The 18th Conference on Functional and Nanostructured Materials

FNMA '22

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ABSTRACT BOOK

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CONTENTS

Effect of sonication treatment on the distribution of the nanoparticle agglomerates dispersed in an aqueous suspension

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Single-domain iron oxide nanoparticles (MNP) can convert AC magnetic field energy into heat. However, as recently observed [1], thermal fluctuations lead to an increase in the frequency of particle collisions and their subsequent sticking due to magnetic dipole interactions. This leads to the agglomeration of the magnetic material and its sinking to the bottom, which in turn reduces the heating efficiency of the magnetic suspension. To break up the aggregates and facilitate the dispersion of nanoparticles, we decided to use the sonication technique. When investigating its influence on magnetic colloids, it turned out that the hydrodynamic diameter as a function of sonication time appeared to have a power-law character [2]. Moreover, the values of the mean hydrodynamic diameters of the nanoparticles converge to the final value, which is in acceptable agreement with the mean value of a single nanoparticle diameter determined by the TEM technique. Overall, it was found that extending the sonication time of the MNP suspension results in a noticeable increase in its heating efficiency.

Acknowledgement

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Microscopic auxetic hierarchical mechanical metamaterials showcasing tunable mechanical properties and shape morphing

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Shape morphing [1-3] and the ability to control mechanical properties of functional materials [4, 5] remain some of the biggest challenges in the field of materials science. This stems from the fact that these properties, with the emphasis on the unusual types of mechanical behavior such as the auxeticity or negative stiffness, are of great significance in the case of numerous applications. Some of these applications include protective equipment, vibration damping and biomedical devices. Particularly important in this regard is a recent progress made in the field of hierarchical mechanical metamaterial [6, 7], i.e. structures composed of components being able to deform irrespectively to the rest of the system. The concept of hierarchy implemented in mechanical metamaterials enables them to exhibit a range of different mechanical properties without being reconstructed. This in turn makes it possible to potentially construct mechanical metamaterials capable of adjusting their mechanical response depending on the external stimulus. Nevertheless, despite several significant achievements reported in this field, studies related to hierarchical mechanical metamaterials are still at the very early stage and hierarchical structures reported in the literature normally share several limitations. First of all, it is worth mentioning that a vast majority of known hierarchical metamaterials are two-dimensional which significantly limits their applicability since they cannot respond to the stimulus applied from an arbitrary direction. However, an even larger limitation is the fact that the behavior of the currently known hierarchical mechanical metamaterials has been primarily studied at the microscale. On the other hand, the propensity of such a system to exhibit the programmable shape morphing would be of great significance at the much lower scales including the microscale where it could be utilized in the design of novel robotics and biomedical devices.

In this work [8], a novel microscopic 2D and 3D hierarchical metamaterial is proposed that is capable of exhibiting a wide range of auxetic behavior depending on the variation in its geometric parameters. It is shown that the considered system is

capable of shape morphing at the micro-scale where it can assume an arbitrary predefined shape. Finally, it is demonstrated that in addition to the auxetic behavior, the considered hierarchical structure can exhibit very different rates of energy absorption and different values of stiffness. These results indicate that the proposed concept can be utilized in the design of novel types of robotics as well as biomedical devices and vibration damping materials.

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Magnetic nanoparticles in a thin elastic film for detecting mechanical deformation

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We consider a system composed of single-domain magnetic nanoparticles that are densely packed within an ultrathin elastic nonmagnetic film. We further analyze the effect that magnetic dipole interactions have on the process of heating of the magnetic nanoparticles by an external magnetic field, $H=H_0 cos(2)$, where f denotes the frequency of the field. Some of the results of this study were published recently in Physica Status Solidi B [1], where it was shown that magnetic dipole interactions between the nanoparticles can be used to detect the mechanical deformation of the elastic film that is hosting the nanoparticles. The temperature of the heated magnetic nanoparticles, which changes in time due to the presence of the pulses of an external radiofrequency magnetic field, depends on the extent of the mechanical deformation. Thus, in this work, a theoretical model of the magnetic sensor of elastic deformations is shown where the heating power of the film is expressed in terms of the specific absorption rates (SARs).

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Effect of twist on indentation

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Materials with low stiffness that can gradually decelerate colliding bodies when contact area is high, but have relatively high indentation resistance to resist penetration when contact area is low, are useful in protective equipment. It is known that classical Hertzian indentation resistance increases with a material's (2D) plane Cauchy stress modulus ($E/(1-\nu 2)$ for isotropic materials), where E is Young's modulus and ν is Poisson's ratio. The isotropic limits of Poisson's ratio are between -1 and 0.5. Based on their potentially high magnitude Poisson's ratio, auxetic (negative Poisson's ratio) materials have often been studied under indentation and impact [1].

Force torque coupling (known herein as twist – Figure 1a) is not considered in Cauchy continuum mechanics but is possible in various micropolar continuum theories. Interestingly, twist increases 2D plane stress modulus [2]. So, we hypothesised that indentation resistance would increase with twist.

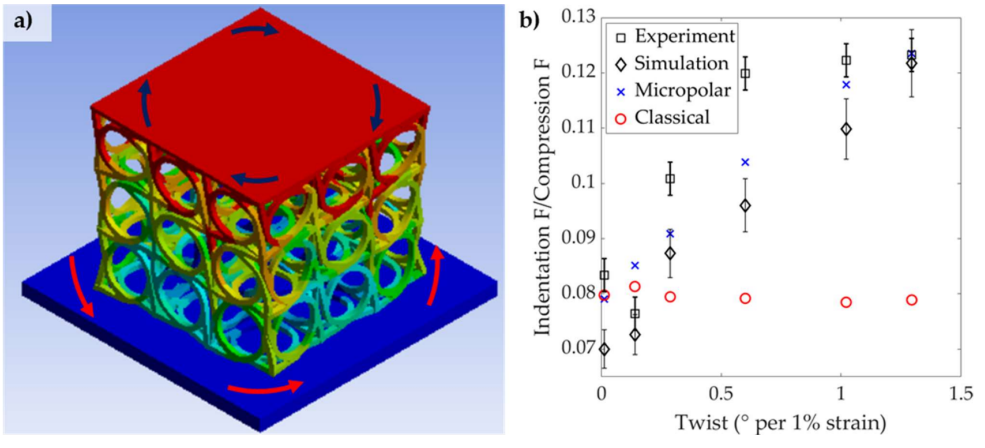

Figure 1: a) Model of twisting lattice; b) Normalised indentation forces. Error bars show load cell precision (of 0.333 N) and simulation uncertainty (from a mesh convergence study).

We simulated, calculated and tested spherical indentation resistance of twisting and non-twisting lattices (based on [3] – Figure 1a), finding reasonable agreement between micropolar calculations, finite element simulations and experimental data

(Figure 1b). Twist increased indentation force, so could be targeted to develop better protective equipment, analogous to (negative) Poisson's ratio.

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Radiative properties of emitters embedded into negative index materials

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The radiative properties of emitters (e.g. atoms or quantum dots) located close to the surface between dielectric or conducting materials can be significantly modified compared to those in vacuum [1, 2]. The modification results from the presence of surface EM modes known as surface plasmons. At the interface between a different category of materials, so-called meta-materials, which are characterized by specifically designed geometrical structures, a guided high density modes can be generated by the surface plasmons [3, 4]. Due to the high density of modes, emitters located close to the surface between two materials can interact strongly with the surface field which may significantly change their radiative properties. In this presentation, we discuss in details the radiative properties of two independent emitters, two-level systems located close to the interface of two meta-materials, one of a negative permeability and the other of a negative permittivity. We show that surface plasmon polaritons, i.e. nonradiative electromagnetic excitations associated with charge density waves propagating along the interface, are generated. The radiative systems located close to the interface can excite the surface plasmon polaritons. Thus, the interface behaves as a directional guiding plasma field mode propagating in one direction, with a formal analogy being a plasmonic waveguide. Our focus is on showing how the plasmon field induced at the interface between the materials may change the dynamics of the emitters, in particular, the population transfer and entanglement. The mathematical approach adopted in this work is based on the Greens function method which leads to remarkably simple analytical expressions for the probability amplitudes valid for an arbitrary initial state, arbitrary strengths of the coupling constants of the emitters to the plasmon field, and arbitrary distances between the emitters [5]. A number of interesting general results on the population transfer and entanglement between the emitters will be discussed in both strong and weak regimes of the coupling to the surface plasmon field.

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Auxetic metamaterials: Negative Poisson's ratio in high pressure crystals

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Carbon dioxide has a rich phase diagram boasting numerous high pressure polymorphs such as CO_2-II and CO_2-V. This polymorphism has intrigued researchers in various fields such as chemistry, planetary sciences and geophysics [1-3]. For example, high pressure polymorphs of CO_2 are thought to be found in the interior of planets, making research on high pressure polymorphs of CO_2 essential to understand the dynamics of planet interiors [4]. Moreover, the field of high pressure polymorphism has also attracted the attention of researchers due to the formation of non-molecular substances from compounds which are typically molecular at ambient conditions.

Despite numerous studies on high pressure polymorphs of CO_2, work on the auxetic potential of these substances in lacking. In view of this, the Poisson's ratio of CO_2-II and CO_2-V will be studied through the use of first principles DFT simulations. The auxetic potential of these polymorphs, together with its pressure dependence, will be studied through the use of spectroscopic techniques, namely infrared and Raman spectroscopy.

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Negative materials: be ready for the unexpected

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We are used to seeing things becoming thinner when stretched, expanding when heated, and getting smaller when placed under pressure. Does this need to be the case? Can the opposite happen? If so, what causes such unusual behavior?

This presentation will provide an overview of recent developments in the field of unusual materials and metamaterials, with a focus on negative Poisson's ratio (NPR, auxetic), negative thermal expansion (NTE) and negative compressibility (NC). It will be shown how such behavior can be achieved, controlled and enhanced. The presentation will also show how we are already benefitting from these "unusual" materials and discuss some possible applications which could benefit from the use of such anomalous materials.

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DC magnetization hybrid nanocomposites containing nanocrystalline TiO_2 and graphene-related materials

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In this work, DC magnetization of nanocomposites modified with graphene oxides was investigated with this study being a continuation of the other project focused on dynamic magnetic interactions [1]. In this study, the dynamic magnetic interactions showed a complex nature. In particular, it was shown that titanium dioxide modified by RGO, in addition to the classical magnetic ordering, in some areas may also exhibit the superferomagnetic ordering.

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Entanglement generation via a series of external pulses in a system of nonlinear coupler

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The ability to create and manipulate quantum states is relevant for developing quantum information theory and its applications. Maximally or almost maximally entangled states play a crucial role at that point. Such states have found applications in quantum communication, cryptography, and quantum computing.

As a source of maximally entangled states, we consider the system consisting of two mutually interacting anharmonic quantum oscillators. Both oscillators are externally driven by a series of ultra-short coherent pulses. For such a system, we discuss the influence of excitations on the generation of entangled states. We show that the efficiency of the creation of maximally entangled states strongly depends on the time between two subsequent pulses and the scheme of excitations. Additionally, we present that this efficiency in a system excited by a series of pulses is higher than in a continuously excited system [1, 2].

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Material research engineering laboratory

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The presentation concerns the plan of how to use the scientific and research infrastructure of the new laboratory hall to conduct both scientific research as well as research and development works for industry. Individual laboratories will be described and an offer of industrial research and development works for partners from the industry will be proposed. As the laboratory is designed to work with industry partners, potential partners will be identified and case studies described, which will be carried out in collaboration with companies.

3D printing laboratory

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The industry is constantly looking for innovative ideas that give a competitive advantage through the rapid introduction of new and innovative products and the use of new manufacturing technologies. Recent years show the growing interest of the industry in additive manufacturing technology (AM, 3D Printing). 3D printing of plastic parts is widely used due to wider availability of technology and lower prices of devices.

The implementation of additive manufacturing of metal parts involves significant investment costs in machines and highly qualified staff. This is why additive manufacturing is less frequently used for metal than for plastics. The lack of knowledge about the potential and possibilities offered by additive manufacturing of metal parts is also significant.

The 3D Printing Laboratory established as part of the RID project implemented at the University of Zielona Góra enables the industry to become familiar with the potential and possibilities offered by additive manufacturing without incurring high investment costs. In the 3D Printing Laboratory, it is possible to carry out all the necessary activities related to the preparation and execution of a 3D print of a metal part. In Additive Manufacturing, the 3D printed metal parts are created directly from a computer model without the need for tools or molds.

Scope of activities:

- checking the correctness of the digital model / error fixing
- design consultation - proposals for design changes using the potential of additive manufacturing (DfAM – Design for Additive Manufacturing)
- preparing models for 3D printing - parts orientation on the working platform and design of support structures,
- additive manufacturing/3D printing
- postprocessing: support removal, heat treatment, sandblasting.

The result is an additively manufactured metal part of a quality similar to that of samples manufactured through conventional casting or forging. Additionally, the knowledge about the possibilities offered by additive manufacturing is transferred. Industry can evaluate the suitability of additive technology in its own production processes without incurring significant investments.

The capabilities of the 3D Printing Laboratory regarding cooperation with the Industry in the field of knowledge transfer and the implementation of additive manufacturing projects in the University - Industry cooperation will be presented. Laboratory equipment will be discussed and case studies of cooperation with the industry will be presented.

Cyclic air denoxification utilizing Ag/TiO_2-decorated activated carbon fibre-based filtering cloths

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This work aimed at obtaining the hybrid filtering composite cloths based on various photoactive silver-modified TiO_2 (theoretically containing 3, 5 or 10 wt.% of AgNPs) and activated carbon fibre felts that could be successfully applied in air deNoxification. The Graphite Felt Carbopon B-Active 200 (BA 200) supplied by OJSC "SvetlogorskKhimvolokno" was used for the first time as support for modified TiO_2 photocatalysts, and the cyclic stability of various silver-modified TiO_2 photocatalysts covered BA 200 ACF felts was performed. The structural properties of obtained photoactive hybrids, including AgNPs content, were checked by employing XRD, ICP-OES, XPS, DRIFT, UV-Vis/DRS, and low-temperature N_2 adsorption-desorption analyses.

It was found that the BA 200 cloth used in this study acts as a support for photocatalyst nanoparticles, which additionally adsorbs by-products of NO photooxidation (mainly NO_2) due to the large SBET and the microporous nature of the fabric. It was also noted that AgNPs content and the type of TiO_2 photocatalysts impact the efficiency of deNOxification (5 wt.% of AgNPs and TiO_2 from Grupa Azoty Zakłady Chemiczne "Police" S.A. were the most suitable for NO photooxidation). 5 wt.% of silver in TiO_2 photocatalysts was an optimal content due to the optimal size of the Ag nanoparticles that impacts the efficiency of NO photooxidation. Incorporated AgNPs of optimal size act as electron trapping centres, preventing the recombination of the electron-hole pairs, thus, enhancing the NO removal efficiency. Using a higher concentration of silver nanoparticles (10 wt.% in this case) in the TiO_2 modification process promotes Ag agglomeration on its surface, reducing the denoxification efficiency.

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Thermal dewetting as a method for the manufacture of nanoalloys and nanocomposites

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Over the years, alchemists would try to obtain gold from other non-noble metals. Nowadays, with the help of methods for the manufacture of nanomaterials, it is possible to design materials with defined properties, even to copy the properties of gold by bimetallic nanoalloys or nanocomposites. Thermal dewetting seems to be one of the best choices as a production method of nanoalloys and nanocomposites.

The dewetting of metastable metallic thin films could be used for preparation of bimetallic nanoalloys or nanocomposites. The thermal annealing of nanometric films leads to an isolated island formation. The properties of manufactured nanostructures depend not only on their size, but most of all on their nanostructure and chemical composition. Therefore, wide knowledge about kinetics and formation of nanostructure parameters plays a key role from the point of view of practical applications.

In this work, we would like to present an experimental method for manufacturing plasmonic nanostructures based on gold-silver, gold-copper and silver-copper nanoalloys and nanocomposites. We would also like to illustrate the potential of the machine learning method for controlling the optical properties of bimetallic nanostructures.

Transfer of quantum steering along two non-interacting oscillatory chains

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Quantum steering is one of the most intriguing phenomena in quantum physics. It plays a crucial role in fundamental research concerning the quantum world and has applications related to quantum information theory. For instance, steerable states could be applied in quantum cryptography and communication protocols where they can certify the entanglement between two subsystems. What should be emphasized, studies concerning the propagation of various quantum correlations, including the steering, along the chains of qubits seem especially valid in the context of quantum communication and quantum computation systems design. For instance, the perfect transfer of the steerable states plays a crucial role in quantum information transmission and quantum key distribution.

In our research, we consider a system involving two noninteracting chains of qubits. Each chain is modeled by N interacting anharmonic Kerr-type quantum oscillators. We analyze the time evolution of parameters describing steering between qubits belonging to the same or different chains constituting the system. We show that if the first pair of noninteracting qubits belonging to the two chains are prepared in a steerable state, then such a state can be successfully transferred from the one end of the chain to the second one. Moreover, if we replace the nonlinear oscillators with their linear counterparts, the steering transfer effects remain untouched.

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Thin layer of Fe_3O_4 magnetic nanoparticles

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Preparation of thin uniform films of nanoparticles is of great interest for manufacturing and biomedical fields, including protecting layers and functional magnetic nanodevices or active molecules immobilization. There are various methods of obtaining thin nanoparticles films. The presentation focuses on methods involving the use of nanoparticle suspension, where the key element is the stabilization of such a suspension. It can be achieved by modifying the surface with chemical compounds or changing the electrostatic charge at the nanoparticle surface. In the study, the stable suspension of magnetic iron oxide nanoparticles was tested for thin layer formation during evaporation as a sessile droplet [1], with the spin coating method and Langmuir Schaefer method.

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Analysis and improvement of production processes

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The paper presents an important issue concerning the size and concentration of copper nanoparticles in a nanofluid. The influence of nanoparticles on the stabilization of the nanofluid, tool vibrations during turning of 316L stainless steel and the machined surface topography are described. Four sizes of Cu nanoparticles were used: 22 nm, 35 nm, 65 nm, 80 nm and four types of concentration: 0.25%, 0.5%, 0.75% and 1%. For all prepared types of nanoliquids, the ultrasonic dispersion was obtained after 50 minutes, and the nanoliquids with smaller nanoparticle sizes were the most stable. The lowest values of the initial parameters, both vibrations and selected parameters of 3D surface topography, were observed for the smallest size of Cu with a size of 22 nm and a concentration of 0.5%. The article presents how important the problem is to determine both the size and concentration of copper nanoparticles in the MQL method.

Electrochemical and thermoelectric properties of mixed-conducting oxides

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Triple conducting oxides (TCO) have gained much interest as cathode materials for devices with a proton-conducting electrolyte. This type of materials is a new group of ceramic materials in which total electrical conductivity is determined by the presence of three types of charge carriers i.e. holes/electrons, oxygen ions, and protons [1-2]. There are two strategies for designing a triple conducting oxide. The first possibility is to modify an oxide having high electronic conductivity in such a way that its oxygen ion- and proton conductivities should increase. The second one is a modification of a mixed proton- and oxygen ion conductor leading to an increase in its electron/hole conductivity [3]. The perovskite-type materials (ABO_3) are attracting intense interest for a variety of energy conversion applications. Proton conductivity in a humid atmosphere has been previously reported in many oxides belonging to this material family [4].

Multicomponent oxides (MO), usually contain five or more elements occupying the same crystallographic position. The lattice distortions influence not only the mechanical but also the transport properties of MO materials. In consequence, the electrical and thermoelectric properties, strongly depend on the structural properties [5]. The combination of the high configurational entropy and mixed oxygen ionic, protonic and electronic conductivity (MOs-TCOs) of selected high-entropy perovskites may render them as interesting electrochemical materials.

In this work, the electrochemical and thermoelectric properties for different groups of mixed-conducting perovskite materials were investigated. The structure and microstructure of these materials was analyzed with X-ray Diffractometry (XRD) and Scanning Electron Microscopy (SEM). The transport properties were studied both by the DC four-wire technique and Electrochemical Impedance Spectroscopy (EIS) as a function of temperature and water vapour or oxygen partial pressures. The Electrical Conductivity Relaxation (ECR) method was used to provide information about the chemical surface exchange coefficients and chemical diffusion coefficients of water and oxygen. The temperature dependence of the Seebeck coefficient and the Figure of Merit (ZT) was also analyzed as a function of pH_2O and pO_2.

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SMA-metamaterial actuators

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Shape memory alloy (SMA) based actuators are typically characterized by a high force/stroke ratio and can be activated by an increase in temperature which is usually induced either by passing an electric current or direct heating. SMA composite actuators are designed as two-component systems with an agonistic-antagonistic relationship, where the main role of the second component is to act as a counter-balance and revert the actuator back to its original shape once it has been deactivated. In this work, we present a design for a reusable SMA actuator based on an auxetic metamaterial system which may be used to obtain a tailored biaxial actuation stroke. By taking advantage of the localised internal deformations of the metamaterial, one may obtain an elongation stroke from the actuator through a contraction of the SMA component. We have also realised a fully-functional prototype of the SMA-metamaterial actuator and tested its performance under cyclic activation and deactivation conditions. Furthermore, a theoretical model which may be used to program the actuation stroke of the system according to the geometric configuration of the system and material properties of the SMA and counter-balance components has also been developed.

Poisson's ratio of hard sphere f.c.c. crystals with selected nanochannel inclusions that preserve cubic symmetry

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Auxetics [1] is the name that has been coined to describe a relatively new class of materials exhibiting unusual elastic properties. Their most characteristic aspect is the occurrence of negative value of the Poisson's ratio [2]. This indicates that when stretched, an auxetic will expand its dimensions in one or more directions transverse to the direction of stretching. The growing interest in auxetics is motivated by the vast potential applications for these materials. Their discovery in the late 1980s, is marked by ground braking works: by Lakes [3], who developed the first auxetic foam, and by Wojciechowski [4,5], who presented and rigorously solved the first thermodynamically stable auxetic model.

Since then, negative Poisson's ratio materials have been extensively studied, both theoretically and experimentally. In case of real materials, auxetic effects have been reported in polymers [6], composites [7], but also in cubic crystals [8]. These studies are backed by theoretical studies of various model structures that also show similar properties. Apart from the aforementioned particle models related to the papers published by Wojciechowski, other most notable examples include models of rotating rigid units proposed by Grima [9]. The search for new auxetic materials can be roughly divided into two approaches: (i) studies of new materials and models or (ii) modification and optimization of existing materials and models in order to induce or enhance the auxetic effects. Recently studied models of f.c.c. hard sphere crystals with cylindrical inclusions of other hard spheres with different diameters [10] pose an example of the latter. It has been shown that such nanochannel inclusions on the structure level can significantly modify elastic properties of the system and strongly enhance its auxetic properties. In this talk, an extension of these studies will be reviewed. Systems with multiple nanochannel inclusions, oriented in different crystallographic directions, have been studied. The systems with nanochannels oriented in either of the two high symmetry directions ([100] [11] or [111] [12]) have been investigated, as well as, models containing inclusions in [110]-directions [13] (which is the direction in which auxetic effect occurs in cubic systems). The inclusions were designed such that they preserve cubic symmetry of the model (as opposed to [10], where the system's symmetry changed to tetragonal). The elastic properties, and in particular, the Poisson's ratio have been investigated with respect to: the changes of size of particles

that form the inclusions, the size of the inclusions them self, and their orientation and layout inside the crystal structure. The impact of these parameters on the Poisson's ratio of hard sphere f.c.c. model is the subject of this talk.

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Self-organization in amorphous-nanocrystalline Fe-based alloys induced by pulsed laser heating and Joule heating

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The structure evolution of amorphous metallic alloys under various kinds of thermal influences is an important problem of disordered structure physics due to the fact that almost all material properties are sensitive to structural changes. Thus, predicting the formation of such a structural state would provide the necessary set of physical and mechanical alloy properties. One of the most important questions of metal glass physics is the transition from an amorphous to a crystalline state. At different thermal conditions, the process of structure formation in metal glasses can differ vastly, and crystallization would result in significantly different final structures. Hence, the aim of this research is to study of processes of structure-forming in metal glasses of the system Fe-B under extreme heating and cooling induced by pulsed laser heating and Joule heating.

The amorphous state is metastable and the processes of self-organization of the structure occur under the impact of external influences. The metastable configuration of the atoms causes the possibility to prefer one among various pathways to change its free energy when the system is pushed to modify the quasi-equilibrium states in one of the multiple states. The self-organization leads to a new structure for the non-crystalline materials, the so-called nanostructure. Self-organization such as nanocrystallization or, in some cases, the formation of laser-induced periodic surface structures (LIPSS), takes place in nonequilibrium conditions under laser irradiation or Joule heating. Our research is devoted to the impact of laser irradiation (λ=1.06 m) and current annealing on the structure evolution of amorphous FeNbCuSiB [1, 2, 3]. Structure and phase transitions have been studied using X-ray diffraction, AFM, Mossbauer, and SEM methods.

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Spectroscopic and luminescent properties of the Pr-doped and Pr-Ag co-doped glasses with $Li_2B_4O_7$ basic composition

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Spectroscopic and luminescent properties of the Pr-doped and Pr-Ag co-doped borate glasses with $Li_2B_4O_7$ (or Li_2O–$2B_2O_3$) composition were studied in detail using electron paramagnetic resonance (EPR), optical absorption, photoluminescence (emission, excitation, decay kinetics) spectroscopy, and Judd–Ofelt analysis [1]. Optical absorption spectra of the studied glasses reveal $4f$ – $4f$ absorption bands, characteristic for Pr^{3+} ($4f^2$, $^3H_4$) ions. Silver co-doping leads to a significant increase of the optical absorption in visible and partly near infrared (NIR) ranges due to effects of light scattering and surface plasmon resonance (SPR) absorption induced by silver nanoparticles.

The orange-red Pr^{3+} emission band with a maximum at 601 nm ($^1D_2 \rightarrow {}^3H_4$ transition) and lifetime 22 μs dominates in the photoluminescence spectra. Increasing of intensity of the Pr^{3+} luminescence in 40% and in 3 – 4 times is observed in the $Li_2B_4O_7$:Pr,Ag glass upon excitation respectively at 445 nm ($^3H_4 \rightarrow {}^3P_2$ absorption transition) and different photoexcitation in UV range. Based on the obtained experimental results and the Judd–Ofelt theory, experimental and theoretical oscillator strengths (f_{exp} and f_{theor}) were calculated as well as phenomenological intensity parameters (Σ_2, Σ_4, Σ_6), radiative parameters (A_{rad}, β, τ_{rad}), and quantum efficiencies (η) of the Pr^{3+} luminescence.

Presence of the isolated Ag^+ ($4d^{10}$, $^1S_0$) ions, small non-plasmonic Ag aggregates (Ag_m^{n+} nanoclusters), and plasmonic Ag metallic nanoparticles in the $Li_2B_4O_7$:Pr,Ag glass was proposed based on detailed analysis of optical absorption and photoluminescence spectra as well as decay curves. Observed enhancement of luminescence intensity and increasing of stimulated emission cross-section and quantum efficiency

of luminescence in the $Li_2B_4O_7$:Pr,Ag glass is explained by energy transfer from single Ag^+ ions and Ag aggregates to the Pr^{3+} ions as well as local-field effect induced by Ag metallic nanoparticles. Silver co-doping is a promising approach for improving of luminescent properties of the Pr^{3+} and other trivalent rare-earth ions in tetraborate glasses.

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Real time effects of a Gaussian wave packet impinging on square well

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The wave function emanating from an initial Gaussian wave packet approaching a square well is obtained, space-time wise in case the overlap of the initial wave packet with the square well region is ignorable. From the wave function, in question, follow the corresponding probability and current densities. In particular, we obtain the corresponding spatial densities at given times and, furthermore, the time evolution of the probability and current densities at the well entrance and exit. There follows comparison of the corresponding effects of the same initial wave packet impinging on a square barrier with height equal to the well depth. Classically a particle approaching a potential well region crosses it irrespective of its initial momentum, something forbidden in the barrier case for incoming kinetic energy below the barrier top potential energy. However, quantum mechanically, the so-called tunnelling case, allows probable partial crossover in the barrier case with incoming kinetic energy smaller than the barrier potential energy height. On the other hand, in the case of well potential the classical total passage gets reduced. As far as the picture obtained for the probability and current densities is concerned in both cases, well and barrier, there appears similarity. E.g. spatial distribution of the current density in the incoming region, at a given time, in both cases appears reversal. Furthermore, the time evolution of the current densities at the potential entrance exhibit reversal, which in the barrier case is repeated. At the exit the corresponding densities are unidirectional in both cases. Finally, one could remark that the quantum mechanical state of affairs relative to the classical one acts in a way enabling disallowed classical processes to evolve partially and at the same time completely allowed classical processes to appear in reduced form.

CO_2 sorbents based on spherical carbon and photoactive metal oxides

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In this work, the adsorption properties of microporous spherical carbon materials obtained from the resorcinol-formaldehyde resin, treated in a solvothermal reactor heated with microwaves and then subjected to carbonization, were checked. The potassium-based activation of carbon spheres was carried out in two ways: solution-based and solid-based methods. The effect of various factors, such as chemical agent selection, chemical activating agent content, and the temperature or time of activation, was investigated. The adsorption performance of carbon spheres was evaluated in detail by examining CO_2 adsorption from the gas phase. The influence of modification with zinc chloride on the physicochemical properties of the obtained materials and CO_2 adsorption capacity was investigated and discussed. The research on the new composites consisting of carbon spheres and photoactive compounds is justified due to the possibility of obtaining materials allowing for the simultaneous adsorption of carbon dioxide and, due to the presence of semiconducting zinc oxide, its processing into useful products in the process of photocatalytic reduction.

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Randomly poled nonlinear crystals as a source of photon pairs

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Generation of photon pairs from parametric down-conversion in randomly poled nonlinear crystals is investigated using analytically soluble model and numerical calculations. Randomly poled crystals are presented as sources of entangled spectrally ultra broad-band signal and idler fields. Their photon-pair generation rates scale linearly with the number of domains. Entanglement times as short as several fs can be reached assuming suitable phase compensation. Strong temperature dependencies are observed. Comparison with chirped periodically-poled structures is given and reveals close similarity.

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Dynamics of electric dipole in non-homegenous electromagnetic fields

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Storage and trapping of charged and neutral particles are extremely important for modern ultracold physics and its various applications. Confinement of charged particles (electrons, protons, ions etc) is commonly achieved in electromagnetic traps where their motion is controlled by properly configured electric and magnetic field. Among such traps the most important are the Penning and the Paul traps. More difficult is confinement of neutral particles. Here we consider neutral particles with non-zero permanent electric dipole moment modeled by a dipole. Because building of traps is very expensive understanding the dynamics of such particles in electromagnetic fields is important. We have started to investigate general qualitative and quantitative properties of appropriate equations of motion in papers [1,2,3]. Analysis of equations of motion of a dipole in stationary homogeneous electromagnetic fields in [3] show that such fields are not appropriate for trapping. In [1] the non-relativistic equations of motion for a dipole in arbitrary stationary non-homogeneous electro-magnetic field are derived and analyzed. Certain novel design for a trap for confinement of neutral particles having a permanent electric dipole moment is presented in [2]. The device uses a combination of a sextupole electric and quadrupole magnetic fields superimposed with a strong constant electric field perfectly aligned along the z-axis. We use the extended dipole model to study the dynamics of particle in this position dependent electromagnetic field. The motion of the centre of mass of the dipole is nonlinearly coupled with its rotation. We present the results of studies of analytical properties of motion equations and several numerical simulations which illustrate trapping and confinement of an electric dipole in this device.

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Mechanical properties of silumin $AlSi_{11}$ in relation to structure changes after modification

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The paper presents the results of the research on the influence of modification on the structure of silumin $AlSi_{11}$. The $AlSr_{10}$ master alloy was used as a modifier in an amount from 0.05% to 0.30%. In order to show the influence of changes in the structure on the mechanical properties, an impact test was performed. The research shows that the highest impact toughness value was obtained for the $AlSi_{11}$ alloy modified with $AlSr_{10}$ master alloy in the amount of 0.30%.

Polish bridges

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Outstanding bridge structures by Polish engineers of the 19th and 20th centuries, built on the Polish territories and - above all - outside Poland: in both Americas, in the Russian Empire, and in several other countries, will be discussed. In addition to these structures, the profiles of the bridge designers, who often made their contributions in other areas as well, and who - as it unfortunately usually happens - are not known in the Western studies devoted to the history of technology, will be presented.

Polymer brushes: new polymeric materials in experiments and simulations

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Brushes are complex macromolecular structures composed of polymer chains densely tethered to another polymer chain or to a surface [1]. Although numerous techniques have been applied for the characterization of polymer brushes, some parameters still cannot be determined, especially for very densely grafted systems. The brushes were synthesized by atom transfer radical polymerization with varied degree of polymerization of the side chains, poly(methyl methacrylate) and were characterized by Gel Permeation Chromatography Multiangle Laser Light Scattering, Pulsed-field Gradient Spin Echo Nuclear Magnetic Resonance, and combined Static and Dynamic Light Scattering methods [2]. A novel calculation strategy employing the Dynamic Lattice Liquid algorithm executed on a dedicated machine ARUZ was applied for theoretical studies [3-4]. The experimental values concerning the structure and dynamics were compared and confronted with simulation results.

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Structural differences between activated carbon spheres (ACS) obtained in environments with different pH values

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Carbon sorbents with high microporosity and spherical symmetry intended for the removal of CO_2 from the atmosphere were obtained using a modified Stöber synthesis [1][2]. The starting materials for carbon were resorcinol and formaldehyde, which were mixed for 24 hours in the presence of ammonia water in an aquatic-alcoholic environment. Different materials were obtained using various pH values of the environment calibrated using ammonia water. The study investigated pH values of 7.50; 8.85; 9.00; 9.25; 9.50 and 10.00. Selected samples after carbonization were also activated with a KOH solution in a way, that allowed 70% of the activator to be incorporated into the weight of the sample.

The morphology of the obtained materials was examined using a scanning electron microscope, which showed that RF spheres obtained in environments with pH values in the range 7.50-9.25 have a spherical shape and develop into solids with a smooth outer surface. Comparatively, the structures obtained in the mixture with increased contents of ammonia water (pH = 9.50 and pH = 10.00) are less regular. Only partial formation of spheres can be observed in them, as the material has an increased tendency to agglomerate.

Thermogravimetric analysis revealed that the structure of the sphere and its thermal resistance during the process depends on the pH value of the environment in which the synthesis was performed – this is shown by the displacement of the DTG peak by about 80°C to higher temperatures for ACT.K.70 pH = 10.00 compared to ACT.K.70 pH = 7.50. The pH value used also influences the shape of the obtained peak due to the different graphitization of the samples. The characterization was further supplemented by the measurement of the specific surface using low-temperature BET nitrogen adsorption and the analysis of the porosity diagrams drawn with the NLDFT model.

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Aging of thin films under interplanetary space conditions

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Space exploration demands hardware with reliable system components. They are built of materials that must be examined with regards to their response to the harsh space environment. Interplanetary space is much more challenging in the context of material aging than the environment in the close vicinity of the Earth. It causes degradation of materials due to their presence in a vacuum and the fact that they are exposed to corpuscular and electromagnetic radiation with a wide energy range.

The aim is to show how thin films degrade under corpuscular radiation of the interplanetary medium. Thin films are commonly used in the space industry. They found their application as solar reflectors and the so-called second surface mirrors. A typical solar reflector material, a polyimide foil coated on both sides with an Aluminum layer, was exposed to a stream of low-energy protons.

A set of samples was exposed to a well-defined flux of 2.5 keV protons in the Complex Irradiation Facility [1] at the Institute of Space Systems of the German Aerospace Center in Bremen. Samples were examined under the Atomic Force Microscope at the University of Zielona Góra before and after the test. Also, a hand-held reflectometer and a Bruker FTIR spectrometer were used to measure the thermo-optical properties of the specimens.

The proton irradiation test revealed that metalized films exhibit the formation of tiny blisters. They are filled with molecular hydrogen gas. The gas results from recombination processes of the incident protons and electrons from a top Aluminum layer of a specimen. A joint experimental effort of the German Aerospace Center (DLR) and the Institute of Physics of the Zielona Góra University reveal that the size and the number of blisters strongly depend on the proton flux [2] and fluence [3] magnitudes. High proton fluence results in an increased number and large size of blisters. However, high proton flux magnitude de-accelerates the blistering process [2]. Such effect is caused by a native Aluminum oxide layer that cracks above a certain

proton flux magnitude and releases the recombined hydrogen gas preventing blisters' formation.

Two conclusions can be drawn. First, the blistering process changes the material's thermo-optical properties [4]. It directly influences the thermal stability of any satellite with a reflector material exposed to the corpuscular radiation of the solar wind. Second, irradiation tests where a high proton flux was used show that laboratory conditions can dictate the material aging process and lead to false conclusions. One can have an impression that a material can degrade much faster than it would under real space conditions. A careful selection of particle flux magnitude is required.

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Conception of a big data architecture to optimize and make automobile production more flexible

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In the age of digitalization, the automotive industry is faced with internal challenges that affect both the technologies used and the people involved. The aim is to maximize efficiency in the production process based on existing data by making optimum use of existing resources. The goal of this work is to develop a Big Data architecture that applies a predictive maintenance approach to production.

Heat conduction of liquid argon in nanochannels and argon nanowires from molecular dynamics simulations

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Recent developments in nanoscience and nanotechnology provide methods to design various devices at the nanoscale. Further progress demands developing fundamental knowledge on the control of thermal transport at the nanoscale. One of the critical issues concerning heat conduction at the nanoscale is the influence of strong geometrical confinement on thermal conductivity [1]. Studies of the heat transfer process in such simple systems, such as liquid argon in nanochannels or argon nanowires, allow us to understand better the influence of strong geometrical confinements on the thermal conductivity of confined systems [2,3,4,5]. The thermal conductivity of liquid argon in nanochannels [3,4] and argon nanowires [5] was determined using two independent methods by molecular dynamics (MD) simulations. The influence of transversal size and shape of a nanochannel and a nanowire on the thermal conductivity of the system was investigated. The studies show that thermal conductivity increases with an increase in the transversal size of the sample and scales well with the cross-sectional area of the system [3,4]. The thermal conductivity of argon in nanochannels reaches its bulk values for some characteristic size of channel that depends intensely on density. Good agreement of the calculated values of the thermal conductivities of liquid argon with the experimental data allowed the value of the characteristic size of the channel as a function of density to be estimated [3]. In the case of argon nanowires, MD simulation results match the theoretical predictions reasonably well. The studies show that the phonon confinement effect influences the thermal conductivity of nanowires. Still, boundary scattering is the dominant factor decreasing the thermal conductivity with the thickness of nanowires. Furthermore, the estimation of the interface specular parameter as a function of the thickness of nanowires at a wide range of temperatures shows that specular phonon-boundary scattering prevails over diffuse phonon-boundary scattering [4].

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A comprehensive study on the mechanical properties of 2D epoxy materials by the Monte Carlo simulation method

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In this research, the effects of shape (equilateral triangle and square), and size $L_{\mathrm{x}} \times L_{\mathrm{y}}$ (10×9, 20×19, 30×29, 40×39 and 10×10, 20×20, 30×30, 40×40) on the mechanical characteristics of 2D (two-dimensional) epoxy material such as shape, strain (ε), stress (σ), Young stress (E), and shear stress (G) are studied by means of the Monte-Carlo (MC) method. It can be noted that after the change of the shape of structural elements from equilateral triangles (honeycomb structure) to squares, the strain (ε) increases, and stress (σ) decreases from 39.05 to 9.85, while the Young stress (E) decreases from $E_{h1} = 3.39$ GPa to $E_{s1} = 1.60$ GPa, and shear stress (G) decreases. Also, it can be seen that an increase in the size $L_{\mathrm{x}} \times L_{\mathrm{y}}$ from 10×9 to 20×19, 30×29, 40×39, and from 10×10 to 20×20, 30×30, and 40×40 is observed to have an opposite effect. The obtained results are completely consistent with the previous experimental and computational results in this field and can be considered a base for the experimental results for epoxy materials.

Hydration and proton conductivity of ternary transition metal oxides

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Barium lanthanide cobaltites with a perovskite structure have been extensively studied due to their potential application in electrochemical devices, such as Proton Ceramic Fuel Cells (PCFCs) and Electrolyzers (PCEs). They exhibit high electrical conductivity, good catalytic properties, and protonic defect formation upon exposure to water vapor [1]. On the other hand, recent reports suggest that more basic transition metals, such as Fe, promote protonic defects formation [2]. Furthermore, cobaltites exhibit high Thermal Expansion Coefficients (TEC), which makes them thermally incompatible with the most common electrolytes [3]. Therefore, the addition of iron can increase the proton concentration and alleviate the high TEC problem.

In this study we present structural, thermal, and electrical studies of $Ba_{0.5}Ln_{0.5}CoO_3$ -$Ba_{0.5}Ln_{0.5}FeO_3$ solid solutions. The main focus of this study was to evaluate the protonic defect formation and protonic conductivity. In order to do so, water uptake was measured in thermogravimetric experiment in which the atmosphere was switched from dry to wet conditions at a constant temperature and oxygen partial pressure. Water uptake was studied both in oxidizing (air) and inert (N_2) conditions. Additionally, the Hebb-Wagner polarization method was used to determine the protonic conducitivty of selected materials.

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A new approach to simulating the deposition of thin films realistically by combining Molecular Dynamics and time-stamped force-bias Monte Carlo methods

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The properties of thin films (TFs) often differ considerably from those of the bulk materials of the same composition. By offering new functionalities and capabilities, TFs find applications in many areas, such as electronics, optics and electrochemistry, attracting constantly growing attention.

Physical vapour deposition (PVD) is a widely used technique for the fabrication of TFs. It is known that the properties of a TF strongly depend on how the deposition process is carried out. However, the limitations of experimental techniques (in particular, those of spectroscopic and imaging methods) prevent a better understanding of the mechanisms governing the deposition of very thin films (several nm thick). This, in turn, hinders understanding of how the parameters of the manufacturing process translate into the produced TF characteristics and its resultant properties.

Atomistic simulations constitute an indispensable tool for predicting the behaviour of matter and interpreting experimental observations. The Molecular Dynamics (MD) method permits predicting the time evolution of an interacting atomic system and, therefore, constitutes a perfect tool for studying the deposition from the gas phase. In fact, the MD method has already been used many times for simulating PVD [1-4], allowing observing how the growth of TF depends on the critical parameters of the deposition process, such as the energies and angles of the incident atoms. However, the deposition simulations carried out so far had a number of limitations. The most important was the use of extremely high deposition rates (exceeding those used in the experiments by several orders of magnitude) and the lack of adequate accounting for the long-time relaxation, which occurs in the growing TF as a result of, e.g., diffusion.

During the talk, we will present a new approach that solves the above problems, allowing a more realistic simulation of the deposition of thin films from the gas phase. The developed method combines two simulation techniques: the MD method and the time-stamped force-bias Monte Carlo [5-6] (tfMC) method. Within the proposed simulation protocol, the first method (MD) is used to simulate the collisions of the incident atoms with the substrate surface and to model the fast relaxation that occurs

immediately after the collisions. The latter method (tfMC) – as it significantly extends the time scale accessed [7] – is used to simulate long-time relaxation. The proposed approach also accounts for other aspects equally important for reliable modelling of the growth. Among others, the energies and angles of the incident atoms follow realistic distributions known from the theory and experiments [8].

The proposed method was implemented from scratch and applied to simulate the growth of a thin (3 nm thick) Au film on the dc Si (001) substrate. The use of the tfMC method allowed us to obtain a deposition rate which was even 1000 times lower than those used by other authors in the last years [1-4]. Consequently, the carried simulation provided a much more realistic TF structure, and this was confirmed with a detailed analysis. It showed that the TF obtained from the hybrid MD+tfMC simulation had much lower energy, was more ordered (containing a lower number of defects: stacking faults, dislocations, grain boundaries), and possessed a more dense morphology, than the TFs obtained from simulations which used the MD method only. The carried out simulations also allowed us to characterize the growth process. It was found that the deposition of Au on crystalline Si proceeded through a layer-by-layer (Frank-Van der Merwe) mode and consisted of three very distinct stages:

1. initial destruction of the substrate surface layer, leading to significant Au-Si intermixing;
2. growth of the mixed Au-Si interface layer, accompanied by the formation of the nuclei of the Au fcc phase;
3. ordered growth of the formed fcc Au nanograins.

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Extremely non-trivial effects in some almost trivial models

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The hard potential is one of the simplest potentials. It describes interaction between purely geometrical objects, called hard bodies. These objects are defined by their size and shape only. Their interaction energy is assumed to be infinite when they overlap and zero otherwise. Despite its simplicity, the hard potential qualitatively describes a very wide class of phenomena and structures observed in nature, ranging from non-ideal gases, through liquids, liquid crystals, plastic crystals, glasses, and ending with crystals.

In this lecture a few examples of hard bodies, treated as molecules, will be presented. Some highly unusual effects found in theoretical studies and computer simulations of the systems of such molecules will be discussed.

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Modeling the interactions of magnetic nanoparticles in aqueous solution

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Nanotechnology is an important topic. Self-organization of nanoparticles is one of the methods of creating nanostructures in the form of nanolayers. Stable solutions of separated nanoparticles are required to ensure the highest quality of constructed nanostructures. Although Derjaguin, Landau, Verwey, and Overbeek's (DLVO) theory describes nonmagnetic nanoparticle interactions, the magnetic interactions between nanoparticles significantly reduce the stability of nanofluids. Therefore, we have to take them into account. Hence, in this study, we enhanced the DLVO model by adding dipole interactions integrated over thermal fluctuations. More specifically, in this presentation, it will be shown how magnetic interaction influences the total energy between nanoparticles. This model allows finding the pH value and salt concentration for which particles with a given size will form a stable or multi-stable solution.

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