stress-strain path dependent algorithm calibrated to a set of experimental data. An algorithm of the sand density increment dependency on the previous density and the step-wise loading history, i.e., a sequence of stress increments, number of steps and hold time duration is formulated in form of a recursive function. It is based on a parametric analysis of a series of tests with constant stress increments and hold periods. The validity of the proposed algorithm is verified by applying the calibrated model to predict independent tests results. Observations and analysis of solid-like state transition into an anisotropic liquid-like states are also discussed. Applications of reported studies are briefly addressed.

## METAMATERIALS WITH AUXETIC AND ULTRA-WIDE BAND GAP PROPERTIES

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Metamaterials are special micro-structured materials ad-hoc designed to obtain properties usually non existing in standard materials. Two meaningful examples are auxetic materials [1] with negative Poisson's ratio and phononic crystals with wide-band gap that filter elasto-acoustic wave transmission [2].

The lecture will be devoted to recent findings in the field of metamaterials with a particular focus to future applications at the micro-scale, typically for innovative microsystems.

Auxetic structures [1] seem very promising for applications in microsystems especially as motion conversion mechanisms. The most popular feature of auxetic structures is, in fact, that they can expand in the direction perpendicular to an externally exerted tension thus showing an equivalent negative Poisson's ratio. In addition, they enhance material properties related to negative Poisson's ratio, such as increased shear modulus, indentation resistance, fracture toughness, energy absorption, porosity/permeability variation with strain and synclastic curvature. The lecture presents three auxetic structures obtained as results of different optimization procedures. All of them are based on the maximization of the ratio between the displacements obtained in one direction (i.e.  $y$ -direction) as a consequence of the displacements imposed in the orthogonal direction (i.e.  $x$ -direction) and the imposed displacements themselves. Some 3D extensions of the optimized 2D auxetic structures are, then, also proposed as 3D motion conversion mechanisms in microsystems.

On the other side, periodic structures and micro-structures may exhibit bandgaps, i.e. portions of frequency domain in which there is no propagation of waves. Such phenomena are well known when dealing with electro-magnetic wave transmission. Recently, there has been a growing interest in the mechanical counterpart, namely elastic or acoustic waves [3-4]. Applications of such periodic structures in the elastic and acoustic domains span all the mechanical frequency domain ranging from very high frequency (i.e. heat conduction) to very low frequency (i.e. seismic insulation). Generally, the widest the bandgap the most robust the wave attenuation around a certain frequency, therefore all the applications take advantages from very wide bandgaps. The lecture presents strategies to improve the bandgap width from the mechanical point of view as well as modeling and experimental validations of the widest bandgap in literature for three dimensional elastic phononic crystals [2]. Particular attention is devoted to the role of additive manufacturing techniques in this kind of applications.

Finally, combination of auxetic and phononic properties in the same structured material are illustrated, in order to exploit tunability of the insulation properties.

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## **FRACTURE AS A RESULT OF SOLID AND FLUID INTERACTION, EFFECTIVE NUMERICAL MODEL**

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Many natural and technological processes involve fluid – solid interaction. A specific class of them may exhibit fracture of solid as a result of strong impact from the fluid. One of such processes is Hydraulic fracturing. It happens when a fluid is pumped at high pressure into a solid material. The push of the fluid makes the fracture propagating. This coupled problem is very difficult to solve. The strong non-linearity of the model requires the use of an iterative algorithm and the presence of singularities requires an intensive use of asymptotics to get good results. Added to this, other aspects of the problem make it more difficult, such as moving boundaries or possible leakage of the fluid inside the material (the so called leak-off phenomenon).

There are a number of numerical simulators (mostly commercial ones) dealing with such problems but their accuracies have not been externally verified while performance still needs a significant improvement [1]. Even for the simplest 1D models (PKN, KGD and radial fracture) there is still room for improvement and understanding. Recently, several groups are working on the improvement of existing numerical techniques used in the HF simulators. The most successful ones are [2, 3, 4].

In this work we consider an improved algorithm for the case of local elasticity operator and Non-Newtonian fluid which makes use of proper choice of variables (velocity and crack opening), accurate asymptotic behaviour of the solution in various regimes, exact implementation of the speed equation (Stefan type propagation condition at the crack front) and added support for higher order quadrature formulas. A new efficient time integration strategy using higher order backward scheme has been implemented. This allowed us to achieve better performance (higher accuracy in the computation of the solution, and, in general, much faster and stable algorithm).

Now our work is focused on bringing all these upgrades into the non - local framework of linear elasticity and then to implement the new important feature, shear stress induced by fluid on the crack surfaces [5]. This will fully resolve the problem of small toughness and the compatibility between viscosity dominated regime and the leak-off models like Carter's one [1]. Another improvement that we are going to implement is related to the treatment of the crack propagation. Finally we are also considering another local version of the HF problem when the fluid opens a gap between the rigid support and a thin non - elastic tissue.

The project for the future is to put together all the knowledge acquired working on the classic 1D models and to use it for adapting our solver to the case of 2D model.

*GD gratefully acknowledges the support of the EU project H2020-MSCA-RISE-2014-644175-MATRIXASSAY.*

*GM is thankful for the support of the EU project IRSES-GA-2013-610547-TAMER.*

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## **SURFACE ENGINEERING FOR PROPERTY ENHANCEMENT OF PHARMACEUTICAL POWDERS**

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Research innovations applicable to pharmaceutical industry based on particle surface engineering that exploits interactions at the nano and micro scales are discussed. Our work involves development of practical methodology employing dry mechanical processing, called dry coating, to create nano-rough surfaces onto micro drug powders. Methodology includes development of models to better understand cohesion and its subsequent impact on key properties of surface modified powders. This has led to development of dry coating toolbox as a predictive, model-based approach to mitigate problems posed by fine pharmaceutical powders due to high cohesion, leading to improvements in flow, packing, fluidization, dispersion, and charging. Examples of its applicability to pharmaceutical

products are presented. Open issues such as prediction of the bulk behavior based on individual particle properties are discussed along with the need to develop models that allow predicting properties of multicomponent mixtures.

### **ADVANTAGE OF SOIL REMEDIATION FROM VOLATILE CONTAMINANTS BY HOT AIR INJECTION**

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The study is on the merit of conducting soil vapor extraction (SVE) operations with hot air as compared to operations with unheated air. In general, SVE are operated with air at ambient temperatures with or without thermal soil warming. Thermal enhancement of soil vapor extraction (TESVE) is usually attained by electrical heating of the soil and is conducted with or without steam injection. Here the focus is on using hot air to enhance the vapor extraction rate. The study shows that this soil remediation technique is highly attractive, particularly when the soil pore saturation drops to low levels (say under 0.1%). At this low saturation levels, cleanup rates of regular SVE methods are markedly slow. To demonstrate the advantage of the hot air TESVE technique, a sandy soil containing contaminated water is studied. The effectiveness of SVE processes is measured by the contaminant mass-removal rate and the removal-capacity limit. As expected, the heating indeed drives a higher vapor pressure of volatile contaminants as well as both, higher vaporization and diffusion rates, thus providing a faster soil-remediation process. The governing equations are based on the Darcy law and are applied to an expanding compressible flow. The equations were solved analytically to determine the minimal time required for complete soil remediation. An approximate closed form solution was obtained based on the assumptions of local equilibrium (owing to low flow rates) and a linearized representation of the vapor to air density-ratio dependence on temperature (reasonable approximation for non-excessive air heating). The characteristic reduction of time necessary for SVE completion is calculated as function of the injected air temperature. Likewise, the corresponding additional energy consumption requirements are also calculated. For example, it is shown that for a certain realistic condition, elevating the injected air temperature by 17°C can reduce the required SVE process time by 50%, while increasing the total energy consumption by 30%. The cost of this added energy consumption is insignificant considering other cost savings, such as equipment utilization and manpower, which are cut by 50%. In essence, the model provides a tool that can be easily used to estimate the potential gains of TESVE operations with hot air for various soils properties and characteristic dimensions.

### **ON THE THEORY OF ELECTROMAGNETIC SEPARATION OF GRANULAR MATERIALS**

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The aim of this work is to determine statistical properties of motion of paramagnetic particles in the layer of non-magnetic particles, by solving the model problem. Since the paramagnetic are weakly magnetic substances and it is practically difficult to achieve strong magnetic field gradients, it is necessary to take into account effects of collisions on the motion of paramagnetic particles. A closed system of equations describing this motion is obtained. Analytical calculations give relatively simple equations that provide qualitative assessment of the paramagnetic particles extraction process. The corresponding insights into the process facilitate numerical modeling of magnetic segregation and can be also of use for setting up the related natural experiments.

### **MICROMECHANICS BASED FRAMEWORK WITH SECOND ORDER DAMAGE TENSORS**

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Using the harmonic decomposition of an elasticity tensor, we investigate the induced anisotropy due to the presence of (non-interacting) cracks in an initially isotropic linear elastic material.

In 2D, we recently obtained the following results in the case of closed cracks: the microcracking state is represented by a single 2nd order crack density tensor, the compliance tensor is square symmetric, and two cracks arrays allow to represent the effects of any arbitrary closed microcracks systems, the angle made by the two cracks arrays being  $\pi/4$ . Moreover, the irreducible part of fourth order change in compliance tensor is found to be an harmonic square of an

harmonic (i.e. symmetric and deviatoric) second order tensor.

In practical case of 3D in-plane measurements, the concept of harmonic factorization allows us to factorize, similarly to the 2D case, the irreducible part of fourth order damage tensor as an harmonic square of an harmonic second order tensor.

With this result, we derive a 3D micromechanics based framework with second order damage tensors. An illustrating example of a family of phenomenological anisotropic damage models compatible with this framework is given.

## **MOLECULAR DYNAMICS STUDY OF THE SPATIO-TEMPORAL EVOLUTION OF VORTEX-LIKE ATOMIC MOTION IN A LOADED SOLID BODY**

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The process of the redistribution of internal stresses and atomic displacements in preliminary loaded solid body is studied by means of the molecular dynamics. A possibility of self-organized system of vortices involving the atomic motion at a stage of relaxation is demonstrated. It is shown that the typical sizes of such dynamic defects vary in interval from 1 to 5 nanometers. At that their life-time depends on the size and can be found between from some part to the dozens of picoseconds. A new approach to the identification of the vortex motion of vector variable discretely distributed in space with random distances between nodes is developed. The used methodology makes it possible not only to visualize the vortex motion of particles in space, but also to analyze evolution of the dynamic defects. It is shown that the system of the dynamic vortices and anti-vortices can move inside the crystallite and provide the stresses redistribution from the bulk to free surfaces in order to conserve continuity of the material.

## **DISCRETE BREATHERS IN CRYSTALS: NEW RESULTS AND OPEN PROBLEMS**

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Discreteness and nonlinearity of media are the two ingredients necessary for the existence of the spatially localized, large-amplitude vibrational modes called discrete breathers (DBs) or intrinsic localized modes. During the last decade a great deal of attention has been focused on the study of DBs in crystals [1,2]. They have been identified in alkali-halides, ordered alloys, pure metals, covalent crystals (diamond, silicon, and germanium), and in 2D nanomaterials such as graphene and graphane (fully hydrogenated graphene). Several general approaches for finding initial conditions to excite DBs in molecular dynamics simulations have been developed. There exist experimental evidences for existence of DBs in crystals. Uncovering the role of DBs in formation of physical and mechanical properties of crystals is the next step of the research in this field. This report is devoted to the review of existing results on DBs in crystals and to the description of the open problems.

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## THE ANALYSIS OF STRESS-STRAIN STATE OF A COMPOSITE PLANE WITH INTERFACE CRACK FOR JOHN'S HARMONIC MATERIAL

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The solutions of some nonlinear problems for bi-material plane with an interface crack (cut) are obtained. The plane is formed by joining of two half-planes made from different materials. On the coats of crack an external loading is applied. The constant nominal (Piola) stresses are known at infinity. Mechanical properties of half-planes are described by the model of John's harmonic material. The application of this model has allowed to use the methods of the theory of complex functions. The stresses and displacements are expressed through two analytic functions of a complex variable, defined by the nonlinear equations on a contour of crack. The exact analytical solutions of some problems on interface cracks are obtained. In particular, the problems for the plane with a free interface crack subjected to constant nominal stresses at infinity and the problems for the plane with interface crack on which coats uniform pressure is set are solved. A particularity of this problem is the dependence of boundary conditions on a crack from the deformation of its coats. A pressure is directed along a normal to the deformed surface of coast, and the coast form is unknown. The exact analytical formulas for stresses and displacements are found. The asymptotic expansions based on the global solutions have been constructed for the stresses and displacements in vicinity of a crack tip.

In nonlinear problem of uniaxial extension of a plane with free crack it is established, that the formulas given the crack opening and the stress intensity factors near the crack tips completely coincide with the similar formulas derived from the equations of the linear elasticity. The nominal stresses have the root singularity at the tips of a crack; the Cauchy stresses have no singularity. The displacements have logarithmic singularity.

It was found out, that in the problem of the crack under action of uniform pressure some critical pressures proportional to the shear module exist and their excess leads to loss of a material stability and large supercritical stresses and strains.

## THE APPEARANCE OF NONLINEAR DEFORMATION WAVES IN THE ELASTIC POROUS MEDIUM UNDER NON-STATIONARY UNIAXIAL LOADING

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The formulating and solving features of non-stationary boundary value problems are discussed for porous materials under their dynamic deformation. When deformations are small, the porous material can be considered as perfectly elastic different strengths medium having a singular point in the reversible deformation area [1]. The dynamic transition through the singular point in the "stress-strain" diagram of the simplest piecewise-linear mathematical model (collapse or disclosure of pores) is actually accompanied by changes in mechanical properties of the material (elastic moduli). As a result, the model allows both weak and strong discontinuities deformations. When solving the non-stationary boundary value problem about uniaxial loading of the perfectly elastic porous half-space, the boundary mode leading to the serial occurrence of strong and weak strain discontinuities with different propagation rates was specified. This effect corresponding to the load oscillations in the neighborhood of the model singular point is achieved using the continually increasing boundary displacement function which changes its convexity direction at some time point. We investigate various forms of boundary conditions, including those that lead to the emergence of the strong discontinuity with the constant propagation velocity, as was done for multimodulus isotropic elastic media [2].

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## **EXACT COHERENT STRUCTURES: FROM TRANSITIONAL PIPE FLOW TO FULLY DEVELOPED TURBULENCE**

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The transition to turbulence in pipe flow and other shows flows have puzzled scientists for centuries: a linear instability analysis suggests that they are stable against small perturbations for any Reynolds number. Observations of the transition differ widely in the Reynolds numbers where the transition occurs. Above the onset of turbulence, the flow is spatio-temporally intermittent. Numerical and experimental studies that built on judiciously adapted concepts from dynamical systems theory have contributed to unravel much of the puzzle of this transition. The onset can be related to sub-critical bifurcations in which fully three-dimensional exact coherent structures (ECS) appear. The differences in transitional Reynolds numbers and the sensitive dependence on initial conditions is a consequence of the fact that the ECS typically are unstable and part of a chaotic saddle. The spatio-temporal intermittency is a consequence of the transience of the dynamics in the transitional region.

For higher Reynolds numbers, localized ECS together with a scaling of the Navier-Stokes equation that combines length and Reynolds number can be morphed into smaller scale coherent structures. As the Reynolds number increases, more of these states with ever smaller scales appear, all the way down to the Kolmogorov scale. Some of them remain localized in the bulk of the flow and help to build the turbulence cascade, others are localized near the walls and contribute to shaping the boundary layer profile. ECS not only provide the key to understanding the transition to turbulence but also for the dynamics and the transport in the fully turbulent flow.

## **MODELING THE STATE PECULIARITIES OF THE POLYMER CHAINS AROUND THE CARBON BLACK NANOPARTICLES**

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Carbon black in elastomers is typically reinforced with specific physical and chemical interaction of the binder with the filler's particles. The paper describes two hypotheses on a possible mechanism for elastomers to be reinforced by carbon black.

A hypothesis on the key role played by a potential interaction of the polymer with carbon black, which takes place at a distance of one to a few nanometers near filler's surfaces, is rather popular. This view considers the Van Der Waals interaction between carbon atoms of the filler's particles with the units of polymer chains to be very important. The paper identifies serious problems in applying this hypothesis to explain the effect of the material reinforcement.

The second hypothesis states that free radicals on the carbon filler surface make the interfacial interaction possible. Carbon black particles have a developed rough surface with a large amount of free radicals in the cleavage of graphite regions. They are able to initiate the chemical cross-linking near the interface phase. This gives rise to free radicals in the polymer chains which interact with other adjacent polymer chains to form chemical cross-linking. The process spreads further into the polymeric matrix.

The paper describes an algorithm to construct the geometry of the carbon black particles with due regard to roughness and activity of the particles' surface. A computational experiment allows us to analyze the process of the chemical cross-links formation between the polymer chains. Computer experiments showed that the chemical cross-linking between the polymer chains can be extended to a considerable distance from the surface of the filler's particles. In other words, the layers with special properties may be thick enough to significantly affect the macroscopic behavior of the material.

*The RFBR project # 16-08-00914 provided financial support to this research.*

## **MECHANICAL BEHAVIOR OF FE-CR STEELS FOR GENERATION IV NUCLEAR REACTORS. NUMERICAL SIMULATION**

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The high demand for heat-resistant and low-activated materials for use in different Gen-IV reactor components makes high-chromium steels a material of great interest to study [1-4]. Their use in high-temperature and high-pressure

applications raises the necessity of a detailed study of their mechanical behavior over a wide range of loading conditions.

Fe-Cr steels are known to be related to a precipitation hardened materials type. Precipitation hardening has a strong influence on mechanical properties of the material. Therefore, it should be accounted for in the model describing the deformation response of precipitation hardened materials. This work aims at predicting the mechanical behavior of precipitation hardened Fe-Cr steels in the temperature range up to 1115 K and pressures up to 10 GPa. A two-level model that takes into account the effect of grain boundary hardening, hardening due to inclusions of the  $\alpha$ - and  $\sigma$ -phase, hardening through dislocation substructures, and hardening from neutron irradiation on the dynamics of dislocations is developed for this purpose.

With the use of the multilevel modeling, the adiabatic curve was obtained. It demonstrates a good correlation with the experimental data for a Fe-Cr-Ni alloy [4] in the pressure range up to 10 GPa. Yield stress values of precipitation hardened Fe-Cr steels were predicted in the above range of temperatures and pressures. The calculated yield strengths are in reasonable agreement with the experimental data for 316 FR SS steel [5]. A discrepancy of the calculated and experimental yield strengths of Fe-Cr steel can be explained by a sharp decrease of the  $\alpha'$ -phase concentration within the temperature range from 500 to 750 K.

The authors would like to thank their scientific supervisor Prof. Dr.-Sci. Vladimir A. Skripnyak for fruitful discussions and valuable suggestions. This work was supported partially by the Grant from the President of Russian Federation and Grant from the Foundation of D.I. Mendeleev's National Tomsk State University within the Program of increasing the competitiveness of TSU. The authors are grateful for the support of this research.

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## THE INFLUENCE OF DISLOCATIONS AND POINT DEFECTS ON THE SPATIAL LOCALIZATION OF NONLINEAR WAVES PROPAGATING IN MATERIALS

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The problems of nonlinear wave dynamics of materials with dislocations and point defects are discussed.

In this paper were obtained the governing equations describing the propagation of ultrasonic waves in a medium with dislocations. It was shown that the propagation of ultrasonic waves is characterized by two dispersion branches ("acoustic" and "optical"). With increasing wave number the phase velocity of the wave, belonging to the "acoustic" branch, from the final value asymptotically decreases to zero, while the velocity of the wave, belonging to the "optical" branch, from the infinity asymptotically decreases to the final value corresponding to the speed of propagation of longitudinal waves.

With the help of the Lighthill criterion, the modulation instability was investigated. The wave packets, the quasi-harmonic wave was split on due to of modulation instability, was defined. It was shown, that there may exist as a periodic, stationary waves of envelopes and stationary solitary wave of the envelope. The dependencies of the height and width of a wave packet, formed because of self-modulation of quasi-harmonic waves with main characteristics of dislocation structure were identified.

When exposed the laser radiation or particle flux to the material (for example, by ion implantation) it creates point defects (vacancies, interstitial). Propagating of the intensive longitudinal acoustic wave contributes to the change in the areas of tension and compression of activation energy of formation of point defects, leading to their spatial redistribution. Defects migrating in the material recombine on different kinds of centers. The role of these centers can play dislocations, interstitials, impurities and others.

It was shown that the problem of the propagation of acoustic waves in the material with the point defects should be considered as a self-consistent, which includes, along with the dynamic equations of elasticity theory, the kinetic equation for the density of defects. This system can be reduced to a nonlinear evolution equation. The exact analytical solutions to the evolution equation were found and analyzed.

## **ANALYSIS OF TEMPERATURE REGIMES FOR HIGH-TEMPERATURE CURING OF AN INFLATABLE ANTENNA IN THE EARTH ORBIT**

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Today a new trend in uncrewed cosmonautics is progressing rapidly. This innovation suggests launching of nano-satellites, being auxiliary payloads, from Russian, American or European carrier rockets or space stations. Many different research centers, private companies and academic institutes have taken interest in the development and manufacture of such nano-satellites. For communication with the Earth, ordinary satellites are equipped with different space antennas and divided into groups according to the method of their deployment and design concept. Large-size metallic antennas cannot be installed within the above-mentioned nano-satellites and therefore the development of suitable inflatable antennas remains an urgent need.

In this work we present a cylindrical shaped inflatable antenna made of a fiber-epoxy prepreg and investigate conditions for its hot curing, which starts even in the earth orbit immediately after the antenna is made operational. The transformation of the prepreg into a solid structural material considerably increases the strength and service life of the antenna. This antenna is not susceptible to the blows of small-sized powder particles moving at cosmic velocities. It requires no permanent gas injection into the inflatable elements of the antenna and, consequently, no additional tanks with gas or vessels with chemicals for its production.

Temperature differences of the antenna, when it is on the sunny and shadow sides of the Earth, were explored. This suggests the possibility of high-temperature curing during the flight of the satellite in the Earth orbit (the period of one revolution of a nano-satellite was about 1.5 hours).

It is shown that the use of a fiber-epoxy material alone (without an aluminum foil) does not allow one to reach temperatures necessary to cure the inflatable antenna. Coating of the entire surface of the cylindrical elements of the antenna with a thin aluminum foil makes possible its heating to very high temperatures, which provides hot curing of the prepreg in the absence of special heating.

It takes approximately 15 minutes to reach the stationary temperature state.

*The study was supported by the Russian Foundation for Basic Research (projects № 16-48-590844 p\_a and № 15-01-07946 a).*

## **A STUDY OF THE RELATIONSHIPS AND MATHEMATICAL MODELLING OF DEFINING FUNCTIONAL PHYSICAL AND MECHANICAL PROPERTIES OF ADVANCED MATERIALS AND NANOMATERIALS**

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An important area of experimental and theoretical study of the functional properties of metal, polymer and other homogeneous, composite, isotropic and anisotropic, bulk and layered materials and nanomaterials include the issues of establishing the relationships of these properties with each other and identification of the dependence of these properties on the parameters, structure of the material and manufacturing technologies (influence) [1-5]. Such characteristics as coefficient of thermal linear and volume expansion, heat capacity, thermal conductivity, density, compliance (modulus of elasticity), yield stress and strength, electrical resistance, magnetic permeability, the optical index of refraction, coefficients of the reduction of time on temperature-time compliance, the friction coefficients, the values of the fracture toughness (crack resistance), and other linear and nonlinear properties of materials.

In the present work it is shown that in many cases relationships of these characteristics can be transformed into an approximately s-shaped form (functions) of their changes on temperature or constructed generalized (synchronized) time, the branches (segments) of which correspond to different structural (physical, phase) states of materials. The most simple spline method of mathematical description of the entire s-shaped functions based on the application of simple mathematical models for each branch is shown. The possibilities of determining the relationships of various functional properties are shown by applying generalized time on the parameters of structure, manufacturing technologies and influence, the ways of calculating some properties on the other, which is important to determine and predict the characteristics of nanomaterials, the experimental definition of which can be a difficult task. Examples of interconnections are given.

*The work is executed at partial support of the grant of the Government of the Russian Federation Decree 220, the Agreement 14.V.25.31.0017.*

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## WAVES WITH THE NEGATIVE GROUP VELOCITY IN CYLINDRICAL SHELL OF KIRCHOFF – LOVE TYPE

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Cylindrical shells of different types are the often used models in modern engineering. It is the element of different line tubes, supports, oil rigs and so on. The problems of preventing from damaging of such the constructions, reducing the vibrations of them are the actual problems of modern technique. The exact calculation of such objects from one side needs great computational resources and from another side often mask some important effects. For example the effects of propagating of the waves with negative group velocity better to analyse on the simplest mechanical models which have the exact analytical solution. In report such the analyses is fulfilled on example of infinite thin cylindrical shell of Kirchhoff – Love type.

The problem of free oscillations of such the shell is considered. The statement of the problem is considered in the rigorous statement. The dispersion equation is found on the base of exact analytical solution. The propagating waves are analyzed. The exploration of waves with negative group velocity in the neighborhood of bifurcation point of dispersion curves is fulfilled. The analysis of arising effects is fulfilled in terms of kinematic and dynamic variables, and in the terms of energy flux. The relative advantages and disadvantages of these approaches are discussed. The comparison of contributions in the integral energy flux of various mechanisms of energy transmission in the shell is fulfilled.

The dependence of subzero energy flux, dynamic and kinematic variables on the relative thickness of the shell, the mode number and other parameters of system is discussed. The possible fields of applicability of the gained effects are established.

## EQUILIBRIUM TWO-PHASE MICROSTRUCTURES AND OPTIMAL COMPOSITE MICROSTRUCTURES

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We relate two problems which arise from different branches of mechanics of materials: construction of limiting phase transformation surfaces in strain space and stress-strain diagrams for stress-induced phase transitions and optimal design of two-phase 3D-composites in the sense of minimizing its energy. Following [1], we demonstrate that, given new phase volume fraction and depending on average strain, the strain energy of a two-phase linear-elastic composite is minimized by microstructures which are either direct or inclined simple laminates, direct or skew second-rank laminates or third-rank laminates. Then we apply these results for construction of direct and reverse transformations limiting surfaces in strain space for elastic solids undergoing phase transformations by additional minimization with respect to the new phase volume fraction and finding strains at which minimizing volume fraction equals zero or unit. We note that direct rank-2 and 3 laminates are energy equivalent to microstructures with elliptical cylinders and ellipsoids, respectively, and skew rank-2 laminates do not correspond to any of nuclei which would be known as the Eshelby inclusions.

Then we construct stress-strain diagrams on various straining paths at which a material undergoes phase

transformations. We demonstrate that an additional degree of freedom – new phase volume fraction – may crucially result in instability of two-phase microstructures even if the microstructures are energy minimizers for composites with given volume fractions of phases. This in turn may lead to incompleteness of ‘monotonic’ phase transformations and broken stress-strain diagrams. Finally we discuss stability problems which arise from the considerations of two phase states with smooth interfaces and note that such interfaces may not be stable since, given boundary conditions, they do not deliver energy minimum to any two-phase states.

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## DETERMINATION OF THE SHEAR VISCOSITY OF THE SCLERA BY USING DIFFERENT RHEOLOGICAL MODELS

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The human eye is a complex structure with different biomechanical properties of its tissues. The eyeball consists of three concentric layers: a fibrous tunic, including the sclera behind and the cornea in front; a vascular pigmented tunic called choroid and a nervous tunic called retina. There are many works devoted to the determination of elastic modules of all this layers and far less papers representing viscosity coefficients. However, sclera and cornea are viscoelastic systems. This work investigates a method for determination of the shear viscosity of sclera based on a comparison of results of the mathematical modeling and the experimental data on intraocular pressure (IOP) discrete measurements for several minutes after the intravitreal injection. Experimental curves based on measurements of IOP for several minutes after the intravitreal injection have the IOP jump immediately after the injection and then go down. Biomechanical properties of sclera play a leading role in problems of determining eyeball shape or volume under the IOP, therefore we can consider only sclera in the modelling of eye behavior after the intravitreal injection. We offer to explain IOP reducing by two facts: sclera viscosity existing and intraocular fluid outflow existing. Wherein we suppose that function of intraocular fluid outflow velocity is known. Eyeball behavior follows the laws of mechanics. To solve the problem we consider viscoelastic spherical layer under the centrally symmetric load: external pressure is absent, displacement of the inner boundary are specified and take into account the intravitreal injection volume, the intraocular fluid inflow and outflow. Material of the human sclera is linear transversally isotropic. We consider problem in the framework of 3D-dimensional linear viscoelastic theory. We use Kelvin-Voigt and Maxwell rheological models to take into account viscoelastic behavior of the sclera. We compared the obtained values of the shear viscosity. We also compared the experimental plot of the IOP reduce during the time of the experiment with plots based on mathematical modeling and corresponding to different shear viscosity coefficients. On this basis, we can conclude which of considering rheological models corresponds to the best coincidence between experimental and theoretical functions of the IOP.

## A POSTERIORI ERROR ESTIMATES FOR APPROXIMATE SOLUTIONS AND ADAPTIVE ALGORITHMS FOR PLANE PROBLEMS OF ELASTICITY THEORY

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This work is devoted to functional approach [1-3] to a posteriori error control in classical [2] and Cosserat elasticity [4-5]. The approach yields reliable majorants that are valid for all conforming solutions of problems regardless of methods used for numerical implementations of a solution process. Estimates include additional free fields and mesh-independent constants. It is shown that a reasonable and natural choice of conforming finite element approximation in the Hilbert space  $H(\text{div})$  for the additional variables provides efficient implementations of the error control. Efficiency of the above technique is shown on a set of numerical examples including consequent mesh adaptations with standard MATLAB tools as in [6]. We are mainly focused on the ability of the functional type a posteriori estimates to provide upper bounds for general approximations (Galerkin and non-Galerkin) and a quality of indication of local distributions of computational errors.

*Work is partially supported by the Grant of the President of the Russian Federation MD-1071.2017.1.*

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## MODAL DESCRIPTION OF CAPILLARY JETS AND REDUCED MODELS

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Capillary jets have both practical and theoretical interest: practical because of their many technological applications (inkjet printing; food, textile, chemical and pharmaceutical industries, etc.); theoretical because they constitute a highly nonlinear system whose description is challenging in many ways. Paradoxically, linear theories usually predict very well some aspects of their behaviour, like their breakup lengths, as in most part of the evolution of perturbations traveling from the exit, these perturbations keep small in amplitude.

The simplest basic configuration is a capillary jet not affected neither by gravity forces nor by the surrounding air, and issuing from a circular exit with plug velocity profile. Under these idealized conditions, the unperturbed jet is a liquid cylinder having uniform axial velocity in every stream station. Two linear descriptions are classical: (i) the temporal approach, introduced by Rayleigh, in which we see the jet as an infinite column spatially perturbed with a definite wavelength, and (ii) the spatial approach, due to Keller and co-workers, for which the jet is harmonically perturbed at the exit and convectively develops a spatial pattern. For each of both approaches our group has completed the modal analysis of the axisymmetric jet. On one hand, the temporal modes are the two so-called capillary modes and the infinite family of hydrodynamic modes. The capillary dominant mode (unstable for low wavenumbers) and the subdominant one (always stable) have surface deformation and net flow rate. Conversely, the hydrodynamic modes are recirculating and have negligible shape deformation. On the other hand, the spatial analysis reveals a set of modes richer scenario, primarily classified in modes living downstream and upstream from any jet station. Among the downstream modes generated at the jet exit, some modes (the two capillary modes and the hydrodynamic modes) are the spatial counterparts of the temporal modes, and others (the inertial modes) are genuinely spatial.

For the temporal scheme, the two relevant conditions are the initial deformation and mean axial velocity, and the two capillary modes are enough to account for the subsequent linear evolution of the jet. Similarly, for the spatial scheme the two relevant conditions are the deformation and mean axial velocity at the jet exit. In this way, we can deal with reduced models. In each case, we have explicit formulae relating the amplitude of the capillary modes with initial/exit conditions. The spatial model, valid for any Weber number in the convective instability regime, agrees with the temporal model in the limit of high Weber numbers. Numerical simulations with Gerris have validated the findings of the reduced spatial linear model.

## GAUSSIAN PRESSURE PULSES ON CAPILLARY JETS

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We have experimentally explored the formation of drops in a millimetric capillary jet by means of Gaussian pressure pulses. The associated deformation yields an intermediate breakup of the jet, leaving two intact portions of it at both

sides of a group of droplets.

Our findings demonstrate that the production of isolated drops by this method is possible. The formation of secondary droplets can be delayed far downstream by proper selection of the pulse.

In parallel, we have developed a simple theory that can predict the linear evolution of the deformation and the position of the intermediate drop formation.

## STUDIES OF MECHANICAL PROPERTIES OF RUBBERS WITH A LAYERED CLAY NANOFILLER

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It is known that one of the main and most common fillers of rubbers based on natural and synthetic caoutchoucs are carbon black (black soot) and oxides of zinc (white soot). Putting into an elastomer such substances can significantly improve its mechanical properties (especially strength and deformability). To date, these effects are well understood and can be said that this method of modifying the properties of the rubber reached the ceiling. Further progress requires a search for new nonconventional types of fillers. One of perspective directions is the use of various clay minerals [1].

The paper presents the results of experimental studies of elastomeric nanocomposites containing a new (for elastomers) type of filler — montmorillonite (MMT). This material, in particular processing, is capable to be dispersed nanoparticles of ultrafine flakes with a minimum thickness of up to 1 nm, that may form individual packs of parallel plates - tactoids.

Two types of nanofiller were used in the experiment: 1) MMT: montmorillonite treated as surfactants by chloride of disteardimethylammonium. Average particle size was about 68 nm, the average distance between the layers in tactoids  $d_{\text{MMT}} = 2.9$  nm. 2) EMMT: mixing MMT with docosanoic acid in a ratio of 1 to 1 by weight was made to increase the degree of intercalation of filler particles to  $d_{\text{EMMT}} = 4.3$  nm. Vulcanizates of natural rubber (NR) were used as a matrix.

Experimental studies conducted by a special technique, based on cyclic deformation of the sample with a stepwise variable amplitude of the deformations. Tests of this kind are used in when it is necessary to receive in one experiment comprehensive data about the viscoelastic and elastic-plastic material properties [2]. In addition, all samples were tested in uniaxial tension until rupture.

It was found that the addition of clay nanofiller rubber contributes to significant dissipative losses increase, indicating that the development of viscoelastic processes in the composite during its deformation. Also, the relative softening of material (compared with pure vulcanizate) occurred at large cyclic strains (more than 3-4 times). And these effects were stronger than for fillers with a larger basal spacing.

By computer simulation shows that an increase in the hysteresis curves of cyclic loading can be explained by the distortion of shape due tactoids nanoplates slip relative to each other. This does not require much energy and contributes to a more easy rearrangement of the composite structure under external loading.

*This work is executed at a financial support of RFBR Grant 16-08-00756.*

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## LEVERAGING INTERNAL VISCOUS FLOW TO EXTEND THE CAPABILITIES OF SOFT-ROBOTS

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Elastic deformation of beam-shaped structures due to embedded fluidic networks is mainly studied in the context of soft-actuators and soft-robotic applications. Currently, the effects of viscosity are not examined in such configurations. In this work we introduce an internal viscous flow and present the extended range of actuation modes enabled by viscosity. We analyze the interaction between elastic deflection of a slender beam and viscous flow in a long serpentine channel, embedded within the beam. The embedded network is positioned asymmetrically with regard to the neutral plane, and thus pressure within the channel creates a local moment deforming the beam. Under assumptions of creeping

flow and small deflections, we obtain a fourth-order integro-differential equation governing the time-dependent deflection field. This relation enables the design of complex time-varying deformation patterns of beams with embedded fluidic networks. Leveraging viscosity allows to extend the capabilities of beam-shaped actuators, such as creation of inertia-like standing and moving wave solutions in configurations with negligible inertia and limiting deformation to a small section of the actuator. The results are illustrated experimentally.

## NUMERICAL STUDY FOR THE HYPERSONIC SHOCK-BOUNDARY-LAYER INTERACTION FLOW WITH ABLATION

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Through solving the Navier-Stokes equations of thermochemical nonequilibrium flow coupled with the ablating boundary condition, the ablative boundary flow with shock-boundary-layer interaction, which is typical in hypersonic reentry flow, is numerically simulated, and the effects of the wall conditions on the flow properties are investigated. 16 chemical species and 29 chemical reactions are adapted in the simulation. The oxidation and sublimation of C, as well as the recombination of O catalyzed by C are considered at the wall surface.

In the simulation of hypersonic flow over plate with incident shock wave, both ablating and non-ablating surface condition are used to investigate the effects of ablation on the flow separation properties. The results show that: (1) the possibility of flow separation and the separation range become larger as the strength of the incident shock wave and the freestream velocity are increased. (2) As compared with the cases with low-temperature wall, the flow separation zones are larger with ablating wall or with high-temperature wall in radiation equilibrium, and this leads to further effects on the flow properties of the downstream.

The hypersonic flow over  $15^\circ$ ,  $18^\circ$ ,  $24^\circ$  compression corners are calculated with Mach number varied from 10 to 30 and total enthalpy from 6 to 55 MJ/kg. Both ablating and non-ablating surface condition are used to investigate the effects of ablation. The flow structure, the characteristics of shock—boundary-layer interaction, the separation properties, and the distribution of the thermochemical properties are analyzed.

*The research is funded by the National Natural Science Foundation of China (11572348).*

## HEAT CONDUCTIVITY IN ONE DIMENSION - MICROSTRUCTURE VERSUS HYDRODYNAMICS

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The talk will review the state-of-the art in a problem of heat transport in classical one-dimensional lattices. This is a classical problem in nonlinear dynamics, which started from seminal paper of Fermi, Pasta and Ulam. After this work it became clear, that mere anharmonicity of the interparticle interaction in a model of atomic chain is insufficient for proper thermalization. Later, with the help of numeric simulations, it was revealed that heat conduction coefficient in the one-dimensional models with conserved momentum diverges in thermodynamic limit according to power law with model-dependent exponent. These numeric results received sound theoretical support through a variety of approaches, such as renormalization group theory, kinetic equations, as well as mode-coupling theory in hydrodynamics.

In the same time, it has been known for long that in some 1D chains, for instance, in the chain of rotators the heat conduction coefficient converges in the thermodynamic limit despite the momentum conservation. This anomaly is attributed to the difference in a number of conservation laws; for the chain of rotators, only total (angular) momentum and energy are conserved. In FPU, and similar chains, in addition, a total length of the system is conserved. Broader set of the conservation laws is believed to lead to different transport properties.

There exist numeric data for certain models that challenge this conclusion. For a group of models, including Lennard-Jones chain, some other chains with possibility of dissociation, as well as in the chain of colliding particles with finite stiffness, the heat conduction coefficient saturates at some finite scale. In these models the number of conservation laws is the same as in the FPU chain. However, the models with the observed saturation of the heat conduction coefficient have one common feature, absent in other models. In these special models, the behavior in the saturation regime can be interpreted in terms of simple kinetic theory. In other terms, one can identify the heat carriers, the scattering events, and predict, for instance, observed dependence of the heat conduction coefficient on temperature and density with the help of almost naïve basic kinetic arguments.

The talk will address this apparent contradiction and possible ways for its resolution. In addition, it will describe and

discuss the findings in a problem of nonstationary heat conductivity.

## **SHOCK FOCUSING AND PRESSURE JUMPS EFFECTS FOR THE INTERACTION OF BLUNT BODIES WITH GAS BUBBLES IN A SUPERSONIC FLOW**

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The numerical investigation of axially symmetric interaction of blunt bodies with low density and high density gas bubbles in a supersonic flow is carried out. The effects of appearing of anomalous pressure and density jumps in a critical point of a body essentially exceeding values calculated for Riemann problem are studied. In case of the interaction with low density gas bubbles the effect was observed but was not enough clearly explained in [1]. Similar results were noticed both experimentally and theoretically for the interaction of a body with high temperature plasma formations induced by pulsed laser energy deposition in supersonic upstream flow [2–3].

Now it is shown that the main reason for appearing of anomalous pressure and density jumps in a critical point of a body was the preceding fast process of focusing of transversal shock wave in small zone on the symmetry axes ahead of a body. The mechanism of fast focusing processes is in general agreement with well investigated shock focusing scenarios [4] for the interaction of plane shock with low density and high density gas bubbles.

For low density gas bubbles according to the “divergent” scenario of the interaction the “weak focusing” regime was realized. The secondary weak convergent-type shock wave propagating inside a shock layer was focused along the symmetry axes. For high density gas bubbles the “strong focusing” regime was realized. According to “convergent” scenario of the interaction the bow shock wave was diffracted around the bubble. Then the strong converging diffracted bow shock wave and the transmitted shock wave were collapsed in a very small zone at the rear pole of the bubble on the symmetry axes. For both cases the collapsing process was accompanied by formation of thin supersonic upstream and downstream cumulative jets. The interaction of downstream jet with a body surface was resulted in anomalous pressure and density jumps.

Parametric investigations for different gas bubbles of ellipsoidal shape were carried out. To realize the cumulation effect the density ratio should be more than some critical value, the gas bubble shape should be closed to spherical and the longitudinal size – about a bow shock wave distance. There were no focusing or cumulation effects for the interaction with a flat layer or ellipsoidal gas bubbles of too large cross size.

*The investigations were carried out in the Institute of Mechanics of Lomonosov Moscow State University and were financially supported by the Russian Foundation for Basic Research (projects 16-29-01092-a) and the Russian Science Foundation (project 14-11-00773).*

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## **ON INTERACTION OF UNLOADING WAVE WITH A MOVING ELASTOPLASTIC BOUNDARY IN CYLINDRICAL TUBE**

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The present work deals with propagating of converging cylindrical unloading wave in a rigid tube of radius  $R$  filled with elastoviscoplastic material. The model of large elastoplastic deformations with account of viscous medium properties in the process of plastic yielding is used to describe elastoviscoplastic medium [1,2]. Material is initially free of strains and begins to be deformed quasistatically under increasing pressure difference, with reversible strains being small. The material remains in the tube due to dry friction on its wall with the formation of near-wall viscoplastic flow and elastic core. Unloading wave is initiated upon overcoming friction when material starts to slip along the inner tube

wall.

The possibility of writing equation of motion for the unloading wave in terms of the displacements was pointed out in [3]. Exact solutions of boundary-value problems of the theory of large deformations on collision of unloading wave with a moving elastoplastic boundary in a flat heavy layer located on inclined plane and subjected to loading at the free surface were obtained in [4,5].

As long as wave equation arisen cannot be solved exactly for the present case of cylindrical symmetry, we find stresses, velocities, and displacements by means of the ray method of constructing approximate solutions for strong discontinuities surfaces. Besides, aspects of interaction of the unloading wave with the moving elastoplastic boundary followed by wave pattern change were considered.

*The work was partly financed by fundamental research program of Far Eastern Branch of the Russian Academy of Sciences «Far East» (projects 0262-2015-0064, 0262-2015-0065).*

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### VARIANTS OF LAGRANGE MULTIPLIER METHOD IMPLEMENTATIONS FOR TWO-DIMENSIONAL CONTACT PROBLEMS

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Two-dimensional elastic contact problem with isotropic and transversely orthotropic materials is considered. Finite element method with triangular second order elements is used. The Lagrange multiplier method for contact conditions implementation with middle line as contact surface is used. A plane problem of contact interaction of the metal rail and composite orthotropic shell in cross-cut section with gasket of the electromagnetic accelerator barrel (railgun) is considered (three bodies contact). Parallel software package for sparse linear systems of equations solving with MPI technology is designed.

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### DETERMINATION OF THE PORE SIZE DISTRIBUTION IN INHOMOGENEOUS NANOPOROUS MEDIUM FOR REPRODUCING THE LIQUID FRONT PROPAGATION

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In the last decade the possible applications of nanoporous materials have been the subject of great scientific interest. One of the problems in this field is the determination of the optimal configuration of the nanoporous medium. Many problems in filtering and biomedicine require the front of the liquid, which permeates the media, to have concrete

shape and position in the given time. We propose the method of finding the nanoporous medium for the realization of the specific liquid front propagation.

The technique consists of two steps: numerical modelling of the liquid front propagation in inhomogeneous nanoporous media and minimizing the difference between modelled results and sought-for one. To numerically model the liquid front propagation we use the combination of the continuity equation for the incompressible flow and the approximation of Darcy's law [1]. It should be noted that the model was made for inhomogeneous nanoporous media with non-constant porosity and pore size distribution so that any needed liquid front shape could be reproduced [2].

Then, assuming that the porosity of the medium is set, the pore size distribution can be presented as a polynomial with unknown coefficients. By using the variation of the Nelder-Mead method [3] we minimize the standard deviation between modelled liquid front profile and given one, thus obtaining the needed result.

The program, which simulates the two-dimensional liquid front propagation in inhomogeneous nanoporous medium, has been written in C++. The specific liquid front propagation has been reproduced for different water front profiles.

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### A CRACK PROPAGATION AT A CONSTANT SPEED IN A DISCRETE BI-MATERIAL

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The treatment of cracks at microlevel is a progressive topic in dynamic fracture mechanics nowadays. This scope is aimed in the better understanding of fracture processes that happen right at the crack tip in solid materials. The mathematical study of such problems is able to make some predictions and draw some explanations for physical phenomena.

In this particular work we are concerned with a problem of an interfacial crack propagation in a brittle bi-material. The fracture process is supposed to be brittle and the model itself may be applied for the consideration of failure of bi-material ceramics.

We present the solution of the problem, derive the relation between the loading parameters and crack speeds. We show the peculiarities that are detected due to the microlevel and additionally due to the material parameters mismatch.

*This work was supported by FP7 Marie Curie ITN transfer of knowledge programme under project PITN-GA-2013-606878-CERMAT2.*

### ELECTRICAL ACTIVITY IN THE ATMOSPHERE OF THE EARTH AND OTHER PLANETS OF THE SOLAR SYSTEM

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In this contribution, we will present an overview of the atmospheric electricity phenomena in the atmospheres of the Earth and other planets of the Solar System. In the Earth, lightning activity in the troposphere drives the occurrence of a zoo of enormous transient electrical events in the upper atmospheric layers (stratosphere and mesosphere) of our planet that can potentially change the electrical and chemical properties of the atmosphere of the Earth. Upper atmospheric electrical discharges could also be taking place in other planets of the Solar System where lightning activity is confirmed (giant gaseous planets) or suspected (Venus). After a brief motivation and historical introduction, the talk will be mostly devoted to the kinetic and spectroscopic aspects of the research done towards the understanding of the so called Transient Luminous Events (TLEs), which are a diversity of weakly ionized low temperature plasmas occurring in the upper atmosphere of the Earth between the thundercloud tops (15 km) and the lower ionosphere (95 km) and recorded for the first time 25 years ago (in the summer of 1989). Our research tries to answer questions such as, what are the chemical and electrical impacts of TLEs in the Earth atmosphere?. What are the physical (kinetic and electrodynamic) mechanisms underlying the ignition of TLEs?. What are the key spectroscopic features of TLE optical emissions, how can they be detected and what can we learn by analysing TLE optical signatures and spectra?. What are the expected optical fingerprints of lightning-driven upper atmospheric discharges in other planets and how do they look like?. Finally, we will conclude by commenting the future missions where we participate to investigate all sort of TLEs, lightning and associated terrestrial gamma ray-flashes (TGF) from the space.

## CONTACT INTERACTION MODELS TAKING INTO ACCOUNT ELASTIC AND SURFACE PROPERTIES OF CONTACTING BODIES

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The internal stresses within contacting bodies as well as normal and shear contact stresses essentially depend on the mechanical and surface properties of the bodies. The surface properties include both a surface microgeometry and surface energy. In contact interaction of dry surfaces adhesive stresses between the interacting bodies arise due to molecular interaction. In case of existence of a thin film of fluid in the gap between the surfaces, the capillary adhesive forces arise due to a meniscus of fluid formed near the contact regions. Surface microgeometry also plays a significant role in contact interaction of deformable bodies. Due to surface roughness the contact is discrete, and the real contact area is much smaller than the nominal one calculated from the classical contact mechanics.

Models are developed to study the normal discrete contact of elastic bodies taking into account their microgeometry parameters, and the molecular or capillary adhesion in the gap between them [1]. These models are based on a solution of the mixed boundary problem for the elastic half-space taking into account an additional loading outside the contact region due to adhesive pressure represented by a piecewise-constant multistep function. This allows one to consider arbitrary forms of the adhesion interaction potential (including the case of capillary adhesion), as well as of taking into account the presence of another additional load, in particular, the effect of neighboring asperities on adhesion of both rough bodies and bodies with a regular surface relief.

An analytical solution is obtained and is used to analyze the influence of a form of the adhesion interaction potential, surface energy of interacting bodies or films covering them, their shapes (parabolic, higher power exponential function), volume of liquid in the meniscus, density of contact spots, elastic modulus and Poisson ratio on characteristics of interaction of the bodies in the presence of adhesion [1-3]. The contact problem for two nominally flat surfaces with regular microgeometry is also solved. The dependence of the approach of the surfaces on the nominal pressure for various microgeometry and adhesion parameters, and also for different mechanical properties of contacting bodies is analysed. This dependence is also used to study the contact characteristics of the bodies with given macroshape taking into account the surface microgeometry parameters.

*The work was partly carried out under the financial support of Russian Foundation for Basic Research (grant No. 17-58-52030 MHT\_a).*

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## WAVE DISPERSION IN GRANULAR MEDIA: HETEROGENEOUS PACKING?

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We present results of the experiments on wave propagation in powders: magnetite (diameter 30  $\mu\text{m}$ , 50  $\mu\text{m}$ , 60  $\mu\text{m}$ ) beads, steel beads (diameter 35  $\mu\text{m}$ , 50  $\mu\text{m}$ , 110  $\mu\text{m}$ ), and cornflour (diameter 15  $\mu\text{m}$ , particle density 1550  $\text{kg/m}^3$ , asperities of the order of 100 nm). The sample is put in a rectangular parallelepipedal cell. Wave propagates in the horizontal direction. The medium is excited with a quasi-static swept-sine signal from 3 to 20 kHz. The size of the sample is 2 cm (in the direction of wave propagation) x 10 cm (approximate height of the sample) x 8 cm. In all the experiments we observe a strong wave dispersion at relatively low frequencies: the group velocity in the powder decreases with the frequency and becomes almost constant at higher frequencies. This cannot be predicted by a classical elastic theory of a homogeneous medium. We discuss various possible reasons of this dispersion and suggest that its most probable reason is heterogeneous packing of the powder caused by the gravity and the influence of the walls. We introduce a simplistic model supposing that in the horizontal direction linear density and effective Young modulus change by the same law similar to a bell shape. We approximate it by a cosine function in the horizontal co-ordinate containing two parameters: the sound velocity at high frequencies and the period of the cosine. We adjust theoretical dispersion curve to the experimental results and obtain a good accordance of the theory and experiment.

*This work has been partially funded by Spanish Government Agency Ministerio de Economía y Competitividad (project No. FIS2014-54539-P) and by Junta de Andalucía. F. Ruiz also acknowledges financial support from the University of Seville (Spain) through the FPI-2012 PhD grant.*

## **INFLUENCE OF STRESS-DEPENDENT DIFFUSION AND CHEMICAL AFFINITY ON CHEMICAL REACTION FRONT KINETICS UNDER MECHANICAL LOADS**

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The problem of the thermal silicon oxidation nowadays is one of the most important problems in chemistry, due to the importance and large use of silicon integrated-circuit technology. Since the volume of a molecule of silicon dioxide is larger than that of a silicon atom, silicon oxidation is accompanied by an increase in volume, this produces internal stresses and strains. In addition, chemical reactions in deformable solids often go under external mechanical loads.

The influence of mechanical loads is taken into consideration through the dependence of chemical affinity on mechanical loads, or through the dependence of diffusion on mechanical loads. In the case of diffusion, stresses are taken into account through the dependence of diffusivity coefficient on stresses. This dependence is usually defined empirically, and there is no certainty of which scalar function of stress tensor should enter this dependence. In this work, we suggest the reasonable diffusion coefficient, which depends on the deformations of the solid skeleton, which leads to the model of the tensodiffusion. We compare the model of stress-dependent chemical affinity and stress-dependent diffusivity coefficient for the various boundary value problems to figure out, how stress-driven diffusion affects the chemical reaction front propagation, investigate, which diffusion coefficient has a stronger influence on the process of chemical reaction front propagation, and obtain a range of the stress values when we can neglect the dependence of diffusivity coefficient on stresses.

## **DEVELOPMENT OF KINETIC MODEL OF DYNAMIC INELASTIC BEHAVIOR OF BRITTLE SOLIDS**

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It is known that the mechanical properties of brittle materials are sensitive to strain rate, namely their dynamic values may significantly differ from the corresponding “static” values.

The traditional approach to development of dynamic plasticity models is introducing the strain rate dependencies of inelastic and strength properties of material. However, strain rate (as opposed to physical mass velocity) is a technical parameter that characterizes the volume-averaged value of sample (or fragment) size change. Local values of strain rate may differ significantly from the integral value. An alternative way of describing the behavior of materials under dynamic loading is the kinetic approach developed in the works of Zhurkov, Regel, Petrov, Morozov and so on. Within this approach the time of material degradation  $T$  is used as a primary parameter of dynamic models of plasticity and fracture. Parameter  $T$  is physical and usually characterizes the process of initiation and growth of the main crack in the sample (or in a fragment of the material) or the formation of the system of microcracks providing macroscopic inelastic behavior of material.

The main idea of the kinetic model of dynamic inelastic behavior of brittle materials that developed in the present work is the account of the finite time of the process of relaxation of local stresses caused by the appearance of cracks of various scales. Modern kinetic models of inelasticity and fracture of brittle materials use integral fracture criteria based on the calculation of increment loading impulse for some time  $\tau$ , called the time of fracture incubation.

In this work the simplified version of dynamic criterion (in term of stresses) is proposed:  $\sigma = \sigma_c^{dyn}$ , where  $\sigma_c^{dyn}$  is dynamic value of material strength. Such a formulation of the criterion implies that when the scalar stress parameter  $\sigma$  reaches the value of static strength ( $\sigma_c^{st}$ ) at time  $t_0$ , the process of fracture begins.

The duration of fracture process is determined by the dynamics of change in the parameter  $\sigma$  during  $t > t_0$ . At the time of the formation of main crack (at  $t=t_{fr}$ ) the value of  $\sigma$  is equal to the some value  $\sigma_c^{dyn} \geq \sigma_c^{st}$  ( $\sigma_c^{dyn}$  depends on the dynamics of the stress state changing during the time period  $(t_{fr}-t_0)$ ). Assume that during the course of crack formation the value of strain rate does not significantly change. In this case the rate of increase of the parameter  $\sigma$  during the period  $(t_{fr}-t_0)$  also does not change significantly. According to this assumption the fracture time period  $(t_{fr}-t_0)$ , local strain rate and corresponding value of dynamic strength are uniquely linked. The value of any parameter of the three ( $\sigma_c^{dyn}$ ,  $(t_{fr}-t_0)$ ,  $\dot{\epsilon}$ ) can be uniquely determined if we know the values of the other two parameters.

Experimental data suggests that not only strength, but also the rheological properties of brittle materials are also sensitive to the value of strain rate. This is due to the fact that inelastic behavior of brittle materials is associated with the nucleation and development of the system of discontinuities (damages and cracks). The formation of such discontinuities also lasts for a finite time. In the paper we describe one of the ways of numerical implementation of kinetic theory of strength within the framework of non-associated plastic flow law.

*The work was carried out in the framework of the Fundamental Research Program of the State Academies of Sciences for 2013–2020.*

## **FREESTANDING HIGHLY CRYSTALLINE ALN LAYERS GROWN ON EVAPORATING SiC SUBSTRATES**

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The best substrates for group-III-nitrides-based devices are Gallium Nitride (GaN) and Aluminum Nitride (AlN). AlN is superior for the device structures with high Al content, e.g., deep-ultraviolet light-emitting diodes (UV LEDs), which are expected to be broadly applicable to medical diagnostics, environment protection, microfabrication technologies, etc. AlN single crystals of large area are grown on SiC substrates by the sublimation technique called physical vapor transport (PVT) [1–2].

In this paper, we compare microstructures revealed using transmission electron microscopy and synchrotron radiation imaging with the x-ray diffraction measurements. The observations reported here were made using special samples, i.e., thick freestanding AlN layers grown in one process with the evaporation of SiC substrates. Typically, AlN layer growth on SiC shows some problems, such as the generation of cracks at cooling due to great thermal stresses caused by the difference in the thermal expansion coefficients of AlN and SiC. Cracking is prevented when the SiC substrate is evaporated and the crystalline quality of AlN layer can be improved.

To explain the experimental observations we suggest a theoretical model which describes the misfit stress relaxation in AlN layer growing on evaporating SiC substrate. The model is based on the action of pyramidal slip mechanism for generation of misfit dislocations [3] and takes into account that dislocation density drastically decreases from the interface to the surface of the AlN layer [1–2]. Our general idea is that glide dislocation half-loops nucleate on the free surface of a growing AlN layer being under biaxial in-plane compression due to the lattice misfit with a polar SiC substrate. These dislocation half-loops glide to the AlN/SiC interface and expand along it. Reaching the interface and propagating along it, they partly accommodate the lattice misfit. As a result of the half-loop nucleation, surface steps appear on the growth surface, which can become favorable sites for further dislocation generation by the same mechanism on the adjacent pyramidal slip planes. Then some “secondary” dislocation half-loops are emitted by the surface, in which case the corresponding surface steps disappear. When these “secondary” dislocation half-loops reach the interface, novel  $\Lambda$ -shaped dislocation configurations form, which consist of two dislocation half-loops, “primary” ones and “secondary” ones, connected together by dislocation segments parallel to the surface. It is worth noting that during the evaporation of the SiC substrate, the distribution of misfit stresses drastically changes and the upper regions of thick AlN layers become stretched. In this case, the top segments of the  $\Lambda$ -shaped dislocation configurations, which create compressive stresses in these regions, partly compensate the tensile stresses there. On the other hand, the  $\Lambda$ -shaped dislocation configurations partly compensate the compressive stresses in the AlN layer near the AlN interface and the tensile stresses in the evaporating SiC substrate. Thus, the formation of  $\Lambda$ -shaped dislocation configurations seem to be energetically favorable process at the every stage of the AlN growth on evaporating SiC substrates.

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## STRESS RELAXATION AND FRACTURE IN HOLLOW DECAHEDRAL SMALL PARTICLES UNDER CHEMICAL ETCHING

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The physical origin and the relaxation mechanisms of residual stresses in pentagonal small particles (PSPs) of face-centered cubic crystalline materials have been in the focus of many studies in over the world. To describe theoretically the residual stresses in these particles, a disclination-based concept [1-3] occurred to be the most natural and productive. By using this concept, the stress-strain states and strain energies were calculated for decahedral [1] and icosahedral [2] particles, and for pentagonal whiskers [1] as well. It was shown, both experimentally and theoretically, that the residual stresses can relax in PSPs through many different modes [3-12]. Some of these modes are obviously stimulated by the external influence. A good example in this sense is cracking and fracture of hollow decahedral and icosahedral small particles (DSPs and ISPs) of electrolytic Cu at chemical etching [6]. Based on these experimental observations, we advanced disclination-based theoretical models describing a two-stage process of fracture in hollow DSPs under chemical etching. The first stage of the process is assumed to be nucleation of cracks on the outer surface of the DSP along the planes of twin boundaries (TBs), at the places of maximal tensile stresses and dilatation in the vicinity of the disclination line [13] at the quintuple junction of TBs. Our examination of this possibility shows that it is quite realistic. The second stage of the process could be association of these cracks in a five-fold star-shaped crack, which would include the disclination line. We showed that this scenario can work if the length of the first-stage cracks is larger than a critical value  $L_c$ , which means that the DSP radius  $R$  must be larger than a critical radius  $R_c$ . For the case of electrolytic copper, our upper estimates are  $L_c \approx 0.3 \mu\text{m}$  and  $R_c \approx (0.5 - 0.6) \mu\text{m}$  that well corresponds to experimental observations in Ref. [6].

*This work was supported by grant from the Ministry of Education and Science of the Russian Federation (Decree No. 220) obtained by the Togliatti State University under the contract No. 14.Z50.31.0039.*

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## HEAT FLUX FOR FINITE LINEAR CHAIN OF N-PARTICLES

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This article is linked with investigation of heat flux passing through a one dimension chain of N-particles. The content of the work is motivated by investigations of authors [1-4] who proposed to use a homogeneous harmonic chain in contact with stochastic Langevin heat baths. This model allowed them to simulate stochastic heat reservoirs at different temperatures of the "left" and "right" parts of the crystal. It was found that in the stationary state the heat flux is proportional to the temperature difference and not to the gradient. This means in particular that Fourier's law is not obeyed.

In our work we decided to analyze the model [1-4] on the foundation of the exact solution of the stochastic equations. In contrast with [1-4] the solution wasn't constructed by passing to the Liouville equation that corresponds to the Fokker-Planck equation. We obtained presentation for the Green function of the stochastic problem. For the analyzed model the heat flux is proportional to expectation of the product from displacement and momentum of the neighboring particles. It was shown that in an arbitrary state of the chain the heat flux is calculated through the components of the Green function.

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### INFLUENCE OF THE TREATMENT PARAMETERS ON THE EVOLUTION THE PROPERTIES OF THE ELASTICITY, PLASTICITY AND STRUCTURAL OF POLYCRYSTALLINE ALLOY 43300

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The purpose of this study is to determine the influence of the parameters of treatments on the evolution of the behavior and the damage in tension, the Brinell hardness, the microhardness, the resilience and the microstructure of the alloy of chemical designation AlSi10Mg and numerical 43300 considering three states of the material: crude of casting noted: F, hardened noted: T and matured followed by an artificial aging designated T46. The addition of 10% silicon which gives excellent casting ability and a percentage of magnesium ( $\leq 1\%$  Mg) to aluminum are the main agents for improving the mechanical properties in addition to specific thermal treatments which reveal precipitates of different kinds which hinder the movement of dislocations.

We studied the influence of structural hardening, Mg addition and casting method: sand and shell metal on the elasticity and plasticity characteristics of the polycrystalline Al-10% alloy. This alloy supports mean mechanical stresses. Parts made from this alloy are part of the components and realizations of the SNVI (Unit Aluminum of Rouiba) and Electro-Industries (Unit Freha Motors in Tizi-Ouzou), Algeria.

### THERMAL EXPANSION COEFFICIENT OF AL + 1.5%NTCM

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The Dilatometric curve of the nanomaterial Al + 1.5% NTCM show an anomaly extending over a wide temperature range 160-340°C. The values of the coefficient of thermal expansion are high in comparison with those of classical aluminum alloys. They are even twice as large as those of aluminum-based nanocomposites containing fewer multi-walled carbon nanotubes prepared under the same conditions and studied in the same laboratory.

Also, we find this anomaly on the curve of differential scanning calorimetry. It is intense and appears at the same temperature as before. The curve of variation of the length increases the ambient temperature to 350°C, then stabilizes and becomes linear up to 600°C.

The thermogravimetry of the nanocomposite tends to increase to 300 ° C and then becomes constant over the rest of the temperature range. In the Raman spectrum the peaks D and G appear clearly. The anomaly D is intense before that of G. Infrared reveals the presence of different bands that overlap with those of pure aluminum produced under the same conditions. They tend to become less spread out to take the form of peaks.

## A PLASTICITY COSSERAT MODEL FOR GRANULAR MATERIALS AND SOILS

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It is well known that it has proven to be a difficult problem to develop equations of continuum mechanics which successfully model the deformation and flow of granular materials and soils. This is often ascribed to the obviously discrete nature of such materials and has led to the development of such models as the Discrete Element Method. However, for a large bulk of such material containing very large numbers of grains discrete methods fail due to limited computing power. It also seems reasonable to suppose that a continuum averaged model should be able to provide some information concerning bulk deformation and flows. Indeed, plasticity models are widely used to model soils in geotechnical engineering. However, there are limits to the applicability of standard plasticity models for granular materials, e.g. they are restricted to steady-state problems and elasto-plastic deformations. This led to the development of another type of plasticity model called the double-shearing model and which has solutions closer to experimentally observed flows. Unfortunately both types of model, for different reasons, are mathematically ill-posed which effectively prevents numerical approximations to solutions from being calculated in time-dependent problems. Both models do appear to successfully describe some aspects of granular material behaviour and it seems a desirable aim to retain the equations which describe those aspects and to embed them into a new model which may be used in a wider variety of contexts. It also appears that a classical continuum is indeed sufficient to describe granular materials with the exception of the interior of shear-bands and in the immediate vicinity of boundaries.

We present a model which can be used in the context of a classical (sometimes called a Boltzmann) continuum and incorporates the concepts of pressure dependent yield and dilatation which does not fully match the pressure dependence (i.e. allows so-called non-associated behaviour). For the Mohr-Coulomb yield criterion the model is hyperbolic for planar steady-state flows. This classical continuum version of the model contains a degenerate case of the relative spin (i.e. the difference between the velocity spin or vorticity and the intrinsic spin) in which the intrinsic spin is everywhere and at all times constant (which may be chosen to be zero relative to an appropriate frame of reference). In the interior of a shear band or in the vicinity of a boundary the intrinsic spin is no longer constant and then the classical equations may be augmented with extra quantities and equations appropriate to a Cosserat continuum. The intrinsic spin is here interpreted as the average grain spin in a small representative volume element and in regions where it is not constant in either space or time there will exist non-zero couple stress tensor and non-symmetric Cauchy stress tensor.

In this talk we shall describe the model, discuss some of its more important properties and consider some applications of the model.

## RAY SERIES METHOD IN MULTIDIMENSIONAL PROBLEMS OF SHOCK DEFORMATION OF ELASTIC ARRAYS

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Is necessary to use a nonlinear mathematical apparatus for modeling many technological processes which use methods of intensive shock treatment. This allows to describe the effect of the relationship of volume and shear deformation, the influence of post-impact process, the non-linear properties of the motion of deformations forefronts confirmed by experiments. Approximate methods are the basic methods of theoretical analysis of nonstationary dynamic deformation problems in solid mechanics. Among them, the ray series method [1] is known as one of the most effective. This method is used in dynamic problems in the form of series with respect to the special spatial ray coordinate or time. The coefficients of these series are the discontinuities of the corresponding derivatives in the forefront of the wave process [1, 2]. They are calculated from the recurrence system of decay equations, which are consequence of the dynamics equations. The presence of shock waves in the boundary value problems is a limitation of this scheme, as decay equations cease to be recurrent. In order to remove this limitation a modified method of ray series [1], which includes additional internal series for functions of coefficients of discontinuities was developed. Previously this method was applied to one-dimensional problems of impact deformation [3 - 5], and also to the two-dimensional problem of antiplane deformation. Additional work should be done to generalize the method in order to the method scheme became suitable for solving boundary value problems, which include the disintegration of the initial discontinuity and the motion through the medium of a few shock waves with an arbitrary previously unknown geometry. In particular, coordination between several ray coordinate systems becomes very important. In this paper, a generalization of the ray method [1] for a multidimensional impact deformation with several shock waves was carried out. This work has been

done on the example of solving of two-dimensional problem of plane deformation of nonlinear elastic half-space bounded by the surface of a non-zero curvature. The difference between the solved problem and [3] is nonlinear divergence of ray directions and the presence of two shock waves with previously unknown geometry. The solution for each of the shock wave in the neighborhood of its wavefront is determined on the base of ray coordinate, agreed with this wave. Fundamentally important for the ray method mechanism of transforming one ray coordinate system to another is presented.

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## INVESTIGATION OF ELASTIC-PLASTIC DEFORMATION IN POLYMER NANOCOMPOSITES BASED ON STRUCTURAL MODEL OF SPHERULITES

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The work is devoted to mathematical modeling of the mechanical properties of polyolefins based on the availability in the structure of the supramolecular crystallite structures. These materials (polyethylene, polypropylene, etc.) are partially crystallizable polymers, and structural heterogeneity is well expressed in ones at the nano, meso and micro level. The most common type of crystallite entities - spherulites (typical size ranges from 0.1 to 1000 microns). It consists of lamellas and the amorphous phase therebetween. The spherulite lamellas emanate radially from a common core, filling the spherical space. From the viewpoint of mechanics of spherulites can be considered as a composite, wherein the lamellas are rigid inclusions in the form of long thin plates embedded in an soft amorphous matrix.

Spherulite was presented in the form of a radially anisotropic inclusion. The material in this case was considered as mechanically inhomogeneous medium with a regular ordered structure. Spherulite structure was modeled as a regular hexagonal lattice (plane strain) consists of a radially anisotropic hexagonal inclusion with mechanical characteristics, selected from the condition of compliance with the real macroproperties of material.

To evaluate the correlation of the values of radial and tangential elastic stiffness of spherulite we solved the problem of the periodicity cell extension. Uniaxial deformation of the system was realized by spreading the lower and upper boundaries in the vertical direction with the simultaneous convergence of the left and right sides in the horizontal direction with the implementation of the invariance of volume. At the same time the cell boundaries remained flat during deformation (to perform the condition of periodicity). The problem was solved by finite element method. Associated flow law was used for the solution of problems. It was assumed that plasticity in the spherulite develops isotropically and anisotropy is appeared only in elasticity.

*The work was supported by RFBR grant № 16-08-00756.*

## ON THE MECHANICS OF CRACKS HAVING PARTIAL CONTACTS BETWEEN CRACK FACES

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Contacts between crack faces are common in various materials, particularly the brittle ones (ceramics, geological materials). They produce strong stiffening effect, even if they are small, and hence they constitute microstructural factor of the primary importance that cannot be ignored. This effect also depends on geometric factors such as the distance between contacts and the center of the crack, as well as contact sizes. The said factors also affect the contribution of the crack to the effective conductivity. These issues are examined by numerical means, and simple models are suggested.

*The research was carried out in Nizhny Novgorod State Technical University n.a. R.E. Alekseev (NNSTU), with the*

*financial support of the state represented by the Ministry of Education and Science of the Russian Federation under the agreement №14.Z50.31.0036. Theme: "Creation of a scientific laboratory of composite and ceramic materials with application to Arctic vehicles (LCCM)".*

## **GENERALISED LANGEVIN EQUATION (GLE) AS A TOOL TO STUDY DYNAMICS OF NON-EQUILIBRIUM OPEN NANOSCALE SYSTEMS**

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The Generalised Langevin Equation (GLE) method, which was initiated by Zwanzig, Mori and others [1], is designed for calculating the dynamics of classical open systems described at the atomic level via molecular dynamics (MD) simulations. The method effectively considers the system and its environment or a bath (held at a constant temperature), although in practice only trajectories of atoms of the open system are calculated explicitly, while the environment is shown to be "mimicked" by non-Markovian Gaussian stochastic noises and a memory friction. Since our method explicitly takes account of the environment surrounding the open system of interest, it enables one to consider rigorously dissipation effects. Hence, this method can be applied to a wide class of atomistic problems, such as tribology, radiation damage, crack propagation, etc., where considerable energy is released in the open system and which dissipates into the environment. Note that the method is exact and can be used both in non-equilibrium and equilibrium MD simulations, i.e. as a thermostat in the latter case.

Our GLE scheme [2-4] goes beyond the commonly used bilinear coupling between the open system and the bath, and permits us to have a realistic description of both the dissipative open system and the surrounding bath. We have developed an original simulation scheme whereby complicated non-Markovian equations with the coloured noise are mapped onto white noise Langevin type equations in which the bath is represented by fictitious degrees of freedom. These equations in turn are mapped onto an appropriate Fokker-Plank equation, which enables one to work out an efficient computational discretisation scheme for calculating atomic trajectories numerically. A special method has been developed which allows "fitting" the fictitious degrees of freedom to represent faithfully the actual vibrational properties of the realistic bath.

We have used this methodology for systems with one and two temperature baths. In the latter case, our technique provides a realistic description of the heat transport through an open nano-system (e.g. a molecule or nanowire) sandwiched between two baths.

In this talk, I will present an overview of our methodology and the results of the method we applied to model heat transport in realistic nano-systems.

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## **ISOGEOMETRIC ANALYSIS OF MINDLIN'S FORM II SECOND STRAIN GRADIENT ELASTICITY: FROM NANO TO MACRO SCALES**

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In the present contribution, we propose a simplified model of Mindlin's Form II second strain gradient elasticity theory with second velocity gradient inertia [1,2,3,4]. Within this model, the strain energy density is enriched by four additional elasticity moduli and the kinetic energy density contains two higher-order inertia parameters. The resulting higher-order continuum model is governed by 6th order partial differential equations replacing the corresponding 2nd order ones of the classical elasticity demanding  $C^2$ -continuous conforming Galerkin methods [5]. NURBS-based isogeometric methods provide a  $C^{p-1}$ -continuous approximation for one patch domains, where  $p$  is the NURBS order, and hence offers a natural framework for solving higher-order problems. The proposed simplified second strain gradient model is implemented as isogeometric user elements in a commercial finite element software Abaqus [6] and verified by benchmarks, and finally used for numerical simulations.

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## THE FILM COOLING FROM CYLINDRICAL AND ROW TRENCH HOLES WITH ALIGNMENT ANGLE OF $\pm 60$ DEGREES AT THE END OF GAS TURBINE ENGINE COMBUSTOR SIMULATOR

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This study was done to study the effects of cooling holes restructure on the film cooling effectiveness under blowing ratio of  $BR=3.18$ . The gas turbine industries attempt to get higher engine efficiencies. To have better engine efficiency, the combustor's outlet temperature must increase. However the turbine inlet temperature increasing creates harsh environment. In this research a three-dimensional representation of a Pratt and Whitney gas turbine engine was analyzed. The findings of the study indicate that the combustor with row trenched holes gave almost doubled cooling performance compared to the baseline case.

Gas turbine industries try for higher engine efficiencies. Bryton cycle is a key to this purpose. According to this cycle, the turbine inlet temperature should increase. However increasing the turbine inlet temperature creates harsh environment. Film cooling is the best technique to cool down this area. In this system, a thin thermal boundary layer is formed. Cylindrical and trenched cooling holes are two schemes of the holes. With trenching the cooling holes, the injected coolant is suddenly spread and attached better on the surface. Stitzel and Thole [1] indicated that dilution jet injection is the dominant feature at the combustor exit. The objective of the present study was to analyze the effects of restructured cooling holes.

In this study a three-dimensional representation of a Pratt and Whitney engine was simulated [2]. The combustor simulator design length, width and inlet height was 156.9 cm, 111.8 cm and 99.1 cm. The contraction angle was 15.8 degrees. The inlet and exit cross sectional area were 1.11 m<sup>2</sup> and 0.62 m<sup>2</sup>. The combustor simulator included four film-cooled stream wise panels. The starting point of these panels was approximately at 1.6m upstream of the turbine vanes. Two different rows of dilution holes with a diameter of 8.5 cm and 11.9 cm were considered within the second and third cooling panels. The diameter of the film cooling holes was 0.76 cm and drilled at an angle of 30 degree from the horizontal surface. The present combustor simulator included three configurations of cooling holes. The length of film cooling holes in the baseline was 2.5 cm. For two other cases the cooling holes embedded within a row trench with depth and width of 0.75D and 1.0D and the alignment angle of  $\pm 60$  degrees.

The results shows the laterally averaged film cooling effectiveness distribution along z axis for different measurement observation planes at  $BR=3.18$ . They declared that for the observation planes of 0p, 1p and 2p, restructuring the cooling holes has positive effects on the film cooling effectiveness. For the planes of 1p and 2p, the film cooling effectiveness increased 116% and 48% respectively by trenching the cooling holes.

The purpose of this research was to extend the knowledge about the film cooling variation near the combustor end wall. To sum up, for the trenched case, the temperature near the wall and between the jets was significantly cooler especially for the planes 1p and 2p.

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## THE EVOLUTION OF THE SYSTEM OF GRAVITATING BODIES

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A natural physical approach to the analysis of the structure of closed gravitating systems has been formulated in the scope of classical mechanics. The approach relies on the interrelation between densities of nested spheres inscribed in the circular orbits of the system bodies. An empirical law has been defined for the evolution of closed gravitating systems differing in mass, time scale and distance from the ground-based Observer. The gravitating systems undergo modifications and evolve from their initial state, namely, a gas-and-dust formation of almost constant density over the entire volume, to a certain terminal phase of the process when the system structure becomes similar to the planetary system (like the Solar system) where almost all the gravitating mass is concentrated in the vicinity of the system center of gravity. Using the proposed method of nested spheres, it is possible to reveal for the gravitating system the character of radial distribution of matter density in the system symmetry plane, quantitatively evaluate the density of medium containing the gravitating system under consideration, and assess the current phase of the system evolution. The research results have led us to a conclusion that introduction into the scientific practice of such an entity as “dark matter” has no physical background since it is based on a wrong interpretation of an “unordinary” distribution of star orbital velocities in galaxies.

## WAVE DISTURBANCES OF THE MICROPOLAR RANKINE VORTEX

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The goal of our study is to assess the effect of an additional rotating degree of freedom for a particle – gyration – on the unsteady development of swirling viscous jets. We devote main attention to one of the simplest basic flow models, namely the plug flow axial velocity profile to which is superimposed a solid body core rotation. It is well known, that the Rankine vortex is neutrally stable for small disturbances (both for axisymmetrical and spiral modes) if an axial core flow, viscosity and a surface tension is ignored. The instability develops if the axial flow in the core is imposed upon the Rankine vortex.

In this study we restrict consideration to the effects of the viscosity and micropolar properties of only core fluid on the stability. Inviscid liquid occupy the external region. The surface of separation between these two liquids would be a surface of tangential discontinuity. We also take into account different densities of immiscible liquids in the inner region and in the external region. It is found exact solution represented an inertial normal mode. From boundary conditions we obtain a dispersion equation. An examination of the roots of the dispersion equation gives us the criterion for the stability of the system. The absolute/convective nature of the instability and effects of varying the Kibel number, the Ekman number and non-dimensional number characterizing micropolar properties are investigated.

## ECCENTRIC PARALLELEPIPEDAL INCLUSION WITH DIFFERENT DILATATION EIGENSTRAINS IN A LONG ELASTIC CYLINDER

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Nowadays the preparation, characterization and application of radially inhomogeneous nanowires are among the hottest topics in modern materials science and applied physics. This is caused by their excellent electronic and optical properties, which encourage their use in various devices of optoelectronics, nanoscale field effect transistors, storage and data transmission devices, logic devices, sensors, etc. [1, 2]. Physical properties of nanowires depend on shape, size, chemical composition, and types of crystalline lattices of the composite components as well as on presence of various defects in their structure. In particular, the shape effects can be tightly related with peculiarities in misfit stress distribution over the nanowires and with the mechanisms of misfit stress relaxation in them. However, in theoretical description of these mechanisms, they commonly use the model of cylindrically symmetric core-shell nanowires [3, 4] as it is much simpler for analytical modeling. The problem is that this simple approach strictly limits the variety of possible relaxation mechanisms available for theoretical examination. For example, it excludes the glide of straight misfit dislocations along the flat areas of the core-shell interface that is sometimes observed in experiments [5, 6]. It is

worth noting that flat interface regions often form in radially inhomogeneous nanowires [7, 8].

It seems that the simplest case of a core with flat faces is the core in the form of a long parallelepiped. To our best knowledge, today there are only two analytical solutions which describe the elastically strained state in elastic cylinders with parallelepipedal inclusions of square cross section, which are placed symmetrically with respect to the free surfaces [9, 10]. The first one [9] addressed the plane strain case, while the second one [10] deals with the case of 3D homogeneous dilatation eigenstrain. Both the solutions were found through the complex potentials method and illustrated by stress maps in Cartesian coordinates.

Here we present an analytical solution to the boundary-value problem in the classical theory of elasticity for a cylinder with the inclusion in the form of a long parallelepiped of a rectangular cross section, which is placed in an arbitrary position in the cylinder and characterized by three different dilatation eigenstrains. In real nanocomposites, this case corresponds to three different values of crystal lattice mismatch in 3D space. The problem solution is given by a sum of the stress field created by the inclusion in an infinite medium [11], and an extra stress field which is needed to satisfy the boundary conditions on the shell free surface. The extra stresses are found through the complex potentials method in a closed concise and transparent form. We show the analytical formulas for the stress components applicable for practical use in theoretical modeling of misfit stress relaxation processes and demonstrate stress distribution in the composite cross section, from which the fulfillment of boundary conditions on the free surface is evident.

*SAK and AMS got the support from RFBR project No. 16-32-00521.*

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## FINITE ELEMENT ANALYSIS OF COUPLED-FIELD ELECTROELASTIC PROBLEMS OF MEMS

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In this work we investigate finite element analysis methods of MEMS – pressure sensors, accelerometers, micromechanical gyroscopes, resonators, rf switches, etc. Occurring nonlinear coupled-field problems of electroelastics are analyzed by the program ANSYS. An analysis of static and dynamic responses of a one-dimensional MEMS-oscillator is performed by using the TRANS126 element (an electromechanical transducer). A finite element computation is performed with various boundary conditions for basic elements of MEMS such as beams and membranes. Their equilibrium forms are calculated in electrostatic fields of various configurations. The next methods are utilized: a generation of layers of TRANS126 finite elements; a coupled-field electroelastic computation («Electroelastic analysis») using the elements PLANE223, SOLID226, SOLID227; an iterative computation with a separate simulation of electrical and mechanical domains («Multi-field analysis»); a calculation using numerical procedures of a modal decomposition («ROM - Reduced order modelling»). A comparison of numerical and approximate analytical results is completed.

## ADJUSTMENT FOR DECREASE OF MAGNETIC MOTOR NOISE

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The electric motor inside volume formed by the winding stator and several rotor core elements is considered. Electromagnetic interaction between stator field winding and the rotor field winding, mechanical motor vibrations and

air fluctuations from ventilation motor impeller excite the basic components of air noise in a wide frequency range. Magnetostrictive forces causing radial deformation of the stator core rings under alternate field action bring the special addition in motor noise. The dependence of the sound noise pressure from electromagnetic vibrations inside of the small volume chamber SVC is considered. The greatest linear size SVC less than half of wave length of the longest eighen frequency is installed. The construction of the stator core of the alternate bipolar commutator motor having two acoustic channels with determinate diameters in the center of each magnet poles is shown. Except of external surface stator core fluctuations there are two acoustic sources excited by internal surface stator core and influence through two channels in antiphasis according external surface stator core fluctuations into SVC. The effective decrease of the carrying basic 100 Hz frequency magnetic motor noise is carried out. The method of the equivalent generator for symmetric parts in the electric analogue scheme is advanced. Equivalent generators as two sources of acoustic fluctuations switched on towards each other are described. The spectrograms illustrating of magnetic motor noise decrease are shown and the adjustment for decrease of magnetic motor noise is supported.

### **COLLECTIVE MIGRATION OF TWO LOW-ANGLE GRAIN BOUNDARIES IN NANOCRYSTALLINE AND ULTRAFINE-GRAINED METALS DRIVEN BY PERIODICALLY APPLIED MECHANICAL LOAD**

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In recent years nanocrystalline (NC) and ultrafine-grained (UFG) metals have been the subject of many research efforts due to their unique mechanical and functional properties. Athermal migration of grain boundaries (GBs) is one of deformation modes effectively operating in these advanced materials. We propose a model that describes collective migration of two low-angle tilt boundaries in NC and UFG metals driven by periodically applied mechanical load.

To consider such process we used the method of two-dimensional dislocation dynamics [1-3]. In doing so we modeled low-angle GB in its initial state before migration as perfect walls of edge dislocations. Triple junctions of GBs were considered as containing wedge disclinations. Through the simulation we calculated the evolution of dislocation ensembles composing the migrating GBs. While shear stress is applied dislocations that form the migrating GBs move to their equilibrium positions or reach high-angle GBs. In the periods of the absence of mechanical load migrated dislocations that haven't reached high-angle GBs tend to return to their initial positions.

The analysis of the obtained data revealed several possible GB migration modes that can occur with different values of the applied shear stress and misorientation parameters of migrating low-angle GBs. The results obtained are in good agreement with experimental data [4].

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### **A POSTERIORI ERROR BOUNDS FOR NUMERICAL SOLUTIONS OF PLATE IN BENDING PROBLEMS**

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For the efficient error control of numerical solutions of the solid mechanics problems, the two requirements are important: an a posteriori error bound has sufficient accuracy and computation of the bound is cheap in respect to the arithmetic work. The first requirement can be formulated in a more specific form of consistency of an a posteriori bound, assuming that it is not improvable in the order and, at least, coincides in the order with the a priori error estimate. Several new a posteriori error bounds are presented, which improve accuracy and reduce the computational cost. Also for the first time a new consistent guaranteed a posteriori error bound is suggested. The presented a posteriori bounds bear on the counter variational Lagrange and Castigliano principles which are valid for a wide class of problems.

## STUDY OF PREBREAKDOWN PROCESSES IN LIQUIDS WITH THE HELP OF KERR EFFECT

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Prebreakdown processes determine pulse electrical strength of liquids. One of the powerful methods of prebreakdown processes study is Kerr effect application. It performs to see both optical picture and electric field change before breakdown. Optical and electrooptical studies of breakdown and prebreakdown processes in water and nitrobenzene are presented here. Charge appearance, charge movement, bubble generation, electrohydrodynamic flows at high electric field action are registered as the main prebreakdown processes.

Moreover in case of screening electrodes due to conductive near electrodes layers it was recorded streamers that didn't originated on electrode surface but in the bulk of liquid. This is some kind of partial discharges. These streamers have form of two semistreamers, One streamer is similar to usual cathode streamer and other semistreamer is similar to usual anode streamer. Interesting events occur after breakdown. Space charge in conductive layers couldn't disappear instantly that leads to generation of strong electric field near breakdown channel that, in turn, leads to generation of postbreakdown streamers. This mechanism is discussed in the presentation.

*This work was supported by the grant № 16-19-10229 funded by the Russian Science Foundation.*

## DYNAMIC MODELS OF PROPAGATING INTERFACES

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The optimal modeling of extended defects propagating in condensed matter is a fundamental problem both for analytical and numerical research. During last two decades a phase-field model approach seems to be the most widespread and powerful to solve the problem. It has been successfully applied to a number of various difficult issues in the context of crystal growth, electro deposition, crack propagation to name a few. However, the approach has certain deficiencies.

Due to its purely phenomenological basis it turns out that one may try to make use of some phase-field model from a very large family of possible candidates, that's the strict criterion to select the most adequate model is simply absent. In practice, it happens very often that the model choice is dictated by some conveniences of a preferred numerical algorithm instead of a deep physical insight. To a large extent the situation takes place due to the fact that generally phase-field models are very difficult to be treated analytically so the computer becomes to be a dominant tool. As a consequence, the proper understanding of physics behind the obtained numerical results is seriously impeded.

In my talk I will discuss some field-theoretical tricks that allow to transform the bulk phase-field models description into so-called interface models. The latter are functionals defined in a space of a lower dimension than the former. Hence, the interface models are much easier to deal with as numerically as especially analytically. To elaborate the general ideas I will demonstrate several examples including rapid directional solidification of dilute alloys, overcritical brittle crack growth and laser-induced crystallization of amorphous solid.

## RELATION BETWEEN DELOCALIZED AND LOCALIZED NONLINEAR VIBRATIONAL MODES IN CRYSTALS

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Delocalized nonlinear vibrational modes is a type of nonlinear lattice vibrations being exact solutions of equations of motion defined by the symmetry of the crystal and independent of interatomic potential and amplitude of the mode. Chechin with co-authors have described four possible delocalized short-wave vibrational modes found recently for the two-dimensional hexagonal lattice with the help of a group-theoretic approach [1]. The important feature of those modes is the fact that their amplitude-frequency dependence behavior is defined by external conditions and they can demonstrate hard/soft nonlinearity type in case of constant volume/zero pressure conditions respectively. The interest to those modes is caused by their possible impact on lattice dynamics and elastic properties. Thus it was demonstrated that the large-amplitude, short-wavelength vibrational modes excited in the honeycomb lattice with  $\beta$ -FPU interaction potential can change its elastic properties due to physical and/or geometric nonlinearity of the lattice bonds. It was also

shown that the excitation of a large-amplitude vibrational mode in combination with equiaxial tensile strain can change the sign of the Poisson's ratio from positive to negative, thus leading to the auxetic property of the lattice [2]. Another notable feature of delocalized nonlinear vibrational modes is the phenomenon of modulational instability. The analysis of modes behavior revealed the decay of the mode resulting in the modulational instability followed by formation of long-lived DBs that radiate their energy slowly until thermal equilibrium is reached [3]. A thorough investigation of superposition of a planar nonlinear phonon mode with the wave vector lying at the edge of the Brillouin zone with a bell-shaped localization function revealed the possibility of excitation of discrete breathers of different symmetry [4]. The results obtained make it possible to approach the search for highly symmetric discrete breathers in three-dimensional crystals.

In general one can conclude that delocalized vibrational modes have a great impact potential for modification nonlinear lattice dynamics, their elastic properties of crystal lattices and initiation of new topological defects. New possible roles of delocalized modes in lattice dynamics are discussed.

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### ANALYTICAL MODEL OF NONLINEAR WAVE INTERACTIONS BETWEEN THERMAL ACOUSTIC AND OPTICAL PHONONS IN CRYSTAL LATTICE WITH CUBIC ANHARMONICITY

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In crystal lattices with cubic anharmonicity, two transverse modes can couple with a longitudinal wave. On the other hand, there are no intrinsic localized modes (discrete breathers), the time-periodic and spatially localized solutions of the nonlinear equations of motion, in the lattice with only cubic anharmonicity [1]. In the recent paper [2], the formation of a dispersionless optical mode in the acoustic phonon frequencies as well as a kink in the dispersion of the longitudinal acoustic branch was predicted to exist at finite temperature in crystal lattice of PbSe with only cubic anharmonicity. This dispersionless optical-like mode was related in Ref. [2] with the intrinsic localized mode. Here we present an analytical model, which describes the interaction of longitudinal acoustic mode with two transverse optical-like branches in the crystal lattice with only cubic anharmonicity. The proposed model describes the thermal excitation of the bulk dispersionless mode through the decay of thermally excited transverse optical mode into high-speed longitudinal acoustic mode and dispersionless (immovable) transverse optical-like mode at one-half frequency. This model does not imply the excitation of the intrinsic localized mode in crystal lattice with only cubic anharmonicity. The considered model of the excitation of subharmonic mode has some similarities with the subharmonic transmission at one-half frequency of high-frequency phonon through the interface, caused by nonlinear interactions with thermally excited anharmonic intermediate layer [3].

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### THE COMPARISON OF TWO TYPES OF BOUNDARY CONDITIONS FOR THE ACTIVE ELECTRODE IN SIMULATION OF IONIC WIND

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Ionic wind is generated by a corona discharge due to the momentum transfer from ions moving into the inter-electrode gap to neutral molecules. The phenomenon underlies a number of notable modern technologies, for example, it enables the creation of silent coolers and efficient electrostatic precipitators. However, the actual development of such equipment pivots on a detailed insight into the physical processes that cause ionic wind. Computer simulation of the

processes requires significant computational power; therefore, different simplified models are relevant. The work aims to compare two models of ionic wind. The simulation involved the needle-plane electrode system with the positive polarity of the active electrode. The first method utilizes a common approach in the scientific community, when the density of the flow of positive ions is set at the active electrode as the linear function of the electric field strength. Defining the function requires experimental values of ignition voltage of corona discharge measured for each electrode system under simulation. The second method uses a more complicated boundary condition for the ion flow, which is based on calculation of the number of ionization collisions near the electrode surface. The advantage of the model is that requires no experimental input data at a change of the electrode configuration. To verify the performance of the models, the structure of ionic wind in the needle-plate electrode system was studied experimentally. The I-V curves of corona discharge were measured over a wide range of voltages. Air velocity distributions in the inter-electrode gap were obtained by the Particle Image Velocimetry method. Distributions of the electric field, charge density and integral value of the current were calculated for both models. Air velocity distributions in the ionic wind jet were obtained and analyzed. The results from simulation and experiments were compared.

## **TWO AND THREE HARMONICALLY COUPLED PENDULUMS**

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We present analysis of the nonlinear dynamics of the system of two and three harmonically coupled pendulums without restrictions on the oscillations amplitudes. This model is a basic one in many areas of Mechanics and Physics (paraffin crystals, DNA molecules and others). We obtained stationary solutions of the equations of motion corresponding to the Nonlinear Normal Modes (NNMs) of the system. We have found inversion of the NNM frequencies when the amplitude of the oscillations increases. Supposing the NNMs resonant interaction we introduce “slow” time-scale which determines characteristic time of the energy exchange between the pendulums. Essentially nonstationary process of the energy exchange is described in terms of the Limiting Phase Trajectories (LPTs), which obtained effective analytical presentation. We found explicit expressions for the threshold parameter values which correspond to NNM instability and transition (in the parametric space) from the full energy exchange between the pendulums to energy localization. In the system of three pendulums a regime of intensive periodic energy exchange between the first and the third pendulums is thoroughly studied. In this case the middle-pendulum serves for the energy transport between the ends of the short chain. The frequency of its energy oscillations is doubled one of the energy pulsations of the ends. The significance of the nonlinearity type (“soft” or “hard”) is revealed. Obtained analytical results are verified by the simulations of the initial system

## **EFFECTIVE ELASTIC PROPERTIES OF A COMPOSITE MATERIAL CONTAINING RIGID TOROIDAL INHOMOGENEITIES**

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Calculation of the effective elastic properties of materials containing inhomogeneities of non-ellipsoidal shapes represents a challenging problem in materials science. In analytical modeling of heterogeneous materials inhomogeneities are usually assumed to have ellipsoidal shape. This unrealistic assumption is largely responsible for insufficient linkage between methods of micromechanics and materials science applications. In this work, we study effect of toroidal inhomogeneities on the overall elastic properties of composite. Such kind of inhomogeneities occur both in natural and man-made materials. For instance, toroidal particles represent preferred morphology of Li<sub>2</sub>O<sub>2</sub> deposition on porous carbon electrode in lithium-oxygen batteries [1, 2]; polymeric “microdonuts” are used in bioengineering [3]; toroidal shape of nanoparticles is reported to be preferred for microwave absorption properties of BaTiO<sub>3</sub> [4].

To the best of our knowledge, there are two approaches to describe effective properties of a composite with toroidal inhomogeneities: contribution of a thin rigid toroidal inhomogeneity into overall stiffness has been evaluated by asymptotic methods in [5] and overall thermal conductivity of a material with toroidal pores was evaluated in [6]. Eshelby tensor of a toroidal inclusion was calculated in [7], however this result cannot be used for calculation of the effective properties.

We solve an elasticity boundary-value problem for an infinite elastic medium containing a rigid toroidal inhomogeneity

subjected to remotely applied uniform strains. The solution is obtained in explicit form of associated Legendre function's series using the approach proposed in work [8]. The averaging over the inhomogeneity volume leads to calculation of the stiffness contribution tensor of the inhomogeneity. The analytical approach is verified by comparison with FEM simulations. The expression for stiffness contribution tensor yields the possibility to calculate effective elastic properties of a material containing multiple toroidal inhomogeneities. It is done using non-interaction approximation, Mori-Tanaka scheme, and Maxwell scheme.

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### STRESS RELAXATION IN DECAHEDRAL SMALL PARTICLES THROUGH FORMATION OF CIRCULAR PRISMATIC DISLOCATION LOOPS

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Small FCC metal particles is one of the most interesting objects in materials science due to possible existence in their atomic structure of five-fold symmetry axes which are prohibited in bulk crystals [1]. In the latter case, they say about 'five-fold twinned' or, shorter, 'pentagonal' small particles (PSPs). They have been studied intensively over the last sixty years and still demonstrate new original and unique properties [1-7]. It is commonly known that PSPs have residual stresses, and their strain energy is proportional to their volume. There are many possible ways for the stress and energy relaxation, which include the formation of various defects such as dislocations, disclinations, low-angle grain boundaries, voids, etc. The reasons for such variety are still left unexplained. Some of them are developed consistently with increasing particle size. Nevertheless, the stress relaxation in PSPs usually starts with nucleation of single defects, in particular, circular prismatic dislocation loops (CPDLs) [8].

In the present work, we analyze the stress relaxation in the simplest PSP that is a decahedral small particle (DSP), by formation of a CPDL. The initial stress-strain state in a DSP is modeled as that created by a positive wedge disclination of strength  $7^{\circ}20'$ , which is placed in an elastic sphere along its diameter. The corresponding boundary-value problem in the theory of elasticity is solved in [9]. On the other hand, a similar problem for a CPDL in an elastic sphere is solved in [10]. Based on these two solutions, we analyze the change in the total energy of the DSP, caused by the nucleation of a CPDL, and show that its formation is energetically profitable when the DSP radius  $R$  is larger than a critical value  $R_{cr}$  which strongly depends on the dislocation core parameter  $\alpha$  ranging from 0.5 to 5 in various materials [11]. We also study the optimum radius  $c_{opt}$  of the CPDL as a function of  $R$  and show that  $c_{opt}/R$  increases with  $R$  and tends to 0.3 when  $R \rightarrow \infty$ . Enlargement of either  $\alpha$  or the Poisson ratio  $\nu$  leads to reduction in  $c_{opt}$ . It is also worth noting that  $R_{cr}$  for a DSP is about 2 times larger than that of a pentagonal whisker [12], which shows a greater stability of DSPs with regard to CPDL formation.

*This work was supported by grant from the Ministry of Education and Science of the Russian Federation (Decree No. 220) obtained by the Togliatti State University under the contract No. 14.Z50.31.0039.*

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## **DNS OF TURBULENT FLOWS IN SPHERICAL LAYER, DRIVEN BY TORSIONAL OSCILLATIONS OF BOUNDARIES**

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We have numerically studied the transition to turbulent flow in a layer of a viscous incompressible fluid confined between concentric spherical boundaries performing counter-rotational oscillations relative to the state of rest. The rotation speeds of both spheres were modulated at the same frequency and amplitude with the phase shift  $\pi$ . We used an algorithm of numerical solution based on a conservative finite difference scheme of the discretization of the Navier–Stokes equations in space and semi-implicit Runge–Kutta scheme of the third order integration accuracy in time. Discretization in space was performed on grids nonuniform in radial and meridional directions with concentration near the boundaries and equatorial plane. The transition to turbulence was caused by an increase in the amplitude of velocity modulation. Using the concept of instantaneous frequency/phase of flow (based on the building of the analytical signal of the velocity time series by means of Hilbert transform), it is established that the turbulence develops in a limited region of liquid layer, outside which the flow remains laminar. The turbulent region of flow exhibits intermittency of the chaos–chaos type with random alternation of weak and strong turbulence.

## **NONLOCAL INTERACTION AND ANOMALOUS HEAT CONDUCTION**

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Influence of nonlocality on the processes of heat conduction in one-dimensional harmonic crystals is analyzed. Method for obtaining the thermal transport laws for the systems with an infinite range of interaction is presented. Each atom of the considered crystal interacts with an infinite number of neighbors. In particular, the exponential and inverse power laws of interaction are considered. The method allows also solution of the inverse problem: obtaining the interaction laws for the desired law of heat conduction. The obtained laws demonstrate combined properties of the ballistic and diffusive thermal behavior. In the case of localized heat disturbance, the interaction nonlocality results in weakening the heat front. It is shown that in the case of a strong nonlocal interaction the heat front can be absent, similar to the classical heat conduction. Applications to the problems of the thermal transport in nanowires, nanotubes and other low-dimensional nanostructures are considered.

## **DESTRUCTIVE ATMOSPHERIC VORTICES AND THE EARTH'S ROTATION AROUND ITS AXIS**

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The results of theoretical and experimental studies of destructive atmospheric vortices, tornadoes and tropical cyclones. Suggestions S.P. Bautin [1] scheme of the functioning and sustainability of such flows. This pattern is confirmed as the results of analytical studies of the relevant decisions of the initial-boundary value problems for the equations of gas dynamics for the full Navier-Stokes equations [1-4], and conducted physical experiments to create a tornado flow [3-6]. Numerically and analytically constructed solutions of equations of gas dynamics, taking into account the action of the Coriolis force to simulate the flow of air in the bottom parts of the tornadoes and tropical cyclones (one-dimensional and three-dimensional non-stationary, stationary), and in general in these streams (three-dimensional non-stationary). All these decisions are consistent with the data of field observations indicated natural air currents. Analysis of geometric, high-speed and power characteristics of these flows showed the following: destructive are those observed in nature tornado in which the kinetic energy of motion of the district in the bottom part of the greater kinetic energy of radial movement of air in this part of the stream.

With the results presented experimental and theoretical studies proved the fallacy of proposals not to take into account the effect of the Earth's rotation around its axis for those flows for which the Rossby number is much greater than unity. Offered specific recommendations on introduction of the practice of the results developed by the gas-dynamic theory of destructive atmospheric vortices. Including made recommendations for early detection of tornadoes and tornado destruction and tropical cyclones with reasonable energy costs [7].

The studies established a new natural scientific fact: for tornadoes and tropical cyclones mathematically rigorous proof that only the rotation of the earth around its axis is the cause of occurrence of twist in these flows and the kinetic energy of the rotational movement of air in them is taken only from the kinetic rotation of the Earth energy around its axis.

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## ROLE OF PARTIAL DISLOCATIONS AND TWINS IN MECHANICAL RESPONSE OF COPPER NANOCRYSTAL DURING SEVERE PLASTIC DEFORMATION

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In this work we investigated atomic mechanisms of the structural response of the copper nanocrystal during severe plastic deformation. It is well known that the plastic deformation of fcc metal nanocrystals is much contributed by partial dislocations and mechanical twins. Partial dislocation motion and twinning provide high plasticity at stresses close to their theoretical strengths. The mechanical features of plastically deformed nanocrystals are largely due to suppression of the ordinary dislocation mechanism. Clarifying the causes of these features requires an analysis of the mechanisms by which partial dislocations and twins nucleate at local stresses close to the theoretical strength of a perfect crystal.

Here we provide the results of computer simulation of dislocation generation and twinning in fcc copper based on the molecular dynamics method. The interatomic potential was described in the scope of the embedded atom method. The loading was simulated as uniform tension in [110] direction, the initial temperature of the specimen was 300 K. Performed computer simulation gave detailed dynamics of local structural changes during partial dislocation nucleation and movement, and nanotwin propagation. It was revealed that the atomic cells can rearrange in the sequence fcc-bcc-hcp at the front of a  $a/6 \langle 112 \rangle$  partial dislocation. The restoring of the fcc structure in the trace of dislocation movement occurs as a result of the reverse hcp-bcc-fcc transformation.

## MODELLING HYDROTHERMAL SYNTHESIS IN AUTOCLAVE WITH OPTICAL ACCESS

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The hydrothermal synthesis is one of the most effective methods of obtaining nanoparticles [1]. This method allows to produce nanoparticles with various composition and morphology, characterized by a narrow size distribution. The efficiency of the nanoparticles synthesis under hydrothermal conditions is determined, in particular, by the spatio-temporal characteristics of the temperature in the autoclave. The team of authors has at its disposal a unique autoclave

with sapphire windows for the studying the process of nanoparticles synthesis using optical radiation. However, all autoclaves, which are experimenting with high pressure, are a kind of "black box", since there is no immediate opportunity to observe what is happening inside. In 1973, Kuznetsov and Lobachev overcome this problem [2]. Theirs model of autoclave had sapphire windows made on opposite sides of the walls of the autoclave. This allows carrying out experiments and optical control, highlighting the fusion process, and recording it on camera. Also, it allows the circuit to assemble a holographic imaging process for the synthesis of nanoparticles in an autoclave.

Since the process of hydrothermal synthesis takes place at high temperatures in the force of gravity, one of the main components of its effects is the convective motion of the fluid. This process defines on of the main parameters of system – distribution of temperature. Experimental setup allows manipulating the initial conditions of temperature distribution. To achieve the most effective results of synthesis needed to find relations between initial distribution of temperature and final distribution of nanoparticles. The first step to find these relations is modelling convection inside autoclave.

Modelling of free convection inside autoclave convenient make using system of Navier-Stokes equations under Boussinesq approximation. OpenFOAM provides standard solver for this problem buoyantBoussinesqPimpleFoam. The mathematical model of problems described by following equations [4]:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial x} = 0,$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \eta \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right),$$

$$u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial x} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \eta \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + g\beta(T - T_c),$$

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial x} = \alpha \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

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## AN ANALYTICAL DESCRIPTION OF UNSTEADY HEAT TRANSFER IN HARMONIC SCALAR LATTICES

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An approach for analytical description of unsteady heat transfer in harmonic lattices is presented. Evolution of initial temperature field in infinite lattice is investigated. Dynamics equations for scalar lattices are written in a form valid for longitudinal and transverse vibrations of chains and for out-of-plane vibrations of two-dimensional lattices. The description of heat transfer is based on analysis of velocity covariances for all pairs of particles. The general solution of the unsteady heat transfer problem is obtained in integral form. The solution shows that temperature is represented as a superposition of waves having a shape of initial temperature distribution. The waves propagate with group velocities depending on the wave vector. The heat front propagates with constant speed equal to the maximum group velocity. The general solution is reversible with respect to time, i.e. it is invariant with respect to substitution  $t$  by  $-t$ . Closed-form fundamental solutions for one- and two-dimensional lattices are obtained. The problem of thermal contact of two half-spaces having different initial temperatures is considered. It is shown that effective heat conductivity linearly diverges with length for all harmonic scalar lattices. This fact is consistent with results obtained in literature for stationary heat transfer problem. An example of unsteady heat transfer in a stretched square lattice performing out-of-plane vibrations is given. Analytical solutions of problems with stepwise and sinusoidal spatial distributions of initial temperature are presented. Numerical simulations show that presented theory describes the unsteady heat transfer in harmonic scalar lattices with high accuracy.

## SEISMIC BARRIERS UTILIZING CONCEPT OF A BROADBAND PHONONIC CRYSTAL: MATHEMATICAL MODELS AND NUMERICAL SIMULATIONS

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The basic idea of seismic barrier is to protect an area occupied by a building or a group of buildings from seismic waves. Depending on nature of seismic waves that are most probable in a specific region, different kinds of seismic barriers are suggested.

For example, vertical barriers resembling a wall in a soil can protect from Rayleigh and bulk waves. The FEM simulation reveals that to be effective, such a barrier should be (i) composed of layers with contrast physical properties allowing “trapping” of the wave energy inside some of the layers, and (ii) depth of the barrier should be larger than half of the considered seismic wavelength. Considerable reduction in geometry of the vertical barriers can be achieved if barriers are filled in with dissipative metamaterials resembling broadband phononic crystals.

Another type of seismic barrier represents a relatively thin surface layer that prevents some types of surface seismic waves from propagating. The ideas for these barriers are based on one Chadwick’s result concerning non-propagation condition for Rayleigh waves in a clamped half-space, and Love’s theorem that describes condition of non-existence for Love waves. The numerical simulations reveal that to be effective the length of the horizontal barriers should be larger than half of the considered seismic wavelength. Analogously to vertical barriers, horizontal barriers can also be filled in with the dissipative metamaterials allowing for both decrease in the barrier overall geometry and increase in reduction ratios.

## CALCULATION OF EFFECTIVE ELASTIC PROPERTIES FOR SOLIDS WITH RANDOMLY ORIENTED CRACKS

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Calculation of the effective elastic properties of materials with a random distribution of cracks is considered. At low crack densities, the elastic properties are well described by the non-interaction approximation. In particular, it is known that the effective elastic properties are orthotropic. In the present paper, we numerically study the range of applicability of the non-interaction approximation. We focus on effect of crack interactions on orthotropic symmetry of elastic properties. The effective properties are calculated using the displacement discontinuity method in the two-dimensional statement. Computer simulations show that interactions between cracks significantly influence the effective elastic properties. However even at high crack densities, the effective properties remain orthotropic as predicted by the non-interaction approximation. Moreover, axes of orthotropic symmetry are accurately determined using the non-interaction approximation.

## FULLY LAGRANGIAN METHOD FOR SIMULATION OF AXIALLY SYMMETRIC GAS-PARTICLE VORTEX RING-LIKE FLOWS

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A combined fully Lagrangian approach for meshless modeling of unsteady axisymmetric vortex flows of a gas-particle mixture with an incompressible carrier phase is developed. The approach proposed is based on the combination of a meshless vortex method for calculating axisymmetric flows of the carrier phase described by the Navier-Stokes (or Euler) equations and the full Lagrangian method for calculating the parameters (including the concentration) of the dispersed phase. The combination of these methods reduces the problem of modeling the two phase flows to the solution of a high-order system of ordinary differential equations for the coordinates of toroidal vortex elements in the carrier phase and the particle trajectories, the velocity components, and the components of the Jacobian of transformation from the Eulerian to the Lagrangian variables in the dispersed phase. The proposed method has a clear advantage as compared to the standard Eulerian-Lagrangian approaches: it makes possible to avoid the cumbersome procedure of the recalculation of the parameters from the Eulerian to the Lagrangian grid. The method is particularly

convenient for accurate calculations of the dispersed phase concentration fields in vortex flows with crossing particle trajectories.

The application of the method is illustrated by modeling the behavior of an admixture of inertial particles with a small mass concentration in unsteady flows like solitary vortex rings in a viscous carrier phase and groups of vortex rings in an effectively inviscid carrier phase. These flows involve the formation of local zones of particle accumulation, regions of multiple intersections of particle trajectories, and multi-valued particle velocity and concentration fields. The proposed combined Lagrangian mesh-free approach enables one to reproduce with controlled accuracy all these flow features without excessive computational costs.

## DISLOCATION MECHANISM OF MICROSTRUCTURAL CHANGES IN DUCTILE SINGLE CRYSTALS

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The present paper considers two problems: i) martensitic phase transition involving dislocations, ii) formation of grain boundaries during severe plastic deformations. Both problems turn out to be non-convex variational problems of energy minimization that will be solved within the continuum dislocation theory (CDT). In the first problem it will be shown that the co-existence of phases having piecewise constant plastic slip in laminates is possible for the two-well free energy density. The jumps of the plastic slip across the phase interfaces determine the surface dislocation densities at those incoherent boundaries. The number of phase interfaces should be determined by comparing the energy of dislocation arrays and the relaxed energy minimized among uniform plastic slips. In the second problem we interpret the grain boundary as surfaces of weak discontinuity in placement but strong discontinuity in plastic slip. The set of governing equations and jump conditions are derived for the energy minimizers admitting such surfaces of discontinuity from the variational principle. By constructing energy minimizing sequences having piecewise constant plastic and elastic deformation in two examples of ductile single crystals deforming in plane strain simple shear or uniaxial compression, it is shown that the formation of lamellae structure with grain boundaries is energetically preferable. The number of lamellae is estimated by minimizing the energy of grain boundaries plus the energy of boundary layers.

## CREEP AND VISCOPLASTIC FLOW IN THE CYLINDRICAL LAYER OF A MATERIAL AT NONUNIFORM ROTATION OF AN INTERNAL BOUNDARY SURFACE

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The construction of a mathematical model of such a process as cold forming because of slow regime of creep requires a researcher to pay attention to the creep of a material and the development of plastic flow in it. This process is the most perspective technology of material processing and producing of a finished work. Intensive forming of the deformed material causes necessity of applying a model of large deformations which considers elastic, plastic and viscous properties of the material.

This study considers a boundary value problem of deforming of an incompressible material with nonlinear elastic, viscous and plastic properties. We assume that the material is placed in the gap between two rigid cylindrical surfaces and deformed at the rotation of the internal cylinder. The solution is constructed in the context of the theory of large deformations [1, 2]. Irreversible strains are initially accumulated because of slow process of creep. At some instant, due to an increase of the rotation velocity of the internal cylinder, in its neighborhood the stress state reaches the yield point, and a region of viscoplastic flow begins to extend. The dissipation mechanism is determined by the associated plastic flow rule. The generalized Tresca yield criterion is used to consider viscous properties of the material. The first step of numerical calculation procedure is the determination of a moving elastoplastic boundary which separates the area of elastic and creep strains and the area of viscoplastic flow from the instant mentioned above till an instant when the latter area reaches the internal cylinder. Components of reversible and irreversible strain tensors are determined with the help of obtained elastoplastic boundary distribution and also by the integration of the system of partial differential equations constructed on the base of constitutive relations of the theory used. The deforming process is considered sequentially at increasing, constant, decreasing and zero rotation velocity of the internal cylindrical surface.

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## **PLANE LONGITUDINAL WAVES IN A LIQUID SATURATED POROUS GEOMETRICALLY NONLINEAR MEDIUM**

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Mathematical models of deformable porous materials date back to the classic works of M.A. Biot, Y.I. Frenkel, L.Y. Kosachevsky, and their subsequent modifications. These models are widely used in the study of processes in geophysics and mechanics of natural and artificial composites. Most authors are limited in their research by the linear theory of poroelasticity, however, nonlinear effects in the liquid saturated porous media are essential and are of interest.

In this paper we consider the propagation of plane longitudinal waves in a liquid saturated porous medium, taking into account the nonlinear dependence between deformations and displacements of the solid phase. A liquid saturated porous medium is considered within the framework of Biot's theory. It is shown that the mathematical model, which takes into account the geometric nonlinearity, can be reduced to a system of evolution equations concerning displacements of a skeleton of the medium and fluid in the pores. Further, the system of evolution equations is reduced to the equation of the simple Riemann's wave, if the viscosity of the medium is missing, and to a generalised Burgers' equation when the viscosity is present in the medium. The solution of the Riemann's equation is obtained by the method of characteristics for a bell-shaped initial profile. The wave breaking time is found. The solution of the Burgers' equation is obtained in the form of a stationary shock wave resulting from mutual compensation of nonlinearity and dissipation effects. The dependence of width of a shock wave front on the saturating fluid viscosity and the shock wave amplitude is determined.

*This work was supported by the Russian Science Foundation (project number 15-19-10056).*

## **DETONATION CONTROL IN A SUPERSONIC GAS FLOW IN A PLANE CHANNEL**

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Using a detailed chemical kinetics, detonation combustion of a stoichiometrical hydrogen-air mixture flowing at a supersonic velocity into a plane symmetrical channel with a constriction was investigated with the purpose of both determination of conditions that provide detonation stabilization in the flow and study of methods of stabilized detonation location control.

The conditions of detonation stabilization in the flow in a plane channel with a constriction, the outflow section of which is smaller than the inflow one, have been investigated in [1]. The stability of the formed gas flow with detonation to strong disturbances excited by an energy input has been examined in [2]. However, in cases under consideration the gas flow does not develop thrust.

In the present research the study of stabilization of energy input initiated detonation in the supersonic gas flow in the channel with a constriction, the outflow section of which exceeds the inflow one, has been carried out with the purpose of determination of conditions that guarantee formation of a thrust developing flow with stabilized detonation in the channel.

The influence the inflow Mach number, the dustiness of the inflowing gas mixture and the width of the outflow channel section variations on location of the stabilized detonation wave was studied. Some methods of stabilized detonation location control that provide the increase of the detonation combustion efficiency have been proposed.

In addition, the possibility of detonation initiation and formation of the thrust developing flow with the stabilized detonation wave in the channel with a constriction without any energy input has been detected.

This research has been supported by the Russian Foundation for Basic Research (14-01-00742, 16-29-01092), by the President Grant for Support of Leading Science Schools of Russian Federation (NSh-5436.2014.1). The software package development and study of dusty mixture detonation combustion were carried out with the support of the Russian Science Foundation (14-19-01759 and 14-11-00773, respectively). This research has been supported by the Supercomputing Center of Lomonosov Moscow State University [3].

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## ON USING FAST MULTIPOLE METHODS FOR SOLVING PROBLEMS OF CONTINUUM MECHANICS

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Modern computational physics tends to account for mutual interactions in systems with multiple (up to millions) degrees of freedom. Two major distinct approaches are used for two distinct types of interactions, which are (i) short-range and (ii) long-range interactions. Specifically, since short-range interaction requires accounting for merely close neighbours, the resulting matrices are sparse, which suggests highly efficient techniques employing this feature in methods of molecular physics, smooth particle dynamics, etc. In contrast, long-range interactions, like gravitational or of Coulomb type, lead to fully populated matrices, while providing options of using properties of the corresponding potentials. The key idea consists of representing far-fields of a group of neighbouring sources by their summary effect via so-called multipole expansions. This gives rise to fast multipole methods (FMM). They use the expansions to obtain the total effect of all distant sources on a particular element by proper translations in upward and downward passes over a hierarchical tree.

Respectively, the same distinction transfers to computational continuum mechanics. The methods based on the discretization of the entire volume, like FEM, DEM, FDM, employ elements with short-range interaction. These methods lead to sparse matrices with the possibility to benefit from this feature. On the other hand, the methods with meshes, which cover merely interfaces and external boundaries, such as the boundary element methods (BEM), require accounting for long-range interaction between parts of the surfaces. They result in fully populated matrices, while far-fields of their potentials suggest using the FMM. These methods are of prime significance when there is need in accounting for non-trivial interface conditions on multiple contacts and/or in accurate evaluation of local fields near sources of strong field concentration, like cracks, edges of grains, thin inclusions, notches. In this work, we focus on such problems and develop FMM for their solution in frames of the BEM.

The presentation starts with a brief review of the two major types of the FMM: analytical (A-FMM), and kernel-independent (KI-FMM). Then the reasonable parameters of these methods are summarized. The comparison of the A-FMM and KI-FMM is given with emphasis on the reasonable ways of using the highly perspective KI-FMM. The conclusions are as follows. (i) To account for far fields when solving a BIE it is sufficient to use the equivalent density of merely that integral which has the highest order at infinity. (ii) The KI-FMM is equivalent to the A-FMM (to the accuracy of terms kept in analytical expansions) if the equivalent density is evaluated in the basis generated by the expansion of a kernel. (iii) When employing the KI-FMM, it is reasonable to take circular (in 2D) and spherical (in 3D) equivalent surfaces with circular-arc (spherical) boundary elements on them. The exposition is illustrated by examples and numerical results obtained by the authors for a number of benchmark and applied problems.

## NUMERICAL STUDY ON HIGH-LIFT MULTI-ELEMENT CONFIGURATIONS WITH FIFTH-ORDER ACCURATE HWCNS

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The flow field of high-lift multi-element configurations is characterized by complicated flow physics such as boundary layer separation, shock/boundary interaction. Accurate prediction of high-lift aerodynamics remains a challenge to Computational Fluid Dynamics (CFD). In this paper, fifth-order accurate explicit Hybrid cell-edge and cell-node Weighted Compact Nonlinear Scheme (HWCNS) is used to solve Reynolds Averaged Navier-Stokes (RANS) equations for the study of the three-element airfoil 30P-30N and the trapezoidal wing. Numerical simulations of both configurations use the SA turbulence model and multi-block structured grids. Surface pressure distribution and velocity profiles at typical stations of 30P-30N are presented without regard to transition, the pressure distribution agree well with the experimental results, the velocity profiles are qualitatively consistent with the experimental results while

differs little quantitatively. The force coefficients and the surface pressure distribution of the trapezoidal wing are in good agreement with the test data, and the wing tip vortex is well captured. Computation results indicate the good performance of HWCNS on the numerical simulation of high-lift configurations.

## **THERMAL PROCESSES IN A ONE-DIMENSIONAL CRYSTAL WITH REGARD FOR THE SECOND COORDINATION SPHERE**

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The process of heat propagation in a one-dimensional harmonic crystal considering the second coordination sphere are studied in this work.

Initial thermal disturbances in a form of a contact between a cold and hot half-space, an instantaneous heat pulse, and a rectangular pulse are considered. It is shown that the presence of nonlocality leads to the propagation of two thermal waves, one of which is related to the maximum group velocity.

The stiffness of the bond between the particles of the second coordination sphere can take both positive and negative values. Expressions for the wavy dispersion and group velocity were found using a single parameter  $\beta$ , which varies from  $-\pi/4$  to  $\pi/4$ , remains real and does not become infinite for all sets of its quantities. The use of the parameter  $\beta$  makes it possible to obtain graphs characterizing the propagation of waves in the system for any allowed values of the second coordination sphere stiffness. At  $\beta = 0$  the connection with the second neighbors is not taken into account. For  $\beta = \pi/4$ , the connection between the nearest neighbors becomes insignificant: in the chain considered, the distances between the particles are doubled comparing to the original one. The value  $\beta = -\pi/4$  corresponds to the limiting value of the negative stiffness of the second coordination sphere for which the chain remains stable. It is shown that all these cases are described by the one equation of heat propagation.

## **NONLINEAR DYNAMICS AND STABILITY OF ELECTROSTATICALLY ACTUATED ELEMENTS OF MEMS**

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In this work we investigate analytical and numerical methods for solving static and dynamic problems of elastic elements of microelectromechanical systems (MEMS). We consider typical deformable elements of sensors and actuators such as strings, beams, membranes and plates and calculate their equilibrium forms in electrostatic fields of various configurations. Analysis of static stability is performed and bifurcation diagrams are determined. Dynamic coupled-field analysis of aforementioned MEMS elements is carried out using method of reduced order modelling (ROM). Frequency and voltage response curves are calculated taking into consideration strong physical and geometrical nonlinearities of the system. Numerical continuation algorithms such as AUTO and MATCONT are utilized, accordingly qualitative (parametric) analysis of static and dynamic stability of MEMS elements is performed.

## **MODELING OF PROPERTIES OF MULTIFUNCTIONAL COMPOSITES WITH CNTS "FUZZY" FIBERS ACROSS THE LENGTH SCALES**

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The applied correct gradient theories of elasticity [1] are used for the simulation, at micro/nano-level of physical and mechanical properties, of whiskerized interfacial layers formed by carbon nanofibers (nanotube forests) grown on the surface of the cylindrical fibers along the normal direction with respect to the surface.

First, we discussed the applied nonlocal second gradient models and show the examples that the accounting the specific

correctness conditions for the gradient models are extremely important for applied problems. Then we elaborated for the nonlocal theory of elasticity the generalized self-consistent Christensen-Eshelby method of the definition of effective mechanical characteristics of fiber composites in the framework of corrected second gradient model [2].

We estimate the effective storage and loss moduli of bristled fiber composite materials, where the surface of the fibers is coated with nanostructures such as carbon nanotubes (fuzzy fiber). We investigate the effects of nanofiber length, density of nanostructure near surface of fibers and changing of density of nanostructure near surface of fibers on the effective mechanical and dynamic properties of a multifunctional fiber composites by employing a self-consistent Eshelby method of a multi-phase model using a viscoelastic correspondence principle. We show that these factors play important role in determining the effective dynamic properties of bristled fiber composite materials.

We develop the methods of modeling, allowing to take into account more fully the properties of multifunctional composites structures at various scale levels. . To receive solution we develop the method of radial multilayers [3] for layered cylindrical inclusions.

We give an assessment not only of the effective mechanical characteristics but also of the dynamic dissipative properties of fiber composites on the basis of the method of complex modules [4,5]. We study also the stress field near the inclusions on the micromechanical level.

*This work was carried out with the particular support from the Russian Foundation for Basic Research Grant No. 15-01-03649-a and 16-01-00623-a.*

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## GEOMETRICAL MODELS OF STRUCTURALLY INHOMOGENEOUS SOLIDS

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Structural inhomogeneity in materially uniform solids may be caused by a variety of physical and technological reasons. Layer by layer (LbL) film synthesizing, surface growth, remodeling, etc are among them. Structural inhomogeneity is closely related to laminar or fibrillar distribution of defects and specific spatial structure of deformation incompatibility. The latter results in unwanted features, particularly, in residual stresses and distortion of geometrical shape of desired structure. These factors are associated with critical parameters in modern high-precision technologies, particularly, in additive manufacturing, and considered to be thereby essential constituents in corresponding mathematical models.

In present communication the methods of geometrical mechanics and their application in modeling of stress-strain state in structurally inhomogeneous solids are developed.

It is known for simple materials that theory of affine connections gives an elegant mathematical formalization of the concept of a materially uniform (in particular, stress-free) non-Euclidean reference form. One can obtain affine connection on material manifold by defining parallel transport as the transformation of the tangent vector, in which its inverse image with respect to locally uniform embeddings does not change. This leads to Weitzenbock space (the space of absolute parallelism, or teleparallelism) and gives a clear interpretation of the material connection in terms of the local non-degenerate linear transformations which return an elementary volume of simple material into uniform state.

The methods in question are based on the representation of a body and physical space in terms of differentiable manifolds. These manifolds are endowed with specific Riemannian metrics and affine connections, which are non-Euclidian in general. Affine connection on the physical manifold is defined a priori by considerations which are independent from the properties of the solid, while the connection on material manifold is defined by intrinsic properties of the body.

Deformation, stress and power measures are formalized by smooth mappings defined on smooth manifolds which represent the body and physical space or vector bundles over them. Tangent map, which locally represents embedding of body into physical space, plays role of deformation gradient. The measures of local deformation are introduced as pull-back of spatial metrics which defines generalized right Cauchy-Green tensor and push-forward of the material metrics, which defines generalized left Cauchy-Green tensor. Forces are interpreted as covectors, i.e. as a linear functionals, which act on the velocity vectors of material points and results power. Accordingly, the stress fields are interpreted as covector-valued exterior two-forms and body forces as scalar-valued three-forms.

Tensor fields of different types are considered as elements of the uniformly graded structure over pair: the material manifold and the physical one. The abstract theory of integration based on exterior forms formalism can be adapted to the elements of this structure which allows one to formulate the power balance equation on the material manifold

(similarly to reference description in the classical mechanics of compatible deformation) and on the physical one (similarly to the spatial description). The balance equations in terms of Cartan's exterior covariant derivative can be obtained from the general principle of covariance.

## **FREE OSCILLATIONS OF DISCRETE MEMBRANE IN THE CONDITIONS OF ACOUSTIC VACUUM**

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We present the analytical and numerical results relating to nonlinear dynamics of the finite discrete membrane consisting of longitudinal and transversal strings vibrating in the conditions of acoustic vacuum. Such conditions are provided by absence of the preliminary strings stretching that leads to zeroth values of normal frequencies and sound velocity in linear approximation. We begin from the solution of the nonlinear normal modes (NNMs) problem. It is shown that, in spite of the presence of strong nonlinearities this problem admits exact solution in significant particular cases and accurate approximate solution in the general case. Using the modal representation of the basic equations adopted to the conditions of acoustic vacuum we introduce the complex variables which are complex combinations of the velocities and displacements (in the modal representation). Then, it is shown that the system under consideration admits a plenty of the intermodal resonances, and that its non-stationary resonance dynamics can be investigated with using the two-mode models. A closeness to resonance leads to existence of the slow time- scale in which all significant regularities of the non-stationary resonance dynamics have been revealed. This time- scale determines, in particular, a characteristic time of the energy exchange between the coherent domains of the membrane. This essentially non-stationary process is described in terms of the Limiting Phase Trajectories (LPTs). We have found the explicit expressions for the threshold parameter values which correspond to NNM instability and to transition (in the parametric space) from the full energy exchange between the coherent domains to energy localization.

## **ON NUMERICAL SOLUTION OF PROBLEMS FOR LAYERED MEDIA WITH HOLES, CRACKS AND INCLUSIONS**

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Problems for layered media arise in different fields of science. For example, accounting for the layered structure of rock is of special significance for modeling hydraulic fractures. The work aims to develop a numerical method to solve such problems.

The efficiency of the solution is provided by considering layers as a chain-like system [1, 2]. It is possible due to the fact that each layer has boundaries that are common with only its two neighbors. This serves to find Green function applying Fourier transform and sweep method to three very similar problems for layers without inhomogeneities. Finally, the problem reduces to the singular integral equation formulated only on boundaries of inhomogeneities.

Key features of the numerical solving problems for multi-layered media are investigated and formulated. It is shown numerically that high efficiency and reliability of the sweep method, combined with the advantages of complex variable boundary element method [3], allows solving such problems with high accuracy for any number of layers and inhomogeneities. The accuracy of the solution is checked by comparison with two classical benchmark solutions. Some test results for Laplace equation are presented in detail.

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## **HYPERBOLIC THERMOELASTICITY IN GAS MEDIUM UNDER LASER IMPACT**

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This paper presents numerical approach in solution of laser radiation on thin layer of gas medium. Aim of article is to

investigate coupled thermal and acoustic waves propagation accounting heat flux time relaxation and therefore damping and finite velocity of thermal wave due to hypertonicity in heat conduction's equations. Spatial description is used in order to describe continuum fields. Density, temperature, heat flux and velocity are evaluated through the system of balance equations: mass, energy and momentum balances are taken in integral form. High speed thermal impact is modeled by defining the distribution of heat sources in the volume for the semitransparent medium. The power of the laser pulse depends on time as the Dirac delta function or as the Heaviside function do. Number of problems with different speed of air is considered which leads to different boundary and initial conditions. For numerical calculation both explicit and implicit techniques' scheme are applied; in attempt to verificate method similar issue of laser interaction on solid continuum was chosen that have analytical solution to compare with.

## MICROSTRUCTURE EVOLUTION IN METALS AND METAL MELTS DURING DYNAMIC TENSILE FRACTURE

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Dynamic tensile fracture can be observed in solid or molten metal; it is referred as cavitations in the letter case. Tension wave with negative pressure can arise at a compression pulse reflection from a free surface or as a result of powerful ultrafast irradiation by electron or laser beam. Development of the dynamic fracture is connected with evolution of micro-voids interacting with other microstructure elements. Basing on the molecular dynamic simulations, we develop a macroscopic model describing the microstructure evolution during the dynamic tensile fracture of solid metals with accounting of other structural heterogeneities, such as initial voids, inclusions [1], dislocations and grain boundaries. The model allows one to predict the metal strength, the fracture progress and the characteristic sizes of the microstructure elements of the fractured metal. It includes the kinetic equations for formation, growth [2] and interaction of voids. The model is verified by means of comparison with the taken from literature experimental time profiles of the free rear surface velocity in the problems of the high-velocity plate impact. Also basing on the molecular dynamic simulations, we develop a macroscopic model of the dynamic tensile fracture of metal melts, both initially homogeneous [3] and with initial voids or inclusions [4]. Our investigations show that both solid and molten material reaches the tensile strength much earlier the complete fracture, which occurs as a fragmentation or a main crack formation. It is also remarkable that the work required for fragmentation exceeds several times the work on reaching the maximal tensile strength [5].

*The main part of this work was supported by the grant from the Russian Science Foundation (Project No. 14-11-00538); investigations for magnesium was supported by the grant from the President of the Russian Federation (Project No. MD-7481.2016.1).*

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## DYNAMICS AND BUCKLING ANALYSIS OF A THIN VISCOUS SHEET

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Understanding of viscous sheet's dynamics is essential in many manufacturing processes (for example, glass and polymer production) as well as in describing natural phenomena (e.g. global plate tectonics, cell membrane, and others). In contrast to elasticity theory, where different thin plate models have been studied for a long time, viscous sheets are undeservedly less examined. One of the main difficulty is non-linearity of Navier-Stokes equations for a viscous sheet with free boundaries.

The present work deals with dynamics of a thin nearly planar viscous incompressible sheet submitted for body forces (e.g. gravity) and surface forces (surface tension or external pressure). The theory starts from scaling analysis of the

general Navier-Stokes equations. Then a small parameter, height to length ratio, is introduced and used for asymptotic expansion. Existence of asymptotic solution requires satisfaction of compatibility conditions, which physically imply media continuity, in-plane stress balance, and bending moment balance. With the derived simplified constitutive relationships, one comes up with a non-linear reduced system which describes dynamics of a viscous sheet. Although the focus is on low Reynolds flows, the presented method resolves inertial effects, which may be essential in some applications. In particular, they allow damped oscillation of a sheet. Besides the dynamics, the approach may be used for buckling analysis of a viscous sheet. It is done via linear stability analysis of a plane sheet. This analysis helps to find buckling shape and growth rate.

The obtained governing equations can be solved with FEM for various sheet's geometry.

## **SIZE INFLUENCE ON THE TENSILE RESPONSE OF SINGLE-CRYSTAL NANO-SIZED COPPER BEAMS**

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It is well-known and experimentally confirmed that the mechanical response to loading of small enough structures differs from what applies to the macro-scale. This is valid for structures of linear measures at the nano-scale, typically below about 50nm. At this scale the number of surface atoms constitutes a non-negligible part of the total number of atoms in the structure, and due to the lack of some neighboring atoms these surface atoms are left in an energy state differing from that of bulk atoms. This will affect the load carrying capacity distribution between the atoms and thus the mechanical response to loading, both as regards elastic and plastic properties.

In addition to pure size effects also the crystallographic orientation becomes important at this scale. As regards elastic properties the orientation i.e. determines if the Young's modulus increases or decreases with decreasing size. Since the crystallographic orientation introduces anisotropy in the structure, also the Poisson's ratio is affected. As regards plasticity, which is built from dislocation formation and slip along closed-packed planes, the crystallographic orientation determines the slip pattern.

This study demonstrates the mechanical response to displacement controlled tensile loading of solid nano-sized fcc single-crystal Cu beams of square shaped cross sections. The investigation was performed through 3D molecular dynamic simulations using the free-ware LAMMPS. Two different crystal orientations and different loading rates were considered. Deformations and stress-strain curves were obtained and the necking behavior was studied in detail. The elastic behavior showed to be non-linear and in some case substantial hardening was observed. Further multiple necking, leading to rupture of the beam at two different positions, was observed.

## **EFFICIENCY OF IONOCRAFTS: EXPERIMENTAL INVESTIGATION**

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Ionocraft is a flight facility which lifting force is created by means of ionic wind. Ionic wind is air flow caused by corona discharge. The flux of momentum which is whirled away by ionic wind jet may be used for propulsion. A significant difference from ion thrusters – perspective spacecraft engines – is that working ionocraft does not lose ions. In ionocraft charged particles are generated in the corona sheath due to impact ionization and afterwards are absorbed on electrodes. Propulsion issues due to momentum of neutral air jet passing out of the electrodes pair. Ionocraft conception is known for decades but efficiency of the prototype models is still low. The main efficiency parameter for ionocraft is the relation of consumed electric energy and lifting force (“Thrust specific energy consumption” - as an analogy to “Thrust specific fuel consumption” which is a commonly used term in aviation). It is necessary to reach a certain level of thrust specific energy consumption for practical applications.

The experimental part of the work consists in direct measurement of lifting force of an ionocraft segment by the weight sensor based on the strain transducer. A classical construction of ionocraft segment – wire-cylinder – is considered. The ionocraft segment is hanged in such a way that its thrust is directed in the upper direction. So the thrust value supplements the ionocraft's weight and this summarized value is measured by the weight sensor which ionocraft is fastened to. Voltage and discharge current are measured as well.

Dependence of thrust specific energy consumption on base geometric parameters is presented. Presumable ways of efficiency improvement are discussed. Formally thrust specific energy consumption of ionocraft may be rather low especially for large interelectrode gaps. However it usually leads to large air volume occupied by construction with significant total lifting force. Consequently more sophisticated criteria should be used such as: thrust specific energy consumption level by fixed lifting force from unity volume. An alternative way of ionocraft efficiency improvement: variation of active electrode form for lowering corona threshold voltage. This way is also considered and discussed.

Possible characteristics of flight facilities are estimated and analyzed.

## **ON THE THEORY OF THE VIBRATION SYSTEMS WITH A HEREDITARY TYPE DRY FRICTION FORCES AND AN OSCILLATION LIMITER**

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The issue of modeling and studying dynamic systems, accounting for dry friction forces, is still vital due to considerable problems with adequately mathematically describing processes in realistic objects. This is reflected in the early works by academicians A.Yu.Ishlinskiy and I.V.Kragelskiy on jumps in the conditions of friction, by professor N.V.Butenin on the hypothesis of "jump" and some others, whose results are currently being actively developed and used.

The present paper analyzes the dynamics of a vibration system, accounting for hereditary type dry friction forces and an oscillation limiter. The vibration system and the oscillation limiter interact either according to Newton hypothesis or accounting for the elasticity of the (limiter) wall.

A mathematical model (MM) of the system, accounting for hereditary type dry friction forces, has been developed, which is a strongly nonlinear non-autonomous system with a nonlinear structure. The dynamics of the MM is numerically and analytically studied, using the mathematical apparatus of the point mapping method. The specific approach of the study is that a point map is formulated not in the classical way (mapping a Poincare surface into itself), but using times of relative rest of the vibration system, which significantly simplifies the process of constructing a point map and of its detailed study. The presence of floating boundaries of the sliding motion plates in the phase space of the MM necessitated developing an original approach to constructing a point map and interpreting the results obtained. Using the developed investigation methodology and the software product, the structure of the phase space of the MM as a function of the characteristics of the forces of sliding friction and rest, as well as of the type and location of the limiter, has been analyzed.

Judging by the character of changes in the bifurcation diagrams, the main laws of the process of changes in the motion regime have been determined for the changing parameters of a vibration system (occurrence of periodic motion regimes of arbitrary complexity and possible transition to chaos via the process of doubling the Feyhenbaum period).

The results of the analysis in the presence and in the absence of an oscillation limiter have been compared.

The work has been done with financial support from the Russian Scientific Fund. Project № 16-19-10237.

## **AUGMENTED AND VIRTUAL REALITY IN MECHANICS. ABOUT THE PROFESSIONAL USAGE IN TEACHING AND SCIENCE COMMUNICATION**

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In industry 4.0, engineers are specialists for hardware and software. Mechanics, electronics and IT are no longer separate worlds. The specialist areas complement each other, influence each other and ultimately merge (cf. Löwer (2014)). Higher education should prepare future engineers to create this complex process and adjust demands for competences and learning outcomes. Not only wide basic and specific knowledge, but also methodological, digital and social competences, as well as the ability to develop cross-curricular thinking, self-organized and collaborative work and the visual and interactive presentation of work results are expected.

This contribution wants to explore the professional usage of augmented and virtual reality in the context of mechanical engineering education to counter the situation described above. As an example, it refers to the finite element method (FEM) as an universal tool for computational analyses of mechanical structures, that rises teachers and learners to a challenge equally. The question is how to combine basic theories and underlying models of these computational method with a competent application of the respective software to reach the learning target: to understand, use and evaluate analyses of mechanical stresses and deformations based on the FEM critically. Furthermore, increasing complexity and abstractness, missing 3-D-surroundings and contexts of visualizations are one of the biggest hurdles to use these computational analyses professionally.

In this framework, applications of virtual reality as simulations of real environments and augmented reality, which extend "the real world environment with a certain amount of synthetic information, ideally just enough to overcome the limitations of the real world for a specific application" (Kalkofen et al. (2014):65), can create inspiring visualizations to get a deeper understanding of computational analyses of mechanical structures. The contribution will introduce how you can implement FEM in augmented and virtual applications to enrich computational analyses and to provide

expertise in a discursive and interactive way. True to Murray Gell-Mann, Winner of Nobel Prize in Physics in 1929,: “We need to move from the sage on the stage to the guide on the side“ (quotation from Vest (2007: vi)).

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## DISLOCATION EMISSION FROM THE EDGE OF A PARALLELEPIPEDAL INCLUSION EMBEDDED IN A NANOLAYER

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Synthesis, study and application of heterogeneous planar nanostructures form one of the main directions in modern materials science and applied physics. Nowadays, much attention is paid to one-dimensional nanostructures, such as nanowires and nanobelts, embedded in two-dimensional substrates and nanolayers. The difference in the structure and properties of materials composing such nanostructures leads to the appearance of thermal and misfit strains and stresses in them. Under several conditions, these strains and stresses start to relax through generation of various defects which cause negative influence upon the properties of the nanostructures. Thus, the study of the relaxation mechanisms and the critical conditions of their activation is of primary importance for these nanostructures. At the moment, there is a number of works dealing with such problems [1-4]. In particular, theoretical models describing stress relaxation by formation of misfit dislocations at the boundaries of subsurface parallelepipedal [1, 2] and cylindrical [3] nanowires in semi-infinite solids, and a layer normally crossing a thin slab [4], were invented and analyzed in detail.

In the present work, we considered the stress relaxation at the edge of a long parallelepipedal inclusion embedded in a nanolayer. In doing so, we assumed that the relaxation occurs through emission of dipoles of edge partial (or perfect) dislocations gliding along the inclusion face normal to the free surfaces of the nanolayer. One of the dislocations glides from the inclusion edge to the free surface, while the other one glides to the middle of the inclusion face. Based on the earlier solutions of the boundary-value problems in the theory of elasticity for such an inclusion in a thin layer [5] and for an edge dislocation in a thin two-layer plate [6], we calculated the total energy change caused by the dislocation emission, and analyzed it in dependence on the distances passed by the dislocations. By analyzing this dependence, we studied the critical conditions for the activation of the dislocation emission and determined the equilibrium positions of the dislocations for different values of the system parameters. We showed that this mechanism of stress relaxation is rather effective and should be taken into account in development of relevant nanotechnologies.

*This work was supported by the Ministry for Education and Science (Russian Federation) (Grant No 3.3194.2017/PCh).*

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## STRESS FIELDS AND STRAIN ENERGY OF A CIRCULAR LOOP OF RADIAL DISCLINATION IN AN ELASTIC SPHERE

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Circular loops of linear defects – dislocations and disclinations – are of great importance for both fundamentals and applications of the theory of defects. To date, the most of researchers deals with the Volterra dislocations [1] and disclinations [2] which are characterized by constant Burgers vectors and Frank vectors, respectively. Nevertheless, there is also another kind of linear defects which are called the Somigliana dislocations [3] and strongly differ by their properties from the Volterra dislocations. A list of solved problems for the Somigliana dislocations is rather short [4-11], although there is a common opinion that their use could be very effective in theoretical description of interface problems. A good example in this respect is a circular loop of radial disclination (CLRD, also called ‘ring dislocation’ [5, 6, 9, 10]) which is also one of the types of the Somigliana dislocation loops. In works [4, 7, 8, 11], virtual surface CLRDs were used in solving of a number of boundary-value problems in the theory of elasticity.

In the present work, we solved the boundary-value problem in the theory of elasticity for a CLRD placed in an axially symmetric position in an elastic sphere. The solution was found by the Lurie method [12] in the form a sum of two terms, where the first term is the stress field of the CLRD in an infinite space [4, 7, 8], while the second one is an extra stress field, which provides the fulfillment of boundary conditions on the free surface of the sphere. The first term was expanded in series of Legendre polynomials using the formulas presented in [11]. Then, by using the general solution for the internal axially symmetric problem of the theory of elasticity in spherical coordinates [12], the coefficients of series representing the second term, were determined from the boundary conditions of the problem. As a result, the CLRD stress fields and strain energy were found in the form of series, analyzed numerically by means of stress and energy maps, and discussed in detail.

*This work was supported by the Ministry for Education and Science (Russian Federation) (Grant No 3.3194.2017/PCh).*

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## PREDICTING CURVATURE IN ASYMMETRICAL ROLLING: COMPARING PREDICTIVE MODELS

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Curvature of the workpiece during rolling processes has significant impact on the process design and workpiece quality. In flat-sheet rolling, unintentional asymmetries can cause turn-up/turn-down which can halt the process and damage the rolling table; in asymmetrical rolling, asymmetries are exploited to improve process efficiency and produce curved products; and in ring-rolling, a uniform curvature must be maintained to prevent the formation of elliptical rings and other instabilities. Due to this broad relevance, curvature studies were first published, at the latest, in 1956 and curvature continues to be the focus of current investigations.

The present work begins with a comprehensive review of conclusions from previously published numerical and experimental studies. We find that no trends identified in any individual study are universally applicable, and indeed many studies appear contradictory when naively compared. One example of this is the direction of curvature due to asymmetric roll surface speed, with some studies showing evidence of curvature towards the faster roll and others towards the slower roll depending on the roll gap aspect ratio.

To explain some of these contradictions and understand the full complexity of the curvature phenomenon, the results of at least eight experimental and ten numerical publications have been digitised and analysed as a larger, more complete data set. The results cover a range of geometries, aspect ratios from 0.07 to 0.57 and reductions from 10% to 55%; a range of asymmetries, friction differences up to 20%, roll size differences up to 80% and roll speed differences up to 80%; and materials, including steel, aluminium, lead and plasticine.

From these data, multiple statistical models are applied. These models provide reasonable prediction as well as suggest some key trends: cross-correlation between the asymmetries is only significant for roll size and roll surface speed; asymmetric roll size, surface speed and friction induced curvature are all influenced by both the roll gap aspect ratio and reduction to the extent of changing the direction of curvature; and, the magnitude of curvature is dependent on the ratio of the Young's modulus and the yield stress.

These results are important as they can provide evidence about the mechanism that causes curvature. For example, it has been proposed that curvature is a consequence of the formation of the cross-shear region within the roll gap. This is unlikely given the non-monotonic relationship between the roll surface speed ratio and curvature. Similarly, dependence on both elasticity and plasticity makes it unlikely that proposed rigid plastic models are able to fully capture this phenomenon.

Finally, a review is conducted of analytical models of curvature with at least three implemented to quantitatively compare with the previously collected data. None of the models match well across all three asymmetries. Many achieve a reasonable fit for asymmetric roll surface speeds but few are able to capture curvature for asymmetric roll sizes.

## **BEHAVIOR OF POLAR AND NONPOLAR LIQUIDS IN DIFFERENT CARBON NANOTUBES**

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Using molecular dynamics (MD) simulations, the static and dynamic properties of polar and nonpolar fluids in carbon nanotubes (CNTs) with different shapes of cross section and different structures of bounding walls have been investigated. It has been found that the fluid flows through CNTs with rectangular cross section is slower than those through CNTs with circular cross sections with the same area. It has been also found that fluid flows through CNTs with bounding walls having honeycomb – like graphen structure are faster than those through CNTs with amorphous bounding walls.

## **SYNTHESIS OF SILICON DIOXIDE NANOPARTICLES IN RF DISCHARGE SUSTAINED AT ATMOSPHERIC PRESSURE**

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Plasma enhanced chemical vapor deposition (PECVD) processes based on the use of electric discharges sustaining in various gases at atmospheric pressure have become of particular interest. Atmospheric pressure PECVD processes can be considered as more effective than low pressure PECVD in the case of synthesis of products *via* homogeneous chemical reactions due to higher reactants partial pressures and therefore increased probability of homogeneous interactions. This method doesn't require expansive vacuum pump systems for sustaining a discharge in the synthesis zone and evacuation of reaction products in comparison with the conventional approach based on low temperature plasma processes carried out at low pressures.

Nanoparticles are the most intriguing objects of nanotechnology world. Nanoparticles and nanopowders because of their unique properties have been widely used as components of composites, ceramics, catalysts, functional sensing materials and potentially can be utilized for biomedical applications.

The results of a comprehensive study of the synthesis of nano and microparticles of silica in a atmospheric pressure discharge have been presented. Nanoparticles were synthesized by APPECVD based on the use of RF (13.56 MHz) discharge sustained in helium, a helium-argon, and a helium-oxygen mixtures. Discharge power absorbed in the discharge was varied in the range 5 - 300 W. Tetraethoxysilane was chosen as a precursor. The products synthesized were collected on the substrate located on the refrigerated holder.

Correlation between the process parameters and the size of the synthesized particles, and the morphology of obtained

deposits were found out.

The plasma parameters were determined using the Langmuir probe, the specially designed probe and photoemission spectroscopy. Silica micro- and nanoparticles synthesized were examined by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS) and X-ray fluorescence (XRF).

It has been shown that the parameters of the plasma discharge (electron temperature, potential and concentration of plasma) determine the size of the synthesized particles and the nature of their agglomeration.

The theoretical models describing the formation of particles of a certain size and the formation of agglomerates of particles on the substrate surface have been developed on the basis of the experimental data.

Good correlation of the experimental results with the results of calculations in accordance with the theoretical models developed have been demonstrated.

## **A COMPREHENSIVE STUDY OF WATER TRANSPORT MECHANISMS THROUGH CARBON NANOTUBES**

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Carbon nanotubes (CNT) are one of the most widely used and ideal nanofluidic devices as they allow almost frictionless fluid flow through them. With an ever increasing field of applications, it becomes important to study novel mechanisms used to transport water molecules through carbon nanotubes and to compare the effectiveness and rate of flow provided by them. In this study, we consider three popular non-conventional mechanisms of pumping water through a CNT are, namely, thermally driven flows, rotation of chiral CNT and AC electric field driven flows, and characterize the flow observed.

Thermally driven flows:

Thermal fluctuations in water molecules depend on their temperature. When a passage is provided to the water molecules present in two reservoirs at different temperatures, the asymmetric thermal fluctuations causes the water to flow from one reservoir to another. The phenomenon that causes this flow of water from the hot reservoir to cold reservoir is abstract and forms one of the focus of the current work. In order to understand the phenomenon, a number of simulations are carried out by varying the temperatures of the two reservoirs over a wide range.

AC electric field:

When an electric field is applied to a CNT in the form of a traveling wave, it causes the water molecules to follow the gradients in the electric field due to their existence as dipoles. A traveling wave breaks the spatiotemporal symmetry of the water molecules and creates wave packets by periodically polarizing the water in the direction of the local electric field. The resultant of this localized effect is that the packets of water molecules orient in opposite directions and are forced to travel along with the particular wave packet. As the wave itself travels along the CNT, this causes the water molecules to be dragged along with the wave packets and be pumped out of the tube. The magnitude of electric field is varied so as to establish the trend of the flux of water molecules with the electric field.

Rotation of CNT:

In this mechanism, transport of water is achieved by rotating a chiral CNT. The structure of a chiral CNT is such that there exists an asymmetry in one direction. When a chiral CNT is rotated, this asymmetry of CNT produces an axial force on the water molecules which pushes them out of one end of the CNT. A number of case studies by varying magnitude as well as the direction of rotation are carried out in this work.

Finally, a comprehensive analysis, comparing the efficiencies of flux obtained by the above-mentioned mechanism is presented in this work.

## **STRESS FIELDS IN AN ELASTIC CYLINDER WITH A CYLINDRICAL INCLUSION OF FINITE LENGTH**

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Nowadays much attention is attracted to various composite nanowires which are considered as important elements for both structural and functional applications. Among others, the nanowires containing discrete inclusions (quantum dots)

are of special interest, in particular, for nanoelectronics, optoelectronics, photonics, plasmonics, etc. Functional characteristics of such composite nanostructures strongly depend on residual elastic strains caused by the atomic misfit of material components as well as on misfit defects providing the misfit strain relaxation. To study these effects, theoretical modeling of misfit strains and misfit defects seems to be rather useful. The first step in this modeling is the posing and solution of an appropriate boundary value elastic problem for a misfitting inclusion. The second step is the modeling of possible mechanisms of misfit strain relaxation. Recently, for example, such a problem has been solved for a cylindrical inclusion of finite length with axial eigenstrain in a long cylinder [1]. Further this solution has been used for modeling strain relaxation in pentagonal nanowires [2, 3]. However, the drawback of these models is the one-dimensional axial eigenstrain of inclusions, which naturally limit their applicability for real nanostructures. The main aim of the present work is to pose and solve similar problems in the case of radial eigenstrain and in the general case of axial-and-radial eigenstrain. First, we solve a boundary value problem in the theory of elasticity for a circular radial disclination loop (Somoglian dislocation) [4-6] coaxial with a long elastic cylinder. Then the dipole of such loops gives us a solution for a cylindrical inclusion of finite length with radial eigenstrain in the cylinder. Superposition of this solution with that found in [1] results in a solution for the inclusion problem in the general case of axial-and-radial eigenstrain. We discuss the peculiarities of stress fields with the help of corresponding stress maps and consider various possible mechanisms of stress relaxation in the composite nanowires.

*This work was supported by the Ministry for Education and Science (Russian Federation) (Grant No 3.3194.2017/PCh).*

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## AC ELECTROKINETICS: THEORY AND APPLICATIONS

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AC electrokinetics is the study of the behaviour of particles in AC electric fields. Dielectrophoresis refers to the movement of polarisable particles in non-uniform electric fields and has been widely used both to characterise particles and as a particle manipulation and separation tool. Electroporation describes the rotation of a particle in a rotating electric field and is used to characterise the dielectric properties of single particles. Complementing this approach is the new method of high speed single cell impedance characterisation where particles are measured at high speed in a flow. This talk will review methods used to characterise the dielectric properties of particles and highlight some recent advances in dielectrophoretic technologies for particle manipulation, with a focus on applications in biotechnology.

## NUMERICAL MODELLING TRANSFORMATION FRONT PROPAGATION BASED ON ISOGEOMETRIC ANALYSIS PROCEDURE

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Various experimental and theoretical observations of chemically and phase transforming materials (i.e. [1-4]) show the influence of mechanical stresses on the transformation front velocity. On the other hand, the strains induced by the transformations are the source of internal stresses and, thus, affect mechanical stresses distribution. This leads to a complex coupled problem. It is known that in the case of moving interface a configurational force driving the front is determined by the jump of the normal component of the Eshelby stress tensor. Recently it was shown that a configurational force driving the chemical reaction front is a normal component of a chemical affinity tensor (see, e.g. [3,4] and reference therein). In both cases a kinetic equation can be formulated in a form of the dependence of the transformation front velocity on the configurational force. Then the stresses affect the front velocity through the chemical affinity tensor.

In numerical simulation the front propagation is realized as a front movement in the normal direction proportional to the front velocity [4]. Various approaches can be used for the realization of numerical simulation. In a present work we investigate efficiency of the numerical approach based on isogeometric method [5]. Above-mentioned method has advantages for solving problems of this type, comparing with finite elements method. Firstly, we achieve much higher accuracy with less computational time. Secondly, we always know the exact equation of the boundary, and as a result – an exact orientation of the surface element. Note that high accuracy is required for the normal component of the affinity tensor calculation, especially in case of complex geometries.

We apply the proposed procedure for solving a number of boundary value problems for elastic solids undergoing phase and chemical transformations. We describe propagating transformation front basing on the isogeometric analysis with the use of ABAQUS [6] and Nitsche method [7] implementation. Computational results are compared with analytical solutions and reference solutions obtained by finite element analysis.

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### **STRUCTURAL-MECHANICAL MODEL OF FILLED RUBBER: INFLUENCE OF INTERPHASE LAYERS**

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The new structural-mechanical model of filled rubber is presented. The model takes into account the filler microstructure (including the presence in the material cracks and defects) and interphase interactions. The filled rubber is modeled as the volume non-uniformly filled with rigid inclusions which are connected by damageable hyperelastic links. The hypothesis that the polymer molecules absorb on filler inclusions in matrix and form interphase layer with special properties is studied. Three cases of this interphase layer with different non-linear distribution of the polymer stiffness are modeled and studied: a) the uniform stiffness throughout the matrix (i.e. absence of special layer); b) the polymer stiffness at the boundary with the inclusion = 10 MPa, and in c) = 100 MPa, and then proceeds to the matrix by a nonlinear law.

The modeled structures with random or clustered filler distribution are subjected to fivefold uniaxial tension. The most physically adequate description of the behavior of the real filled rubber gives the case where the properties of the layer are relatively slightly differ from the matrix (elastic modulus of polymer near the surface of inclusion is 10-times higher than the matrix). Namely, the model without special layers gives poor reinforcement effect and small hysteresis loss; in the model with the hard layers (case c) the material in the gaps between filler inclusions start to break even at small extensions of the "sample" that does not give pronounced stress-amplification effect of the composite at high strains. *The work is supported by RFBR-Grant 15-08-0388116.*

### **MICROPOLAR MEDIA WITH STRUCTURAL TRANSFORMATIONS – THEORY AND EXAMPLE PROBLEMS**

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Generalized continuum theories have recently gained high attention. The idea is to capture the behavior of high performance materials with an inner structure. Applications range from the small to the large and involve solids as well as liquids. For example, micropolar theory emphasizes the aspect of inner rotational degrees of freedom of a material. It seems particularly suited for applications to soils, polycrystalline and composite matter, granular and powder-like

materials, and even to porous media and foams.

Continuum mechanics of solids is typically formulated in Lagrangian manner, where the concept of an indestructible “material particle” prevails. This requires neighboring material particles to remain “close” to each other during motion. Traditionally this idea is also used in micropolar theory: Each material point is equivalent to a rigid body, such that its microinertia does not change. Consider now a granular medium during milling. This affects the material particle, because its subunits will be crushed and mass and moment of inertia will change. Consequently, on a macroscopic scale the moments of inertia will change as well. It is for that reason that one should depart from the Lagrangian way and turn to the Eulerian perspective. Originally the Eulerian description stems from fluids. It does not impose strict constraints on the motion of mass-conserved material points. Rather it embraces the idea of an open system, allowing for exchange of mass, momentum, energy, moment of inertia between Eulerian cells. Moreover, recently a kinetic equation for microinertia (the field of the local inertia tensor) was proposed, which in contrast to former theories contains a production term. For a better understanding of this new concept an underlying mesoscopic theory was developed. The idea is to connect information on a mesoscale by taking the intrinsic microstructure within a spatial grid cell into account with the continuum balances of micropolar continua in combination with suitable constitutive equations.

In this presentation we will, first, present foundations and the underlying mesoscopic interpretation. In particular, we will motivate and explain the advent of the kinetic equation for the development of the field for the moment of inertia. Second, various example problems will be examined in order to show how to use the new approach: (a) A mix of pressurized hollow spherical particles initially homogeneously distributed in an isothermal atmosphere, subjected to a barometric pressure distribution, falling down and thereby transporting a flux into new observational points; (b) Fragmentation of spherical particles in a crusher; (c) Change of the state of rotation of a homogeneous mix of pressurized hollow spherical particles undergoing a nonuniform change of external temperature affecting their moment of inertia. Note that within the classical framework of micropolar theory a change of temperature would not influence rotation. Within the to-be-presented theory, however, changes in temperature will influence the inertia tensor and hence couple to rotational speed.

The presentation will end with an outlook of how the developed model can be used for complex engineering applications, which will require a fully numerical investigation. The problems studied in this talk may provide a first orientation.

## **THE DYNAMICS OF A ELLIPSOID WITH DISPLACED MASS CENTRE ON A HORIZONTAL PLANE**

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The problem of the dynamics of an ellipsoid of rotation with a displaced mass centre on horizontal supporting plane with friction is considered. It is assumed that the mass centre of the ellipsoid lies on its symmetry axis and it is the axis of dynamic symmetry of the ellipsoid.

It is proved, that the ellipsoid can make such motions: rotations around of the vertical principal centroidal axes of inertia of ellipsoid and the regular precessions. The conditions for the stability of these motions on the plane with viscous friction are considered. Approximate equations describing the dynamics of transitional processes are constructed. The corresponding numerical experiments are conducted. Multicomponent friction case and corresponding transitional processes also considered.

*This work is supported by Russian Foundation for Basic Research (project 16-01-00338).*

## **THE THERMAL ECHO EFFECT IN ONE-DIMENSIONAL CRYSTALS**

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Analytical and experimental studies show that in the ultrapure materials, anomalous thermal processes are realized, which are of scientific and practical interest. Such nonequilibrium processes can be caused by the passage of shock waves or by the action of ultrashort laser pulses. It is relevant to study similar processes in systems containing a finite number of particles, especially due to the active development of nanotechnology.

High-frequency oscillations of the kinetic temperature in molecular systems are known from the results of numerical simulation a long time. Until recently this phenomenon did not have a theoretical explanation. The use of correlation analysis made it possible to obtain an analytical description of nonequilibrium thermal processes in harmonic crystals. Earlier it was shown that in the case of instantaneous heating of a one-dimensional harmonic crystal, damped oscillations of the kinetic temperature are realized. This oscillations described by the Bessel function with an index

equal to zero. In contrast to previous papers, in which the main attention is focused on infinite crystals, in the present work thermal processes in a finite crystal are studied.

In this paper, we consider the instantaneous spatially uniform thermal perturbation of a finite one-dimensional harmonic crystal with periodic boundary conditions. An analytic solution describing the nonstationary process in a crystal is constructed. In the work, we show that for a finite crystal after reaching a certain time, an abrupt increase of the amplitude of oscillations of the kinetic temperature (thermal echo) is realized. We can give the following explanation for this phenomenon. With instantaneous thermal action, elastic waves propagate to the right and left of each crystal particle. In a finite crystal these waves are encountered and, due to the linearity of the system, they are added together. Since the crystal is originally in a spatially homogeneous state, the waves from each particle meet simultaneously in the entire crystal. So a sharp increase of the temperature of the system—the thermal echo—are causing. Each thermal echo is expressed of Bessel functions.

The abrupt increase in amplitude subsequently occurs periodically, with a period that depends on the crystal size, and each subsequent echo is weaker than the previous one. It is analytically obtained that the change in the kinetic temperature is described by an infinite sum of Bessel functions with multiple indices, and the thermal echo in the thermodynamic limit is described by the Airy function.

## **ROLE OF POWDER MATERIAL PROPERTIES ON THE PERFORMANCE OF PHARMACEUTICAL CONTINUOUS MANUFACTURING SYSTEMS**

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After 50 years of stagnation, pharmaceutical manufacturing is experiencing unprecedented innovation. In the last five years, the pharmaceutical industry has embraced a world-wide transformation from traditional, inefficient batch methods, to Continuous Manufacturing, which is an emerging technology that has been shown to greatly reduce both the time and the cost of developing and manufacturing new medicines, while enabling significant improvements in quality and reliability. However, this comes with a price - the level of scientific understanding required to design, implement, and operate continuous systems efficiently is significantly steeper than what was required in the past.

A critical issue is the role of material properties. Powder flow properties, density, stickiness, and wettability, all affect the performance of the process and the quality of the finished product.

The effects of properties, which vary due to both inconsistency in raw materials and to the effects of the process itself, must be understood and controlled in order to ensure efficient operation.

In this talk, I will describe methods for predicting the performance of process components and the system as a whole based on material property and process parameter measurements. I will then describe in some detail which properties are critical to the performance of the process and the current limitations in measuring them in real time.

## **BIOMECHANICS OF BONES IN A GLOBAL PICTURE**

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The bony skeleton is the load carrying structure of animals and humans. Since Wolff 1892 it is known that bones develop continuously to adapt themselves to the mechanical demand, thus it is characterized as a biomechanical system. The behavior of bone adaption and remodeling got more and more scientific interest since aseptic loosening of bone-implants has been related to bone remodeling. Early finite element simulations based on rather simple remodeling theories have already shown a good agreement with clinical observations.

Nowadays, bone adaption and remodeling is under research at three distinct length scales, i.e. at organ level, at tissue level and cellular level, however, a bridge between these scales is missing so far, c.p. Webster & Müller 2011. Another issue is on patient specific predictions for clinical usage. Here the total modeling chain has to be developed, starting with patient's clinical image data. Open questions for sure are on the individual load history and the patients past surgical activity etc. In addition, to guide the medical doctor a certain probability of the success of a specific treatment for that individual should be provided rather than computing density fields.

This presentation aims to summarize the state of the art of biomechanics of bones and to provide a roadmap for future research directions with a special focus on clinical usability of the computational mechanics approaches. The need for sophisticated modeling techniques and the incorporation into a probabilistic computational mechanics framework will be highlighted.

## DETERMINATION OF DEFORMATION AND FILTRATION PROPERTIES OF COAL BASED ON COEFFICIENT INVERSE PROBLEM SOLUTION USING ADSORPTION TEST DATA

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Designing of optimal borehole pattern and processing sequence for preliminary coalbed degassing in order to reduce sudden outburst hazard, methane content estimation by *in situ* measurements, determination of sorption capacity for injection of industrial waste gases in natural seams for gas disposition and environmental situation improvement — this is short list of problems solvable using the data for coal physical properties.

Within the framework of transversally isotropic poroelastic model [1] we developed the procedure for estimation of strain properties (radial  $E_r$  and axial  $E_z$  Young moduli) as well as permeability  $K$  of coal matrix based on inverse problem solution using lab data on carbon dioxide adsorption by coal core subjected to constant triaxial compression [2]: radial  $e_r(t)$  and axial  $e_z(t)$  strains of specimen ( $t$  is time).

The two dimensional geomechanical model of the aforementioned laboratory experiment with cylindrical specimens and the numerical-analytical method to solve the related boundary problem based on space coordinate-wise averaging of equations of poroelasticity have been developed. Numerical experiments established that:

- the rate of increase in  $e_r$  and  $e_z$  is governed by the value of  $K$ ;
- in the course of time,  $e_r$  and  $e_z$  reach permeability-independent steady-state values;
- $e_r$  and  $e_z$  are directly-proportional to the volume-average adsorption stress.

The coefficient inverse problem “determination of strain characteristics and permeability of coal matrix” was formulated and examined for solvability. The objective function  $F(E_r, E_z, K)$  was introduced — a relative root-mean-square deviation of theoretical and experimental strains. The minimum of  $F$  providing the inverse problem solution was found by modified conjugate gradient technique [3]. It turned out that Young moduli  $E_r=9.7$  GPa,  $E_z=8.35$  GPa (threefold as the values obtained in [2]) and permeability  $K=0.000017$  mD (by three orders less of corresponding value) describe just the coal substance inasmuch as the test cores had the pronounced jointing.

*The study has been partially supported by RFBR, Project No. 15-55-15046, under RFBR-CNRF Agreement (Projet International de Cooperation Scientifique PICS06582).*

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## MASS TRANSFER AND DEFORMATION OF POROUS-FRACTURED MEDIA

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Log data interpretation for the purpose of poroperm properties revelation and producing zone identification, optimized production planning, preliminary coalbed degassing to prevent sudden dynamic phenomena such as coal and gas outbursts — this far from complete list of problems which solution required the development and investigation of adequate models for mass transfer and deformation process description in fluid-saturated stratum treated as element of hierarchical block-structured rock mass [1]. Petroleum reservoirs in Bazhenov formation are the representative example of a porous-fracture medium. In situ identification of such structures in the well environment faces difficulties due to coarse resolution of acoustic well-logging measurement capable to “recognize” particles with linear dimension not less than centimeter [2]. Nevertheless, it is very difficult to implement the model of near-well zone, for example a few meters thick, composed of such elements in particular owing to uncertainty of joint physical properties and high

dimensionality of current task.

The double porosity model [3] represents a fracture porous rock mass as a continuum with the specific properties. This approach was used to develop the hydro-geomechanical model of two-phase fluid (water and oil) filtration and deformation in the near-well zone based on the concepts of representative equivalent volume [4]. We investigated axially symmetrical case “vertical well in horizontal porous fractured stratum” and proposed the original semi-analytical method when the set of filtration equations is solved by suitable mesh scheme combined with the matrix elimination method, while the rest system of poroelastoplasticity turns to be solvable by quadratures. The irreversible deformation domain size  $R$  at each time moment is determined from transcendent equation connecting fluid pressure, rock mass strength properties and horizontal component  $S$  of natural stress field. The numerical experiments have shown that, among other things, at depletion drive:  $R$  raises with an increase in  $S$  and Poisson ratio; water saturation of the blocks decreases with time due to lower viscosity of water as compared to that one of oil.

The developed model (being supplemented with Archy's formulas) is also destined for parametric support of geoelectric well log data interpretation to reveal pay zone and estimate reservoir permeability and porosity.

*The authors are grateful for the partial support provided by the Russian Foundation for Basic Researches (Project No. 16-05-00573).*

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### **SPECIFCS OF CHARGE ACCUMULATION ON AND TRANSPORT ALONG THE INTERFACE BETWEEN A LOW-CONDUCTING LIQUID AND A SOLID PERFECT INSULATOR**

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Today, solid insulation becomes an essential part of various electrohydrodynamic (EHD) systems with increasing frequency. It accumulates charge in thin layers near its surfaces, which screens the normal component of the applied electric field. Moreover, this charge remains mobile in the tangential field and thus can move. To design EHD systems that use solid insulation or to check applicability of the corresponding computer models, one should understand the above phenomena clearly.

In a simple system as «flat electrode – a layer of perfect solid insulator – a layer of low-conducting liquid – flat electrode» charge accumulation near the interface of the layers proceeds until the electric field in the liquid is fully screened by the charge. A level of low-voltage conductivity may only affect the time of charge accumulation. This often causes disregarding of the accumulation and transport processes in the computer models of EHD systems.

However, in case of more complicated geometry, for example, when a hole is made in the layer of solid insulation, depending on the problem parameters, screening of the electric field in the liquid may significantly decrease even far from the hole (at much longer distance than the thickness of the layer of solid insulation and the hole size).

Thus, the present work uses computer simulation to characterize the processes of charge accumulation and transport in the systems mentioned above and, consequently, checks the applicability of assumptions that are frequently made in computer models of EHD systems.

### **DYNAMIC FINITE ELEMENT ANALYSIS OF PEDESTRIAN BRIDGES**

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High strength of modern building materials allows to build pedestrian bridges with increased flexibility, lightness, and span length. This leads to smaller natural frequencies that may be close to the walking and running frequencies of pedestrians crossing the bridge. As a consequence, excessive vibrations caused by resonance with dynamic loads may occur. For light bridges serviceability criteria for pedestrian induced vibrations can become the dominant design criterion. To avoid over dimensioning of the bridge, it is important to use accurate structural models and realistic dynamic load models. In this work, we present a computational dynamic analysis of a model bridge and compare different load and structural models.

## VARIATIONAL FORMULATIONS, MODEL COMPARISONS AND ISOGEOMETRIC ANALYSIS FOR EULER-BERNOULLI, TIMOSHENKO AND HIGHER-ORDER BEAM MODELS OF STRAIN GRADIENT ELASTICITY

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Boundary value problems of Euler-Bernoulli and Timoshenko beam bending models following the strain gradient elasticity theory [1] are studied for both isotropic [2,3,4] and anisotropic [4] material microstructures.

The problems are formulated within variational Sobolev space settings providing a basis for applying finite element and isogeometric methods for numerical approximations with rigorous error estimates. Numerical convergence analysis is accomplished by presenting a series of benchmark problems for statics and free vibrations.

The role of thickness and gradient parameters connected to size-effects are studied thoroughly for both isotropic and anisotropic cases. In particular, it is shown the standard strain gradient model of Timoshenko beams suffers from the so-called numerical locking effect which is cured by proposing two different locking-free formulations.

The variational formulation for isotropic Euler-Bernoulli beams is shown to be extendable to two other generalized beam models which follow a modification of the strain gradient elasticity theory and a modified couple stress theory. A model comparison with observations on the physicality of the models reveals that the beam models demonstrate essentially two different kinds of parameter-dependent stiffening behaviour. One of these kinds provides results in a very good agreement with the size-effects observed in experimental tests.

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## PSEUDO 3D HYDRAULIC FRACTURING MODEL WITH ACCOUNT FOR VERTICAL VISCOUS DISSIPATION

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A great number of hydraulic fracturing (HF) models exists which are differentiated with complexity and physical accuracy. Most straightforward 2D models (PKN, KGD, radial models) are reasonable while express analysis or first estimations fulfilling only as they are restricted with geometrical shapes significantly and consequently are not of interest in HF design treatment. At the same time, fully 3D models or planar 3D models are most accurate ones from physical point of view but cause great times costs in numerical simulation.

Pseudo 3D (P3D) models play a role of compromise between two previously examined cases. Key results of P3D model fracture growth in multi-layered lithology with focus on proppant transport mechanism and tip-screen out are examined in [1]. To reduce the consequences of assumptions various efforts to enhance P3D models are made [2-6]. In particular, pressure profile is assumed to be one-dimensional (along the fracture growth direction) within the P3D model. Consequently, the fluid flow in lateral direction is not examined, viscous dissipation is ignored in this direction and it turns into fracture height overestimating (toughness regime is observed only). To enhance the model authors in [5] account for viscous dissipation via so-called apparent fracture toughness that depends on propagation velocity on both lower and upper fracture tips. However, the case of symmetric three-layers lithology is investigated.

The purpose in the present project is to generalize the concept of apparent fracture toughness for multi-layered lithology with arbitrary properties. Numerical results present significant difference in fracture width profile between classic P3D model and enhanced one (about 10% of difference can be achieved). The enhancement is demonstrated in the frame of the problem of unwanted breakthrough layers that may lead to water or gas coning breakthrough.

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## EFFECT OF INTERACTION BETWEEN ION DRAG AND CONDUCTION ON ELECTROHYDRODYNAMIC PUMPING

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Electrohydrodynamics (EHD) flow is induced by Coulomb force acting on excess charges in a dielectric fluid and can be applied to pumping and heat transfer. Excess charges are generated by charge injection from an electrode and a non-equilibrium state of dissociation-recombination of dissociative molecules. An EHD pump that utilizes the former phenomenon is called the ion drag pump and the one that utilizes the latter phenomenon the conduction pump. However, the effects of the two charge generation phenomena on EHD pump characteristics have not been sufficiently understood. This paper investigates numerically the interaction of the two phenomena on EHD pump characteristics.

The governing equations are the continuity equation, the Navier–Stokes' equation including Coulomb's force, Gauss' law and the charge conservation equations. It is assumed that the injected charges do not affect the dissociation-recombination reaction. Therefore, three charge conservation equations are taken into account to treat injected charges, positive and negative charges generated by dissociation-recombination reaction. The model detail is presented in Ref. [1-3]. To obtain the parameter that represents field enhanced dissociation, electric field dependence of electric conductivity is measured in laboratory.

Two electrode configurations in two-dimensional flow channel of  $1 \times 8 \text{ mm}^2$  are simulated. First one is plate-bar electrode with a positive plate electrode in center and negative (grounded) bar electrodes mounted on channel walls, and the gap between the positive and negative electrodes is 0.2 mm. The second one consists of a 0.5 mm length and a 1.5 mm length plate electrodes embedded on a wall, and the gap between the electrodes is 0.5 mm. Inlet flow rate is imposed from zero to a maximum. Three scenarios are investigated, i.e., only ion drag pump action, only conduction pump action, and both ion drag and conduction pump actions. Working fluid is dibutyl sebacate ( $\text{C}_{18}\text{H}_{34}\text{O}_4$ ).

The positive and negative charges generated by the dissociation-recombination reaction are widely distributed around the negative and positive electrodes, respectively. The injected charge density distribution is significantly varied by the addition of the conduction pump effect. It is considered that the flow generated by the conduction pump effect varied the injected charge density distribution. The developed pressure increases relatively significantly compared to the case of ion drag pump action only and compared to the case of conduction pump action only. When the ion drag and conduction pump actions act simultaneously, the developed pressure is augmented and is higher than the sum of the pressures generated separately by the ion drag pump action and the conduction pump action. The pressure augmentation depends strongly on the electrode configuration.

This paper investigates numerically the interaction between the ion drag pump action and conduction pump action. When the ion drag and conduction pump actions act simultaneously, the developed pressure is augmented and is higher than the sum of the pressures generated separately by the ion drag pump action and the conduction pump action.

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## ON POWER TRANSMISSION OF DRIVE BELT AS ROD WITH SHEAR

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In the present work we consider the quasistatic problem of belt deformation and contact interaction with two equal pulleys with friction. The goal is to analyse the effect of belt deformation and elastic microslip on the transmission ratio in dependence on the applied load (the simpler model of elastic microslip is considered in [1]). The belt is modelled as elastic rod, initially having the form of a circle. We take into account bending, transverse shear and tension as well as friction between the belt and the pulleys in the geometrically nonlinear formulation.

The problem is solved in two stages. At the first stage we model the fitting the belt on the pulleys, determine the stress strain state of belt, and calculate the contact pressure [2,3]. The difficulties of the nonlinear contact problem are overcome by means of computer mathematics. We solve arising boundary value problems for the ordinary differential equations (ODE) systems by the shooting and finite difference methods.

At the second stage we consider the problem with the prescribed small pulley rotations and applied torques from the friction forces. Here we use the equations in variations [4] superimposed upon the stress state calculated at the first stage. We deduce and solve the linear ODE systems with the variable coefficients determined earlier. The state on the pulleys is described by the second-order ODEs, their solution allows finding the contact pressure and friction forces. For the free spans of belt we formulate and solve the sixth-order problems. Finally the boundary value problems for the sixteenth-order ODE systems is formulated and solved. As at the first stage, we use computer mathematics and interpolate the complex dependences – the coefficients of the linear equations – by the built-in functions.

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## RELATIVISTIC GRAVITY IN A NEWTONIAN CONTEXT

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Newton's law of gravity is a non-contact force of attraction between masses transmitted instantaneously across empty space. This is in direct contradiction to Einstein's theory of relativity which states that nothing, whether a particle, wave, means of communication, transmission of force or otherwise can travel faster than the speed of light. However, even Einstein's equations, that describe gravity as a warping of spacetime, reduce to Newton's equations for weak gravitational fields and speeds very much lower than the speed of light. It must be that Newton's equations are right, but their interpretation is wrong.

The simplicity of Newton's equations combined with their accuracy means that this is largely the science we teach to our school children and young university students. Many general physics books quickly state that "Einstein's theory of gravity is beyond the scope of this book" and make brief introductions to his special theory of relativity, which excludes gravity. Indeed, the mathematics that describes Einstein's theory of gravity is beyond the reach of the vast majority of the world population, and Newton's simple but misinterpreted "pull of gravity" persists in its place.

In this context, Galileo's "tower of Pisa" experiment as reinterpreted by Einstein unlocks this contradiction. Galileo was the first to state that we cannot detect the uniform straight line motion of a reference frame. It turns out that Einstein's "free falling lift", which links directly to Galileo's "Tower of Pisa" experiment, is another frame of reference whose motion cannot be detected. Together these two fundamental truths about motion establish the principle that all motion is relative, and absolute motion has no meaning. In this presentation, the author further uses these fundamental principles to derive a frame-invariant version of Newton's classical second law of motion. This redefines gravity as a free-fall motion and not a "pull" force. It also enables the recasting of Einstein's theory of relativity into a Newtonian context and provides a new and simplified means to teach gravity in a consistent manner, thus avoiding the contradiction outlined above. The presentation concludes that understanding gravity is tantamount to understanding the

very nature of motion itself. The author presents an initial outline of how we might present and teach this early stage physics and articulate it to the wider public in the future.

## **PROTEIN MECHANICS: FROM AMINO-ACID TO SWIMMING CELLS**

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Proteins are often referred to as the building blocks of life, playing critical roles in almost all activities and structures in life. At the smallest, atomic length scale, proteins are made out of amino acids. There are 20 different amino acids, each with their own atomic structure, chemical composition and physical properties. The amino acids form long polypeptide chains consisting of hundreds and sometimes thousands of amino acids. Depending on the specific amino-acid sequence the polypeptide chains fold into regular structures, such as alpha-helices and beta-sheets (secondary structure). At a larger spatial level of organization, the alpha-helices and beta-sheets will fold into three-dimensional (tertiary) structures, i.e., the actual protein molecule. Finally, protein molecules can combine to form large protein complexes (quaternary structures). In this presentation I will take you on a journey through protein state space, addressing three different biological functions, each with their own time- and length scale: (i) the beating of cilia and flagella, hair-like structures that propel living cells, (ii) the strain-stiffening of cross-linked cytoskeletal networks that form the mechanical constitution of our cells, and (iii) transport through nanopores in the membrane of the cell nucleus.

## **ON THE MULTI-FLUID APPROACH TO MULTIPHASE FLOW MODELING IN HYDRAULIC FRACTURING APPLICATIONS**

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The technology of hydraulic fracturing of a hydrocarbon bearing underground formation is based on injecting a fluid laden with rigid particles under a high pressure (up to several hundred bar) into the well to create fractures in the porous medium, which are filled with particles. After the end of pumping, fractures closed on packed granular material provide high-conductivity channels to transport hydrocarbons from reservoir to the well and all the way up to the surface. The well may be vertical (when a single bi-wing fracture is formed) or near-horizontal with several perforation clusters providing reservoir contact (the so-called multi-stage fracturing in low-permeability formations). The latter case gives rise to several transversal fractures.

With respect to different stages of the hydraulic fracturing technology, we consider four classes of multiphase flows that can be modelled within the multi-continua (or multi-fluid) approach [1]. In a more detail, we distinguish the following classes: (i) the flow of suspension of fluid with particles in a circular pipe at high Reynolds numbers during pumping, (ii) the flow of suspension in a narrow vertical hydraulic fracture at moderate  $Re$  during pumping [2], (iii) suspension filtration through a packed of proppant particles in a closed fracture during cleanup [3], and (iv) multiphase gas-liquid flow with admixture of rigid particles in a circular pipe during well start-up, cleanup and testing in a wide range of the Reynolds numbers [4]. We discuss the advantages and limitations of the multi-fluid approach based on the simulation examples from each of the four classes of multiphase flows, in comparison with simplified semi-empirical approaches, e.g. drift-flux model for well flows, the effective-fluid model for suspension transport in fractures, and the deep-bed filtration model. The talk ends up with recommendations for future research on the topic.

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## ON IDENTIFYING ELASTICITY CLASSES OF POLYCRYSTALLINE MATERIALS

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An approach to solve the problem of elastic symmetry identification for a generally anisotropic Hookean solid is considered. A formal concept of four-rank tensor class is introduced to provide various elasticity tensor classifications including the symmetry classification. Given all components of an elasticity tensor with respect to an arbitrary basis, it is possible to approximate this tensor by a tensor from a certain class. According to the considering approach, the tensor in question may be refers to this class if there is such approximation that its residual in the Hooke's law is sufficiently small [1]. To find the best-fitting approximation, an upper estimation of the residual is to be minimized. A set of the optimal approximations for each class of interest is then used to form a hierarchy of classes to which the tensor in question belongs with the corresponding error.

Stated framework is applied to research elastic symmetry of single-phased polycrystalline materials. A numerical criteria to estimate a representative volume of such material based on isotropic incompatibility of its elastic properties in the case of uniformly distributed crystallites' orientations is proposed. With the help of the two-level crystal elasto-visco-plasticity constitutive model [2] an analysis of elastic symmetry evolution for polycrystalline copper's representative volume under inelastic loading is performed. It is found that under quasi-axial upsetting non-uniform crystallographic textures resulting in macroscopic elastic isotropy are possible to appear within the process.

*This work is supported by the Russian Federation Ministry of Education and Science (basic part of the state task PNRPU, No. 1208) and the Russian Foundation for Basic Research (grant No. 15-08-06866-a).*

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## ON SIMULATION OF THE ELASTIC BEHAVIOR OF SINGLE-LAYER MOLYBDENUM DISULFIDE

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This work is devoted to the application of both Stillinger-Weber potential [1] and the pair torque interaction potential [2] for the simulation of the elastic behavior of a promising two-dimensional material: single-layer molybdenum disulfide (SLMoS<sub>2</sub>). It is well-known that pair force potentials are hardly applicable to complex lattices, i.e. lattices having more than one atom in the unit cell. Due to the additional terms which stabilize a lattice, torque potentials also allow us to successfully describe the mechanics of complex lattices such as graphene, diamond etc. However, in contrast to the other potentials usually used in MD, e.g. REBO, EAM, SW, torque interactions have a relatively simple form and their parameters possess clear physical meaning.

A mathematical model of SLMoS<sub>2</sub> is constructed using the method of molecular mechanics. The boundary effects in the plane of isotropy are eliminated by the introduction of periodic boundary conditions, whereas the upper and lower boundaries are free. Due to the nearest neighbor interaction assumption, the equilibrium state is stress-free. Hence, in order to determine the components of the stiffness tensor, a set of problems in which the material is subject to a homogeneous strain field with one non-zero component is solved. Note, that the lattice of SLMoS<sub>2</sub> is complex, thus, it is also necessary to calculate the infinitesimal sublattice shift for each deformation so as to maintain the equilibrium. It is demonstrated that the disregard of the sublattice shift results in up to 20% error in the in-plane elastic moduli, whereas the out-of-plane moduli are not influenced.

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## **THE STRUCTURE OF THE INTERELECTRODE LAYERS IN POLARIZED LIQUID FLOWS IN MICROCHANNELS WITH THE ION SOURCE AFFECTED BY THE APPLIED FIELD**

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The interest in electrohydrodynamics of flows in micro- and nano-size channels, which is observed in recent years in the literature, is caused by the need to manage the motion of ultrasmall portions of fluids in various devices employed in biological research, biotechnology, pharmacy, medicine, and other areas of science. This work is focused on the study of the influence of strong non-uniform electric fields on the ionization processes in partially ionized liquid mixtures as they flow through plane microchannels. The effects caused by the action of a non-uniform field on the bulk electrochemical kinetics in highly polarized liquids at moderate values of the Debye number are analyzed. In weakly conducting chemically reacting environments the applied electric field can affect the ionization process both indirectly, through redistribution of reactive charged components, and directly, by means of increasing the kinetic rate of ionization. In the last case, in the near-wall layers with a strong non-uniformity of the field, bipolar structures of uncompensated space charge are formed, which can be affected by the applied longitudinal field. The presence of the layers with the opposite Coulomb forces brings about inflection points in the velocity profile. This may cause instability of the flow and thereby induce the mixing of the liquid in the microchannel. This work was supported by RFBR, project № 16-01-00157.

## **THE NON-ISOTHERMAL MATHEMATICAL MODEL OF ION IMPLANTATION PROCESS WITH ACCOUNT OF INTERNAL BOUNDARY**

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Each stage of technological and technical development is directly connected with the improvement of operational properties of materials. Vacuum ion-plasma methods are widely used for enhancing material properties and also for modifying the surface layer composition [1]. But the achievement of extensive experimental results requires detailed theoretical studies in this area.

The treatment of a metal surface by ion beam is accompanied by a variety of physical and chemical phenomena [2]. It is known that the particle impact on the target surface leads to the appearance of stresses. The implanted impurities can meet internal surface separating several areas with different structure or orientation. Also it may be the border separating coating from substrate material. That is why the propagation velocity of mechanical waves in transition across the border is changed. As a result, the concentration wave velocity is changed too. In [3], the interaction of impurity diffusion and deformation was studied. However, the mathematical model in this work does not take into account the change of the substrate temperature during processing.

The paper is aimed at investigating the initial stage of ion implantation process into target with coating. The model allows considering the processes occurring after interaction of ions flux with target surface. Assume that ions have sufficient energy for generation mechanical perturbations.

*The work was supported by RFBR, grant No. 16-01-00603.*

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## **NONLINEAR WAVES IN MICROSTRUCTURED MEDIA**

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Creation of advanced structural materials with unusual properties is a very urgent scientific problem of the XXI century. Prediction of the characteristics of these materials and behavior of products from them necessitates elaboration of structural models, which, in contrast to phenomenological models, enables one to establish the interrelation between the macroparameters of a medium and parameters of its microstructure.

A two-dimensional model of a monolayer granular medium (composite material), which represents a square lattice consisting of rigid spherical particles, is discussed in this work. Each particle of this lattice has six degrees of freedom: three translational and three rotational ones. The space between the particles is a zero-mass elastic medium through which force and moment interactions are translated that are modeled by elastic springs.

The nonlinear differential equations describing propagation and interaction of waves of different types in this medium have been derived. Dependence of the coefficients of these equations on the microstructure parameters has been found in the analytical form. It is shown that in the limiting case, when the planar particles vibrate only in one plane, the obtained dynamical equations degenerate into the previously derived equations for the dynamics of a square lattice consisting of round particles, which, in its turn, coincide with the equations of the two-dimensional Cosserat continuum consisting of centrally symmetric particles.

For the case of a chain of round particles with account of cubic nonlinearity in the governing equations, numerical investigations of counter and passing interactions of strongly nonlinear soliton-like subsonic and supersonic waves have been performed. In particular, effects of splitting of supersonic solitary waves are demonstrated.

*The research was carried out under the financial support of the Russian Foundation for Basic Research (projects NN 15-08-01836-a, 16-08-00971-a, and 16-08-00776-a).*

## **STRESS-LIFE CRITERIA FOR FATIGUE ASSESSMENT OF STRUCTURES: ADVANTAGES AND DRAWBACKS**

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Presently in rules for fatigue assessment of steel, and in particular, welded structures in different technologies subjected to intensive alternating service loading the Stress-Life (S-N) criteria are recommended in several versions of approaches. These are the Nominal stress approach based on typifying welded joints and representing fatigue resistance of the joints by classed S-N curves; the Hot-spot stress approach focused on evaluation of «structural» stress by the means of finite-element analysis (FEA) and the Notch-stress approach based on the FEA-based assessment of the local stress caused by the geometry of structural detail and the weld shape. The criteria and approaches provide assessment of fatigue properties of structures, however, accompanied with a series of approximations and uncertainties. The nature of drawbacks of the S-N criteria and approaches is commented and feasible means of improvement the fatigue criteria evaluation and applications in fatigue assessment procedures are proposed.

## **PROPERTIES OF TURBULENCE DRIVEN BY RANDOM EXTERNAL FORCE IN THE MODIFIED KLB MODEL**

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Two models for quasi 2D turbulence with global reaction are used: 1. model of decaying turbulence[1]; 2. model of forced turbulence[2]. The paper presents the results of the second model with random external force (REF) assuming that REF is a) small-scale, b)short correlated in time and c)statistically homogeneous in space[3-6]. New element introduced in the paper is REF that allows obtaining solution corresponding to statistically stationary turbulence with global reaction. The model of inverse cascade with the large-scale dissipation mechanism (modification of KLB model [7]) is used. The properties of turbulence driven by random external force in the modified KLB model with global reaction are investigated. It is assumed that turbulence is weak as compared to the mean flow and the Navier-Stokes equation is linearized.

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## CARBON DIOXIDE SPLITTING USING NANOSECOND PULSED CORONA DISCHARGE

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Carbon dioxide is usually seen as an unwanted product, due to its implications on the global temperature rise of Earth. However, new emerging technologies envision CO<sub>2</sub> emissions from waste gas streams as a feedstock for the synthesis of green chemicals. In this context, the reduction of CO<sub>2</sub> molecules using non-thermal plasmas can be particularly efficient, since the electron temperature can be very elevated. Additionally, cumulative vibrational excitations of CO<sub>2</sub> molecules can result in a highly energy efficient stepwise towards dissociation.

In this work, the decomposition of CO<sub>2</sub> using pulsed corona discharge is experimentally investigated. The production of molecular species (CO, O<sub>2</sub>, O<sub>3</sub> and C<sub>2</sub>O), radicals (O and C) and vibrational excited states of CO<sub>2</sub> was simulated using a combination of a 1D and a 0D model. The 1D model simulates the propagation of a single pulsed discharge, and their results are used in the 0D model to simulate the plasma chemistry of corona discharge over long times. Experiments were carried in pure CO<sub>2</sub> and its mixtures with argon at different gas flow rates, using a coaxial wire-to-cylinder corona discharge reactor 30 cm long. A tungsten wire, with radius 125 μm, was used as the corona electrodes, while the outer electrode was a stainless steel cylinder, with radius 17 mm. A high voltage pulse generator was used to energize the inner wire, and the discharge current was measured with the help of a wide band current transformer. The production of carbon monoxide resulting from the decomposition of carbon dioxide was analyzed by means of a Fourier transform infrared spectrometer ex situ.

The results of this investigation have shown that the structure of the high voltage waveform, which is constituted by a first nanosecond sub-pulse of high amplitude (~17 kV) followed by a series of smaller sub-pulses, has important implications on the kinetics of CO<sub>2</sub> dissociation. The best absolute conversion (~14%) was achieved in a gas mixture of 10% CO<sub>2</sub> – 90% Ar, although the best energy efficiency (~80%) was obtained when CO<sub>2</sub> and Ar were in the ratio 1:1.

## DISSOCIATION OF CARBON DIOXIDE USING PULSED DIELECTRIC BARRIER DISCHARGE

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The responsibility of carbon dioxide emissions on the global temperature rise of Earth has boosted the research in a variety of promising mitigations technologies. In that frame, the reprocessing of CO<sub>2</sub> using non-thermal plasmas has the advantage of producing valuable chemicals which can be of interest to the industry. Different plasma sources have been applied to this end, like microwave discharge, corona discharge and dielectric barrier discharge (DBD). Usually, dielectric barrier discharge is powered by AC voltage, operating at frequencies up to a few tens of kHz. A substantial part of the electrical energy is wasted in gas heating, thus limiting the energy efficiency and the production of valuable species, like ozone, which is rapidly decomposed at high temperatures. In contrast, nanosecond-pulsed dielectric barrier discharge injects high amounts of energy into the system in short pulses, thus avoiding gas overheating. In the present study, a high voltage nanosecond pulse generator has been used to power a planar DBD reactor, with both electrodes covered with a dielectric glass. The dissociation of CO<sub>2</sub> and the production of CO and O<sub>3</sub> at different gas flow rates have been measured by means of UV and IR spectrophotometry. Using a fast current transformer, the current intensity was measured in order to evaluate the electrical energy consumed in the reactor. Then, the energy efficiency of the CO<sub>2</sub> dissociation process has been evaluated. The results obtained have shown that the CO and O<sub>3</sub> productions using nanosecond-pulsed DBD are significantly higher than using conventional AC DBD under similar operating conditions.

## LOCAL AND NONLOCAL MODELING OF SQUARE LATTICE

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A generalized two-dimensional square lattice model is considered with additional long-range interactions between particles. The elastic forces between the particles in the lattice are assumed to be nonlinearly dependent on the spring elongations. An analysis of the linearized discrete equations reveals an influence of long-range and nonlocal interactions on the shape of dispersion relation. A comparison with the cubic crystalline model in the continuum limit is used to study an influence of additional interactions on an auxetic behavior. An asymptotic procedure and the formalism of the operators of the shift are developed to obtain continuum two-dimensional nonlinear equations to study weakly nonlinear plane longitudinal and shear strain waves disturbed in the transverse direction. Different character of the transverse instability for both types of the strain waves is studied, and the coefficients of rigidity responsible for instability are revealed. Amplification and localization of nonlinear strain waves are studied on the basis of the model equations derived.

*The work of AVP and AEO has been supported by the Russian Foundation for Basic Researches, grant No 17-01-00230-a.*

## HYDRODYNAMICS OF ONE-DIMENSIONAL PARTICLE SYSTEMS

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One-dimensional particle systems are known to be anomalous with respect to the dynamics of their hydrodynamic conserved fields and their related currents. We review some of the predictions of mode-mode coupling theory and of exact results by Prähofer and Spohn [J. Stat. Phys., vol. 115, 255 (2004)] to derive asymptotic expressions for the time-correlation functions of the hydrodynamic modes and their currents. These results are compared to extensive computer simulations for two simple fluids with non-linear short-range interactions.

## SOME PARADOXES OF MATHEMATICAL THEORY OF CONTINUES MECHANICS AND OF KINETIC THEORY

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The paper presents an analysis of mathematical approximations underlying description in different environments, and will present new models. The self-diffusion and thermo-diffusion which were foretold by S. V. Vallander is obtained from kinetic theory for rarefied gas. The classic presentation continuum mechanics do not preserve the continuity of the environment due to the use of the conditions of equilibrium of forces and the symmetry of the stress tensor.

Our stress tensor is not symmetric. Besides, the delay process is counted, which is important in describing of the discrete space and in describing the relaxation of the complicated molecules. The analysis of the recording the Lagrangian function for the collective interaction of the particles is made with counting of changing position of the inertia center. From these equation should have a modified Liouville equation and the Boltzmann equation. General consideration of all effects gives us cumbrous system of equations. The simplest interaction of two homogeneous flows is studied which move in the same direction at different speeds.

## CHARGE ACCUMULATION AND DISSIPATION IN MICROMETER SIZED POWDERS

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When moving, dry particles tend to acquire electric charge due to collisions between themselves and other solid surfaces, in a process called tribocharging. Provided there is enough number of collisions in a short amount of time, the charge accumulated can be high enough to constitute an electrostatic hazard. However, when the particles finally come at rest, the electric charge tends to dissipate, even if the particles are made of insulating material. In fact, in general the time it takes for the charge to dissipate is much shorter than what it would be expected from the electrical conductivity of the material of the particles. In this work, we present a model that describes the discharge of a powder layer formed by the settling of charged particles based on the assumption that the settled powder has an effective conductivity. We compare the model with the results of an experiment in which particles are charged and collected in a Faraday cage. The value of the conductivity that the model requires to match the experimental results is compared with the electrical conductivity of the bulk powder measured directly.

## FLOW OF ELECTROLYTES INDUCED BY AC ELECTRIC FIELDS IN MICROSYSTEMS

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The manipulation of small fluid volumes in micro-systems is of great interest for the lab-on-a-chip technology. This technology seeks to integrate biochemical laboratory functions on a single chip with the intention of achieving automation and high-throughput detection. The use of electrical forces for liquid handling in microsystems has the advantages of voltage-based control, no moving parts, and dominance over other forces.

DC electric fields have been widely used in microsystems for manipulation of particles and fluids, particularly, by employing electrophoresis and electroosmosis. However, the high voltages required generate electrolysis and the electrodes must be placed outside the device. Microelectrodes mounted inside the microchannels can be energized by AC voltages, generating high electric fields, with the advantages of lower power requirements, simple integration, and little or no electrolysis. In addition, electrical properties of fluids and particles depend on frequency of the applied AC signal, which opens new ways of actuation, such as particle, and fluid, dielectrophoresis.

This talk will deal with the flows of electrolytes that are generated by AC electric fields in microsystems. These AC fields can actuate either in the liquid bulk (e.g., electrothermal flows), or in the double layer at metal-electrolyte interfaces (e.g. AC electro-osmosis). In both cases, the applied electric field induces charge and actuates on this induced charge. Therefore, the electrical force is a quadratic function of the electric field amplitude, which has a non-zero time-average for AC fields. In the liquid bulk, forces in electrolytes arise from the action of an electric field on inhomogeneities in the liquid conductivity and permittivity. These inhomogeneities can be induced by temperature gradients, or at the interface of two-phase flows. In the double layer, flow is usually generated when an AC electric field is both charging the metal solid/electrolyte interface and acting upon this double-layer induced charge. The force that the tangential component of the electric field exerts on the double-layer charge generates the fluid flow, known as AC Electro-osmosis or Induced Charge Electro-osmosis.

## ELECTRO-ROTATION OF SEMICONDUCTING PARTICLES

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AC electrokinetics of small objects in micro-systems is of great interest for the lab-on-a-chip and nanomaterial technologies. In particular, the electrical characterization and control of semiconducting micro- and nano-particles suspended in electrolytes is important because semiconducting nanowires and nanotubes are extensively studied in many areas of research for their potential used as sensors, building blocks in novel nanocircuits, or for the absorption of light in solar cells by means of a dense array of nanowires.

In this work, we study the electrorotation (ROT) of semiconducting particles, i.e. the constant rotation induced on semiconducting particles when subjected to a rotating electric field. We examine theoretically the physical mechanisms responsible for the electrical rotation of semiconducting spheres and nanowires suspended in an electrolyte as a function of frequency of the applied ac electric field. The ac electric field interacts with the induced charge in the electrical double layer at the semi-conductor-electrolyte interface, causing rotation due to the torque on the induced dipole and

due to the induced-charge electro-osmotic (ICEO) flow around the particle. Here we take into account that the double layer between semiconductor and electrolyte is formed by two charge layers with finite lengths: the Debye layers on the electrolyte and semiconductor sides. In general, ROT spectra of semiconductors show two peaks: one positive and one negative. These peaks represent particle rotation either in the same direction of the electric field rotation (co-field ROT) or in opposite direction (counter-field ROT). The differences in ROT between thin and thick double layers will be highlighted.

## **DRAG REDUCTION ON A CIRCULAR CYLINDER BY CORONA DISCHARGE**

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Improvement of aerodynamic characteristics is an important problem of applied aerodynamics. There are various ways to change wake structures of solid bodies. One of them is using a corona discharge. Near the grounded bluff body a thin wire is placed. When the high voltage is applied to the wire, the corona discharge occurs. Generated by the corona ion wind can significantly change the wake structure. This technique has many advantages: it is simple, robust, cost-effective, without moving parts.

In this work, we carried out computer simulation of positive corona in a system of electrodes cylinder-wire and the ionic wind produced by the discharge. Mathematical model of corona discharge includes the Poisson's equation for electric field, the Nernst equation for concentration of positive ions and the Navier-Stokes equations for gas flow. We use original unipolar model with the boundary condition in form of the flux density rate of positive ions. The input parameters of the model include known physical quantities, amenable to independent measurement: the ionization rate, positive ion mobility and diffusion coefficient, the critical number of ionization collisions required for discharge ignition.

The system of electrodes was placed in a model wind tunnel with a given free-stream velocity. The wire was located behind the cylinder at a distance equal to the radius of the cylinder. The flow regimes with Reynolds numbers up to 7880 under which is formed the Kármán vortex street were considered. The flow generated by corona discharge at voltages to 21.2 kV was investigated. In addition, the drag force acting on the cylinder for different corona voltages was calculated.

The simulation showed that using the corona discharge could affect the periodic character of the Kármán vortex street. The discharge was able to significantly reduce the frequency of vortex shedding behind the cylinder compared with the Kármán vortex street without discharge. Thus at high voltages, the vortices could accumulate a large angular momentum, because the ionic wind was pressing them to the cylinder's surface.

The drag force was mainly determined by the pressure to the cylinder and had a periodic character. It was shown that for the studied conditions, its mean value depends linearly on the discharge voltage. As the voltage increases, the force of drag is significantly reduces.

## **EXPERIMENTAL VERIFICATION OF THE COMPUTER MODEL FOR SIMULATION OF WATER DROPLET ELECTRICAL COALESCENCE AND NON-COALESCENCE**

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Electrocoalescence is the process of combining the conductive (water) droplets suspended in a dielectric liquid (oil) by the electric field. The reverse situation is possible, when conductive droplets in the electric field are repelled; the process can be called non-coalescence. The study of the process of transition from coalescence to non-coalescence is not only of scientific but practical importance for the development of efficient electrical dehydrators, the devices that are used to extract dispersed water from the crude oil. The main principle of operation of the devices is the effect of the electric field upon emulsion, which is followed by deposition and coalescence of water droplets. However, designing such a device is difficult because of the lack of a reliable computer model, which allows investigating the process in detail. In view of this, the study aims to experimentally verify a computer model that can explain the cause of the transition from the coalescence to non-coalescence.

The work was carried out on the basis of comparison of experimental research data on coalescence and non-coalescence with those of computer simulation. The simulation was conducted in COMSOL Multiphysics software package using the phase function method. The experimental study was conducted at the setup, in which edge effects were excluded to the maximum and which used liquids with known properties and parameters that entered the computer model.

As the result of the study, the experimental database has been collected and used to carry out the verification of the computer model.

## ACCELERATED NUMERICAL SIMULATION OF SEISMICITY ACCOMPANYING HYDRAULIC FRACTURE AND MINING

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Numerical simulation of seismic and aseismic events is a modern means to increase understanding, to improve design, to conclude on the state of rock mass and to control mining and oil, gas and heat production. Presently the simulation is quite time expensive because of two bottle-necks. The first one is common for any problem of continuum mechanics involving the need to solve algebraic systems with large number of degrees of freedom (DOF). It is overcome by well-developed approaches, which employ either sparse matrices in methods like finite elements, discrete elements, finite differences, molecular dynamics, etc., or fast multipoles in methods like the boundary element method.

The second bottle-neck is specific for numerical modeling of seismic and aseismic events. It is caused by the need to account for the influence of a large number  $N_a$  of already activated flaws (sources of events) on a large number  $N_p$  of flaws, which may be activated by events of the group  $N_a$ . The total number of arithmetic operations on a time step, being proportional to  $N_a \times N_p$ , this leads to extreme time cost when the numbers  $N_a$  and  $N_p$  are of orders used in practical calculations (hundreds and thousands). Our objective is to overcome the difficulty.

The approach developed reaches the objective by employing the fact that mutual influence of flaws decreases as  $1/R^3$  when the distance  $R$  between flaws grows. This suggests following the line of the fast multipole methods, which employ the same feature. Firstly, we build a hierarchical tree of octants with sides decreasing as  $1/2^n$  on the  $n$ -th hierarchical level. Secondly, we properly account for the interaction between flaws on successive levels. As a result, the time needed to account for interactions drastically decreases.

Examples illustrate the improvement provided by the accelerated method. We re-visit problems of hydraulic fracturing and mining, for which simulations of seismicity have been performed in the papers [1] and [2], respectively. When modeling seismicity accompanying the propagation of a hydraulic fracture [1], the time expense for simulation of events on a propagation step of 10 meters decreased two orders, as compared with non-accelerated computation. Of importance is that the number and locations of simulated events practically coincide with those obtained without acceleration. Similar speeding up without distortion of simulated events is observed for the mining problem discussed in [2].

We conclude that the method developed is quite efficient. It is implemented in the code SEISM-3D-FAST. Being combined with the mentioned accelerated methods of solving systems with large number of DOF, it provides a tool to simulate seismic and aseismic events in real time on conventional laptops.

*The authors appreciate the support of the National Science Centre of Poland (Project Number 2015/19/B/ST8/00712).*

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## COMPUTER SIMULATION OF DYNAMICS OF THREADING DISLOCATIONS IN POROUS EPITAXIAL LAYERS OF GALLIUM NITRIDE

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The study of microstructural changes in crystalline materials is one of fundamental problems in materials science and micromechanics of strength and plasticity. One of the practical tasks of great importance in this field is to find the most effective way for reducing the density of defects in heteroepitaxial materials. This mainly concerns so-called threading dislocations (TDs) which are formed during the epitaxial growth and strongly deteriorate the conductive and optoelectronic properties of device heterostructures based on III-nitride semiconductors (in particular, GaN) [1,2]. An effective way to reduce the density of TDs is the formation of intermediate porous GaN layers. Experimental research has shown that the use of porous substrates leads to significant decrease of TD density in growing GaN films [3-6]. Nevertheless, the effect of porosity on the evolution of TDs in GaN layers and its theoretical description is still quite far from total clarity. Only in the most recent years, the first physical models which describe the evolution of TD density in

GaN layers were developed [7-10].

The aim of the present work is to shed some light on the behavior of TDs through computer simulation by the method of 2D discrete dislocation dynamics. Using this approach, we suggest a computer model which clearly demonstrates the collective behavior of TDs in the vicinity of pores in a strained growing layer of GaN. Within the model, the pores are considered as cross sections of cylindrical cavities elastically interacting with unidirectional parallel edge dislocations, imitating TDs. As a result, temporal dependences of coordinates and velocities of the dislocations are obtained. A special software interface is elaborated which provides the visualization of the current structure of the dislocation ensemble at any time. It is shown that the density of final dislocation structures essentially depends on the ratio of the area of the pore cross section to the area of simulation box. For example, when the surface fraction of pores on the layer surface reaches 6% and 25 %, the final dislocation density decreases 2 and 5 times, respectively.

*This work was supported by the Russian Science Foundation (grant RSF No. 14-29-00086).*

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## ON THE REGIMES OF AVERAGE FLOW APPEARING IN AN ELASTIC OSCILLATING SPHEROIDAL CONTAINER

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The work has the aim to investigate the behavior of viscous liquid in spheroidal cavity with elastic wall under the action of periodic deformations in a wide range of dimensionless frequencies of vibrations  $\omega$ . The intensity and structure of averaged motion of liquid generated in the cavity is determined by the amplitude and frequency of vibrations.

It is known that the vibrational action is able to generate the averaged flows in liquid. The mechanism of emergence is described, for example, in [1]. In a viscous fluid oscillating near the rigid boundary the averaged flows appear in a Stokes layer [2] and then generate the secondary flow in the volume of the cavity. In a range of low dimensionless frequency, when the Stokes layer is thick with respect to the cavity size, the primary flow in a form of a pair of toroid vortexes occupies the whole volume of the cavity. With increasing the dimensionless frequency the characteristic size of primary vortexes decreases. Simultaneously in the central area of the cavity the secondary flows appear. The intensity of secondary flow increases with increasing the dimensionless frequency. In a range of high dimensionless frequency (thin boundary layers) the secondary vortexes occupy the whole volume of the spheroid. It is shown that the velocity of liquid in the secondary flows is determined only by the pulsating Reynolds number. In a range of very high values of  $\omega$  the instability of flows in the vortexes is observed.

*The research was supported by the RFBR (project No. 16-31-60099 mol\_a\_dk).*

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## **PREPARATION AND THERMAL PERFORMANCE OF POLYTETRAFLUOROETHYLENE (PTFE)/THERMALLY EXPANDED GRAPHITE (TEG) NANOCOMPOSITES**

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In this study, Thermally Expanded Graphite (TEG) was used as reinforcing nanofiller in a fluoroplastic (PTFE) polymer matrix. The aim of the present work was to determine the impact of TEG on the structure, on the thermal properties and on the degradation process of the obtained polymer nanocomposites. The latter were prepared by manual milling, with TEG particles loading of 2.5 wt%, 5 wt%, and 10 wt%. The structural properties of the PTFE/TEG composites were then investigated using X-ray diffraction (XRD) and infrared spectroscopy (FT-IR). Subsequently, the thermal stability and degradation kinetics of the composites were studied through differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The influence of the temperature during milling was considered as well (milling at 23° C and 160°C). The results reported that milling at high temperature enhanced the dispersion of the nanofiller inside of the polymer matrix. Furthermore, the concentration of TEG was found to impact the increase of the glassy phase transition temperature. This confirms that the degradation of the studied nanocomposite occurs at a relatively higher temperature with a greater TEG loading; displaying the potential of TEG to improve the thermal properties of fluoroplastics.

## **THE OPPOSITE MODE OF STREAMER-TO-LEADER TRANSITION**

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Test with standard lightning pulse impact are generally accepted for high voltage constructions. Streamer form of discharge occurs in air under such conditions. Streamer is a channel of low-temperature (non-equilibrium) plasma growing due to intensive ionization at the tip of the channel. Streamers do not lead to breakdown itself due to their high electric resistance. Breakdown demands that plasma transfers to high-temperature (equilibrium) state. Usually this transfer follows streamers closure of the electrode pair. Solid dielectric barriers are used to stop streamers and increase breakdown voltage without lengthening interelectrode distance. An important topic is – how geometric parameters of solid dielectric parts influence on breakdown voltage.

Two breakdown cases should be distinguished. The simpler one may be called “enveloping breakdown”. In this case streamers turn when coming up to the barrier surface. Reaching the edge of the barrier streamers turn again: in the direction to the opposite electrode. Breakdown voltage increases because the air path between the electrodes lengthens. In this case the main way to increase breakdown voltage is to increase the barrier diameter or to create “labyrinth insulation”.

The second case is present when air path between electrodes is long enough. Experimental data are presented which prove that a pair of high temperature plasma channels (“leaders”) form without streamer closure under such conditions. It gets possible due to intensive heating of streamer channels by capacitive (non-closed) currents charging barrier surfaces. This mechanism may be called “opposite leaders”. Some types of creeping discharges may be an instance of this case.

The experimental investigation is implemented in sphere-sphere and sphere-plane electrodes systems with plane dielectric barriers. Photographs of streamer discharge and breakdown are analyzed as well as current oscillograms. Also surface charge on barrier surface is visualized to get additional information about discharge structure.

A character of barrier parameters influence on breakdown voltage is crucially different in these two cases. That is why it may be of interest for high voltage insulation developers.

## EFFECT OF CONTACT ORIENTATION ON ULTRASOUND VELOCITY IN MAGNETIC POWDERS

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We study the sound propagation velocity of P-waves in granular media made of micrometer sized magnetite particles of different particle sizes when a magnetic field is applied. The sound propagation velocity is measured as the time of flight of a short pulse centered at 20 kHz. At these frequencies we do not observe the wave dispersion in the sample. In each experiment, the material is initialized by fluidization to allow the particles to rearrange their positions. The magnetic field is applied either after fluidization stops and particles settle or while the material is still fluidized. Both procedures result in different particle arrangements, that depend also on the relative orientation of the field with respect to the fluidizing gas flow direction (vertical). Differences in the initialization procedure and the magnetic field intensity and orientation change the sound propagation velocity in the material, increasing the sound propagation velocity when the magnetic field is applied parallel to the sound propagation direction and decreasing it when the magnetic field is applied perpendicular to the sound propagation direction. The relationship between the changes in the particle arrangement and the sound propagation velocity is discussed using effective theory medium (EMT).

*This work has been partially funded by Spanish Government Agency Ministerio de Economía y Competitividad (project No. FIS2014-54539-P) and by Junta de Andalucía. F. Ruiz also acknowledges financial support from the University of Seville (Spain) through the FPI-2012 PhD grant.*

## THERMOELASTICITY OF MICROPOLAR THIN PLATES

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In the present paper three-dimensional theory of thermoelasticity of micropolar body is introduced [1] both in the form of differential equations with boundary conditions and in general variational form. Hypotheses method [2] is developed during the construction of general applied theories of micropolar elastic thin plates and shells. Applied theory of thermoelasticity of strain stress state and bending deformation of micropolar thin plates is constructed on the basis of the accepted hypotheses both in the form of differential equations with boundary conditions and in general variational form. Problems of bending of micropolar rectangular and circular plates are studied on the basis of the constructed applied theory of thermoelasticity of micropolar thin plates. Numerical solutions of the stated problems are obtained. With the help of the analyzing of these numerical results effectiveness of the micropolar material of the body is stated from the point of view of its rigidity compared with the classical material.

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## INSTABILITY OF SHEAR FLOWS IN THE NANOMETER WAVELENGTH RANGE

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The phenomenon of Kelvin–Helmholtz instability (KHI) occurs in many natural and industrial processes. At present, an interest in the study of instability increases in connection with its manifestation in the preparation of surface nanolayers

and the behavior of materials under severe plastic deformation (SPD) [1]. The active research of the viscosity influence on the maximum perturbation growth rate is recent. These studies find the influence of the viscosity on the growth rate of maximum perturbation. However, the numerical analysis of the dispersion equation for the viscous and visco-potential model of KHI is previously conducted, and the mode in which the decrement dependence on the wavelength has two maxima is found. Therefore, the viscosity can fundamentally change the nature of the decrement depending on the wavelength. In this context, the aim of this work is to determine the range of parameters that allow the existence of the second maximum[2]. The mathematical model of formation of nanostructured layers based on the occurrence conception of flow instability of materials under superplastic deformations have been developed. The dependence of a instability decrement on a wavelength which has two peaks was determined. The first maximum is at wavelengths of 100– 400 nm, the second one is at 1 – 10  $\mu\text{m}$ . It was found out that with increasing the speed the second maximum disappeared, and the first one offset in a wavelength range  $<100$  nm. Analytical dependences of the maximum decrements of instability on the parameter values were obtained. The value range of velocities and kinematic viscosities was determined, where the bimodal instability of Kelvin– Helmholtz took place. Conducted parameterization of experimental data on the disintegration cementing layers of steel during SPD and the values of effective viscosity. Of discrete-lattice models the formula for the theoretical viscosity of the fluid. Specify the ranges of parameters under which the viscosity match.

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### ON THE REPULSION OF SOLID, OSCILLATING IN FLUID, FROM THE RIGID BOUNDARY. THE ROLE OF THE AMPLITUDE OF VIBRATIONS

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The dynamics of a cylindrical solid in a rectangular container filled with a viscous incompressible fluid under the action of translational horizontal vibrations is studied experimentally. The experiments are performed with the bodies of a density either greater or less than the density of the liquid.

Another subject of study is the fluid flows appearing in liquid under the action of oscillating body. The velocity fields and averaged fluid currents are studied by PIV (Particle Image Velocimetry). The variations of the amplitude and the frequency of vibrations together with the parameters of liquid change affect both the intensity and the structure of fluid flows generated in the container. It is shown that with increase in the dimensionless amplitude the laminar flow regime is changed by a disruption one.

Theoretical and experimental investigation of the lift force acting on the cylindrical body in the limit of small amplitude and high frequency of vibrations is carried out earlier in [1]. The experimental results in the case of small-amplitude of vibrations for the body in a non-viscous liquid are in good agreement with the theoretical ones.

In the limit of high amplitudes of body's oscillations with the change of flow regime the value of lift force is decreasing. These results suggest that the dynamics of a cylinder, oscillating near the wall, and the magnitude of vibration lift force largely depends on the flow regime and the intensity of flow excited within the fluid volume.

The described effects present the interest for the fundamental and applied studies connected with vibrational control over the solid inclusions in viscous fluids in microgravity as well as for the problems associated with the intensification of the processes of mixing of liquids inside the oscillating cavities.

*The work is supported by the Russian Foundation for Basic Research (Grant 16-31-00201).*

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## ON THE STABILITY PROBLEM OF BULK AND UNFIXED CARGO ON A ROLLING SHIP

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Huge losses from shipwrecks caused by unfixed or bulk cargo remains a big problem. Reason for these shipwrecks is that under rolling effect ship center of mass becomes displaced.

In current article, we suggest a simple model of body (cargo) movement and stability on a coarse carrying surface, which is making rotatory oscillations. The research is a still currently unexplored problem of vibrotransportation theory, in which body is considered to be on a progressively moving surface. Research shows, that ship oscillations (rolling) lead to the decrease of repose angle of the bulk media, and, in turn to the decrease of dry friction angle. It is shown, that exceeding of this angle leads to specific instability of a cargo – increasing from period to period movement in the direction of one of the ship boards.

## A CLOSED STRING AND THE STABILITY OF ITS REFERENCE CIRCULAR CONFIGURATION

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Closed strings are one of the popular objects of research in modern theoretical physics. The study of the closed strings has an objective problem because of the lack of an appropriate mathematical description [1]. There are reasons to believe that the properties of the virtual string objects studied by theoretical physics, should be similar to the properties of its mechanical prototypes. Therefore, the mechanics of solids can help overcome the problem of constructing correct mathematical models of string objects that can be studied by modern mathematical methods.

The properties of closed string in the solid mechanics have not been sufficiently studied up to date. This is due to the rare cases of application of this kind of models.

It is presented closed purely mechanical 1D-object with the decisive property of a mechanical string. The bending stiffness of a mechanical string is equal to zero. Therefore, the natural or reference configuration of such an object can not exist without interaction with its environment. The role of the environment is to provide the string with a pre-tension.

The presentation gives one of the constructive ways to create a pre-tension in a closed string. This is achieved by using a radial Winkler base. Equations of equilibrium of the nonlinear rod theory for a one-dimensional momentless continuum stretched over a radial Winkler base allow a circular static solution. However, the proof of the uniqueness theorem of a static configuration in the form of a circular curve for such an object is not known.

The circular equilibrium configuration of a closed string is investigated for stability. In this paper the circular equilibrium configuration of a closed string is investigated for stability. Dynamical equations in variations are constructed using strictly formal procedures for the mechanics of solids. Conditions for the existence of non-trivial solutions of static equations in variations are found. It is shown that there are values of the system parameters when the circular configuration of a closed string is the only static solution of the system of nonlinear equilibrium equations.

It is also established that for certain ratios of the elastic properties of the radial Winkler base and the elastic and geometric parameters of a circular string, the static equations in variations for a circular mechanical string have nontrivial localized solutions.

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## TERMS OF SEARCH OPTIMAL PARAMETERS OF SHUNT ELECTRICAL CIRCUITS

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In designing and exploitation of modern structures, an effective control of their dynamic behavior is the front-burner problem. Its solution requires the elaboration and development of new approaches to damping of structure vibrations. A relatively new approach is based on the use of structure elements made of smart materials, particularly, of materials with piezoelectric effect. One of the methods of damping the structure vibrations with piezoelectric elements consists in their connection to electrical impedance in the form of external passive electric circuits and is generally known as a

shunt technique. In this case, a piezoelectric element serves as a transformer of mechanical energy of vibrations into electric energy, which is then dissipated in the external circuits.

In this paper, we propose a new approach for choosing the appropriate parameters of the external passive electric circuits, which is based on the mathematical statement of the natural vibration problem. Solving this problem yields complex eigenfrequencies, the real part of which represents the vibration frequency and the imaginary part – the damping coefficient, specifying the rate of vibration damping. For the examined problem, different variants of the objective functions are investigated based on the analysis of the real and imaginary parts of complex eigenfrequencies as a function of the external circuit parameters. The maximum value of the damping coefficient taken as a variant of the sought objective function is considered to be a condition that specifies the optimal parameters for the external passive shunt circuits providing the required dissipative characteristics of the structure. The efficiency of the above approach is demonstrated in the context of example problems on dynamic behavior of plane and spatial objects for two types of external circuits- resistive R-circuit and resonant RL-circuit. The results of solving the forced steady-state vibration problem are used to support the validity of the determined optimal parameters.

*The work is supported by the RFBR (projects No 15-01-03976-a, No 16-31-00094-mol-a).*

## **REPRESENTATION OF SOME INTEGRAL CHARACTERISTICS OF POTENTIAL FIELDS BY THEIR VALUES AT SOME POINTS**

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This work is concerned with potential fields  $\Phi(M)$ , where  $M$  is the point of a plane domain  $D$ . The goal is to study the problem of representation of the integral ( $\Phi(M)$ ) over the contour  $\Gamma$  as a linear combination of values of  $f(\Phi(M))$  at some points  $\Gamma$ . It is assumed that  $f$  is a function and  $\Gamma$  is a contour lying in the domain  $D$ . The properties of the function  $f$  and the contour  $\Gamma$  are determined, and the location of points  $M$ , at which such a representation is possible, is established. As an example of application of the obtained results, the flow of a Chaplygin gas around wing profiles is considered. The results provide evidence of the existence of this point on the profile chord, where pressure-drop and lift coefficients are related via a linear transformation. Techniques for determining the point and the transformation are described. The influence of small variations of the profile chord on the relationship obtained in this study is also investigated. Our simulations demonstrate the validity of the proposed approach for measuring the air-speed performance of flight vehicles (1). At the aircraft conceptual design stage, the developed mathematical models can be used to calculate an aerodynamic pressure field for a whole bearing surface. With these techniques one can reduce the production cost of vehicles by the use of selective cross-sections and points on their surface. The linear relationship mentioned above is taken as a basis for the approach.

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## **CASES OF INTEGRABILITY CORRESPONDING TO THE MOTION OF A PENDULUM IN THE FOUR-DIMENSIONAL SPACE**

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In this activity, we systematize some results on the study of the equations of a motion of dynamically symmetric four-dimensional fixed rigid bodies-pendulums located in a nonconservative force fields. The form of these equations is taken from the dynamics of real fixed rigid bodies placed in a homogeneous flow of a medium. In parallel, we study the problem of a motion of a free four-dimensional rigid body also located in a similar force fields. Herewith, this free rigid body is influenced by a nonconservative tracing force; under action of this force, either the magnitude of the velocity of some characteristic point of the body remains constant, which means that the system possesses a nonintegrable servo constraint (see [1]), or the center of mass of the body moves rectilinearly and uniformly; this means that there exists a nonconservative couple of forces in the system.

Earlier, the author already proved the complete integrability of the equations of a plane-parallel motion of a fixed rigid body-pendulum in a homogeneous flow of a medium under the jet flow conditions when the system of dynamical equations possesses a first integral, which is a transcendental (in the sense of the theory of functions of a complex variable, i.e., it has essential singularities) function of quasi-velocities. It was assumed that the interaction of the medium with the body is concentrated on a part of the surface of the body that has the form of a (one-dimensional)

plate.

The planar problem was generalized to the spatial (three-dimensional) case, where the system of dynamical equations has a complete set of transcendental first integrals. It was assumed that the interaction of the homogeneous medium flow with the fixed body (the spherical pendulum) is concentrated on a part of the body surface that has the form of a planar (two-dimensional) disk.

Later on [2], the equations of motion of the fixed dynamically symmetric four-dimensional rigid bodies, where the force field is concentrated on a part of the body surface that has the form of a (three-dimensional) disk.

In this activity, the results relate to the case where all interaction of the homogeneous flow of a medium with the fixed body is concentrated on that part of the surface of the body, which has the form of a three-dimensional disk, and the action of the force is concentrated in a direction perpendicular to this disk. These results are systematized and are presented in invariant form.

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### SELF-ADAPTED ELASTOMER COMPOSITES PREVENTING TEMPORARY OVERCOOLING OF A SEAL

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Rubber O-rings are widely used in sealing applications in the oil and gas industry. The glass transition temperature ( $T_g$ ) of rubber can be varied by adjusting the composition but is typically in the region of  $-10^\circ\text{C}$  to  $-40^\circ\text{C}$ . When the temperature of the seal drops below  $T_g$ , the rubber becomes brittle and cannot maintain a seal between the counterfaces. In addition, the high thermal contraction of the elastomer seal during cooling compared to the steel housing increases the sealing challenge.

Operational temperature is usually above  $T_g$ , but sometimes sealing materials can be exposed to a sudden cold temperatures during a so-called "blowdown" event. Blowdown is a transient process, when the gas system pressure is rapidly released and it causes rapid cooling of the gas in the pipelines. The cold gas may cool down the seals lower  $T_g$  and therefore the elastomeric seals must be protected to ensure that the seals remain above  $T_g$  at all time.

To prevent temporary overcooling of the seal caused by blowdown or other temporary chilling conditions a novel class of composite is studied. The composite consists of rubber and fillers made of micro encapsulated phase changing materials (MEPCM). The phase changing materials release heat during the phase transformation from liquid to solid at cooling. This heat increases thermal inertia of the composite and delays the cooling down of the seal.

In the research numerical simulation is used to predict both mechanical and thermal response of the composite O-ring during transient blowdown. Performed simulation shows that the MEPCM may successfully protect rubber from temporary overcooling. A sensitivity analysis of thermal properties of the phase change material is also researched to highlight possible avenues of improvement of the MEPCMs for sealing applications. It is shown that the latent heat of the MEPCMs and the thermal conductivity of the solid phase of the MEPCM are the most significant parameters to increase thermal inertia of the composite.

### INVESTIGATION OF THE OCCLUSION BLOOD VESSEL MAGNETIC NANOPARTICLES

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In this work we investigate the process of embolization (occlusion) blood vessel using magnetic nanoparticles under influence on them external magnetic field and laser. Process of embolization occurs in two stages. First stage is introducing into a blood vessel suspension with magnetic nanoparticles, which are deposited on the wall of vessel under the influence of an external magnetic field. Second stage is provide thermal effect by means of laser radiation. Under heating magnetic nanoparticles transfer heat to the blood after that occurs its coagulation and occlusion the vessel in the area where it is needed.

The model for the study process of embolization was created, imitating section of the system circulation and allowing apply magnetic influence and also realize registration of the accumulation magnetic nanoparticles. [1]  
In the experimental setup the magnetic nanoparticles transported due to fluid flow along a tube and deposit on the wall of the tube in the magnetic field of the permanent magnet. This system describes the motion of the individual nanoparticle :

$$\begin{cases} m \frac{d^2 x}{dt^2} = F_x - a \frac{dx}{dt} \\ m \frac{d^2 y}{dt^2} = F_y - a \frac{dy}{dt} \\ m \frac{d^2 z}{dt^2} = F_z - a \frac{dz}{dt} \end{cases} \quad (1)$$

, where  $x, y, z$  the coordinates of nanoparticle,  $t$  is the time,  $m$  is the mass of nanoparticle,  $a$  is the coefficient of friction of nanoparticle on the liquid,  $F_x, F_y, F_z$  are the components of magnetic force.

The system of differential equations (1) is integrated with initial conditions:

$$t = 0 : \quad x = x_0, \quad y = y_0, \quad z = z_0, \quad \frac{dx}{dt} = 0, \quad \frac{dy}{dt} = 0, \quad \frac{dz}{dt} = V(x_0, y_0)$$

For the calculating magnetic force acting on the nanoparticle we use the formula:

$$F = mM(H) \nabla B$$

, where  $M(H)$  is the specific magnetic moment of the particle,  $B$  and  $H$  are the magnetic induction and magnetic field strength.

In the calculation components of the magnetic induction were used the following expressions [2]:

$$B_x = -\frac{K}{2} [\Gamma(a-x, y, z) + \Gamma(a-x, b-y, z) - \Gamma(x, y, z) - \Gamma(x, b-y, z)]_0^h$$

$$B_y = -\frac{K}{2} [\Gamma(b-y, x, z) + \Gamma(b-y, a-x, z) - \Gamma(y, x, z) - \Gamma(y, a-x, z)]_0^h$$

$$B_z = -K[\phi(y, a-x, z) + \phi(b-y, a-x, z) + \phi(x, b-y, z) + \phi(a-x, b-y, z) + \phi(b-y, x, z) + \phi(y, x, z) + \phi(a-x, y, z) + \phi(x, y, z)]_0^h$$

, where  $K$  is the parameter characterizing the magnetization of the magnet,  $a, b, h$  are sides of the magnet,

$$\Gamma(\gamma_1, \gamma_2, \gamma_3) = \ln \left( \frac{\sqrt{\gamma_1^2 + \gamma_2^2 + (\gamma_3 - z_0)^2} - \gamma_2}{\sqrt{\gamma_1^2 + \gamma_2^2 + (\gamma_3 - z_0)^2} + \gamma_2} \right),$$

$$\phi(\varphi_1, \varphi_2, \varphi_3) = \begin{cases} \arctan \left[ \frac{\varphi_1}{\varphi_2} \frac{\varphi_3 - z_0}{\sqrt{\varphi_1^2 + \varphi_2^2 + (\varphi_3 - z_0)^2}} \right], & y \neq 0. \\ 0, & y = 0 \end{cases}$$

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### FINITE ELEMENT MODELING POLARIZATION OF POLYCRYSTALLINE FERROELECTRICS

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In the paper is presented a model, which allows solving the nonlinear problems of irreversible processes of polarization and deformation for polycrystalline ferroelectrics continuum media and for quasi-static processes. Certain difficulties at

solving such problems are consist in formulation of constitutive equations, which are written for the reversible and irreversible parts separately and at the quasi-static process presented in increments. For constructing constitutive equations for increments of irreversible parts a physical model of locked domain wall was used, from which we obtain the desired relations as a system of equations in differentials for the irreversible components of the polarization vector and strain tensor. Constitutive relations for increments of reversible components were derived from the thermodynamics of irreversible processes. Method of finite element brings the solution of a task to a system of linear algebraic equations, for which the elements of the stiffness matrix depend on the elastic, piezoelectric and dielectric modules, which, in turn, depend on the current values of the residual polarization and deformation. The right side of the system includes the increments of external loads and the previously obtained values same residual parameters. The properties of the matrices satisfy the conditions of the unique solvability. After solving system, we find the increment of the searched parameters and proceed to the next state of equilibrium. The process is repeated until the final values of loads are achieved. As an example, the results of calculations of the residual strain fields and polarization were presented within the two-dimensional and axially symmetric cases. This model was implanted in the finite-element complex of software, to solve the problems for piezoelectric bodies with nonhomogeneous polarization.

Work carried out in the framework of the competitive part of state task of Russian Ministry of Ed. and Sci. - project № 9.1001.2017 / PCh.

## COMPETITION BETWEEN DISLOCATION SLIP AND DEFORMATION TWINNING IN ULTRAFINE AND COARSE-GRAINED METALS

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Lattice dislocation slip is the dominant deformation mode in most metallic crystalline materials [1]. Also, deformation twinning effectively contributes to plastic flow in metals especially at low temperatures and high strain rates [1,2]. In a metallic polycrystalline specimen, dislocation slip and deformation twinning can concurrently occur in various grains (with various crystal lattice orientations) of the specimen. The crossover from lattice slip to deformation twinning was observed in coarse-grained polycrystalline titanium in the experiment [3]. Note that deformation twins in nanostructured metals are typically nucleated at grain boundaries [4]. At the same time, the formation of lattice dislocation pile-ups (that stimulate the crossover under discussion) is limited in ultrafine grains composing nanostructured metals deformed by lattice slip [1]. Thus, the two competing structural factors – large amounts of grain boundaries and ultrafine grains – operate in nanostructured metals. This motivates interest in understanding the specific features of the crossover from dislocation slip to deformation twinning in nanostructured metallic materials. Thus, we have suggested a theoretical model [5] which describes the crossover from lattice slip to deformation twinning at grain boundaries in nanostructured and coarse-grained polycrystalline metallic materials. Within our description, the lattice dislocations that mediate dislocation slip in a grain interior are stopped by a grain boundary and form a pile-up configuration. Head dislocations of the pile-up are absorbed by the grain boundary where they split into grain boundary dislocations. Deformation twin is nucleated at these grain boundary dislocations and propagates to the neighbouring grain interior. The energy and stress characteristics of this transformation in nanostructured and coarse-grained polycrystalline metals (Ni, Ti) are calculated. Our theoretical results [5] are well consistent with corresponding experimental data reported in the literature [3].

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## EQUILIBRIUM FORMS BIFURCATION OF THE NONLINEAR NEMS/MEMS

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This work is devoted to analyse the equilibrium form bifurcation of the some nonlinear electromechanical systems in nano- and micro-scale (NEMS/MEMS). These systems may be or membrane, elastic plate, cantilever else the system of

parallel conductive nanolayers, which can be used as a sensor of internal or external mechanical and electrical alterations. The important significance of nano- and micro-actuators has been acquired as the micro-switches with forward or rotary movement or else micro-sensors based on «pull-in» effect. It's important to note that exactly in a case of NEMS and MEMS it is necessary to take in account the nonlinearity of its interaction, which leads to significantly nonlinear effect - the bifurcation of equilibrium elastic forms.

## GENERATION OF RECTANGULAR GLIDE DISLOCATION LOOPS IN CORE-SHELL NANOWIRES WITH PARALLELEPIPEDAL CORES

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Nowadays nanowires (NWs) and nanoparticles (NPs) have attracted much attention due to their unique electrical, optical, mechanical and catalytic properties that are strongly depend on their defect structure which, in its turn, is a function on the size and shape characteristics of NWs and NPs. The size and shape effects are tightly related with mechanisms of misfit relaxation in nanostructures. Good examples are NWs and NPs, which consist of Au cores and Pd shells, and are among the most promising materials for using as catalyst in CO and vinyl acetate oxidation [1-3]. Experimental observations revealed the presence of multiple stacking faults in truncated octahedral NPs with Au:Pd = 1:1 shells and Au cores. The appearance of stacking faults can be explained by Au diffusion from the core to the shell or by the formation of Shockley partial dislocations accompanied by stacking faults [3]. Core-shell NWs with parallelepipedal cores represent the simplest case of cores with flat faces; similar faces can be found in truncated octahedral nanoparticles with Au cores and Pd shells, where the aforementioned new interesting defect structures were demonstrated [3].

To consider a flat core-shell interface, we used a theoretical model of a NW consisting of a parallelepipedal core and a surrounding shell with a cylindrical free surface. Recently, we have obtained a strict analytical solution for the boundary-value problem of a parallelepipedal misfitting inclusion in an elastic cylinder [4], which is a mathematical basis for the present work. Based on the energy approach, we analyze here the possibility of generation of a rectangular glide dislocation loop embracing the core and lying in a plane inclined to the core axis. The loop generation is energetically favorable if the total energy change, i.e. the difference between the total energy of the system after and before the dislocation generation, is negative. Using this criterion, we study the dependences of the total energy change on the system parameters in the special case of the Au/Au-Pd core-shell NW and define the critical conditions for the loop formation. Moreover, we compare the preference of this relaxation mechanism with respect to some other mechanisms of misfit relaxation such as partial and perfect misfit dislocations generation by gliding in the cores and shells from the free surface, perfect misfit dislocation generation by climbing from the free surface, and partial and perfect dislocation dipole generation from a corner of the core.

*SAK and AMS got the support from RFBR project No. 16-32-00521.*

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## ENTROPY PRODUCTION FOR ONE-DIMENSIONAL HEAT TRANSFER

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In the publication [1] the equation describing anomalous heat conduction was obtained. This equation is time reversible (substitution of  $-t$  instead of  $t$  does not change the form of the equation). However, analysis of the solutions for this equation showed that it has both wave and diffusive behavior. Reversibility of the heat conduction process, described by this equation, is the topic of this work. Calculating the entropy production is connected with reversibility of the process.

In case of equilibrium processes the concept of entropy is well discovered and applied. In case of non-stationary heat flow, the concept of entropy is more complicated [2,3,4]. The aim of this work is to find an approach to determine the entropy change by considering several particular problems of non-stationary heat flow. Several approaches for calculating the entropy production are considered. It is shown that for the problem of an initial step temperature distribution the total entropy increases linearly. In the case of rectangular initial perturbation [5] the entropy is calculated numerically. It is shown that in case of rectangular initial perturbation the entropy reaches an asymptotic value, unlike the step solution, where entropy is an unbounded increasing function of time. It was shown that in case when the solution is self-similar, i.e., it has form  $T(x,t) = T(xt^{-\alpha})$ , where  $\alpha$  is dimensionless parameter, the entropy production has a power dependence on time.

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### STRUCTURAL MODELING OF NANOSTRANDS FORMATION IN DISPERSEDLY FILLED ELASTOMERS

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Dispersedly filled elastomeric composites represent a structurally heterogeneous system, consisting of highly elastic low modulus rubber phase (matrix) with embedded solid granular filler particles (dispersed phase). Usually this is carbon black and fumed silica. The particle size varies from tens of microns to hundreds of nanometers. Despite the fact that these materials are widely used in our lives for over a century, there are still questions that there is no single answer today.

The most important of these is the effect of rubber hardening when adding dispersed carbon black particles. Filling rubber by carbon black (20-30% by volume) greatly improves its operational properties: enhances the stiffness, rupture force increases 5-15 times, the limiting deformation in 2-4 times, and the smaller size of the filler particles, the stronger is reinforced material [1-3].

One possible explanation for this phenomenon is that the nanofiller composite creates a huge amount of uniformly distributed micro-breaks to facilitate transfer of the rubber matrix from complex stress state into the system of many uniaxially loaded fibers. Therefore, rupture efforts for them to be much higher than the corresponding values for the same elastomer in an undirected condition.

Appropriate structural model of an elastomeric composite was developed to verify this hypothesis. It is based on a new criterion of deformation strength, taking into account the possibility of an anisotropic hardening of the elastomer under the stretching (by reorientation of the molecular chains in the direction of load). The main feature of the criterion that a tensile or compression biaxial its value will be higher than when a uniaxial deformation (this is at the same strain intensity). That is, when the uniaxial loading material collapses later than in the case of two or triaxial deformation.

The results of computer simulation showed that in case of a new strength criterion using matrix breaks occurred not in the gap between the inclusions, but on some removal from it. Thus, the formation of a weakened zone in the form of a "hollow ring" occurred around the gap between the particles, that is quite be interpreted as a possible appearance of the elastic strand between the particles. Hence we can conclude that the strands appearing in the composite promote an increase in its strength and deformability ("pulling" the moment of global macro-cracks occurrence).

*This work is executed at a financial support of RFBR Grants: 16-08-00756, 16-08-00914.*

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## ANALYTICAL AND NUMERICAL SIMULATION OF THE BEAM BENDING WITHIN 2D AND 3D FORMULATION OF DIFFERENT GRADIENT ELASTICITY THEORIES

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Gradient elasticity theories allows to describe non-classical effects occurring in small-size structures and devices. Different variants of the gradient elasticity theories are known, but the choice of the optimum one remains open questions. In the present study, the comparison of different gradient theories solutions of a beam bending problems in 2D and 3D statements is presented. Pure and cantilever beam bending is considered. Numerical solutions are realized in the frame of simplified gradient models, which contain in the case of isotropy two classical elasticity parameters, and from one to three additional material constants [1]. Aifantis, couple stress, Gusev-Lurie [2] and dilatational gradient models are compared. The influence of scale effects and additional parameters values on the effective stiffness of the beam, on its stress state and on the deformations of its cross sections and outer surfaces is studied. For the obtained numerical results the symmetry of the double stress tensor is verified. The numerical results are compared to the corresponding analytical solutions of 3D problems (for the pure bending) and to the solutions that was found in the frame of the beam theories. Based on this comparison, we investigated, in particular, the correctness of various models of scale-dependent beams. Obtained results also compared to the previous works [3-5]. The possibility of the certain gradient models choice based on the direct experimental measurements of deflections and deformations of the beam in flexural tests is discussed.

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## CONVERSION OF MECHANICAL ENERGY TO THERMAL ENERGY IN A ONE-DIMENSIONAL CRYSTAL

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We discuss a process of conversion of mechanical energy to thermal energy in a one-dimensional insulated crystal: a chain of identical particles, connected by the same nonlinear springs. Random initial velocities and periodic boundary conditions (the Born-von Karman boundary conditions) are set. The velocity dispersion is determined from the correspondence to the required temperature profile.

We are solving the Cauchy problem for the chain using the finite difference method and averaging over the realizations. A mechanical wave in such a crystal will loose its shape and decay as its energy transforms into thermal energy. Conditions of this transition are investigated. Solutions for standing and traveling sine-shaped waves are compared. The law of the mechanical energy decrease is studied as a function of the thermal noise value and time. The irreversibility of the process is demonstrated for the large dispersion of velocity fluctuations. The influence of the thermal noise value on the shape of a mechanical wave and the possibility of solitons formation in a crystal are also investigated.

## ANALYSIS OF DAMAGE ACCUMULATION'S PROCESSES OF COMPOSITES MATERIALS AND IDENTIFYING OF FEATURES FAILURE

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The complex of tests to estimating the residual static strength of composite samples after preliminary cyclic loading. The samples were made from of glass fiber prepreg strips. 23 samples, divided into five groups, were tested. Each group

of samples of different value cyclic loading, which lies in the range of load cycles ( $N=0 \dots 1.75 \cdot 10^5$ ). Cyclic loading was performed on the test system Instron ElectroPuls E10000. The samples were tested at the same amplitude stress level with a maximum value  $\sigma_{\max}=0.5\sigma_b$  of the coefficient of asymmetry  $R=0.1$  and a frequency of 50 Hz. The amplitude of the cyclic loading was  $\sigma_a=0.225 \sigma_b$ . After cycling tests the quasi-static tensile test with the definition of the ultimate strength were carried out. This type of test was conducted using a testing system Instron 5882.

As a result, were obtained depending on the strength limit of the composite material from the duration of previous cyclic loading. The point corresponding to the value  $\sigma=0$  obtained as the mean fatigue life of the material samples. For determine this value three fatigue tests to failure were conducted. The cycle parameters of this fatigue tests is the same as in the previous cyclic loading.

Analyzing the results, we can conclude a reduction of tensile strength by increasing the value of the pre-cyclic loading. The schedule is not linear. In the first range ( $0 \dots 10^5$  cycles) reducing the tensile strength of the material sample is about 20%. The following range ( $10^5 \dots 1.5 \cdot 10^5$  cycles) reduce the tensile strength is not reduced. In the latter range ( $1.5 \cdot 10^5 \dots 2.1 \cdot 10^5$  cycles), a sharp decrease in the limit of the material strength.

*The work was supported by Grant of the Russian Foundation for Basic Research RFBR-Ural (grant № 16-41-590360)*

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## STUDY OF VARIOUS NUMERICAL SCHEMES FOR TRACING HYDRAULIC FRACTURES

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Numerical modeling is an important way to increase understanding and efficiency of hydraulic fracturing (HF). However, because of mathematical difficulties, numerical simulation of HF still remains a very difficult task. The recent comparative study of HF simulators [1] has shown that the inexplicit level set algorithm (ILSA) [3], employing the theory of propagating interfaces [4] in *inexplicit* form, is presently superior over other approaches. The modified theory of HF [2] implies that *explicit* forms may be used as well, what significantly extends options for numerical simulation of HF. This paper aims to employ the new options by further developing efficient algorithms started in [5].

We employ (i) hypersingular elasticity operator not using its inversion; (ii) global coordinates, in which the temporal derivative is singular at the fracture contour; (iii) the speed equation to trace the front propagation at points of the front; (iv) universal asymptotics to evaluate the speed via the opening; (v) combining the speed equations with discretized continuity equations in a joined system of ODE; and (vi) specially tailored schemes for inclusion nodes passed by the fluid front. It is revealed that the latter is of crucial significance for stability of an algorithm.

By using theoretical considerations, the benchmark KGD model and detailed analysis of numerical results for it, the schemes, which provide stable results with acceptable accuracy, are distinguished. They are based on proper using the universal asymptotic umbrella and the causality principle. Their computational efficiency is checked by employing various methods (forward and backward Euler's, Runge-Kutta, backward differentiation) for solving the resulting system of ODE. Remarkably, the forward Euler's method has appeared competitive, to say the least, when compared with the other methods tested. Having positive results for the KGD problem, it became possible to apply the scheme developed for solving the axisymmetric HF problem as a truly 3D problem. The tests have confirmed that the scheme provides stable and quite accurate results even for rough meshes.

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## STUDIES OF FRACTURE IN SHEAR OF A CONSTRAINED LAYER

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Cracks normally propagate in the opening mode associated with a state of local symmetry at a crack tip. However, the micro- or macrostructure of a material or structure sometimes forces cracks to propagate in a shearing mode. An important example is in the motion of tectonic plates that results in earthquakes. Irrespective of the actual material studied, fracture in shear is frequently associated with the formation of a large number smaller sigmoidal-shaped cracks in the propagation direction of the major crack. Propagation of the major shear crack is accomplished by coalescing the sigmoidal-shaped cracks. The shape of these cracks in brittle materials can be understood from the principle of local symmetry. A material class that is especially suitable for studies of shear fracture is polymeric adhesives joining metal substrates. Appropriately designed and loaded specimens can force a major crack in the adhesive to propagate in a shearing mode at a reasonable load level and in a stable manner. Experiments show that the formation of sigmoidal cracks due to shear loading of the substrates leads to a normal separation of the joined substrates. Theoretical studies of brittle shear fracture in adhesive joints show that constraining the local opening of the sigmoidal cracks increases the fracture resistance for the propagation of the major crack; the associated fracture energy increases by about 30% from a completely free to a completely constrained opening. Most engineering materials are however ductile. In the present study, experiments with a ductile adhesive loaded in shear and where the normal separation is constrained are evaluated using the path independent  $J$ -integral. The experimental set-up does not provide a completely free, nor a completely constrained, normal separation. However, the evaluation shows that the fracture energy increases with about 50% due to the constraint. A novel technique is used to extrapolate the experimental data to a state of pure shear, i.e. without a normal separation. The associated cohesive law shows that considerable normal compressive stress develops in the adhesive during macroscopic shear loading. It is also concluded that by ignoring the normal separation in the evaluation of the experiments, the strength of the adhesive is underestimated. Thus, the procedure developed in earlier studies is conservative from a strength analysis perspective. The present technique might be possible to extend to other materials to reveal their properties in shear fracture.

## INERTIAL WAVES AND PATTERN FORMATION IN LIBRATING CYLINDER WITH LIQUID

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The fluid motion in rotating cylinder is investigated experimentally. The cavity rotation velocity changes according to the harmonic law (librations). In the absence of librations the fluid performs a solid-body rotation together with the cavity. Librations of the cavity lead to the appearance of an oscillating motion in the viscous boundary layers. In this case the corners formed by the cylindrical and end walls of the cylindrical cavity generate the inertial waves. The waves propagate in the liquid along the characteristic surfaces in the form of cone; the angle between this surface and cavity walls is determined by the frequency of librations. It is found that in case of small amplitudes of librations on the cylindrical boundary of the cavity the heavy particles of visualizer are accumulated in the rings. The analysis shows that the position of the rings corresponds to the places of the reflection of the inertial waves. This indicates that at the point of incidence the wave generates the average flow in the boundary layer, which leads to a redistribution of particles of visualizer. Pattern formation on the cavity boundary and the structure of the fluid flow in the bulk depending on the frequency and amplitude of librations are studied.

*The research was supported by the RFBR (project No. 16-31-00169 mol\_a).*

## JACOBI STABILITY AND UPDATING PARAMETERS OF THE LORENZ SYSTEM USING HYBRID ALGORITHMS

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Continuously time evolving dynamical systems are widely used as effective theoretical tools for the mathematical modelling of natural phenomena in various fields of physics and engineering. The global stability of dynamic systems is described by the theory of Lyapunov stability. An alternative approach is represented by the local stability (Jacobi stability) analysis. The analysis is based on the Kosambi–Cartan–Chern (KCC) theory. In this approach one describes the evolution of the dynamic system in geometric terms, by considering it as a geodesic in a Finsler space. In the framework of the KCC theory, they reformulate the dynamic system as a set of two second-order differential equations. The geometric invariants associated to the system, and the deviation curvature tensor, as well as its eigenvalues, may be obtained explicitly.

The Lorenz system plays an important role for understanding hydrodynamic instabilities and the nature of the turbulence. The purpose of this work is to find parameters of the Lorenz system from indirect (measured) data. The sought-for parameters of the system can be interpreted as the Prandtl number, the Rayleigh normalized number, and the wave-length number, respectively. Input data are given approximately by eigenvalues of the deviation curvature tensor. The optimization approach has been applied to solve the regularized inverse eigenvalue problem. Two novel hybrid global optimization algorithms combining the stochastic Multi-Particle Collision Algorithm (for scanning the search space) and deterministic techniques (for local descent) are applied. Iterated smoothing approximations are inserted during the local search in the first algorithm. The second algorithm implements the local search procedure by use of numerical approximations to space-filling curves. Results of successful computational experiments are presented.

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## **CONTROL PHASE TRANSITION BEHAVIOR OF POLYCRYSTALLINE MEDIA BY GRAIN SIZE ENGINEERING. ROLES OF INTERNAL AND EXTERNAL LENGTH SCALES**

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We report recent advances in the experimental and theoretical study of effects of grain size (from 1500nm to 10nm) and sample size (from 1 mm to 1 micron) on the thermal, mechanical, cyclic and fatigue properties of NiTi polycrystalline SMAs which have nano-grain and grain-size gradient structures. Particular emphasis is paid to the significant effects of internal and external length scales on the properties and behaviors of the material. It is proposed that the emergence of the observed significant changes in the behavior of the material with the length scale reduction originates from the large increase in the area-to-volume ratios of the interfaces (grain boundary and phase boundary) in the polycrystal and that there is huge potential to improve and control the performance of the existing NiTi SMA by grain size engineering.

## **MULTISLOT LOW-SPEED INTERNAL COMBUSTION ENGINE IGNITION TRANSDUCER**

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The invention relates to mechatronics, particularly, to contactless pickups, and can be used in ignition systems for internal combustion engines (ICE), as well as in other mechatronic systems: switching, telemetry, distribution devices for automation and telemechanics. Multislot low-speed ICE ignition transducer comprises stationary stator, equipped with  $n$  uniformly distributed in circumferential direction sensor pairs, and rotary rotor, equipped with shielding, separating the elements of sensor pairs, which includes  $mn+1$  or  $mn-1$  slots for direct or reverse spark formation relative to direction of rotor rotation, where  $n$  is the number of ICE cylinders, while  $m$  is any natural number:  $m = 1, 2, 3, \dots$ . All these provide:

1. possibility of continuous switching, as well as
2.  $mn+1$  or  $mn-1$ -fold reduction of rotor rotation frequency for forward or backward spark formation, respectively,
3.  $mn+1$  or  $mn-1$ -fold increase in closed state time,
4. multiply higher mechanical and electrical reliability,
5. multiple increase of device accuracy and wear resistance.

## **ON GOAL ORIENTED FEATURE EXTRACTION STRATEGIES FOR PROPER ORTHOGONAL DECOMPOSITION BASED REDUCED ORDER MODELING IN STRUCTURAL DYNAMICS**

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The Finite Element method is frequently applied for the simulation of the dynamic response of engineering structures. However, a detailed model with sufficiently precise discretization of real structures, e.g. bridge buildings, introduces a tremendous number of unknowns that goes ahead with huge computational effort for transient dynamics analysis. For much faster simulations of the long term behavior or even parametric studies, reduced order modeling (ROM) is a suitable approach.

Besides modal reduction and Krylov subspace techniques, Proper Orthogonal Decomposition (POD) is a reduction method that enables for capturing nonlinearities approximately. POD is based on the generation of so-called snapshots of the high-fidelity systems response, from which a projection matrix is generated via main feature extraction. Projecting the original system of equations onto the defined subspace, a smaller set of equations with fewer unknowns is obtained which therefore can be solved more efficiently.

This contribution gives an introduction to the ROM approach in general and focusses on a goal oriented strategy for the snapshot generation for POD in particular. The results obtained using POD are compared to modal reduction results in terms of computational costs, accuracy and applicability. A reality-close bridge building is considered to evaluate the ROM efficiency.

## FORMATION OF TUNGSTEN AND MOLYBDENUM DISULFIDE MICRO AND NANOPARTICLES BY SPRAY PYROLYSIS

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Tungsten and molybdenum sulfides nanoparticles have attracted considerable interest of scientists because of their unique antifriction properties and possibility to use them as solid lubricants for applications when liquid lubricants cannot be used [1]. It has been shown [2] that spray pyrolysis which can be considered as one of the approaches to aerosol assisted chemical vapor deposition (CVD) processes can be successfully used to obtain spherical particles of molybdenum disulfide however influence of process parameters on size and structure of the particles formed has not been studied. As to synthesis by spray pyrolysis of tungsten disulfide nanoparticles only one paper has been published [3] in which formation of nested WS<sub>2</sub> particles exhibiting a rectangular parallelepiped shape with the structure of a closed nanoboxes was described. The aim of our work was to study experimentally the influence of the main process parameters of spray pyrolysis of (NH<sub>4</sub>)<sub>2</sub>MoS<sub>4</sub>-C<sub>3</sub>H<sub>7</sub>NO and (NH<sub>4</sub>)<sub>2</sub>WS<sub>4</sub>-C<sub>3</sub>H<sub>7</sub>NO solutions aerosol particles on the average size of MoS<sub>2</sub> and WS<sub>2</sub> particles, their size distribution, composition, and structure.

Spray pyrolysis was carried out in a tubular reactor with inner diameter of about 23 mm equipped with three inline resistive heaters. The first streamwise zone (T<sub>1</sub>=150-800 °C) was mainly used to evaporate solvent from aerosol particles, the second zone (T<sub>2</sub>=600-900 °C) served as a pyrolysis area, and electrostatic filter was placed in the third one (200 °C) where the particles obtained were collected. An aerosol of precursor solutions was created by piezoelectric nebulizer.

Processes in the first zone of the reactor determine the shape, size and structure of MoS<sub>2</sub> particles formed. It is possible to obtain hollow and solid particles with average size varied over the wide range depending on temperature in this zone. The fraction of hexagonal crystalline phase (the rest is rhombohedral phase) gradually increased from 78-80% to 98-99% and the size of coherent X-ray scattering regions for both phases slightly decreased from 55 till 35 nm with increase of T<sub>1</sub> in the range 300-800 °C. The temperature in the pyrolysis zone does not influence the size and structure of the particles obtained. The average size of MoS<sub>2</sub> particles gradually increased with concentration of (NH<sub>4</sub>)<sub>2</sub>MoS<sub>4</sub> in solution. The main process parameters have no effect on the chemical composition of products synthesized which always correspond to MoS<sub>2</sub>.

Solid particles of WS<sub>2</sub> with spherical shape and average radius varied in the range of 50-100 nm were synthesized by spray pyrolysis of (NH<sub>4</sub>)<sub>2</sub>WS<sub>4</sub>-C<sub>3</sub>H<sub>7</sub>NO solutions for the first time. In contrast to synthesis of MoS<sub>2</sub> the particles with near stoichiometric composition can be obtained only at pyrolysis temperatures above 800 °C. As well as for synthesis of MoS<sub>2</sub> dilution of the solution used for formation of aerosol leads to decrease of the average size of particles obtained and power of piezoelectric nebulizer does not influence the average size of WS<sub>2</sub> particles.

Solid disulfide particles consist of short and randomly oriented fringes of WS<sub>2</sub> and MoS<sub>2</sub>.

*The authors are grateful to the Russian Science Foundation for the financial support of the study (contract N 15-13-00045).*

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## DERIVING CONSTITUTIVE BEHAVIOR LAWS FOR COMPOSITES AND POLYCRYSTALS USING DIRECT MICROSTRUCTURE-RESPECTIVE FINITE-ELEMENT SIMULATIONS AND UNIFORM FIELD HOMOGENIZATION METHODS

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All materials have a scale below which they cannot be considered homogeneous anymore and at that scale the physical properties varies from one point to another. Explicit representation of the microstructure in numerical simulations is often not feasible due to a significant difference between the size the structure and the size of heterogeneity. In such cases, suitable for macroscopic computation effective physical properties and constitutive behavior laws can be obtained by considering a Representative Volume Element (RVE) of its microstructure [1].

Adopting a concept of an RVE one can treat it in two ways. First way employs direct numerical simulations with an explicit microstructure geometry. A finite-element model should be constructed, which is often done using Voronoi tessellation algorithm and its post-treatment. Explicit microstructure representation allows to incorporate many

geometrical and mechanical features in the model: such as material nonlinearities, complex interfaces and also possible local damage behavior. However, incorporating many features into the model may result in its extensive demand for resources and computational time.

Second way of treating the heterogeneous microstructure is adopting the “uniform field” homogenization methods. Such methods estimate an averaged response of a given inhomogeneity, which is seen as a single inclusion in an infinite homogeneous equivalent medium. The starting point of such methods was the solution for stresses and strains in the case of the ellipsoidal inclusion obtained by John Eshelby [2]. Several methods evolved from the Eshelby’s solution, each best suited for a certain type of composite or polycrystal.

In the talk, several examples of employing the above-mentioned homogenization techniques are shown, advantages and comparisons are presented. Issues of thermal residual stresses and energy dissipation due to plastic deformation are addressed.

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## MULTI-FLUID MODELLING OF SUSPENSION FILTRATION IN THE NEAR-WELLBORE ZONE OF INJECTION WELLS

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Injection wells are widely used in the oilfields to maintain reservoir pressure and increase ultimate recovery of hydrocarbons. During injection, water adsorbs solids admixtures from wellbore walls and fine particles from the pores in the near-wellbore zone, which results in the flow of suspension in the near-wellbore zone. Suspended particles are trapped in pores, which results in permeability damage and, as a result, in the decrease in injectivity of the well. In order to maintain the injection flow rate (injectivity), one needs to either increase the pumping pressure or to introduce additional water cleaning equipment on surface. Both results in the increase of the cost of development of the reservoir. To optimize the process of water injection, it is proposed to use a combined approach based on modeling of suspension filtration in porous media with account for permeability damage and recovery.

In order to do so, we present a development of the multi-fluid model of suspension filtration in a porous medium, which was first disclosed by the authors in [1]. The derivation of the governing equations from conservation laws is carried out in the multi-continua approach [2], where the three phases, namely the carrier fluid, the suspended particles, and the particles trapped in pores are treated as three different continua described by different hydrodynamic field variables. Fluid fluxes through large pores of the porous medium and through narrow pores of the packed bed of deposited particles are explicitly taken into account, via two different values of permeability. These are the key novel features, which distinguish it from the classical deep bed filtration model [3, 4]. The model predictions are compared with laboratory data sets on the contamination of a core sample. The most recent progress in the model development is mainly in taking into account particle mobilization, compressibility of the fluid, two-phase filtration (oil/water), and reservoir influx. Applications of the model are primarily in the oil and gas industry: drilling mud invasion and cleanup in the near-wellbore zone, fines migration in porous medium and suspension filtration in propped hydraulic fractures; permeability damage and recovery in the near-wellbore zone of injection wells, which are used to maintain reservoir pressure.

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## DYNAMICS OF THIN ROD AFTER THE LONGITUDINAL IMPACT BY A RIGID BODY

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Longitudinal impact of a rigid body on a thin elastic rod is studied. The opposite end of the rod is assumed to be fixed. In order to find the contact force  $P(t)$  we use the Sears model [1] including both the waves propagation in the rod and the local deformations described by the Hertz contact model [2]. The obtained non-linear integral-differential equation [3] is solved numerically which allows one to determine the force  $P(t)$  and the impact time  $T$  for various values of the problem parameters.

The special attention is paid to analysis of the rod vibration when the impact is over. In this case the rod exhibits free longitudinal vibrations generated by the impact. The longitudinal deflections are expanded in the Fourier series and the corresponding vibration amplitudes of eigenmodes are found. A distribution of the impact energy after the impact is studied. This energy consists of the energy of bounced impactor and sum of vibrational energies of the rod eigenmodes. The next step is to analyze the possible parametric resonances caused by bending vibrations of the rod. There exist a number of works, Refs [4,5] etc, which are concerned with the problem of parametric resonances for the case of prescribed force  $P(t)$ . However the present report differs from the previous ones in that force  $P(t)$  is to be determined as solution of the collision problem.

It is shown that the vibrations have a character of beatings in the resonance case. By using the results of Refs. [4,5] we estimate the maximum amplitude of beatings and determine the impact parameters at which this maximum can be achieved.

*The present report is supported by the RFBR grants No. 16.51.52025 MHT-a and 16.01.00580-a.*

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## APPLICATIONS OF PARTICLE DYNAMICS - FROM THE MOLECULAR SCALE TO THE CONTINUUM

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The Molecular Dynamics (MD) simulation method, invented by Berni Alder in the mid 1950s, provides an essentially exact description of matter at the atomic level once a force law has been specified. In MD, Newton's motion equations are solved numerically for a set of particles, yielding time ordered sets of positions and momenta from which thermodynamic properties can be obtained through the application of Boltzmann's statistical mechanics. Extensions of the basic method involving modifications to the boundary conditions and motion equations have made possible the investigation of non-equilibrium phenomena.

Smooth Particle Applied Mechanics (SPAM) - invented by Lucy, Monaghan and Gingold in the late 1970s to solve problems in astrophysics, also uses particles. In this case, the underlying equations being solved are those of continuum mechanics. The particles act as interpolation points which transform the partial differential equations into ordinary differential equations that are then solved using similar methods to those employed in MD.

Both MD and SPAM are powerful tools which can be used to study the behaviour of matter. MD is at its most powerful when used to generate pseudo-experimental data for testing new statistical mechanical theories or discovering new constitutive laws. It can also be used to yield mechanistic information. SPAM is useful for modelling the behaviour of matter at the scale of interest to the engineer. When the two methods are used together, MD can provide the material properties required as input to SPAM simulations, allowing true multiscale capability.

In this lecture, examples will be given from both these particle-based simulation methodologies including the simulation of confined fluid flow, Joule-Thomson throttling, radiation damage in ceramic wasteforms, filtration, and fragmentation. In the latter example, we show how the MD has been used to parametrise SPAM.

## EFFECTIVE ELASTIC PROPERTIES OF COMPOSITES WITH PARTICLES OF POLYHEDRAL SHAPES

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Regular polyhedra can be used to describe shapes of some crystalline metallic particles that are encountered as precipitates or synthesized as powders to be used as additives in particle-reinforced composites ([1-6]).

In this study, we analyze the effect of shape of several representative convex polyhedral on the overall elastic properties of particle-reinforced composites. We utilize stiffness contribution tensor formalism to estimate overall elastic properties of materials with polyhedral inhomogeneities and compare the results with direct finite element simulations of periodic RVEs. Contributions of 15 convex polyhedral particle shapes to the overall elastic properties of particle-reinforced composites are predicted using micromechanical homogenization and direct finite element analysis approaches. The micromechanical approach is based on the combination of the stiffness contribution tensor (N-tensor) formalism with Mori-Tanaka and Maxwell homogenization schemes. The second approach involves FEA simulations performed on artificial periodic representative volume elements containing randomly oriented particles of the same shape. The results of the two approaches are in good agreement for volume fractions up to 30%. Applicability of the replacement relation interrelating N-tensors of the particles having the same shape but different elastic constants is investigated and a shape parameter correlated with the accuracy of the relation is proposed.

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## DEVELOPMENT OF THE ELECTRO-MECHANICAL MODELS OF THE CARBON NANO-WHISKERS AS MASS DETECTORS

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Carbon nano-whiskers are the monocrystalline fibers made of amorphous carbon. These beam-like structures have the linear size of several hundred nanometers and about 10 nanometers in diameter. Due to small size and good strength, such whiskers were recently proposed to use in micro- and nanotechnology.

This work is devoted to use of carbon whiskers in nanoelectromechanical systems (NEMS). The double-whisker system consists of two parallel carbon nano-beams. The beams are connected with a thin elastic jumper. The beams are considered as the rigid bodies and a jumpers is represented as an elastic spring. As a result, a mathematical model with two degrees of freedom is obtained. The model predicts the beats-like oscillations. Parameters of the beats such as period of an envelope curve, amplitude and frequency show the discrepancy of masses. Due to this, carbon based double-whisker resonators can be used for mass measuring.

The oscillations can be excited in two different ways. Impulse load is the simplest method of excitation, but the amplitude of registered signal wouldn't be enough for precise measurements. Due to this, another method is proposed to solve this issue. It is based on the excitation of oscillations using piezoelectric element. Building-up of the oscillations prolongs during the enough time to reach the maximum amplitude. Hence, the oscillations form is close to the resonance one.

High amplitude can be registered with a sufficient accuracy using the electrical circuit. In this circuit the double-whisker resonator is used as a capacitor such that each whisker serves as one of the capacitors plates. Mechanical oscillations of the whiskers are related to voltage oscillations, which in turn can be registered very precisely.

## **CONTACT PROBLEM ON INDENTATION OF A CONICAL PUNCH INTO AN ELASTIC TRANSVERSELY-ISOTROPIC FUNCTIONALLY-GRADED HALF-SPACE**

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Indentation of an elastic transversely isotropic half-space with functionally graded transversely isotropic coating by a conical punch is considered. Elastic moduli of the coating vary with depth according to arbitrary independent differentiable positive functions. Elastic moduli of the substrate are constant. Cases of free and fixed boundaries of the contact area are considered. The problem is reduced to the solution of a dual integral equation over Hankel image of contact pressure. Kernel transforms of the integral equation is constructed numerically. Using specially design approximation of the kernel transforms the approximated solution of the problem is constructed in analytical form. The solution is asymptotically exact for small and large values of relative coating thickness. Some aspects of modeling of micro- and nano- indentation experiments are discussed. Qualitative differences in process of elastic deformation of bodies with homogeneous and functionally graded coatings are illustrated.

*This research was financially supported by Russian Science Foundation grant no. 15-19-10032.*

## **ON STRUCTURE OF ELECTROHYDRODYNAMIC FLOWS CAUSED BY FIELD-ENHANCED DISSOCIATION IN VARIOUS SYSTEM CONFIGURATIONS**

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Designing electrohydrodynamic (EHD) systems pays special attention to electrode-configuration choice since it determines the flow structure and the device performance. Most EHD systems use a sharp electrode (needle, blade, or wire), which forms the flow with well-studied structure, directed from the electrode towards the counter one. However, other electrode configurations can lead to radically different flow structures and thus to new prospects for the development of various EHD systems.

The present work uses computer simulation to study EHD flows caused by field-enhanced dissociation in relatively high-conducting liquids. EHD flows of the type are still poorly studied and, unlike the injection ones, they can be caused by specific configuration of solid insulation. The work investigates their structures and shows their variety.

The base case is a blade-plane system that shows a flow of classical structure. Next, a hollow tube that can be treated as a rolled blade can give rise to EHD flows of unusual structure. Depending on geometry parameters, the flow structure can be close to the classical one or be as in systems with the major role of solid insulation. At last, the cases of conditioning role of solid insulation, the systems with insulation barriers, complete the study. Specifics of each case is analyzed and discussed.

## **IMPACT OF THE NEW VIBROEXCITATION METHOD TO THE SCREENING PROCESS INTENSIFICATION OF BULK MATERIALS**

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One of the new, and perhaps the most perspective development directions of screening equipment, at present day, in our opinion, are the screens "with complex excitation of the material." Sometimes the term "dynamic excitation" is used.

One example of complex impact on the screened material is spiral vibrating screen design. This screen is an aggregate that combines the principles of drum and vibrating screens.

New excitation principles of bulk material are used in screens using «Kroosher» technology, the screen has the properties of multifrequency resonance oscillation system. Moreover, among the claimed benefits are large capacity, high screening efficiency, guaranteed effect of self-cleaning screens, etc.

Considering the urgency of the research areas in the D.Serikbaev East Kazakhstan State Technical University (EKSTU) research in this area is conducted for several years. The result of this work is series of new solutions for the use of relatively simple designs for devices that implement the principle of complex material excitation on the screen's sieve (hereinafter SS - screening surface).

The effectiveness of the screening process can be enhanced due to the intensification of one or both stages of the

process. But the intensification of the first stage of screening is the most promising way to improve the screens performance.

For this purpose, initially, we proposed new screen design, feed elements (FEs) are fixedly mounted above the screen surface, made in the form of rods, mounted on separate frame. This design allows intensifying the process of mixing the material on the SS, which speeds up the passage of the lower particles class to the sieve.

Intensification of screening stages is provided by: firstly, active motion of FE relatively bulk material particles, resulting in an inhomogeneous behavior of individual material monolayers (active mixing); secondly, more efficient sieve loading that allows creating the conditions to maximize pushing and mixing forces.

As a result of the two screening stages intensification, the productivity increases. Also as a result of more efficient surface use is possibility of metal consumption reduction, and as a result, screen power consumption. The main advantage of the proposed screening method is that it can be used for the modernization of all types of flat screens.

To check the proposed solutions, a number of theoretical and experimental studies were carried out. The obtained data show that the use of renewable energy leads to intensity increasing of lower grade passage of bulk material to the sieve on 6.6 ... 13.3%. Moreover the required screening performance is increased by 10 ... 17%.

Thus, it can be concluded that authors proposed a new way to improve the efficiency of the screening process (by appropriate design of new units), which has a significant effect on the screening process kinetics and the concentration state of fine particles in the granular layer; it increases the overall screening efficiency due to acceleration of the first phase of screening, i.e. time acceleration of particulate material passage to the sieve.

## ON STRUCTURAL TRANSFORMATIONS UNDER MECHANICAL IMPACT

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One of the most interesting and promising areas in the mechanics of solids lies in studying structural transformations of material at high strain rates, when a complex rearrangement of crystalline lattice, caused by its local loss of stability, occurs during extremely short times, not exceeding few microseconds. Recent experiments on high speed deformation demonstrate that these changes in microstructure of material may exert a serious influence on its physical properties. At macroscopic scale they result in energy loss spent on the transformation of crystalline lattice. There is a big experimental data devoted to the problem, but it still requires an appropriate mathematical model. For this purpose we consider two-component medium, assuming that it consists of two lattices connected by nonlinear force with several equilibria. The method of investigation is based on a discrete analogue of continuum model, allowing to predict the time during which the process of structural transformation takes place. Analytical expressions are compared with results of numeric solution performed by finite difference method.

## STUDYING MECHANICAL PROPERTIES OF MATERIALS IN WELDED JOINTS OF THE VT1-0 TITANIUM ALLOY AND THE 12CR18NI10TI AUSTENITIC CORROSION RESISTANT STEEL WITH AN INTERMEDIATE COPPER INSERT BY KINETIC INDENTATION

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The mechanical properties of the laser-welded joint of the VT1-0 titanium alloy and the 12Cr18Ni10Ti stainless steel with an intermediate copper insert are studied in the work. It is known that, after penetration, a welded joint, initially comprising three different components, is characterized by an inhomogeneous microstructure, for which the averaged properties cannot always be considered. The degree of heterogeneity in the weld and the order of the values of the mechanical properties must be clear to investigate further the performance of the welded joint and to state the problem of evaluating its stress-strain state. It is shown that this mode provides for an intensive diffusion interaction of the materials to be joined and the copper plate, allows obtaining a smooth change in the chemical composition, and is characterized by the scatter of the mechanical properties in the bulk of the joint. With the application of a technique for the determination of the strain-hardening diagram by the results of indentation and scratch tests, the strength properties of the surface layers of the different zones of the welded joint were determined. Kinetic indentation and scratching is performed on a TI950 Nanotriboindenter test system. The technique is based on the analysis of the indentation and scratch test results together with the results of a numerical experiment on a fine-grid finite element model of the testing process. The obtained results have been used to plot flow-stress curves for the zones in the welded joint. The investigation results will further be used to simulate the effect of the nonuniform distribution of mechanical properties on the characteristics of the stress-strain state of a welded joint under loading, and they will offer practical

recommendations for further work with this type of welded joints.  
*This work was supported by RFBR grant No. 16-38-00741 mol\_a.*

### **STUDYING MECHANICAL PROPERTIES OF HETEROGENEOUS MATERIAL BASED ON EPOXY OLIGOMER FILLED WITH SILICA BY MICROINDENTATION**

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A promising way to increase the performance, power performance, durability and reliability characteristics of electric machines is to increase the efficiency of electrical insulating materials (EIM). The current trend of a radical improvement of the EIM performance is the use of modifier additives of different nature in a composition comprising an oligomeric base (usually epoxy resins produced by tonnage) and a curing agent, which causes base polymerization. The scope of the work is the study of the mechanical properties of epoxy resin with silica nanoparticles at the microscale level. A Primer 204 epoxy resin with the addition of Tarkosil T-20 silica from 1,2 to 3,5 % volume content with gradual increase of the additive by 0,2 % for every sample was studied. All the experiments were performed using a FISCHERSCOPE HM2000 XYm complex. The introduction of modifying silica nanoparticle additives increases the hardness and reduced elastic modulus of Primer 204 epoxy resin. Load, loading time, hold time and applied displacement have a significant effect on the behavior of the material. The processed experimental data has demonstrated that the test material exhibits viscosity properties at the micro level, manifested in the existence of the creep and stress relaxation phenomena.

*This work was partially supported by RFBR grant No. 16-08-01154 A in terms of developing research methods.*

### **MECHANICAL PROPERTIES AND FRACTURE BEHAVIOR OF THE BIMETAL PRODUCED BY EXPLOSION WELDING UNDER LOW-CYCLE FATIGUE**

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The scope of the work is the study of the mechanical properties of the "copper M1 – steel 09G2S" and "steel 08Cr18Ni9 - steel 09G2S" bimetal obtained by explosion welding under low-cycle fatigue. All the low-cycle experiments were performed using a INSTRON 8801 complex on a sinusoidal cycle with a loading frequency of 5 Hz. It simulates a condition of relatively rare and significant cyclic loadings. The coefficient of cycle asymmetry is zero. By results of tests the number of cycles before damage at different levels of maximum stress was carried out. Furthermore the mechanical properties of single-layer strips of steel 08Cr18Ni9, steel 09G2S, copper M1 were determined at the similar experimental conditions. The following results have been received. The welded seam has a significant effect on the behavior and strength of the bimetal. The processed experimental data has demonstrated that in case of design of bimetal products it is necessary to consider the fact that in case of certain cycle loadings better bimetal works, and in case of others – the initial one-layer metals.

*This work was supported by RFBR grant No.16 –38–60169 mol\_a\_dk.*

### **MATHEMATICAL MODELING OF A MULTIPLY CONNECTED BORDER OF THE STOKES VISCOUS FLUID**

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The quasi-stationary Stokes approximation is used to describe flows with small Reynolds numbers, such as viscous fluid, glass[1] and lava[2]. Two-dimensional mathematical models allow us to qualitatively explore processes occurring in such flows[3]. The pressure distribution of fluid in some two-dimensional area can be found as the expansion in series of harmonic functions [4]. From the pressure distribution, we can calculate the velocity on the boundary and investigate the boundary deformation due to capillary forces, external pressure, centrifugal forces, etc.

The goal of this work is to develop and implement a mathematical model which describes the evolution of multiply connected boundary by capillary forces.

The following results were obtained. First, a theoretical model of evolution of multiply connected boundary was built. Second, the pressure distribution in a particular region was obtained expressed in a basis of the complete system of harmonic functions. Third, from that pressure distribution we computed the velocity of the region border and computationally modeled the process of border deformation.

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### ESTIMATION OF THE MOST PROBABLE ZONES OF DETERIORATION OF THE PIPELINE PULSE PNEUMOTRANSPORTATION

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During processing of the fulfilled nuclear fuel there is a necessity of transportation and recycling of formed firm waste materials, namely insoluble in acid solutions of metal covers of radioactive fuel. These covers are transported by a flow of the compressed gas in pipelines of system of pulse pneumatic transport to collectors and then to a burial place. The factory experience of operation of pipelines of the system shows, that there exist zones of a pipeline (nearby a pipe corner of turn on  $90^0$ ) that are exposed to the most intensive deterioration.

The intensity of the corner wear process, as well as all system of pipelines, depends on many factors: velocity of a gas flow, angle between a direction of gas velocity and pipe surface at the corners (corner of attack), concentration of a firm phase in a flow and some others.

In a paper the results of experimental and numerical modeling of a gas flow in the pipe are presented with the purpose of an estimation of zones of deterioration at constant values of radius of a bend and diameter of the pipeline.

The model is based on conservation laws of mass, momentum and energy for non-steady two-dimensional compressible gas flow in case of axial symmetry. The processes of viscosity, heat conductivity and turbulence have been taken into account.

From the analysis of experimental data received on model and numerical simulations even within the framework of homogeneous approach it follows that there exist three local zones with of highly increased level of deterioration, that may result in violation of the whole device proceeding and may influence safety and serviceability of the system.

### SPECIFIC FEATURES OF GAS IGNITION IN DETONATION CHAMBERS

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The problem of construction of engine based on detonation phenomenon is one of the widely studied in many research centers all over the world. There are many technological and scientific aspects here. Vortex or cylindrical chambers are one of the engine parts. The stability of the flow in the chamber is often interrupted by gas mixture self-ignition observed in experiments, although the value of mean gas temperature in the chamber (after the passage of initial pulse) is essentially lower than the value of self-ignition. The reasons of the effect are not quite clear. The recent paper is devoted to theoretical and experimental study of the problem.

The numerical calculations of the flow field in a planar vortex chamber and cylindrical detonation chamber have been performed. The model is based on conservation laws of mass, momentum and energy for non-steady two-dimensional compressible gas flow in case of swirl axial symmetry. The processes of viscosity, heat conductivity and turbulence have been taken into account. It was found that transition of kinetic energy of gas into heat due to processes of dissipation generates “hot spots” in boundary layers at the chamber walls. The gas temperature at the spots may exceed the temperature of gas ignition ( $T = 1200$  K), while the surrounding regions remain still cold. It may be the reason of

cold gas self-ignition observed in experiments.

For appreciation of the flow geometry on the appearance of the hot spots the three-dimensional approach has been used as well. Three-dimensional numerical simulations revealed the appearance of micro vortexes at the walls of the chamber that cannot be described within the two-dimensional approach. The existence of such a structure may play a decisive role in a flow self-ignition (as well as a generation of a mixing zone in case of separate inlet of a fuel and oxidizer within the chamber).

To appreciate the influence of turbulence on the gas self-ignition, the numerical simulations of laminar flow were performed on the base of Navier-Stokes equations at the same initial values of the problem parameters. For laminar flows the mixture self-ignition may occur as well. Although the maximum value of temperature in laminar hot spot  $T = 1370$  K is significantly less than turbulent  $T = 2110$  K at the same instant. So the flow turbulence may play decisive role in possibility of gas self-ignition.

## **A SPACE-TIME FULLY DECOUPLED WAVELET GALERKIN METHOD FOR STUDYING NONLINEAR STRUCTURAL DYNAMICS**

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Nonlinear dynamic analysis of structures is quite a daunting and costly job using conventional techniques, in which the changing stiffness matrix resulting from the nonlinear behavior depends on the displacement and demands a repeated calculation at each time step, requiring a considerable amount of computations to achieve a steady state. Motivated by such a problem, a space-time fully decoupled Galerkin formulation for analyzing nonlinear structural dynamics is developed through the use of the sampling approximation for a function defined on a bounded interval by combining techniques of boundary extension and Coiflet-type wavelet expansion. In such a wavelet method, all matrices generated from the spatial discretization are completely independent of the displacement, thereby saving considerable computing resources. By solving several widely considered test problems, results demonstrate that the proposed method has an excellent accuracy and efficiency. Most importantly, the study also indicates that the proposed wavelet method is capable of solving the strongly nonlinear problems, such as the extremely large amplitude vibration of circular plates. Even for the bending of circular plates under such a large deformation, finding a convergent solution is also an extremely difficult task for conventional methods. Moreover, a systematic investigation on the nonlinear vibration of beams and plates is conducted.

## **GRAZING INDUCED BIFURCATIONS: INNOCENT OR SINISTER?**

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In this lecture I will examine nature of subtle phenomenon such grazing bifurcations occurring in non-smooth systems. I will start with linear oscillators undergoing impacts with secondary elastic supports, which have been studied experimentally and analytically for near-grazing conditions [1]. We discovered a narrow band of chaos close to the grazing condition and this phenomenon was observed experimentally for a range of system parameters. Through stability analysis, we argue that this abrupt onset to chaos is caused by a dangerous bifurcation in which two unstable period-3 orbits, created at "invisible" grazing collide [2].

The experimentally observed bifurcations are explained theoretically using mapping solutions between locally smooth subspaces. Smooth as well as non-smooth bifurcations are observed, and the resulting bifurcations are often as an interplay between them. In order to understand the observed bifurcation scenarios, a global analysis has been undertaken to investigate the influence of stable and unstable orbits which are born in distant bifurcations but become important at the near-grazing conditions [3]. A good degree of correspondence between the experiment and theory fully justifies the adopted modelling approach.

Similar phenomena were observed for a rotor system with bearing clearances, which was analysed numerically [4] and experimentally [5]. To gain further insight into the system dynamics we have used a path following method to unveil complex bifurcation structures often featuring dangerous co-existing attractors.

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## TWO-DIMENSIONAL THEORY FOR DESCRIBING OF RAYLEIGH WAVE FIELD IN LAYERED CYLINDRICAL SHELL

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The far-field of the non-stationary Rayleigh wave is characterized by jumps, high-frequency vibrations, localization near the surface. The numerical solution of corresponding 3D problems is difficult and requires much time for calculation. On the other hand, the 2D classical and refined theories of shells and derivation techniques for such theories as series expansion of 3D fields in the normal direction, asymptotic integration, variational methods etc. are not applicable in the vicinities of wave fronts. In this work, a two-dimensional asymptotic theory is proposed, which allows to calculate far-field of Rayleigh wave in an infinite layered cylindrical shell subjected to non-stationary surface load. The theory is based on the asymptotic techniques developed in [1-4]. First the asymptotic model is constructed which includes hyperbolic equations describing the propagation of the wave along the surface and a sequence of Dirichlet problems for the Laplace equation describing exponentially decaying wave field in each of the layers. These problems are solved explicitly with Poisson's integral, then all the unknown functions are consequently expressed in terms of the functions defined on the surfaces. Thus a system of two integro-differential equations is obtained for the functions which do not depend of thickness coordinate, so the problem is reduced to two-dimensional one. By deriving of the model it is assumed that the elastic properties of the layers satisfy the following condition: the speed of Rayleigh wave, for which the model is derived, is less than the shear wave speeds in all the layers. The numerical examples are presented which confirm the applicability of the proposed theory by comparison with the exact solution.

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## ELECTROHYDRODYNAMICALLY DRIVEN TWO-PHASE HEAT TRANSPORT DEVICES

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Electrohydrodynamic (EHD) conduction pumping of a dielectric liquid arises from the interaction of the induced electric fields and flow fields via the Coulomb force. The required free charges come from the dissociation and recombination of neutral electrolytes present in the fluid. When the external electric field exceeds a threshold, the rate of dissociation exceeds that of recombination. There is a non-equilibrium heterocharge layer that forms in the vicinity of each electrode due to ion motion caused by the Coulomb force. The attraction of the ions present within the heterocharge layers to the adjacent asymmetric electrodes of a given pair causes bulk fluid motion in the desired direction.

This presentation will illustrate the EHD conduction pumping mechanism and its resultant transport characteristics. Specifically, the heat and mass transport resulting from EHD conduction pumping of a dielectric fluid in macro-, meso-, and micro-scales in the presence and absence of phase change (liquid/vapor) will be described.

EHD pumps are simple in design, light weight, non-mechanical, free of vibrations and noise, and they allow for effective active control of heat transfer and mass transport. EHD pumps require minimal electric power to operate. The resultant heat transport capacity is typically three orders of magnitude larger than the electric input power.

## SKIN EFFECT OF REDISTRIBUTION OF DISSOLVED HYDROGEN IN METALS UNDER TENSION

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Plastic deformation is accompanied by structural rearrangement of the material. Prediction and diagnosis of such adjustment is an important task, since for structural materials, the plastic deformation precedes the destruction. One of the important features of plastic deformation is the redistribution of natural hydrogen that is inside metals. This process is associated with a number of mechanical phenomena, ranging from the diffusion of hydrogen into the zone of tensile stresses and ending with a change in the size of the structural elements of the metal and the appearance of new structural defects.

Studies show that there is a good correlation between the concentration of diffusively mobile hydrogen and the value of plastic deformation, in many cases they are linearly related.

The report describes a new effect, discovered by the authors in the process of investigating specimens broken with different degrees of plastic deformation. A careful study of the distribution of hydrogen concentrations shows that all changes that are associated with plastic deformation occur in the surface layer of about 200  $\mu\text{m}$  in thickness. This thickness is approximately equal to the size of the metal grains.

This result agrees well with the data on the thickness of the layer providing residual stresses after plastic deformation. According to our earlier estimates, the transition to plastic flow is associated with the forces of surface tension of the metal grains.

Thus, this result gives evidence submitted on the surface nature of the damage accumulation during plastic deformation. On the one hand, this is the basis for developing methods of technical diagnostics of damage by the state of a thin layer. On the other hand, the obtained data makes it possible to develop methods for reducing the damage in plastic deformation by treating the metal surface.

## NUMERICAL MODELLING OF SURFACE-REINFORCED TUBE ROD STRUCTURES

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The study treats rod structures consisting of tubes whose external surfaces are reinforced by means of suitable reinforcing material (reinforced composites, special nanomaterials etc.). It is assumed that the technology of reinforcement deposition is diffusive (painting, pulverization, some electrochemical methods of deposition). Thus a transition area of gradual penetration of the reinforcement into the basic material (substrate) emerges. However, to solve the diffusion problem, one needs to find the diffusion coefficient which turns to be a complex experimental task. Hence, the authors use another approach, proposing a quadratic approximation of material elastic modulus, which varies within a range bounded by the elastic modulus of the reinforcement and that of the substrate. A complex tube structural element is thus formed having two areas with smooth transition between them: a substrate (core) and a transition area. It is assumed that the element deformation under loading is non-homogeneous linear-elastic, without damage. Loading is static (axial tension/compression) applied under normal temperature and humidity. The linear axial strains are constant within the core and following a quadratic parabolic law within the transition area-strain transition between both areas is also smooth. Stresses are distributed evenly within the core and non-linearly within the transition area. A rod under tension is separately considered and its strength is calculated. Moreover, a compressed rod is also analysed assuming a possibility of rod stability loss. Tension stiffness and bending stiffness of the complex tube are calculated considering eventual stability loss under bending. The authors outline a possibility to homogenize the tube structural element using the stiffness values and employing FEM codes for complex tube rod structures. The quadratic approximations are performed within an arbitrary thin transition area and their accuracy is close to that of the FEM calculations.

Such an approach yields stress and strain expressions, which involve the thickness of the transition area and the edge axial deformation. Those two parameters of the approximate calculation model are found using the equilibrium conditions and solving 3d degree algebraic equations. Thus, the approach becomes practically useful. A numerical example is set forth in the study proving model applicability and a possibility of decreasing the structure weight by using thinner but appropriately reinforced tubes.

The analysis of the complex structure shows that it is advisable to deposit a material with combined (reinforcing and protective) properties instead of depositing regular anticorrosion and fireproofing layers.

## THE LATERAL STABILITY PROBLEM AND NUMERICAL SIMULATION OF A SLENDER DELTA WING DURING SELF-EXCITED WING ROCK

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The Lateral stability problem of modern combat aircraft in high angle of attack is an important issue related to flying safety. This investigation focuses on the sideslip behaviors of a slender delta wing during self-excited wing rock. The nonlinear double degree of freedoms aerodynamics model is established for governing the coupling movement in combined free-roll and free-sideslip motion. Then, a numerical investigation is conducted on the dynamic characteristics of an 80° delta wing in combined free-roll and free-sideslip by solving flow governing equations and Euler rigid-body dynamics equations simultaneously. Implicit, upwind, flux-difference splitting, finite volume scheme and the second-order-accurate finite difference scheme are employed to discretize and solve these governing equations. The governing equations of fluid and movements are solved alternately with a coupling method, either loosely coupling or tightly coupling, both coupling methods are discussed. Well-regulated sideslip oscillation is observed as expected. The sideslip behaviors are mostly affected by the roll oscillatory properties, i.e., the frequencies and phases. The loosely coupling method achieved considerably efficiency and accuracy. The behaviors of double DOFs motion is more complicate than that of single DOF wing rock.

## EXPERIMENTAL RESEARCH OF VISCOELASTIC PROPERTIES OF HIGHLY-FILLED POLYMERS UNDER COMPLEX HARMONIC LOADINGS

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The topic relevance is due to: the use of highly-filled polymer composites in important aerospace structures and other industries; the action of complex harmonic loadings on structures where highly-filled polymers are used; the need to develop methods of experimental research and to define deformation properties of materials and calculation methods for structures working in extreme conditions.

The aim of this research is to develop methods for conducting the experiment, to define viscoelastic parameters of highly-filled polymer composites under stationary two-frequency (dual-frequency) loadings, and to identify the mathematical model for calculating the stress-strain state of viscoelastic aerospace structures.

As a result of this work, nonlinear representation of stress and strain under two-frequency loadings were presented. It is based on representation developed by Volterra [1-3]. It was used polynomials to describe viscoelastic parameters on frequency, a time-temperature superposition for the accounting of the viscoelastic properties on the temperature, and the Fourier series to determine the viscoelastic parameters. It was also developed experimental design, determined material constants, and checked the model adequacy.

*The work was supported by Grant of the Russian Foundation for Basic Research (grant № 16-31-00230).*

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## FOUR-ION MODEL OF AN ELECTROHYDRODYNAMIC FLOW IN THE TWO-WIRE ELECTRODE SYSTEM

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The structure of an electrohydrodynamic flow of injection type is defined by electrophysical and electrochemical properties of the working fluid, as well as the properties of the electrode-liquid contact. The electrochemical asymmetry of the electrode-liquid contact is required in the symmetrical electrode system to pump fluid through the system, which can be achieved if electrodes made of different materials or with different coatings or using a liquid with an electron-

acceptor impurities.

Previous works analyzed the structure of EHD flow in the symmetric electrode system and ascertained the effect of the injection intensity on each electrode upon the kinematic and dynamic structure of the EHD flow [1, 2]. Computer simulation of generation and development process of the latter showed that charge plug can form behind electrode under certain conditions; this inhibits the through pumping of liquids and can be removed by selecting the impurity composition of the liquid for the injection to proceed on the surfaces of both electrodes [3]. Earlier computer simulation of the EHD flow, observed in the open channel, analyzed the effect of the level of the low-voltage conductivity [4] and dielectric walls on the flow structure [5].

Four types of liquid ions form in the symmetric system of electrodes, where a through flow of the injection type is realized: those resulting from the injection from the electrodes and those dissociated in the bulk. In the connection, the paper presents the results of computer simulation of the generation and development process of the EHD-flows in a symmetric system of two wire electrodes in a closed channel on the basis of a complete set of EHD equations, which takes account of four ion varieties.

As the result of simulation, the main features of the injection-type EHD flow were obtained. A special feature of the model is the capability to analyze the processes of mutual recombination of injected and dissociated ions. In addition, the model with the closed channel allows accounting for the impact of the uncompensated charge on the cyclic development of EHD flows and that of differences in the properties of injected and dissociated ions.

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## MULTISCALE STRUCTURE OF POLYNOMIAL DYNAMICS

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We consider a wavelet based multiscale description for nonlinear optimal dynamics (energy minimization in a high power electromechanical system as a key example).

In a particular case, we have the solution as a series on shifted Legendre polynomials parametrized by the solutions of the reduced algebraical systems of equations. In the general case, we represent the solution via multiscale decomposition in the base of various families of compactly supported wavelets. In this case the solution is parametrized by solutions of two reduced algebraic problems, one as in the first case and the second one is some linear problem obtained from the popular wavelet constructions: Fast Wavelet Transform, Stationary Subdivision Schemes, the method of Connection Coefficients. Such a machinery allows us to consider maximally localized bases in the underlying functional spaces together with most sparse representation for all type of operators involving in the initial set-up.

All that provides the best possible convergence properties and as a result our numerical modeling is more flexible and saves CPU time. In addition, the final representation is parametrized by the reduced pure algebraic construction (the so-called general dispersion relations) and allows us to solve the dynamical or optimal control problems (energy minimization, e.g.) in a most effective way.

## QUASICLASSICS IN WIGNER-MOYAL-VON NEUMANN FRAMEWORK VIA MULTIREOLUTION

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We present the application of our variational-multiscale approach to numerical/analytical calculations in the general quasi-classical set-up. The starting points are Wigner-Weyl-von Neumann framework as well as Moyal (naive)

deformation quantization. Our technique allows to cover all complicated underlying features of complex quantum dynamics based on the proper choice of background functional spaces which determine dynamical properties together with the internal structure of pseudo-differential operators incorporated in the full hierarchy of Wigner-like equations describing the evolution of the quasiprobability beyond trivial gaussian-like area with pure positive Wigner functions. The choice of hidden underlying symmetry and its representation on the orbits of proper actions provide us with the filtration of the background Hilbert space of states which implies the whole tower of internal hidden scales by using multiresolution decomposition.

All that allows to consider maximally localized quantum states and most sparse representation for all set of observables. At the same time the orbit structure allows to consider basic non-local phenomena like entanglement with possible subsequent decoherence.

Our main applications in this consideration are related with a description of quantum properties in nonlinear beam dynamics, both in accelerator and plasma physics but such general background provides all possibilities to describe the modeling of prototypes of any future quantum devices.

### **THEORETICAL AND NUMERICAL ANALYSIS OF THE FLOW SEPARATION CRITERION FOR HYPERSONIC NONEQUILIBRIUM FLOW OVER COMPRESSION CORNER**

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Through combining the Triple Deck theory in the analytical treatment of shock wave boundary layer interactions and the numerical simulation of hypersonic nonequilibrium flow over compression corner, the influence factors on flow separation are analyzed, and a criterion parameter to predict whether the separation occurs is proposed. The criterion parameter ( $S$ ) is the product of the powers of the corner angle, the free stream Ma number and Reynolds number, and the Chapman-Rubensin parameter. It is based on the existing formula of the incept separation angle for calorically perfect gas flow, but the reference temperature and the corresponding viscosity in the calculation of Chapman-Rubensin parameter are determined by the reference enthalpy with chemical equilibrium assumption, which introduces the high-temperature gas effects. The powers in the criterion parameter ( $S$ ) and the critical value of  $S$  for incept separation are determined through large number of numerical simulations of hypersonic nonequilibrium compression corner flow for 3 corner angles (15, 18 and 24 degrees), where the 12 free stream Mach numbers range from 8 to 35, the 36 gas densities are corresponding to the altitudes from 30 to 65km, the freestream Reynolds numbers range from 10000 ~ 500000.

*The research is funded by the National Natural Science Foundation of China (11572348).*

### **THE ROLE OF SYNCHRONIZATION IN TRANSITION TO TWO-DIMENSIONAL AND THREE-DIMENSIONAL TURBULENCE**

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Turbulent flows of a viscous incompressible fluid in a layer between rotating concentric spheres under the action of the modulation of the velocity of one of the spheres have been studied experimentally and numerically. We used an algorithm of numerical solution based on a conservative finite difference scheme of the discretization of the Navier–Stokes equations in space and semi-implicit Runge–Kutta scheme of the third order integration accuracy in time. Discretization in space was performed on grids nonuniform in radial and meridional directions with concentration near the boundaries and equatorial plane. The experimental setup consisted of two coaxial spheres. The space between the spheres was filled with silicone oil to which aluminum powder was added for visualization of flows. The rotation velocity was periodically varied. Agreement was shown to be between the experimental and calculated results, including the integral properties of turbulent flows. The possibility of the formation of turbulence with spectra qualitatively similar to spectra obtained in measurements in the upper atmosphere is established: with the slope close to  $-3$  at low frequencies and close to  $-5/3$  at high frequencies and with the negative longitudinal velocity structure function of the third order. It has been shown that such spectra are formed in the regions of a flow that are strongly synchronized under the action of the modulation of the rotational velocity.

## SOLUTIONS OF MECHANICS PROBLEMS WITH STRONG NONLINEARITY

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A high-order wavelet method is developed for general nonlinear boundary value problems in mechanics. This method is established based on Coiflet approximation of multiple integrals of interval bounded functions combined with an accurate and adjustable boundary extension technique. The convergence order of this approximation has been proven to be  $N$  as long as the Coiflet with  $N-1$  vanishing moment is adopted, which can be any positive even integers. Error analysis has proven that the proposed method is order  $N$ , and condition numbers of relevant matrices are almost independent of the number of collocation points. Examples of a wide range of strong nonlinear problems in mechanics, including the extremely large deflection bending of plates and shells, demonstrate that accuracy of the proposed method is even greater than  $N$ , and most interestingly, such accuracy is independent of the order of the differential equation of the problem to be solved. Comparison to existing numerical methods further justifies the accuracy and efficiency of the proposed method.

## FLEXURAL-GRAVITATIONAL WAVE PROPAGATION THROUGH PERIODIC STRUCTURES IN FLOATING PLATES

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The periodic structure is formed by regularly spaced array of straight-line obstacles in a floating plate of infinite extent. We study transmission of waves having a small amplitude through the structure and derive exact analytical solution for the wave field by applying Floquet theory. In equilibrium the fluid under consideration has the constant finite thickness.

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## THREE-DIMENSIONAL CELLULAR-AUTOMATA FINITE-DIFFERENCE MODEL TO EVALUATE GRAIN STRUCTURE DURING LASER ADDITIVE MANUFACTURING

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Laser additive manufacturing has received considerable attention in recent years due to its successful application in the fabrication of complex three-dimensional parts directly from a computer model. The mechanical properties of the additive manufactured components are known to depend essentially on their microstructural characteristics. Notably, the microstructure of additive manufactured materials differs significantly relative to that of materials produced by conventional methods due to the rapid heating and subsequent cooling during the additive manufacturing processing.

Thus, an accurate prediction of the microstructural evolution will contribute to the design of components with tailored properties.

In this work, a cellular automata model to describe the grain growth in solidification process and a finite-difference method to describe the heat transfer are coupled to simulate the evolution of grain structure during selective laser melting. The Goldak double ellipsoid model is adopted to calculate the heat input produced by a moving laser beam during the process. A polycrystalline substrate with equiaxial grains is generated by simulation of multiple grain growth in the uniform temperature field cooled down at a constant rate. To generate a non-textured substrate, an original approach is used. In the SLM simulations, we consider a unidirectional scanning strategy. Several laser passes in each powder layer treated as a continuous isotropic medium are simulated. Several powder layers are considered. The dynamics of grain growth during SLM in three dimensions is simulated with the use of the approach proposed. Spherical projections and pole figures are used to analyze the grain structure. The simulation results are compared with experimental data presented in the literature. The model developed can be used to analyze and predict the correlation between processing parameters and grain structure of additive manufactured specimens.

Support of the Central Research Development Fund of the University of Bremen is gratefully acknowledged.

### **ATOMIC MECHANISMS OF NUCLEATION AND DEVELOPMENT OF PLASTICITY IN VANADIUM UNDER MECHANICAL LOADING**

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The molecular dynamics simulation of nucleation and evolution of plasticity in the vanadium crystallite with interfaces (grain boundaries and free surfaces) under mechanical loading was carried out. Various schemes of crystallite loading were realized. The volume of crystallite was not changed during mechanical loading in order to simulate its behavior in constrained conditions. Vanadium crystallites with interfaces were deformed by the uniaxial uniform tension. It was shown that thermal fluctuations caused the generation of the structural defects. Abrupt growth of number defects took place when deformation of crystallite reached a threshold value. The characteristic sequence of atomic transformations on the first and second coordination spheres was revealed. The correlation between atomic transformations and thermodynamic parameters at various schemes of crystallite deformation was shown. The influence of the deformation rate and temperature on peculiarities of nucleation and development of the defect structure in the crystallites of vanadium was investigated.

*The work is done in the framework of the Programme of fundamental research of state academies of Sciences for 2013-2020.*

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