Book of Abstracts

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Darya Alontseva	East Kazakhstan Technical University, Kazakhstan

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Viacheslav Barsukov	Kyiv National University of Technologies And Design, Ukraine
Jean-Yves Raty	University of Liege, Belgium
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PLENARY SPEAKERS

Phase Identification in $HfZrO_2$ Ferroelectric Thin Films: DFT and X-ray Absorption Fine-Structure Spectroscopy

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Abstract: HfO_2-based ferroelectrics are important materials for microelectronics applications such as advanced memory, and negative capacitance low-power field effect transistors. With the recent discovery of the ferroelectric phase of HfO_2 these materials become potentially good candidates for integration with silicon based complementary metal-oxide -semiconductor (CMOS) devices. The stabilization this ferroelectric phase and identification of the various phases present in $Hf(Zr,Al)O_2$ thin films are crucial for the implementation of these ferroelectric materials in CMOS processing technology. However, crystalline phase identification for hafnium-based ferroelectrics by diffraction techniques has been elusive. We use density-functional theory (DFT)-assisted extended X-ray absorption fine-structure spectroscopy (EXAFS) to determine the crystal symmetry of thin hafnium zirconium oxide ($Hf_{0.46}Zr_{0.54}O_2$) films grown by atomic layer deposition. Grazing incidence fluorescence-yield mode Hf L_3 absorption edge EXAFS experiments were performed at the 6-BM beamline at the National Synchrotron Light Source II of Brookhaven National Laboratory. Ferroelectric switching in $TiN/Hf_{0.46}Zr_{0.54}O_2/TiN$ metal-insulator-metal capacitors is verified. Grazing-incidence fluorescence-yield mode Hf L_3 and Zr K absorption edge EXAFS data are compared to reference data calculated from DFT-based atomic coordinates for various structural phases of $Hf_{0.5}Zr_{0.5}O_2$. Via EXAFS multiphase fitting, we confirm that the frequently invoked polar orthorhombic $Pca2_1$ phase is present in ferroelectric hafnium zirconium oxide, along with an equal amount of the non-polar monoclinic $P2_1/c$ phase. For comparison, we verify that paraelectric HfO_2 films exhibit the $P2_1/c$ phase.

Keywords: HfO, Thin film, Ferroelectric.

PLENARY SPEAKERS

Manufacturing and Characterization of Tantalum and Zirconium Microplasma Coatings

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Abstract: Currently, along with widely used Titanium and its alloys, the most promising materials for the production of medical implants are Tantalum, Zirconium and Niobium. To increase the biocompatibility of medical endoprostheses that grow into the patient's bone, various surface treatment methods for these implants are used, including coatings made of biocompatible materials applied by spraying. Fotovvati et al. have compared the results of obtaining biocompatible coatings by cold and thermal spraying in favor of thermal spraying. However, despite the advantages and relative cost effectiveness of the method of thermal plasma spraying, its use for the manufacture of medical implants has not yet become as widespread. This is mainly due to the high heating temperatures of the bulk resulted from the thermal spraying process. The microplasma spraying (MPS) avoids the issue of overheating. It allows obtaining coatings from materials with a high melting point, such as titanium and tantalum by a laminar microplasma jet. MPS introduces a very small thermal impact into the substrate. The use of robotic MPS could be considered promising for the production of patient specific implants. The studies proved that it was possible to obtain coatings from biocompatible materials with the desired level of porosity and satisfactory adhesion to the substrate by microplasma spraying. A robotic assisted microplasma spraying of coatings from biocompatible materials of Titanium and Hydroxyapatite onto titanium implants has been implemented. The objective of this work is to consider the advantages and challenges of using robotic MPS for applying Tantalum and Zirconium coatings to medical implants using scanning electron microscopy (SEM) to analyze the effect of various MPS modes on the morphology and structure of coatings. The research has been carried out at a pilot production site with an industrial complex for plasma processing of materials on the basis of Kawasaki RS-010LA, an industrial robot (Kawasaki Robotics, Japan). The robot's arm is equipped with "MPN-004" microplasmatron produced by EWI (Ukraine) for microplasma spraying of wire or powder coatings. The main results of this work are the following: 1) it has been established that the main parameters controlling the size of the sprayed particles and the porosity of the coatings are the electric arc current and the plasma gas flow rate. The parameters of microplasma deposition of Ta or Zi-wire for the

formation of porous coatings with rough surface have been established. 2) The advantages of applying SEM for analysis of the structure of sprayed Tantalum and Zirconium coatings have been shown. The analysis has been successful in assessment of the relation of the morphology and structure of coatings on the processing parameters of the MPS. The results of the research are of significance for a wide range of researchers developing the plasma spray technologies of biocompatible coatings manufacturing. Acknowledgment. The study has been conducted with the financial support of the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan by the project AP05130525 “The intelligent robotic system for plasma processing and cutting of large-size products of complex shape”.

Keywords: Microplasma Spraying, Zr coatings, implants, material utilization rate

INVITED SPEAKERS

Id-1734

Peculiarities of Dipolar Ordering in Mixed Cation Halide Perovskites

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Abstract: The methylammonium (MA) lead halides MAPbX3 (where X = I, Br, Cl) are popular perovskite materials among scientists and industry due to their perspectives in effective and cheap solar cells [1]. During the past decade, the power conversion efficiency of cells based on these hybrid compounds exceeded more than 20%. A high performance of these materials results from several physical properties such as large absorption coefficient, optimal bandgap, long carrier diffusion length, low exciton binding energy, exceptional defect tolerance. However, a successful application of hybrid perovskite solar cells is mainly prevented by their lead toxicity and poor both thermal and water stability. The most stable and efficient solar cells are obtained by using perovskites with mixed cations at the A-site. The most popular alternatives to MA are formamidinium and Cs^+ ions. A Dimethylammonium (DMA) cation has been introduced recently as an alternative A-site modification for these compounds. Several investigations have shown that during certain synthesis procedures high quantities of DMA may be unintentionally introduced into $MAPbI_3$ and $CsPbI_3$. These modifications stabilize the preferable cubic phase of MAPbI3 and leads to the enhanced performance at ambient condition. In the field of classical inorganic perovskites it is well known that mixing may significantly perturb structure of resulting compound. Thus, the long-range order can be suppressed and frustrated phases may appear. The dielectric permittivity behavior of lead halides seem to be especially informative for the performance of the perovskite cells, as their relatively high value of the dielectric permittivity results in a pronounced defect tolerance and low exciton binding energy. However, a complete understanding of mixing effects on the dielectric permittivity dynamics and structural phase behavior is still absent. Here, we present a multitechnique experimental study of the mixed hybrid perovskite $MA_{1-x}DMA_xPbBr_3$. Our results show that structural phase transitions are significantly suppressed even for a low substitution of the DMA cations. For higher DMA levels,

the long-range dipolar order disappears and dipolar glass dielectric behavior dominates in the dielectric spectra.

Keywords: Methylammonium, solar cell, Dimethylammonium, Halides.

INVITED SPEAKERS

Id-1738

SMARTELECTRODES: Electrodeposited Foams/Nanostructured with Large Specific Area Suitable for Catalytic, Sensing and Magnetic Applications

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Abstract: Demand of “smart” electrodes/systems has recently increased due to significant role of various devices/equipment based on these electrodes used for versatile application. The smart-electrodes play significant roles in several areas as catalysis/electrocatalysis, magnetic, sensoring, thermoelectrics, electrowinning. The 3D architecture extends the surface area and properties of such electrodes and leads to improvements across multiple performance parameters. In this view, metal foams offer a substantial specific surface area and sturdy frame, which makes them great candidates for various applications such as catalysts, sensors, heat sinks, etc. Metal foams electrodes as catalysts could replace the expensive Pt, because they could be made from cheaper materials e.g. iron group metals. Thus, cobalt and its various compounds are being considered as a cheaper alternative for precious and rare metal catalysts (like Pt, Ir and their oxides). There are two ways to form metal foam via electrodeposition: i) deposition on polymer template; ii) using hydrogen bubbles as template. In the last case, by manipulating electrochemical deposition parameters (current density, solutions composition, deposition time, temperature etc.) we can obtain different pore sizes and porosity levels. Obtained porous/textured surfaces can be easily modified using various electrochemical techniques, further enhancing their applicability in various fields. Thus, obtained porous materials have been tested for electrochemical catalytic activity in alkaline media – hydrogen evolution reaction (HER) as well as oxygen evolution reaction (OER), including modified foams were evaluated for application as sensors for free chlorine in water detection. Furthermore, the commercial copper foam was used for Fe electrodeposition and has been tested as a catalyst for Fenton reaction applied to methyl orange (MO) dye aqueous solution organic decomposition. Moreover, nanostructured iron group metal electrodes can have tunable magnetic properties depending on temperature and time of electrodeposition. The targeted application can be expanded even more by controlling alloying element and/or surface architecture offering the

most flexibility to tailor not only their magnetic properties, but also their thermal expansion and corrosion resistance. Thus, smartelectrodes generates extensive research that focus on understanding of the controlling mechanisms to build a toolbox to guide applications of new materials in different systems/devices. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement Nº 778357- SMARTELECTRODES.

Keywords: Electrodeposition; Iron Group Metals; Foams; Nanostructured; Specific Area.

INVITED SPEAKERS

Id-1739

SMARTELECTRODES: New Way of Recovering Metals from Electronic Waste by Electrowinning

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Abstract: Electrowinning is a very convenient and robust way to recover dissolved metals such as copper, silver, gold, nickel, cobalt, and other metals that can be electrodeposited from aqueous solutions. Electrowinning comprises an electrochemical cell, where metal ions are reduced and deposited in metallic form onto the cathode, while usually oxygen gas is a main product of anodic process. The most important component in the electrochemical reactor is the cathode. The electrode can be broadly classified into two types, namely 2D or 3D- electrodes. These electrodes can be static or moving, such as the rotating cylinder or disc electrode, cyclone-type design. High mass transfer rates can be achieved with electrode movement, while high surface area can be achieved with the use of porous, three-dimensional electrodes. Three-dimensional electrodes (smartelectrodes) are more superior compared to two-dimensional electrodes when dealing with dilute process liquors, due to the high active electrode area per unit reactor volume leading to more turbulent mass transport conditions adjacent to the electrode surface. Examples of three-dimensional electrodes are porous graphite electrodes, carbon felts, reticulated vitreous carbon, packed-bed electrodes, active fluidized-bed electrodes, metallic foam electrodes. Data on comprehensive investigation of foam electrodes will be provided and compared with 2D copper electrodes applied for electrowinning of Cu and Sn. Using chronoamperometry, and electrochemical impedance spectroscopy (EIS) it was determined, that the copper deposition, under investigated concentrations, and potentials, was controlled by mass transfer. It was also determined that because of superior hydrodynamic capabilities copper electrodeposition occurs 3 times faster on the porous copper substrate, than on the flat one. Using EIS data it was determined that commercial porous electrodes have up to 14 times higher electrochemically active surface area. Using chronopotentiometry and Sand's equation effective diffusion coefficients of Cu (II) ions have been calculated and the average effective diffusion coefficient on a flat copper surface is $6.72 \cdot 10^{6}$ cm²/s and on porous copper foam – 19.67·106 cm²/s. It was also determined that copper foam has lower charge transfer

resistance than flat copper plates, making the electrodeposition faster on the porous surface. Therefore, metal foam electrodes preferentially may be used for electrowinning if electrode processes are controlled by mass transfer, since it shows less hydrodynamic limitations. In order to intensify electrowinning, Sn cementation by Zn can be also concerned. During this procedure the 4 valent Sn is exchanged by 2 valent Zn. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement Nº 778357- SMARTELECTRODES.

Keywords: Electrowinning, Electrodes, Metallic Foam, Tin, Copper.

INVITED SPEAKERS

Id-1803

Measurement of Magnetic Permeability Using Various Methods

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Abstract: Fast kicker magnets are used for the beam injection and extraction out of the European Organization for Nuclear Research (CERN) accelerator rings. These magnets are often ferrite loaded transmission line type materials. For a correct development of accelerator's equipment a good knowledge of electromagnetic properties of materials in the wide frequency range is essential. The sample which was investigated in this work is material sample of a ferrite garnet (low loss commercially available ferrite material AL800), which will be used in a tuner that is installed on the 80 MHz cavity in the CERN Proton Synchrotron machine, as a part of the injector chain for the Large Hadron Collider. Unfortunately, producer does not provide enough electromagnetic parameters of the ferrites. Thus, magnetic properties of ferrites must be investigated. One of most popular measurement method is implemented in Keysight 16454A magnetic material test fixture. It uses approach of lumped inductor, with very simple mathematical model. This approach does not take in to account factors, which are important on the high frequencies as distributed parameters of the system and dielectric permittivity of the sample. Required frequency range exceeds 1 GHz limit of Keysight 16454A. In order to achieve maximal accuracy the text fixture optimized to sample dimensions was made. Real part of magnetic permeability goes to negative values. In order to be sure, does the simple model provide accurate enough results – numerical calculations using finite element method software were performed using the same impedance data as in the simple model, measured by vector network analyzer. We took in to the account detailed geometry of the sample and test fixture as well as dielectric permittivity of the sample. We used Ansoft HFSS commercial software. Simulation software solves direct task – calculates impedance by using electromagnetic properties of the material. In order to solve reverse task, we used optimization function. During optimization, algorithms select permeability values to fit optimization goal, which is the value of measured impedance. It is time consuming, but universal method for relation of measured impedance of the test fixture to electromagnetic properties of the material. We see good agreement between simple model and numerical simulation results. Thus, conventional model and our test fixture perform acceptable accuracy up to 2 GHz frequency.

Keywords: Magnetic Permeability, Finite Element Method, Ferrite, Impedance.

INVITED SPEAKERS

Id-1830

Composite Paints for Electromagnetic Shielding

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Abstract: We have developed composite paint based on graphite, carbon black and some other not expensive components, which can be used as a clay court for sustainable buildings and electronic devices. This paint can reduce sufficiently the problem, which is related to the effects of electromagnetic radiation (EMR) on human health. Cellular and radiotelephones, as well as their broadcast antennas, especially which use of the 5G, 6G communication system, may pose a high risk of cancer, reproductive disorders, memory, cellular stress, neurological and mental disorders. The medical disorders are already often experienced by servicemen working at radar stations, observation posts and other similar facilities associated with high-frequency EMR. The effect of EMR is especially dangerous for children of preschool and school age, so, it is necessary to use similar paints first of all for such buildings. Carbon-based composite paints have been developed, which can be used as a clay court for sustainable buildings and electronic devices. This paint can reduce sufficiently the problem, which is related to the effects of electromagnetic radiation (EMR) on human health. Cellular and radiotelephones, as well as their broadcast antennas, especially which use of the 5G, 6G communication system, may pose a high risk of cancer, reproductive disorders, memory, cellular stress, neurological and mental disorders. The medical disorders are already often experienced by servicemen working at radar stations, observation posts and other similar facilities associated with high-frequency EMR. The effect of EMR is especially dangerous for children of preschool and school-age, so, it is necessary to use similar paints first of all for such buildings. It is also necessary to note the significant impact of EMR on electronic equipment. First of all, this is a well-known problem of providing the so-called "electronic compatibility", when simultaneously operating different electronic equipment (e.g., thermal imager and radio transmitter) interfere with each other. A number of scientific developments have been implemented and work is underway under the NATO SfS international grant in this area.

Keywords: Electromagnetic Shielding, Carbon Composite Paint, Sustainable Buildings, Electronics.

INVITED SPEAKERS

Id-1832

Metavalent Bonding: Characterisation and Implications for Applications in Phase Change Materials, Thermoelectric and Photovoltaic Compounds

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Abstract: In the last two decades, Phase Change Materials have emerged as active components of non-volatile memories thanks to their ability to switch extremely rapidly from a conducting crystal to a semiconducting glass. Ab Initio simulations helped understanding the structure and some properties of the glassy phase, like aging, but also led us to reinvestigate the nature of chemical bonding in the crystalline phase. Using a two electron (pair density) formalism, we develop a two-dimensional map based on a quantum-topological description of electron sharing and electron transfer in binary solids. This map intuitively identifies the fundamental nature of ionic, metallic, and covalent bonding in a range of elements and binary materials. More interestingly, it highlights a distinct region where phase change materials are found and for which bonding has been qualified as 'metavalent'. Extending this map into the third dimension by including physical properties interesting for applications, we show that bonding in metavalent compounds differs from the usual views of bonding. This map could then be used to help designing new materials: by searching for desired properties in a 3D space and then mapping this back onto the 2D plane of bonding. Indeed, the metavalent region of the map encompasses compounds with other enhanced properties, such as high thermoelectric performance or photovoltaic efficiency. We illustrate metavalent bonding for lead chalcogenides and V-VI compounds, and the transition between covalent and metavalent regions of the map is described. Interestingly, we show that it is possible to transform regular covalent bonds metavalent through excitation, which can explain the ovonic threshold switching behavior of some chalcogenide glasses, or sub-picosecond laser induced phase transitions.

Keywords: Metavalent Bonding, Phase Change Materials, Chalcogenides, Ab Initio Simulation, Glasses.

INVITED SPEAKERS

Id-1843

Role of Critical Parameters (Composition, Phase Superposition and Grain Size) on the Electrocaloric Properties of $BaZr_xTi_{1-x}O_3$ Ceramics

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Abstract: In the last years, there is a high interest in developing alternative cooling technologies because: (i) it is important to reduce greenhouse gases that are used heavily in domestic and industrial refrigeration; (ii) high current densities in integrated circuits impose higher demands on cooling systems that cannot met by the fan-based solutions. The main advantage of electrocaloric (EC) refrigeration is that by comparison with magnetocaloric solid-state refrigerators based on another solid-state cooling technology, the big-sized magnet is still a drawback. $BaTiO_3$ (BT) family as EC materials has been studied quite extensively in the past several years in various forms including thin films, bulk ceramics (also multilayer ceramic capacitors -MLCC) and single crystals and a large ΔT has been reported for BT-ceramics in the vicinity of ferroelectric-paraelectric (FE-PE) (tetragonal-cubic T-C) phase transition. Owing to the high transition temperature the using of pure BT as EC materials is limited, but this can be properly modified by incorporation of suitable dopants. In the present work we proposed to study the effect of composition and grain size on the phase superposition and electrocaloric effect in $BaZr_xTi_{1-x}O_3$ ceramics with x=0.02 – 0.20. Ceramics were obtained by sintering at 1500 ^oC the powders prepared by solid state method. X-ray diffraction data showed the phase purity and SEM images demonstrated homogeneous microstructures (average grain size between 10-5 μm) and well-defined grain boundaries. Impedance spectroscopy in the temperature range of (25 to 150)^oC shows a composition-induced ferroelectric-to-relaxor crossover with compositional-dependent shifts of the structural transition temperatures by comparison with ones of the pure BaTiO3. All samples are tunable, DC tunability increasing with x from 2.11 (x=0.08) towards 2.6 (x=0.20) at 25 kV/cm. P(E) loops indicate regular variation with increasing Zr addition, a reducing of loop area, remanent and saturation polarization from P_{sat}=15μC/cm^2 to P_{sat}=9μC/cm^2. ECE was indirect evaluated from P(E) loops with temperature and in case of

Zr addition a maximum of 0.7 K was obtained for x=0.04 at 373K. This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-TE-2019-1689, within PNCDI III

Keywords: $BaTiO_3$ Solid Solution, Ferroelectric-Relaxor Crossover, Electrocaloric Effec.

INVITED SPEAKERS

Id-1871

Modeling Phonons and Mechanical Properties of 2-Dimensional Materials

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Abstract: In the first part of the presentation the phonon spectra of graphene and hexagonal boron nitride (hBN) are calculated through dynamical trajectories obtained by molecular dynamics simulations. Their dependence on temperature or mechanical strain is presented. In the second part, analytical empirical potentials will be presented for efficient atomistic simulations of graphene and then the mechanical response of graphene and graphene nanoribbons of various widths under uniaxial tension is calculated.
Keywords: Graphene, BN, Phonons, Mechanical Response, Molecular Dynamics.

INVITED SPEAKERS

Id-1883

Exploiting Local Field Inhomogeneity for Tunning Functional Properties in Ferroelectric Based Composites

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Abstract: The interfaces between regions with contrasting permittivities in composites modify the local field distribution. The effective macroscopic properties of composites are a result of this local field inhomogeneity and therefore, the properties of ferroelectric-based composites can be tailored by controlling the microstructure characteristics (local field engineering) or by adequate choice of the phase constituents and phase interconnectivity. This approach can be applied to design ferroelectric-magnetic composites with specific dielectric/ferromagnetic properties. Since the local field inhomogeneity increases when the difference in permittivities of the constituent phases is higher, porous ferroelectric structures ensuring a maximum permittivity contrast have a great potential in order to reach desired ferro/dielectric properties, although porosity is usually considered detrimental in electroceramics. Based on this idea, 3D FEM models have been developed to compute local field distributions in realistic microstructures in order to explore the possibility to maximize their ferroelectric (switching) or non-linear dielectric responses (tunability). The role of nanostructuring and of porosity on the macroscopic properties (effective permittivity, tunability, P(E) hysteresis loops and piezoelectric) were studied theoretically and validated for BaTiO3 nanostructured ceramics, for a few types of PZT ceramics with various porosities, including anisotropic, and for PbTiO3 films with vertical nanoporosity. As a first step, different realistic 3D microstructures were generated. Local field distributions were computed by 3D FEM calculation and used as inputs in switching (Preisach and Landau-Ginzburg-Devonshire) or tunability (Johnson) models, in order to derive the ferro/dielectric, piezoelectric and tunability responses. If properly engineered in well-controlled microstructures, porosity may be used as an elegant factor to enhance functionalities as result of the field concentration in specific regions. This work was supported by the Romanian UEFISCDI projects PN-III-P1-1.1-TE-2019-1929 and PN-III-P4-ID-PCE-2020-1988.
Keywords: Local Field Engineering, Composites.

INVITED SPEAKERS

Id-1886

Effect of Porosity on Dielectric, Ferroelectric and Piezoelectric Properties in Batio3- Based Materials

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Abstract: In the last years, piezoelectric materials have attracted a growing attention for energy harvesting due to their excellent electromechanical conversion properties. Thus, taking into account the adopted European legislation to restrict or eliminate the use of lead piezoelectric materials and alternative of these have been stared to be search. The first approach of this study was to prepare a Pb-free material with high piezoelectricity which to possess a combination of physical (figures of merit (FOMs)) properties. The challenging in obtaining these types of materials with enhanced FOM is to reduced dielectric constant, while keeping high the piezoelectric and pyroelectric performances. The recent studies demonstrated the benefits of introducing porosity in ceramics for various purposes and improving of piezoelectric FOM for energy harvesting application. In order to increase the piezoelectric performances, solid solutions of $BaTiO_3$ close to the morphotropic phase boundary like in $Ba_{0.85}Ca_{0.15}Zr_{0.10}Ti_{0.90}O_3$ (BCTZ) was proposed. The aim of the present work was to use Finite Element Method (FEM) for designing porous microstructures and to demonstrate how the porosity influences the permittivity response. Also, the preparation and investigation of the effect of porosity on structural and functional (dielectric, ferroelectric, non-linear and piezoelectric) properties in $Ba_{0.85}Ca_{0.15}Ti_{0.90}Zr_{0.10}O_3$ (BCTZ) ceramics were reported. The microporosity with 0-3 connectivity has been produced by using poly(methyl methacrylate) (PMMA) microspheres as sacrificial template. The structural investigation has shown that the porosity induced phase transition from orthorhombic to tetragonal phase. The role of porosity on the low and high field dielectric properties was studied in BCTZ ceramics with various porosity levels (from 4 to 31% of porosity). The maximum permittivity decreases with increasing porosity, from around 6000 (ceramic with 92% density) down to 3000 (ceramic with 69% density), and a shift with a decrease

of Curie temperature from 65ºC to 70ºC due to the possible structural and strain modifications. The effect of porosity, grain size and specific microstructural characteristics induced by the pore forming addition, from closed porosity with interconectivitty (0-3) type towards (3-3) of microstructures for the most porous ceramics was taken into consideration. All the investigated ceramics preserve a high level of tunability as in the dense material. An enhanced piezoelectric response (d_{33}) with increasing of porosity level in BCTZ ceramic was obtained. Therefore, we have obtained porous BCTZ ceramics with reduced dielectric constant and enhanced piezoelectric FOM, which are leading to the idea for using them as materials for energy harvesting applications. This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS – UEFISCDI, project no PN-III-P4-ID-PCE-2020-1988, within PNCDI III.

Keywords:.Porous piezoelectric ceramics.

INVITED SPEAKERS

Id-1891

Thermo-Mechanical Behavior of AISI 4140 and MMFX Steel at Different Temperatures and Strain Rates

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Abstract: The present paper addresses experimentally the thermomechanical responses of two high strength steels AISI 4140 and MMFX by examining their flow stress under different temperatures and strain rates. To characterize these steels, two distinct test configurations were utilized. The first was conventional uniaxial tensile tests conducted over a wide range of temperatures, i.e., room and three elevated temperatures of 523 °K, 723 °K and 923 °K and three strain rates of 0.0015 s^{-1}, 0.015 s^{-1} and 0.15 s^{-1}. The second test configuration was carried out under dynamic compression using a drop mass bench at room temperature and considering three intermediate strain rates of 300 s^{-1}, 400 s^{-1} and 500 s^{-1}. Scanning electron microscopy (SEM) images were also taken to quantify the density of micro-cracks and voids of fractured specimens. Particular attention was paid to key features related to plastic straining, work-hardening, dynamic strain aging and their connection to the coupling effect of temperatures and strain rates. The flow stresses of AISI 4140 and MMFX steels showed almost insignificant dependence on the quasi-static strain rate at room temperature. However, the strain rate sensitivity increases as the temperature increases with very active regions of dynamic strain aging (DSA) encountered at higher temperatures. The Voyiadjis-Abed (VA) model was utilized to describe the flow stress of these two alloys and was implemented into finite element (FE) software to develop a robust FE model that can accurately simulate different structural responses of AISI 4140 and MMFX steel alloys.

Keywords: AISI4140; MMFX; Temperature, Strain Rate, Mechanical Characterization, Damage, Constitutive Modeling

REGULAR SESSIONS

Id-1736

SMARTELECTRODES: In Situ Study of Chalcogenide Thin Films Growth During Vacuum Thermal Evaporation

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Abstract: The aim of the present work is the in situ characterization of the thin films growth process by optical transmission method. There are several methods capable of accurately measuring the thickness such as ellipsometry, interference microscopy, and normal incidence transmission or reflection spectrophotometry. In order to get in situ thicknesses growth we have implemented a normal incidence optical transmission method because it is relatively simple and requires little modification to the growth chamber. The thicknesses of thin films based on chalcogenide glasses namely As_2S_3 and Se were monitored simultaneously during thermal vacuum evaporation from two boats. We used 945 nm light-emitting diode which is suited for chalcogenide glasses thin film investigations due to weak absorption in this region. In such a case, interference from the light transmitting and reflecting from different interfaces will affect to the overall transmittance. As the film grows, the interference conditions change, causing the sample transmittance to oscillate with a frequency determined by the growth rate, the incident wavelength, and refractive index of the film. Knowing the incident wavelength and refractive index of the film this method was used to monitor growths in real time. First of all the refractive index dispersion of As_2S_3 and Se films were evaluated from transmission spectra proposed by Swanepoel. Refractive index, in this case, is represented using Cauchy approximation $n(\lambda)=A/\lambda^2+B$ that works well for chalcogenide glasses in the visible and NIR range. Assuming a refractive index of 2.285 and 2.415 at 945 nm for As_2S_3 and Se films correspondingly, which were extrapolated from the obtained refractive index dispersion spectra, we modelled the optical oscillations during the film thickness growth. Each oscillation period corresponds to the determined value of film thickness. This is within 1% of what was obtained by transmission spectra after evaporation of film. The authors acknowledge the financial support of the 778357-SMARTELECTRODES project (H2020) and Moldavian National Agency for Research and Development grant No. 20.80009.5007.03.

Keywords: Thin Films, Chalcogenide Glasses, Thermal Vacuum Evaporation, In Situ Measurement

REGULAR SESSIONS

Id-1744

SMARTELECTRODES: Scaling up from 2D to 3D Electrodes and Unifying Methods of their Catalytic Activity Characterization Using EIS

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Abstract: In the renewable energy field, molecular hydrogen is considered a feasible alternative to fossil fuels due to its high energy density and environmentally friendly characteristics. Electrochemical water splitting is an economical route to produce H_2, but a catalyst is needed to lower the kinetic barrier of the hydrogen evolution reaction. Broadly speaking, there are two ways to enhance the catalytic performance of an electrode – modifying the catalytic material's intrinsic properties, or increasing the electrocatalytically active surface area. The latter is a much simpler way, as it relies on the homogeneous dispersion of a given catalytic material over a conductive substrate with a high geometrical surface area. However, it is also preferable that the electrode have a small volume. For this reason complex-shaped 3D electrodes (metallic foam, carbon cloth, nanostructured, etc.) are widely used in the construction of catalytic cells. It is often almost impossible to measure the geometrical surface area of such electrodes, which complicates the characterization of their catalytic efficiency. In this study catalytic MoS_2 films have been electrochemically deposited onto copper wire (2D) and metallic copper foam (3D) substrates by varying the catalyst loading as measured by charge passed during deposition. The prepared electrodes were used for HER electrocatalysis in 0.5 M H_2SO_4 media. Their characterization included typically-used methods: linear sweep voltammetry (LSV), Tafel slope calculation, galvanostatic stability, as well as a non-stationary electrochemical impedance spectroscopy (EIS) study. LSV measurements revealed that better electrode activity (higher HER currents at lower overpotentials) were achieved by electrodes with higher catalyst loading. In contrast, the lowest Tafel slope was achieved only at an optimal catalyst loading. Finally, the EIS study revealed that total electrode activity is decisively linked to one parameter – hydrogen adsorption resistance – which is directly related to charge passed during electrodeposition regardless of the substrate used (2D or 3D). It is therefore proposed that this method can be used to characterize and compare catalytic electrodes regardless of geometric surface area

uncertainties. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement Nº 778357- SMARTELECTRODES.

Keywords: Hydrogen Evolution Reaction, Catalysis, Electrochemistry, Molybdenum Sulfide.

REGULAR SESSIONS

Id-1749

The Effect of Graphene Structural Integrity on The Thermoelectric Behavior of Bismuth Telluride

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Abstract: This study examines the effects of the structural integrity of graphene on the thermoelectric properties of p- and n-types bismuth telluride nanocomposites. These nanocomposites were prepared via mechanical alloying and spark plasma sintering techniques. Different graphene concentrations were added at different time intervals during mechanical milling. The thermoelectric properties were measured and the results showed that the milling time significantly affected the structure and the defect level of graphene as well as its agglomeration. It is revealed that the optimum time to add the two-dimensional filler is during the last phase of mechanical milling as it will preserve graphene's structure and boost the electrical conductivity. The results also showed that as the milling time of graphene increases, the Seebeck coefficient improves. Even though an increase in the thermal conductivity is expected due to the high electrical conductivity, a clear reduction in the lattice thermal conductivity part was obtained due to the increased scattering at the new interfaces. In the n-type $Bi_2Te_{2.7}Se_{0.3}$ matrix, the figure-of-merit for the optimum sample with 0.05 wt.% graphene added in the last 10 minutes of milling had an improvement of 19% at room temperature and 25% at 160 degrees Celsius achieving a final value of 0.81.

Keywords: Graphene; thermoelectric; Bismuth telluride, nanocomposite; Figure of merit.

REGULAR SESSIONS

Id-1781

Optimization of Ball-Milling Parameters for The Processing of Samarium-Cobalt Magnetic Compound Using Taguchi Approach

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Abstract: High temperature resistant Sm-Co intermetallic magnets find many applications in high tech industry. The popular route for the manufacturing of these magnets is powder metallurgy route where ball milling is an important mechanical process having lot of parameters influence the final magnetic properties of the product. It is therefore, important to optimize the ball milling parameters to make a better control over the reproducibility of the final product. Taguchi orthogonal array is well known statistical tool to reduce the large number of experiments. In this study L9 orthogonal array is used to observe the effect of four prominent ball milling parameters i.e. ball milling time, ball milling speed, ball:powder ratio and ball size ratio, at three levels. The results identify the maximum influencing individual parameters and the interaction of these parameters on coercivity and ramanance of the final product.

Keywords: $SmCo_5$, Ball Milling, Taguchi Array, L9 Orthogonal Array.

REGULAR SESSIONS

Id-1805

Preparation and Characterization of Dielectric, Ferroelectric and Piezoelectric Properties of Lead-Free Ceramics on the Base of Sodium-Bismuth Titanate and Sodium-Potassium Niobate

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Abstract: Lead-free perovskite oxide materials are among the most intensively studied in order to replace widely used toxic lead containing ones last ten years. We studied influence effects of cation substitutions in A- and B-sites on stoichiometry, structure parameters, microstructure, dielectric, ferroelectric, and piezoelectric properties of ceramics based on sodium-bismuth titanate $(Na_{0.5}Bi_{0.5})TiO_3$ (NBT) and sodium-potassium niobate $(K_{0.5}Na_{0.5})NbO_3$ (KNN) perovskite ceramics. Ceramic samples in the systems $(Na_{0.5}Bi_{0.5})TiO_3$ - $BaTiO_3$ (NBT-BT) and $(K_{0.5}Na_{0.5})NbO_3$ – $BaTiO_3$ (KNN-BT) with compositions close to the Morphotropic Phase Boundaries (MPB) were prepared by the two-step solid-state reaction method at high temperatures up to 1500 K. The samples were additionally modified by Li^+, Ag^+, K^+, Mn^{3+}, Ni^{3+}, and Fe^{3+} cations. Over stoihiometric additives KCl, LiF, Bi_2O_3, CuO and ZnO were additionally used to improve sintering of ceramics. The samples were characterized using complex of physico-chemical methods using the X-ray Diffraction, Scanning Electron Microscopy (SEM), Second Harmonic Generation (SHG), Dielectric Spectroscopy, and Piezorespone Force Microscopy (PFM) methods. Changes in the unit cell volume of the KNN- and NBT-based ceramics were observed correlating with radii of A- and B-cation substitutions. In the dielectric permittivity versus temperature curves anomalies related to ferroelectric phase transitions marked by steps at ~ 450 K (NBT) and by peaks at ~ 550 K (NBT) and at ~ 700 K (KNN) were revealed of the compositions studied. Phase transitions near 450 K revealed typical relaxor-type behavior attributed to the presence of polar nanoregions in a nonpolar matrix. Non monotonous changes in the spontaneous polarization value were checked in modified ceramics using the

SHG method. Local PFM hysteresis loops for the KNN- and NBT-based ceramics were observed indicating ferroelectric polarization switching at nanoscale. At the room temperature, non monotonous changes of the dielectric parameters ε_{rt} and $\tan\delta_{rt}$ and maximum effective d_{33} values were observed in modified BNT- and KNN-based ceramics, thus confirming their prospects for new lead-free materials development. In addition, a decrease in the magnitude of the coercive voltage in the modified samples, which is important for measurements of piezo- and electrocaloric properties of processing samples was observed.

The work was supported by the RFBR and DFG (Project 21-53-12005).

Keywords: Perovskites, Piezoelectrics, Modification.

REGULAR SESSIONS

Id-1809

Scanning Magnetometer Based on A Magnetoimpedance Sensor for Nondestructive Evaluation of Materials Containing Magnetic Nanoparticles

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Abstract: The glass coated Co-rich amorphous ferromagnetic microwires with small metallic core diameters d = 5 – 30 μm are promising for various technological applications. In particular, Co-rich microwires with a negative nearly zero magnetostriction show giant magnetoimpedance (GMI) effect with a high GMI ratio. A new generation of sensitive miniature GMI magnetometers is being developed on the basis of such microwires. As has been shown recently, the off-diagonal GMI sensor based on the microwire was used as a measuring head of a scanning magnetometer. The important characteristics of scanning magnetometer are magnetic sensitivity and spatial resolution. These parameters are determined by the measuring sensor. In this work, the GMI scanning magnetometer with a magnetic field sensitivity of better than 1 nT and a spatial resolution of less than 1 mm was used for magnetic nondestructive evaluation of material containing magnetic nanoparticles. The off-diagonal GMI-sensor was based on a 4 mm microwire segment and a measuring coil wound around the microwire. The GMI-sensor was placed perpendicular to the sample surface. The minimal distance ***h*** between the microwire's tip and the sample surface could be up to 0.1 millimeters. Relative movement of the sample and the GMI-sensor was performed by means of X-Y-Z positioner. Measurements were carried out within a magnetic shield to reduce the effects of external magnetic fields. To check the main characteristics of the developed scanning magnetometer, single and double current lines of different sizes were used as the samples. The samples were made of copper wire 0.04 mm in diameter and supplied with a DC current of 3 mA to 30 mA. It is known that laser printer toners contain up to 10% magnetic iron oxide nanoparticles. In this work, as samples, we used lines of different widths, which were printed on a black and white laser printer HP 2200. Before

measurements, the samples were magnetized in a perpendicular or longitudinal magnetic field. Magnetic nanoparticles contained in the sample can retain residual magnetization and generate weak local magnetic fields. During the measurements, magnetic images of various samples printed on a laser printer were obtained. The results show that the GMI scanning magnetometer can measure the local magnetic fields of samples containing micrograms of magnetic nanoparticles. The authors gratefully acknowledge the financial support of Russian Science Foundation, grants 20-19-00607.

Keywords: Amorphous Microwires, Scanning GMI Magnetometer, Magnetic Toners, Magnetic Images.

REGULAR SESSIONS

Id-1821

Role of R&D Toward Fossil Fuels to Clean Environmentally Friendly Fuels

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Abstract: The need of using fossil fuel is increasing due to many factors. The era of producing heavy oil became a fact. This is observed based on the importance of growing up in the advanced technologies worldwide on the upstream related to heavy oil production. The major reason behind this is the depletion of the light, high-quality crude oils, at the same time the demand for fossil fuel is in the continuous increase. At the same time, fossil fuels are considered to be more than 90% of total energy demand in the coming decates for production of clean and envirnmentally friendlay fuels. Fossil fuels is the major cause for CO2 mitrogen & sulfur Oxides emission and particulates. Efforts have to be made to enhance the usage of clean fuels from fossil fuel to reach zero level emission. Based on the above, required studies and investigations are substantially needed in order reach different means and ways of utilization of fossil fuels to produce clean fuels. Research & Development (R&D) has a significant impact to countermeasure and mitigate the issues related to this matter.Among these studies are the following: characterization and crude oil assays of typical crude oil, utilization by blending, partial upgrading & full upgrading schemes, distillation of heavy crude oil, advanced characterization on the molecular level of different fraction including the middle distillate and residual portion, process scenarios, technology advancement including key parameters associated in processing the fossil fuel, reactor configuration, target product specification, and catalysts, utilization associated such as hydrogen….etc, environmental impact and comply with the regulations and guideline worldwide.This paper will address the above through an overview, elaboration, highlighting the various issues, problems, solutions through cases studied and investigation. Workplan and topics to be considered for future will be also given as part of the paper.

Keywords: Fossil Fuel, Crude Oil, Emission, Technologies.

REGULAR SESSIONS

Id-1834

Interlocking and Welding Effect on the Electrical Machines

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Abstract: The report demonstrates experience in implementing instrumentation to define characteristics two-phase flows for helium, hydrogen, liquefied natural gas (LNG), and oil-water-gas mixtures. Two types of such devices are presented. The first type is flow-meters based on combination of a void fraction RF-sensor and a narrowing device. They can be applied for superconducting accelerators cooled with two-phase helium, refueling hydrogen system for space ships and oil production industry. A feature of the cryogenic RF-sensor is that its sensitive part is made of metal-ceramic tube. A combination of a gamma-densitometer and a narrowing device is employed for the second type. These systems can be used for the diagnostics of LNG and oil-formation water flows. Temperature sensors with negative and positive temperature coefficients for wide range of application (from 1.5 to 373 K) and a measuring system based on a modular industrial computer, are presented as well. In particular, the composite TVO sensor is made of nanoscale grains of carbon within micronized alumina oxide substrate. The obtained characteristics for different flow-meters are discussed. It is shown that the experience gained allows separationless flow-meters for three-phase oil-gas-formation water flows to be produced. Some features of its operation are also considered.

Keywords: Multiphase Flows, RF-Sensors, Gamma-Densitometer, LNG, Oil Industry, Cryogenics

REGULAR SESSIONS

Id-1841

Photosynthesized Extra Small Silver Nanoparticles: Structural Evaluation and Antimicrobial Potential

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Abstract: Recently, increase bacterial resistance to antimicrobial and antifungal compounds issue constitutes a real threat to human health. One of the useful materials for fighting against pathogens is silver nanoparticles (AgNPs). However, the use of AgNPs in medical fields remains somewhat limited due to their probable cytotoxic effects. To reduce the toxicity, AgNPs can be functionally modified by biocompatible polymer composition such as cellulose, chitin, agarose, starch. Moreover the targeting properties of AgNPs are also can be enhanced by attaching functional biodegradable attachments. The principal aim of this study was to synthesize AgNPs in novel Carboxymethyl cellulose (CMC)/poly (maleic acid-alt-acrylic acid)/ octadecyl amine (ODA) hybrid hydrogel and to find out their antimicrobial ability to Enterococcus faecalis 29212, E.coli 25922, Pseudomonas aeruginosa 27853 as well as against Candida albicans ATCC 10231 yeast. wLED light as an ecofriendly and harmless approach used for conversion of Ag ions to AgNPs in aqueous biopolymer composite suspension. Prepared biocapsulated and functionalized AgNPs were characterized by Ultraviolet–Visible (UV–Vis) Spectroscopy, Transmission electron microscopy (TEM), Dynamic Light Scattering (DLS) and Zeta potential. TEM imaging showed monodispersed extra small spherical nanoparticles of 1–5 nm. The antimicrobial activity novel biofunctionalized AgNPs were evaluated against pathogenic microorganisms using the agar disk diffusion method. The highest antibacterial activity of AgNPs was noticed against Pseudomonas aeruginosa 27853, followed by Enterococcus faecalis 29212 and E.coli 25922 at 0.05 mg/mL. The antifungal activity was determined against Candida albicans 10231 at 0.1 mg/mLWe conclude that used wLED approach gave us a unique opportunity to maintain the compatibility of AgNPs with biopolymer

environments. The synergistic effect methylcellulose modified AgNPs was proved by having antimicrobial effect at such as low concentration of 0.05 mg/mL against examined bacteria and yeast at 0.1 mg/mL. Given the current findings, biofunctionalized AgNPs mediated by harmless wLED approaches have positive antibacterial and synergistic powers. Therefore, they might be considered as a promising candidate to combat the multi-drug resistance bacteria and some fungi.

Keywords: Extra Small Agnps, Light Mediated Nps, Biocompatible Polymer Nanocomposition, Antimicrobial and Antifungal.

REGULAR SESSIONS

Id-1841

Study of Physico-Chemical Properties of Refractory Materials Synthesized from Metallurgical Waste

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Abstract: The aim of the research was to investigate the utility of components of metallurgical wastes in the production of high temperature refractory bricks based on rich and poor chromium waste produced by self-propagating high-temperature synthesis method. The series of experiments on the obtaining of carbon containing refractories based on the waste of rich and poor chrome spinel powder were conducted in a muffle furnace. The following reagents were used for the synthesis of carbon-containing refractory materials: PA-4 grade aluminum powder (99% of purity), bag filter dust, rich and poor chrome spinel powder, carbon in the form of electrode graphite (purity 95%), silicon powder (purity 98.5%). The samples were thoroughly mixed and, to obtain a dense material, were compacted in a mold in the form of cylindrical pellets (30 cm in diameter) using a hydraulic press with a force of 30 kN. Then, the samples were left on a special table for natural drying at room temperature (18–22 °C) for 24 hours, after that dried at 100 °C for 6 hours. Next, the samples were placed in a muffle furnace. Samples' inflammation was initiated at 950 °C and lasted for 2-5 minutes. A detailed assessment of the basic equations of the expected chemical reactions in SHS process of the studied samples based on the waste compositions with different binders were carried out. Silica sol and 15% of $MgSO_4$ aqueous solution were used as a binder. The phase composition of the materials obtained was determined by X-ray phase analysis on a Dron-4M diffractometer using cobalt Ka-radiation. The completeness of the reaction was determined by the phase composition of the synthesis products. Thermal conductivity dependent on different content samples has been measured by a Lasercomp HFM Fox-50 heat flow meter device measuring under the conditions given in ASTM C518, EN 12664 and ISO 8301 standards. Thermochemical modelling studies were done by using HSC Chemistry 6.12 software to simulate possible products for increasing reaction temperature from 900 °C to 1650 °C. Compression strength of the samples was determined in accordance with the requirements of ISO 844 standard by using Zwick-Roel Z020. The test specimens are cut into cubes of dimensions of around 30 mm×30 mm × 30 mm.

Keywords: Chrome Spinel Powder, Thermal Conductivity, Thermochemical Modelling, Compression Strength.

REGULAR SESSIONS

Id-1857

Interlaboratory Pressure Comparison Measurement in Hydraulic Medium up to 400 MPa Range

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Abstract: Results of interlaboratory comparisons and proficiency tests are a significant parameter for the calibration and testing laboratories for assuring the quality of test and calibration results performed by those laboratories. Accredited and non-accredited laboratories that have a quality system for their working areas are expected to join into inter-comparisons and proficiency tests in certain periods to show a degree of equivalence among the participant laboratories and assure their service quality. The necessity of participating in comparison measurements (ILC) and proficiency tests (PT) are stated in the EN ISO/IEC 17025 International Standard that accredited laboratories or laboratories applying for accreditation must participate in ILC and PT from parameters related to measurement quantities within the scope of accreditation and have achieved successful results, and it is also a requirement sought by accreditation bodies. This comparison was organized and piloted by TUBITAK National Metrology Institute (UME). The participant laboratory was an accredited laboratory (AL) in rubber industry. The comparison was conducted in accordance with the Technical Protocol that was prepared and agreed upon by all participants before the comparison measurement. The comparison measurement was performed at 10 different pressure points which were equally distributed from 40 MPa to 400 MPa. The measurement results of the pilot laboratory were taken as the reference value in the comparison. So, the results from the participant laboratory were compared across the results for reference values for each pressure point. Degrees of equivalence values versus pressure values were calculated according to ISO/IEC GUIDE 43=1:1997(E). A digital pressure gauge instrument was used as a transfer standard. Both laboratories measured the same transfer standard (TS) at different times and results were compared. The short-term stability of the TS was obtained by making extra measurements on the TS before the comparison measurements start. This study gives the organisation steps and the obtained results of a bilateral pressure comparison measurement of digital pressure gauge in the hydraulic medium between UME and an accredited laboratory in rubber industry up to 400 MPa.

Keywords: Pressure, Comparison, Calibration, 17025, Uncertainty.

REGULAR SESSIONS

Id-1858

The Influence of Liquids on Dynamic Pressure Transducers Performance by Using Dropping Mass Method

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Abstract: Dynamic pressure measurement is a big necessity for some industries like defense, aerospace, medicine producing and etc. In this type measurement, pressure value changes by time and it has short period of time as a few miliseconds. In dynamic pressure measurement includes a pressure sensor, signal conditioning amplifier and data acquisition system. Dynamic pressure measurement by using dropping mass is one of the methods. This method uses a dropping mass on to a piston cylider unit that is known its effective area, increasing the pressure in the hydraulic medium by up to some hundreds of MPa. Measurements of such dynamic pressure sensors can be done with different pressure transmission fluids using various reference devices. However, whether the pressure transmission fluids with different physical and chemical properties have an effect on the performance of the dynamic pressure sensor has been among the subjects studied. In this study the influence of the process conditions on dynamic pressure transducers such as the effect of different process parameters like pressure transmission medium in liquid on dynamic pressure sensors performance have been investigated. The pressure points in the measurement are (100, 200, 300, 400, 500) MPa. To see the effect of different fluid media on the performance of selected dynamic pressure sensors, two different pressure transmitting fluids have been selected for comparison. They are sebacate and glycerol. For each pressure point, measurements have been repeated 5 times for both liquids. The produced voltage outputs proportional to applied reference dynamic pressure values for dynamic pressure sensors have been recorded during the measurements. For the measurements, a Kistler dynamic pressure sensor has been used. Its measurement range is 500 MPa. In summary, in this study the influence of liquids on dynamic pressure transducers performance has been investigated and the results have been shared.

Keywords: Dynamic, Pressure, Calibration, Measurement, Dynamic Pressure Sensor.

REGULAR SESSIONS

Id-1859

Calibration of Pressure Balances

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Abstract: Piston cylinder units known as pressure balances are used as primary and secondary level standards in the field of pressure metrology all over the world. The pressure balances work according to the principle of obtaining the reference pressure value applying force by using mass sets on the piston-cylinder unit whose area is known with high accuracy. Both gas-operated and liquid-operated pressure balances are available. The calibration method of the pressure balances is a comparative method. The balances can also be used for calibrating other pressure balances. A pressure balance consists of a piston that freely rotate in a cylinder. The piston-cylinder unit has a well machined surface called as effective area. The calibration of a pressure balance nearly means determining the effective area of the piston-cylinder unit. The comparison is carried out using the cross-floating procedure which include three different methods like falling rate method, differential gauge method and pressure gauge method. We examined the compatibility of the measurement results in each method with each other in this study.

Keywords: Pressure Balance, Piston Cylinder Unit, Deadweight Tester.

REGULAR SESSIONS

Id-1865

Metallo-Supramolecular Assembles based on Terpyridine and Ferrocene Units: Formation, Composition and Properties in Solution

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Abstract: A promising approach in today's polymer chemistry is the conjunction of covalent linked polymer species with non-covalent interactions to establish new polymeric systems. For this purpose, supramolecular polymers containing reversible metal–ligand interactions have been widely studied in the past decades. However, in spite of the strong attention on such polymer systems their detailed molecular analysis in solution remains scarce. In the here presented study the attention is focused on the detailed macromolecular analysis of differently structured copolymers embedding terpyridine and ferrocene units by the complementary methods of molecular hydrodynamics namely analytical ultracentrifugation (AUC), viscosity and light scattering approaches. The copolymers were synthesized using the controlled radical addition-fragmentation transfer (RAFT) polymerization technique. Subsequently the macromolecules were treated with Eu^{3+}, Co^{2+}, Fe^{2+}, and Pt^{3+} metal ions. The intercorrelation of obtained results was evaluated via the concept of the hydrodynamic invariants. The special attention was paid to the investigation of the intra- and inter molecular complexation behavior of the metal ions with the ligand containing methacrylate copolymers at different conditions by the sedimentation velocity analysis applying modern solutions for the AUC data treatment.

Acknowledgments. The reported study was funded by RFBR and DFG, project number 21-53-12034. The authors are grateful to the St. Petersburg State University Research Park for providing of some necessary scientific equipment.

Keywords: Metallo Polymers, Hydrodynamics, Characterization, Polymer Solutions.

REGULAR SESSIONS

Id-1880

Electrochemical Behaviour of High Molybdenum Maraging Steel in Neutral, Acidic and Alkaline Media

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Abstract: Maraging stainless steels (MSS) are a class of high strength stainless steels with excellent comprehensive performances including high strength, superior corrosion resistance and good weldability. In this present study electroslag refining process have been employed for the production of cobalt free maraging steel with high amount of (5.8%) molybdenum (Mo). Mo is an important alloying element which gives strength and durability to this steel. Electrochemical studies that is potentiodynamic polarization resistance properties of this alloy were studied in three different solution i.e. in acidic, alkali and neutral solution in room temperature. For this 1M H_3PO_4 solution, 0.5M NaOH solution and 3.5% NaCl solution were taken respectively. The corrosion rate of maraging steel sample increases with increasing pH of the medium. SEM of the samples were done after corrosion performance to study the changes of the surfaces due to corrosion attack in different medium. Raman spectroscopy of these samples were also done to identify the phases due to corrosion reaction.

Keywords: Maraging Steel, Potentiodynamic Polarization Resistance, 1M H3PO4 Solution, 0.5M NaOH Solution and 3.5% NaCl Solution, Raman Spectroscopy.

REGULAR SESSIONS

Id-1884

Process Improvement with Using Biodegradable Material in Scope of Sustainability

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Abstract: Sustainability is one of the topics that is at the top of the agenda of today's companies and investors. Companies are expected not only to have achieved financial success with their services or sales, but also to be sensitive to the environment and to do things that will not harm human life. Unfortunately, the global warming we face today, the loss of biodiversity, the rapid consumption or pollution of resources, the rapidly increasing population and the resulting environmental problems force humanity to seek a new order or to find solutions that will stop the increase of these problems. For all these reasons, companies adopt corporate sustainability approaches by considering economic, social and environmental sustainability as a whole in order to implement their sustainability strategies in the long term, and they tend to change classical business models according to these models. In this study, the products produced with ABS raw material in the current situation and the products produced with sustainable additive ABS are compared and reviewed. The effects of the biodegradable additives used in the products on the manufacturing process and bio-degradable polymer products durability were examined. It is aimed to improve the process by providing the current product requirements.

Keywords: Mass production, Quality Assurance, Sustainability, Bio-degradable Polymers.

REGULAR SESSIONS

Id-1898

Recent Results of New Additive Technology CMPS of Manufacturing Elements of Vacuum Electronic Devices

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Abstract: The development of vacuum electronics is strongly linked to manufacturing capabilities. The complexity of many products does not allow or greatly complicates their realization, which is why many ideas remain theoretical. Modern 3D printing technologies can radically solve this problem, since, in comparison with modern CNC machines, they have great capabilities in accuracy, productivity and cost. However, this only applies to dielectric products, since metal 3D printers are currently significantly inferior to CNC machines in all respects. Therefore, special methods are required to realize metal products. In this paper, we propose a method for multistage chemical metallization of photopolymer structures (CMPS) printed using stereolithography technologies. Experimental testing of various elements of vacuum devices manufactured using this technology demonstrates great prospects for this approach. The work is supported by the Russian Science Foundation under grant #21-19-00884.
Keywords: 3D-Printing, Microwave components, Chemical metallization, Waveguides.

POSTER SESSIONS

Id-1718

Growth Conditions Influence on Quantum Cascade Lasers

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Abstract: Quantum cascade lasers (QCLs) are considered now as standard light sources for many chemical sensing applications in the mid-infrared range above 3 μm. Alas, QCL formation using molecular beam epitaxy is very complicated because even the smallest fluctuations in growth conditions can cause catastrophic crystal failure. High arsenic overpressure should be used during the native oxide desorption process due to the very strong arsenic desorption rate temperature dependence. On the other hand, the high group V overpressure may cause anti-site defect formation and increase defect density in the grown structure. Very careful balancing between these two parameters is required adjusting the oxide desorption and structure growth conditions. In this work, we investigate how the InAs wafer oxide desorption and heavily Si-doped cladding layer growth conditions as well as the wafer temperature distribution influence the defect density in the grown structure. The defect density is a very important QCL wafer crystal parameter since it directly correlates to lasers performance and can even deny coherent light emission by creating high amount of non-radiative centers. Defect density is observed using differential interference contrast microscopy. The first observed effect was wafer temperature distribution influence on QCL growth. 2 inches wafers exhibit very even temperature distribution in 525±25 ℃ range. The situation is different using 3 inches wafers – during preliminary growths, the halo of wafers had very high number of defects due to the contamination from the wafer holder. Then the holders were sanded to clean them from any contaminants. This changed the holders surface roughness which increased it heat absorbance from both effusion cells and wafer heater. We assume, that this created very uneven temperature distribution. The temperature scan across the wafer revealed about 25 ℃ difference from center to edge. This temperature shift impacted quality of the deoxidation process by overheating the periphery of the wafers and it was not possible to control the deoxidation by RHEED pattern observation during the growth as only central part of the wafer is accessible for this technique. This caused failure in cleaning procedure which led to high defect density with unusual distribution. High temperature gradient across the wafer had also a strong impact on the growth of the heavily silicon doped cladding layer which resulted in formation of the regions with extremely high defect

density. To combat this effect the growth conditions were carefully modified maintaining the balance between arsenic overpressure and the growth temperature. However, setup modifications were inevitable to reduce the wafer temperature gradient. This had a strong impact on reduction of the defect density in InAs-based quantum cascade laser structures.

Keywords: QCL, Bismides, Lasers, Photonics, MBE.

POSTER SESSIONS

Id-1732

Naphthalene Based Fluorophores in Organic Electronics

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Abstract: 1,8-Naphthalimide compounds are an attractive class of electron-deficient organic materials for OLEDs. They have high electron affinities, and related naphthalenediimide compounds have electron mobilities as high as 0.16 $cm^2/(Vs)$. 1,8-Naphthalimides can have wide energy gaps and low reduction potentials, making them good candidates for use as n-type materials in OLEDs. While many 1,8-naphthalimide derivatives have low luminescent efficiencies at room temperature, due to strong intersystem crossing to their triplet states, 1,8-naphthalimides substituted at the 4 and 5 positions with electron-donating groups can have high fluorescent quantum yields. Naphthalimides have been utilized in both small molecule and polymer-based OLEDs. In our laboratory we have developed several new building block molecules that have found wide application for the synthesis of various naphthalene based fluorophores and chromophores. The new dyes are promising candidates for high-tech applications such as OLEDs[1], OFET, visualization of cellular organelles[2], bimodal diagnostic imaging, etc.Authors are grateful to the Bulgarian National Science Fund project NSF KP 06-N29/12 and "EXCELLENCE IN COLLOID AND INTERFACE RESEARCH & INNOVATIONS FOR BETTER QUALITY OF LIFE" A project within the program "EUROPEAN SCIENTIFIC NETWORKS", funded by the Bulgarian Ministry of Education and Science

Keywords: 1,8-Naphthalimide, Fluorophores, Chromophores, OLEDs, OFET.

POSTER SESSIONS

Id-1733

New Efficient Method for Weak-Nucleophile Derivatization of Functional Dyes

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Abstract: 1,8-Naphthalimide and its derivatives with a strong electronwithdrawing imide group are a specific series of environmentally sensitive fluorophores, widely utilized in various fields due to their good chemical stability, large Stokes shift, and high fluorescent quantum yield. They have been widely used as biological, biomedical, optical, and electronic materials. 1,8-Naphthalimide have high electron affinities and the introduction of electron donating group at the 4- or 4,5-positions of 1,8-naphthalimide would increase the fluorescence quantum yield and shifted the absorption and fluorescence maxima to the longer wavelength. 1,8-Naphthalimides have been used with considerable success as intracellular markers in a wide variety of systems. Furthermore, some naphthalimide have been used for monitoring the interactions between single stranded deoxyribonucleic acids and proteins. Here we present the new efficient method for weak-nucleophile derivatization of 1,8-naphthalimide. This method allows the introduce a weak nucleophiles, such as water, alcohols and fluoride anions to the 1,8-naphthalimide core. In addition, the method works with short reaction times with high yields in relatively mild conditions. The obtained compounds are highly fluorescent in solution and in the solid state and make them very suitable for OLED application.Authors are grateful to the Bulgarian National Science Fund project NSF KP 06-N29/12 and "EXCELLENCE IN COLLOID AND INTERFACE RESEARCH & INNOVATIONS FOR BETTER QUALITY OF LIFE" A project within the program "EUROPEAN SCIENTIFIC NETWORKS", funded by the Bulgarian Ministry of Education and Science.

Keywords: Welding, Interlocking, B-H Characteristics, Electrical Machines, Ferromagnetic Materials.

POSTER SESSIONS

Id-1735

Kinematics of the “Ai-Gerim” Robot Arm

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Abstract: In this paper, the direct and inverse kinematics of the "Ai-Gerim" humanoid robot arm are solved. "Ai-Gerim" is a remotely controlled social robot, and it is used to perform contactless medical and other services. Each robot arm has six degrees of freedom. For the study of kinematics of the robot arm, the Denavit – Hartenberg transformation matrices are derived. The pose of the end-effector (hand) in the direct kinematics is determined by multiplying these matrices. For the study of the inverse kinematics of the robot arm, a reverse decoupling method is used to analytically determine the joint angles.

Keywords: Social Humanoid Robot, Direct and Inverse Kinematics, Denavit-Hartenberg Transformation Matrices, Reverse Decoupling.

POSTER SESSIONS

Id-1740

SMARTELECTRODES: Pre-Sulfurization Assisted Defect Treatment in CZTSSe Absorbing Material

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Abstract: The research on a pre-annealing of Cu_2ZnSnS_4 (CZTS) films in sulfur vapor atmosphere at low temperature has been caried out in order to assess its influence on the quality of $Cu_2ZnSn(S_xSe_{1-x})_4$ (CZTSSe) based films and solar cell devices. We deposited the absorbing CZTS material on an FTO glass substrate coated with Sb_2Se_3/TiO_2. The CZTS films were deposited at 320 °C and then sulfurized at 380, 420 and 450 °C. The density of point defects was evaluated using XRD and Raman spectroscopy. We have shown that by replacing the CdS buffer layer with Sb2Se3 improves the adhesion of CZTS to TiO_2 and, more importantly, that Sb as a dopant in CZTS films decreases the density of Cu_{Sn} antisite defects and compensates for Sn losses during CZTS sulfurization and selenization at high temperatures. From the Raman analysis, it was found that when excited at near-infrared (785 nm), the intensity ratios between Q (I_{288}/I_{304}) and Q‘ ($I_{337}/(I_{366}+I_{378})$) can be studied as a sensitive measure of Cu/Zn disorder in CZTS samples. The relative increase in the magnitude of Q and Q' indicates an increasing order in the CZTS films. Despite the complex spectral pattern and overlapping bands, the annealing temperature-dependent change in Q and Q' ratios was found to be consistent with the FWHM of the A mode at 337 cm^{-1}. The highest Q and Q' ratios, and hence the least disorder, were found for the 420 and 450 °C samples. In our previous work, we have shown that the distance between XRD peaks of kesterite (CZTS) corresponding to 200 and 004 allows an evaluation of the amount of point defects Cu_{Zn} or the degree of disorder in the positioning of Cu and Zn ions in the 2d plane of the tetragonal crystal lattice of kesterite. A larger distance corresponds to a lower degree of disorder. We have also applied this method to the assessment of disorder in (CZTSSe) kesterite, selecting the peaks at $2\theta \approx 66.5°$ corresponding to the 400 and 008 planes in CZTSSe. The smallest spacing ($2\theta_{008}–2\theta_{400}$ = 0.261 °C) and consequently the highest degree of disorder was determined for CZTSSe films sulfurized at a temperature of 380 °C, while the largest spacing ($2\theta_{008}–2\theta_{400}$ = 0.288 °C) and the lowest degree of disorder was determined for

the sample sulfurized at a temperature of 420 °C. In summary, we have shown that the pre-annealing temperature of CZTS has a significant effect on the quality of both CZTS-based films and solar cells. The best film quality and efficiency were obtained by pre-annealing CZTS films in sulphur vapour atmosphere at 420 °C. This additional step allows to obtain CZTS(Se) films with larger crystallites, since the residual solvent is removed more efficiently and also saturated with sulphur. In addition, the defects that occur during the selenization process when selenium is replaced by sulphur are reduced, and the antimony in the coating potentially compensates for the tin lost during selenization. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement Nº 778357- SMARTELECTRODES.

Keywords: CZTS, CZTSSe, Kesterite, Spray Pyrolysis, Solar Cell.

POSTER SESSIONS

Id-1742

SMARTELECTRODES: Electrochemistry Of Bismuth Interlayers in $(Bi_2)_m(Bi_2Te_3)_n$ Superlattice

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Abstract: Electrodeposition and electrochemical modification of bismuth telluride based nanostructures attract a lot of interest since it allows improving physical properties of the materials using electrochemical transformations inherent to the structure. Bismuth telluride-bismuth $(Bi_2)_m(Bi_2Te_3)_n$ superlattices have layered structure built up of two types of alternating blocks: Bi_2Te_3 quintuple and bismuth interlayer (bilayer) (Figure 1a) [1]. We have shown recently [2] that bismuth of the interlayers is electrochemically labile and can be selectively oxidized at the potential above the potential of metallic bismuth oxidation but bellow the oxidation potential of bismuth telluride. In this work, we have studied the selective bismuth anodic dissolution from the interlayers in $(Bi_2)_m(Bi_2Te_3)_n$ superlattices and the subsequent cathodic reintroduction into the electrochemically created voids by in situ Raman spectroscopy, electrochemical microgravimetry and potentiodynamic electrochemical impedance spectroscopy. The selective oxidation of bismuth in the interlayers proceeds synchronously with the decrease in mass; the potential scan reversal allows partial reintroducing of bismuth from the electrolyte by underpotential deposition above the reversible potential $E(Bi^{3+}/Bi)$ (Figure 2b). The anodic and cathodic reactions have been examined in more detail using Raman spectroscopy and potentiodynamic electrochemical impedance spectroscopy at variable initial amount of bismuth in the interlayers with the goal of development of electrochemical means of the superlattice composition control. Authors acknowledge funding from H2020 project MSCA-RISE-2017-778357-SMARTELECTRODES.

Keywords: Bismuth Telluride, Bismuth, Superlattices, Electrodeposition.

POSTER SESSIONS

Id-1743

SMARTELECTRODES: Influence of the Composition on the Properties of the Modified Surface Layer Generated on Steel by Electrospark Alloying

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Abstract: Electrospark alloying (ESA) is a method to obtain a material with advanced characteristics, e.g. as wear resistant coating. One of the advantages of these coatings is a very strong adhesion to the substrate as a result of electric spark discharge. Moreover, it was shown that due to intensive thermal and dynamic action of ESA, the obtained surface layer contains significant part of the substrate material. This layer is conventionally called a composite layer. In order to achieve desired characteristics of the composite layer, a detailed study on interdependencies between the treated substrate composition and the resulting properties of the layer was performed. Thus, the influence of the steel composition on the transfer coefficients of the tool-electrode (TE) material, roughness, microhardness and wear resistance were evaluated. Steels with different carbon and manganese content (St3, 45 and 65G) were used as substrates. The T15K6 and VK8 hard alloys were used as material for TE. ESA was applied on samples at different fixed discharge energies in the range 0.07 J to 1.58 J. The elemental composition was determined by X-ray fluorescence analysis, up to 3-5 μm in depth. The surface roughness was estimated by Surtronic-25 profilograph-profilometer. Vickers microhardness measurements (PMT-3) were performed with a load of 50 g. In order to evaluate weight loss, the reciprocating sliding friction tests were carried out at 180 double stroke/min under dry conditions. The performed study on the obtained by ESA composite layer using various steels and tool-electrodes (T15K6 and VK8) enable to draw following conclusions: the resulting composite layers have various composition, which depends on TE and type of steel used, where iron concentration can reach up to ~ 70 wt.%, while W and Ti carbides transferred from TE ~ 20-25 wt.%. The Co content exceeds 50 wt.% and can reach ~ 90 wt.% depending on the initial content in the TE; the mass transfer coefficient K depends on the discharge energy E, namely, with increasing E the K increases and its value depends on the substrate composition (minimal

for steel 45). Nevertheless, when the value of discharge energy E is exceeding a value at which K~1, than K start to decrease; the surface roughness and microhardness depend on the mass transfer coefficient K. The thermophysical properties of TE and substrate materials have a complex influence on these characteristics; the wear resistance is determined mainly by the steel composition, while the microhardness and roughness of the obtained composited layer has minor impact on a wear loss. The wear can vary by an order of magnitude and the layer with maximum wear resistance is obtained using steel 45. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement Nº 778357- SMARTELECTRODES.

Keywords: Electrospark Alloying, Steel, Discharge Energy, Wear Resistance

POSTER SESSIONS

Id-1751

New Bimodal Sensors for Diagnostic Imaging

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Abstract: Multimodal imaging agents were first introduced a decade ago and consist of a targeting moiety that is dually labelled with radioactive and fluorescent contrast. These compounds allow whole-body and intraoperative imaging to be performed through administration of a single agent and provide complementary diagnostic information that can be used to guide tumor resection. Among the existing optical imaging methods, fluorescence imaging that uses near-infrared (NIR) light (650 − 900 nm) has found widespread application both in vitro and in vivo. Various chelators such as DOTA, NOTA, etc., were developed for various radiometals (111In, 68Ga, 64Cu). In our laboratory we have developed several new Monomolecular Bifunctional Imaging Probes (MoBIP) as the main unit for new bimodal sensors for diagnostic imaging of various disease states. Their design is based on a combination of strategically selected fluorescent dye and a macrobicyclic chelator that will enable the simultaneous application of optical and nuclear imaging modalities by the use of one and the same molecule. The radiotracer which was employed consists of a sarcophagine cage that has recently been proved as the best chelator for Cu(II) ions. As fluorescent dyes we have used naphthalene- and perylene-based derivatives with electron-donor substituents at the peri-positions leads to formation of a push-pull system with desired optical properties. The new MoBIPs were characterized by various spectroscopic techniques and their applicability as bimodal sensors for diagnostic imaging was demonstrated. Authors are grateful to the Bulgarian National Science Fund, project NSF KP 06-N29/12.

Keywords: Bimodal Probes, İmaging, Fluorescence, PET.

POSTER SESSIONS

Id-1754

How Stenosis Can Influence the Hemodynamics Flow in a Coronary Artery

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Abstract: Invasive coronary angiography is the current “gold standard” for the identification of CAD. Injection of a contrast agent into the circulatory system provides a good visualization of the location and relative degree of narrowing in the coronary arteries. In some cases, however, such information is not enough to develop an adequate strategy for patient treatment. A decision regarding the treatment plane based on coronary angiography is often subjective. Generally, the correct decision should be based on an understanding of the extent to which narrowing of the artery lumen affects the myocardial function. In other words, it is necessary to know the hemodynamic significance of a stenosis. To improve the accuracy of the planning of IHD treatment, many modern instrumental methods are implemented for the needs of practical cardiology. Although these approaches have demonstrated the increase of treatment effectiveness, their use is not widely introduced in clinical practice. The main reasons are the high cost of equipment, the significant labor and time costs required for the procedures and the additional risk of death. A well-known method for studying blood flow is a technology based on measuring the rate of filling of an artery with a contrast agent. The known disadvantages of this technique are low accuracy due to the low motion speed of video recording during the angiographic examination and the impossibility of determining the distribution of blood flow velocity in the section. These problems can be overcome by the approach of computer simulations of hemodynamics in the artery. The greatest success was achieved using the Navier-Stokes model to describe incompressible blood flows. However, in cases of native artery geometry and plausible boundary conditions, it turns out to be necessary to use advanced software. Non-Newtonian fluid models are also studied but mostly in order of theoretical researches. In the present study, we discuss a technique using the basic Navier-Stokes model and non-Newtonian fluid model as well in comparison with recent theoretical researches. We

present a physical and computational model of the non-Newtonian liquid flow in a channel, which mimics the blood in a coronary artery with stenosis. This model allows computing the field of the liquid velocity in the arteria as well as the volume velocity for an arbitrary shape and size of the stenosis and realistic dependence of the blood pressure difference between the artery inlet and outlet. The theory and computations under consideration were made possible due to the support of the Russian Science Foundation (project no 20-61-46013).

Keywords: Stenosis, Hemodynamic flow, Coronary artery, Navier-Stokes Model.

POSTER SESSIONS

Id-1755

Towards Nucleation and Evolution of Ellipsoidal Particles in Metastable Liquids

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Abstract: The processes of phase transformations from a metastable liquid state of matter to a solid state underlie many technological processes and natural phenomena. Therefore, the establishment of laws governing such processes is an important practical task that allows one to control the microstructure and properties of solid materials by changing the physical and operational parameters of the phase transformation process. When a substance crystallizes from a highly supersaturated or supercooled liquid, there is a bulk phase transformation associated with nucleation and subsequent growth of solid particles. As this takes place at the intermediate stage of the phase transformation, the nucleating particles are far enough away from each other and can therefore be considered as non-interacting. Mathematical models of such processes consist of integrodifferential kinetic and balance equations and corresponding boundary and initial conditions. In addition, the boundaries of growing crystals move with time. This means that, in general, the mathematical model of the phase transformation process is also a problem with a moving boundary. This means that there are no general methods for solving such problems, and each individual model requires the development of special approximate approaches to its solution. In the last decade, significant progress has been made in the mathematical description of bulk nucleation and growth of spherical crystals. For example, a solution of such a problem for the first-order kinetic equation was constructed in a series of papers. A generalization of the theory to fluctuations in crystal growth rates leading to the kinetic equation of the second order was made in works. A theory taking into account the runoff of product crystals in the kinetic equation and the presence of external sources in the balance equations was developed in references. However, as is shown in experimental works, the shape of nucleating and growing crystals is not always spherical. To account for the non-sphericity of particles, a natural step in the development of the theory is to use an approximation about their ellipsoidal shape. This study develops a theory of bulk nucleation and growth of a polydisperse

ensemble of ellipsoidal particles in supersaturated solutions. This study was supported by the Russian Science Foundation (project no 18-19-00008).
Keywords: Nucleation, Crystal growth, Metastable liquid.

POSTER SESSIONS

Id-1757

Radiation Resistance of Synthesized Under Different Conditions ZrO_2 Micro- and Nanostructured Compacts

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Abstract: Zirconium dioxide (ZrO_2) (band gap 5.0-5.5 eV) is considered today one of the most important materials used in modern measuring technology, nanoelectronics and photonics. It has a significant luminescence yield, high reflectance, low phonon energy, and high thermal and chemical stability. Phosphors based on ZrO_2 are used for the manufacture of oxygen sensors, biological sensors, laser technology devices, optoelectronic devices, UV and ionizing radiation dosimeters, scintillators, high-energy radiation visualization devices, etc. For these applications, an important task is to ensure the stability of the luminescent properties of the material when exposed to various types of radiation. This problem is especially relevant when using ZrO_2-based devices in military and space technology, as well as in the nuclear industry. Micro- and nanostructured compacts were prepared by uniaxial cold pressing of monoclinic ZrO_2 nanopowder and tested using SEM (Carl Zeiss Sigma VP), and X-ray fluorescent analysis (ARL QUANT'X). Based on the results of X-ray fluorescent, the chemical composition of all types of samples was determined. The compacts were irradiated by 130 keV electron beam, 4.5-75 kGy (Linear Electron RADAN Accelerator, Yekaterinburg, Russia), 10 MeV electron beam, 209-1256 kGy (LERA-10-10C Accelerator, Yekaterinburg, Russia) and 200 MeV Xe ions, 10^{10}-10^{14} ion/cm^2 (cyclotron DC-60, Nur-Sultan, Kazakhstan). Samples were irradiated at room temperature. Thermostimulated luminescence (TSL) of irradiated samples showed the presence of different peaks. Several TSL peaks have been identified. The kinetic parameters of the TSL were also calculated. Dose dependence of TSL was analyzed. We can conclude which samples are promising for high-dose TSL dosimetry of electron and ion irradiation.

Keywords: Zirconium dioxide, Electron beam, Swift heavy ions, Thermostimulated luminescence, Kinetic parameters.

POSTER SESSIONS

Id-1759

In-Depth Raman Spectroscopy Study of Radiation Damages Induced by Swift Heavy Ion Irradiation in Polycrystalline Si_3N_4

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Abstract: Radiation-resistant materials play an important role in nuclear energy: structural materials, composite nuclear fuel matrices, and materials for storing radioactive waste. All these materials must work and function for a long time in a radiation medium with various particles, such as gamma radiation, neutrons, electrons, ions. Currently, as a result of intensive research, dielectric materials – ceramics based on nitrides and carbides, which demonstrate increased radiation resistance against high-energy heavy ion irradiation, simulating the effects of fission products of nuclear fuel, have been found. As is known, the structural sensitivity of solids to this kind of radiation is determined, first of all, by the possibility of the formation of latent tracks, extended defects in the nanoscale region surrounding the ion trajectory. Si_3N_4 is the only nitride ceramic in which latent tracks have been detected. The present work is aimed to study the mechanisms of radiation damage formation in polycrystalline silicon nitride irradiated by ions with fission-fragment energies. The depth-resolved Raman spectroscopy technique has been used to study the structural disorder and associated residual stresses in polycrystalline silicon nitride across of 167 MeV Xe and 710 MeV Bi ion irradiated layer at fluences ranged from 1x 10^{11} to 4.8x 10^{13} ion/cm^2. To evaluate stress level the peak shifts of the 862 cm-1 band have been converted to stress via piezospectroscopic coefficients knowing from the literature. As was found from Raman spectra and SEM images the amorphization of Si3N4 is induced in surface region and expands toward the depth with ion fluence. Ion track sizes deduced from the threshold ion fluences needed to transform material into amorphous phase are in good agreement with those found from TEM examination.

Keywords: Silicon nitride, Swift heavy ions, Raman spectroscopy, Amorphization, Stress.

POSTER SESSIONS

Id-1760

Impregnation of Benzyl-L-Cysteine into Silica Gel for the Removal of Cadmium(II) Ion from Water

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Abstract: The silica gel has been successfully impregnated by S-Benzyl-L-cysteine (S-Bn-Cys) using the sol-gel method. The new material of inorganic-organic composite of general formula SG-(S-Bn-Cys) has been fully characterized by SEM, ATR-IR, PXRD, MP, and EA. The IR spectra of SG-(S-Bn-Cys) prove the physically presence of the S-Benzyl-L-cysteine molecule within the silica gel matrix, and the occurrence of a hydrogen bond at 3617 cm^{-1}. The XRD shows the successful formation of SG-(S-Bn-Cys) material by appearing new peaks. Furthermore, the change in the degradation point of SG-(S-Bn-Cys) (217 ºC) compared to SG (296 ºC) indicates the successful impregnation of S-Bn-Cys into the silica gel matrix. The new material of SG-(S-Bn-Cys) composite has been tested for the sorption of Cd^{2+} ion from water. The maximum removal of Cd^{2+} ion is a ca. 95% upon the study conditions of C_i = 0.5 mg L^{-1}, T = 55 ºC, 80 rpm, pH = 7, and dosage = 2 g L^{-1}. Thermodynamically, the sorption behavior of Cd^{2+} ion onto SG-(S-Bn-Cys) follows Langmuir isotherm models (R^2 > 0.9993). Kinetically, the sorption mechanism follows the pseudo-second-order model (R^2 = 0.9918). The new composite material can be used for the removal of low level Cd^{2+} ion concentrations from water.

Keywords: Silica gel, Cadmium(II) ion, Langmuir isotherm, S-Benzyl-L-Cysteine.

POSTER SESSIONS

Id-1761

Synthesis, Spectral Characterization, Thermal, Computational and Antibacterial Studies of Lanthanide Complexes with 2-Fluorobenzoic acid-(5-R-2-hydroxy-benzylidene) hydrazide {R = Chloro or Bromo)

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Abstract: Tridentate Schiff base ligands, 2-Fluorobenzoic acid-(5-bromo-2-hydroxy benzylidene) hydrazide {H2LCl} and 2-Fluorobenzoic acid-(5-bromo-2-hydroxybenzylidene) hydrazide {H2LBr} have been used to prepare a variety of lanthanide complexes [HNEt3][LnLx(NO3)2(H2O)]H2O, Ln = La, Pr, Nd, Sm, Eu, Gd, Tb, Dy and Er. The 1H and 13C NMR of lanthanum in conjunction with the infrared, elemental, thermal and conductance measurements enable the assignment of the formula to these complexes. The anionic unit [LnLx(NO3)2(H2O)]- contains one tridentate ONO-donor, L2-, which coordinates the metal ions via the phenolate-O, the imine-N and the deprotonated amide-O atoms in enol tautomeric form. The coordination environment around central metal ion is completed by two bidentate nitrate ligands and one coordinated water molecule to give a coordination number of eight for Ln(III). In order to get a better insight into the structural features of the complexes, their molecular geometries were fully optimized using density functional theory calculations at the M06-2X/6-31G∗ level of theory. The antibacterial activity results, on a panel of six different bacterial strains, show that the activity of the complexes is higher than that of the free ligands and in some cases higher than that of amoxicillin which is taken as standard reference drug. Compared to the free ligands, the emission spectra of the complexes exhibit a blue-shift with a clear enhancement in the emission intensity.

Keywords: Lanthanide complexes; ONO donor ligands; DFT computation; Photophysical properties; Biological activity

POSTER SESSIONS

Id-1763

Carbon/Coke Formation on The Various Synthetic and Natural Carrier-Based Nickel Oxide Catalyst Surfaces in The DRM Reaction

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Abstract: The present research deals with the comparative study of carbon/coke formation processes in the DRM reaction temperature range 500÷850˚C on nanostructured nickel oxide catalyst, synthesized on the surfaces of various granulated synthetic (γ-$Al_2O_3$and NaX zeolite) and natural (clinoptilolite and bentonite from Georgian deposits) carriers. The above synthetic and natural supporter materials-based catalytic systems with ~3mas% NiO catalyst were prepared via impregnation of the granulated micro/nano-porous carriers according to their moisture capacity with the aqueous solution $Ni(NO_3)_2 \cdot 6H_2O$ as a metal precursor. The obtained samples of NiO-based catalyst systems, after drying a 300˚C/2h and subsequent calcination at 500˚C/3h, have been tested for the catalytic activity in the reaction of carbon dioxide conversion of methane in the temperature range 500÷850˚C. A complex study of the developed samples of the catalyst systems, before and after catalytic reactions, were conducted using SEM-EDX, Auger-electron spectrometry (AES) and X-ray diffractometry in order to determine the influence of nature of the carrier materials on the carbon/coke formation on the surfaces of nanostructured NiO catalyst. It is shown that in the case of equal amount of (3mas%) of nickel oxide on the various carriers, the nature of the carrier material significantly affects the carbon/coke formation process in the wide range of the DRM reaction temperatures. Particularly, it was determined that at high reaction temperatures, deposition of a free carbon in the form of whiskers (CNWs) and multi walled carbon nanotubes (MWCNTs) with Ni/NiO clusters on the tip or bottom of the above 1D carbon nanoforms (CNFs), occurs more intensively in the case of the catalyst systems on the base of the synthetic carriers than in the case of the catalyst systems on the base of natural carriers. The comparative study of the fine structure of the carbon KLL Auger-transition peaks in the AES spectra recorded from the surfaces of the samples of the investigated NiO-based catalyst systems before and after DRM reaction, showed that at low reaction

temperatures (<700˚C) a continuous nanofilm (~1000Å) of carbon gum and multi-layered graphene are formed on the surface of the NiO catalyst, simultaneously realized in short-range ordered deposits which can exist in the form of carbon atom groups distinguished in sp^2, (sp^3+sp^2) mixture, and even in the linear sp electronic hybridization, with the different ratio of the above carbon phases in the polymerized gum-like carbon nanofilm on the surface of NiO catalyst, depending on the nature of the carrier materials. The authors propose that in contrast to the synthetic carriers, the presence of ~1÷2mas% of the oxides of Mg, Fe, Ca etc, in the composition of natural carrier materials may play the role of the promoters and cause the observed increase in the ratio of active carbon, and at elevated reaction temperatures enhance the anti-coking performance of the above natural carriers-based nickel oxide catalyst. This work has been done with the financial assistance of the International Science and Technology Center within the project GE-2606.

Keywords: Carbon coke, Ni oxide catalyst, Carbon nanotubes, MWCNT, MWCNW.

POSTER SESSIONS

Id-1765

The Boundary Integral Equation for The Growth of a 2D Dendrite in The Presence of Convection

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Abstract: Crystal growth under natural conditions is always accompanied by convection. Fluid flow can be caused both by external and internal causes (density gradient of liquid resulting from a temperature gradient, impurity concentration gradient, and even surface tension gradient). The convective contribution to the heat transport may exceed the contribution from heat diffusion, which results that the flow near the crystal will determine the dynamics of interfacial boundary motion. For example, instabilities of the forced flow caused by rotation of the crystal and crucible when pulling a single crystal from the melt (Czochralski method) lead to the growth of spiral shapes of single crystals of some oxides. The boundary integral theory is one of the effective methods for solving heat and mass transfer problems with a moving boundary. Existing boundary integral solutions do not take into account the contribution of convection, which becomes critically important for crystallization occurring at a rate close to the melt flow rate. The extension of this theory to the case of convective fluid flows allows us to significantly expand the class of moving boundary problems to be solved. The boundary integral approach based on Green's function allows one to pass from a linear heat conduction equation, with given boundary conditions, to a general integro-differential equation defining the form of the interface, depending on the total undercooling of the system. Taking the interface function as a parabolic cylinder, we can calculate the convective integral. Note that Green's function depends on two points, one of which defines the position of the heat source and another one defines the position of the "observer" and lays at the interface. Since the parabolic dendrite retains its shape during growth, its surface can be considered isothermal. Then, the convective contribution should not depend on the position of the interface point. Thus, the integral can be simplified by choosing and fixing the observation point at the top of the dendrite. A comparison of the undercooling found from the solution of the heat diffusion differential equation and from

the boundary convective integral verifies the application of Green's function to problems of crystallization with a moving melt.

Keywords: Phase transitions, Kinetics, Crystal growth, Formation of structures, Mathematical modeling.

POSTER SESSIONS

Id-1772

Influence of the Nature of Carriers on The Activity of the Iron Catalyst in The Decomposition of Methane

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Abstract: In connection with the transition to "green" technology, intensive work is underway all over the world to find alternative energy sources and energy carriers. Hydrogen is one of the most promising modern energy carriers, which is determined by its ecological purity, versatility and high efficiency of energy conversion processes with its participation. The most common technologies for hydrogen production are steam reforming of methane (STR), catalytic decomposition of methane (CRM), partial oxidation of methane, gasification of coal and other hydrocarbons, water electrolysis, photocatalytic water splitting, etc. The catalytic decomposition of methane is a promising technology for the production of hydrogen and nanocarbon without emissions of carbon oxides (CO, CO2), and at the same time is a promising replacement for steam reforming of methane to produce hydrogen. Therefore, the creation of a technology for producing hydrogen and nanocarbon from methane without emissions of carbon oxides using inexpensive, highly active and stable catalysts is an urgent task. The aim of this work was to study the effect of the nature of the supports on the activity of the iron catalyst in the decomposition of methane. As is known, the catalyst carrier serves to stabilize the particles of the active phase of the catalyst on its surface. In heterogeneous catalysis, the role of the support is to prevent the coarsening of catalyst particles or sintering of the active component, which makes it possible to maintain a high contact area of the active substance and reagents. Typically, the amount of carrier is much greater than the amount of active ingredient applied to it. The main requirements for carriers are a large surface area and porosity, thermal stability, chemical inertness, and high mechanical strength. Both natural (zeolites, clays) and synthetic materials (aluminum and silicon oxides, etc.) are used as carriers. In this work, carriers of various natures were studied as carriers, such as: alumina gamma modification (Al_2O_3), synthetic silicon oxide (SiO_2 (synth)), silicon oxide obtained from rice husk (SiO_2 (RH)), zeolites. Testing of the activity of supports and synthesized catalysts in the CRM was carried out on a

laboratory flow-through unit. Determination of the concentration of the starting reagents and analysis of the reaction products of methane decomposition were carried out on a chromatograph (Chromos-1000). Iron oxide catalysts (Fe /Al_2O_3, Fe /HZSM-5, Fe /3A, Fe / SiO_2 (syn.), Fe /SiO_2 (RH)) were prepared by capillary impregnation of the support with an aqueous solution of iron nitrate salt according to moisture capacity. Thus, it is determined that the deposition of iron oxide leads to an increase in the activity of the composite. On the 5 wt % Fe / HZSM-5 composite, methane begins to decompose starting from 700 °C, the methane conversion is 1.8%. On a 5 wt% Fe / ɣ-Al_2O_3 composite, methane also decomposes starting from 700 °C, methane conversion 2%, hydrogen concentration 0.8 vol.%. The greatest conversion of methane (13%) is observed at 850 ° C, hydrogen with a concentration of 5.8 vol.% Is formed in the reaction products.

Keywords: Nanocarbon, Natural carriers, Methane, Catalytic reforming.

POSTER SESSIONS

Id-1774

Degradation Diagnosis and Durability Assessment of a SRT Composite Material Submitted to Endurance Test

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Abstract: Self-regulating temperature (SRT) heating materials based on *electroconductive polymer composites* (CPCs) with positive temperature (PTC) present nowadays large interest for various technical applications, including heating elements for buildings, deicing of pavements, sidewalks or vehicles, constant temperature chambers for foods or medical items, self-limiting circuits a.s.o. Even the specific service temperature of such devices is rather moderate, the high number of cycles near to a specific transition temperature combined with the electric field and presence of air would result in increased degradation of the polymer matrix as compared to normal conditions, such as in storage or continuous presence of either thermal stress or low electric fields. Therefore, the aim of this work was to detect if increased degradation occurred during the operating conditions and to evaluate the lifetime of a CPC-PTC material in these conditions. A composite consisting in radiation-crosslinked HDPE-EVA matrix and CB-graphite binary filler was subjected to continuous operation for 7300 h at 9V cc, at a superficial temperature of 50.5...51.4 ^{o}C. The states of the aged and initial materials were compared using different physico-chemical measurements, namely: (i) FTIR spectroscopy was applied for detection of the possible changes in chemical composition, such as increase in oxygen containing groups content due to possible oxidation processes; (ii) DSC was used to observe the changes in physico-chemical transitions of the polymer matrix; the oxidation induction time was calculated from ramp experiments at different heating rates; (iii) SEM was applied to observe the eventual changes within the polymer matrix, such as filler distribution or morphology; (iv) mechanical testing – elongation, resistance and modulus values were measured for initial and aged materials in order to detect eventual alteration of the mechanical properties of the composites. The lifetime value of $\geq$ 40000 hours was estimated using a kinetic model based on a first order kinetics for oxidation induction time decay.

The financial support was provided by Ministry of Research, Innovation and Digitization through contracts: PN 19310101-46N/2019, Dubna 04-4-1140-2020/2022 and 446PED/2020.
Keywords: Composite, Self-regulatin Temperature, Gamma radiation, Degradation.

POSTER SESSIONS

Id-1775

Cu-Au Nanoparticle Solutions with Broad-Spectrum Antimicrobial Properties Used as Disinfectants for Highly Contaminated Surfaces

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Abstract: Given the current global situation, caused by the Sars-Cov-2 virus, with major socio-economic effects, it is necessary to develop materials that control or prevent microbial colonization with various pathogens. The use of nanotechnologies in the applied biomedical sciences can offer a new way in treating viral infections and in disinfecting of surfaces, materials and products contaminated with various types of viruses, bacteria and fungi. The Cu-Au nanoparticles were obtained by an eco-friendly method, namely, radiochemical synthesis, that allows the obtaining of controlled size, well dispersed, fully reduced, highly stable particles at very mild conditions, in a one-step process, in an aqueous system of Cu^{2+}/Au^{3+}/Sodium Dodecyl Sulfate (SDS)/Ethylene Glycol using high energy ionizing radiations (γ-rays) at a dose of 30 kGy. The nanoparticles were characterized by UV-Vis spectroscopy, Dynamic Light Scattering (DLS), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and zeta potential. After irradiation, the change of color to red-wine was a first indicator for the formation of nanoparticles. Moreover, the UV-Vis spectra shown a maximum absorption peak at 532 nm ant the nanoparticles presented nearly spherical shapes, average sizes bellow 5nm and a zeta potential of about -44 mV, respectively. The antimicrobial properties performed according to various standards applied in medical area, in dirty conditions, shown a log 5 reduction (EN 13727 +A2:2016) for Staphylococcus aureus, Pseudomonas aeruginosa and Enterococcus Hirae, log 5 reduction (14476:2013 +A2:2019) for enveloped viruses such as Adenovirus type 5, Murine Norovirus, and human Corona virus 229E and log 4 reduction (according to EN 13624: 2014) for Candida albicans, respectively. These nanoparticle solutions have the potential to be used as disinfectant solutions with direct applicability in decontamination of hospital surfaces, as well as in public spaces characterized by high levels of microbiological contamination and, also, helping to fight against SARS-CoV-2 effects.

The financial support was provided by Ministry of Research, Innovation and Digitization through contracts: PN 19310101-46N/2019, 22Sol/2020 and 446PED/2020.
Keywords: Metal nanoparticles, Gamma radiation, Antimicrobial, Disinfection.

POSTER SESSIONS

Id-1777

Formation of Surface Self-Assembled Organosilicon Nanolayers on Carbon Steel and Its Effect on Electrochemical and Corrosion Behavior of the Metal

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Abstract: With the using Fourier transformed infrared (FT-IR) spectroscopy, scanning electron spectroscopy (SEM) and energy dispersive x-ray spectroscopy (EDX), the adsorption of vinyltrimethoxysilane on the surface of carbon steel from an aqueous solution and surface self-assembled organosilicon nanolayers formation have been studied. The mechanism of formation of the surface self-assembled nanolayer is proposed. It has been shown that during adsorption organosilanes interact with hydroxil radicals of a metal surface with Fe-O-Si bonds formation. The effect of organosilicon nanolayers on the electrochemical behavior of carbon steel was studied by obtaining anodic polarization curves. It is shown that the presence on the surface of vinyl and diamine-containing siloxane nanolayers on the surface leads to a significant reduction in the critical passivation current of steel, i.e. surface organosilicon nanolayers contribute to passivation of steel. In addition, it has been found that in the presence of organosilicon nanolayers on a metal surface causes the shift of critical potential of pitting formation of steel to the region of positive values, which indicates the inhibition of localized anodic dissolution of the metal. Accelerated corrosion tests of steel samples in the climatic chamber were carried out and the corrosion inhibiting effect of vinyl-containing surface nanolayers was shown. It has been established that vinyl-containing soiloxane surface self-assembled nanolayer is resistant to anodic polarization action, which usually contributesunifiorm and localized dissoltution of metals. As have been shown by FT-IR spectroscopy, the surface nanolayer is presented on a metal surface after anodic polarization. The results obtained indicate on the stability of siloxane nanolayers to water and corrosion-active components of an electrolyte action and to change of surface morphology due to dissolution of surface metal atoms with the release of metal ions into solution.

Keywords: Corrosion Inhibition, Carbon Steel, Benzotriazole, Organosilanes, Coupling Agents.

POSTER SESSIONS

Id-1782

The Mechanical Properties of Mediterranean Wild Silk Fibres

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Abstract: Pine processionary, Thaumetopoea pityocampa Schiff, is a moth that belongs to the family Thaumatopoeidae, subfamily Thaumatopoea Hbn. The larvae of pine processionary moth are the main pest of pines all over the world, but mainly in Mediterranean region. Pine processionary is considered a serious pest because caterpillars graze pine needles necessary for life of the tree, and significantly reduces the total value of riparian forests. The defence mechanism of the pine processionary caterpillar is the release of tiny needle-like hairs, which inject poison into whatever the caterpillar feels threatened. Therefore, the contact with pine processionary caterpillar can produce a strong inflammatory reaction on skin and mucous membranes what can be dangerous for both humans and animals. As a moth, it has no means of causing a harm; it is only during the development as a caterpillar. There are only a few ways to control the pine processionary caterpillar: mechanical control (mechanical removal of nests and destroying the caterpillars), chemical control (applying insecticides) and biological control (by predators, parasites and viruses). By applying any of these methods, complete eradication of one pest species is impossible. From an ecological point of view, they could be even harmful by disturbing the biological balance necessary for normal functioning of ecosystems. It is therefore obvious that today's research is based only on the mass appearance of Mediterranean wild silk, without destroying the natural balance and their attention was not focused on the fibres. Systematic studies of fibres from unconventional sources, such as Mediterranean wild silk, opens up the possibility of exploiting raw materials that are a special problem in today's ecosystem. Finding technology isolating the fibres from the nest, raw materials can be obtained for further processing with removing pests at the same time. The aim of this article is to increase knowledge about the mechanical properties (fineness, tenacity and elongation at break) of Mediterranean wild silk and compared with the cultivated raw silk fibers, Bombyx mori. Investigations were performed on Mediterranean wild silk taken from two silken nests mechanically separated from the pine tree in 2018. Prior to the study, a fibre demineralization procedure was performed. Mediterranean wild silk cocoons are difficult or impossible to reel

under conditions that work well for cocoons of the Mulberry silkmoth, Bombyx mori due to the presence of mineral deposits and difficulty in removing sericin. Therefore, it is necessary removed minerals from the surface of silk fibres without removing or modifying the sericin. Prior to the study, a fibre demineralization procedure was performed. Analysis of mechanical properties of Mediterranean wild silk fibres shows that Mediterranean wild silk fibres are finer with much higher elongation at break compared to cultivated raw silk fibres. Its tenacity is lower than the tenacity of cultivated raw silk. Silk fibres produced by wild Thaumetopea insects have properties suitable for commercial applications. However, further research is necessary to study the chemical and physical composition and potential applications for the wild silk. In addition, it is necessary to exam and find a safe way circumventing defence system of the pine processionary caterpillar. This work has been supported by the European Union from the European Regional Development Fund under the project KK.01.2.1.02.0270 Development of biodegradable nonwoven agrotextiles from natural and renewable sources.

Keywords: Mediterranean wild silk, Pine processionary moth, Thaumatopoea pityocampa schiff, Cultivated silk fibres, Properties.

POSTER SESSIONS

Id-1784

Improvement of Liquid Sulfur Filtration Process

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Abstract: The filtration of liquid sulfur is a key operation in the production of sulfuric acid. This operation aims to remove solids from liquid sulfur, which could clog the sulfur burner spray nozzles, leading to the reduction of life cycle production of sulfuric acid units. In fact, the standard life cycle operation for sulfuric acid unit is 24 months, while with the clogging issue life cycle operation can be reduced to less than 18 months. During liquid sulfur filtration, filter aid is used as a precoat for liquid sulfur filtration, mainly diatomaceous earth is the most used as a filter aid. The objective of this conference is to share the results study of the substitution diatomaceous earth by cellulose-based filter aid using industrial liquid sulfur filtration unit. The results shows that the two type of filter aid gives the same performance, in terms of ash content in filtered liquid sulfur. However, replacing the diatomaceous earth filter aid with the new cellulose-based lead to the extension of filtration cycle production from 24h to 72h accompanied by an easy de-building of the cake without a degradation of the filter cloths. Other results show that filtered liquid sulfur in case of cellulose based filter aid is not contemned by silicate one of the main sulfur spray nozzles clogging elements

Keywords: Sulfuric Acid, Liquid Sulfur, Filtration, Diatomaceous Earth, Filter Aid.

POSTER SESSIONS

Id-1785

Improvement of Phosphoric Acid Concentration Unit by Scale Reduction

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Abstract: Phosphoric acid generated by the di-hydrate process, usually characterized by a concentration between 25% and 32% P_2O_5. While merchant grade or fertilizer raw phosphoric acid need to have a concentration up to 42% P_2O_5, that way it's very important to concentrate the resulting dihydrate phosphoric acid using a flash concentration process technology. Fouling on heat exchanger surfaces is one of the serious and complex problems of this technology. During phosphoric acid evaporation, various impurities increases to supersaturation conditions and crystallizes into scale deposit composed mainly of gypsum both dihydrate ($CaSO_4.2H_2O$) and hemihydrate ($CaSO_4.1/2H_2O$) in addition to Sodium hexafluorosilicate (Na_2SiF_6), this lead to the decrease of life cycle operation of the concentration unit. Most companies try to avoid scale problem by reviewing equipment design and conception however, this solution cannot prevent scale formation. Our work aims is to increase the concentration unit life cycle operation by preventing scale formation using antiscalants agents. For that three commercial calcium sulfate scale inhibitor were tested in a batch evaporator pilot plant with a capacity of 20 liters, equipped with two graphite tube heat exchangers. The evaporation is conducted under vacuum pressure at 60 mmHg, and the heating is assured by hot oil recirculation trough the graphite type heat exchanger. After batch operations at the same conditions with fresh acid, the formed scales on heat tube surfaces are recovered then quantified and analyzed with XRD for study the effect of inhibitors (antiscalants) on scale morphology and mineralogy (nature of the precipitated phase). The results shows a decrease of scale formation by 40% to 50% after the addition of the three antiscalants in a concentration range between 2ppm and 5ppm. Furthermore, the uses of antiscalants affect the concentration process by increasing the evaporation rate and phosphoric acid concentration, for the same conditions of evaporation.

Keywords: Phosphoric Acid, Concentration, Antiscalants, Fouling, Scale Deposit.

POSTER SESSIONS

Id-1789

Ship Loading and Capacity Utilization

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Abstract: People have been shipping and loading cargoes in large amounts for 100 years. In order to get the most benefits of bulk carriers, i.e., get the maximum profit, bulk carrier must be able to be loaded with different cargo types. The overwhelming majority of these shipments are prepared easily without any restraints so there are a great loss of ships and lives. The reports show that in order to get the most benefits of bulk carriers, it must be loaded with different cargo types after applying the stability and strength criteria. In this research paper, the result of the existing bulk carrier's case study has been carried out computationally to investigate the effect of the loading conditions. Also, the effect of bulk cargoes types on the ship's stability conditions. Then, the significant factor has been taken into consideration. This factor has an impact on loading various cargoes with different characteristics in different stability and strength conditions. The results of the calculations have been observed in the graphical curves that can be used for enabling the loading on the board of the ship within minimum time, less cost, and maximum profits. This research paper gives the seafarers some graphical curves that help the ship's captain to obtain a sufficient ship's loading, freight rate and efficient ship's capacity. In this research, a bulk carrier vessel has been investigated by using Auto hydro and Auto ship programs. Some considered calculations have been done properly about the ship stability in both cases, intact and damaged. So, the results indicate that the research idea can improve the accuracy of applying some specific curves for the suitable cargoes. There are three dominating types of merchant ships which are bulk carriers, tankers and container ships. The tonnage of the world fleet consists from 33% of bulk carriers nowadays. The demand for raw materials has greatly increased such as coal, steel, copper, etc., since the beginning of the millennium. The proportion of bulk cargoes, which carried by sea, has increasingly varied recently as they form an important part of the international sea borne trade. Huge amounts of grains, coals, animal foodstuffs, fertilizers, ores and minerals are shipped by sea on daily basis. They face a great loss of lives and ships as a result of the vast shipment that are prepared without any restraints. Many problems have been arisen because of the inappropriate cargo distribution which caused capsizing and structural failure and deficiency of using the maximum capacity as well. The first

priority for the ship owner is earning capacity (freight rate) and capacity which is affected by the stowage factor. Consequently, capacity utilization and freight rate are studied and exposed carefully in this paper to suit the primary stage of design. There are a lot of new types of bulk cargoes or new categories of existing cargoes which having different characteristics such as stowage factor. As a result, an important factor which has been taken into consideration in this work. This factor has an impact for loading different cargoes having different stowage factors and angle of repose on the intact and damage stability and longitudinal strength.

Keywords: Bulk carrier, Freight rate, Capacity utilization.

POSTER SESSIONS

Id-1791

Development of Biodegradable Nonwoven Agrotextiles from Natural and Renewable Sources

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Abstract: Approx. 90% of the agrotextiles are made of synthetic polymers of PP, PE to a lesser extent from petroleum products such as PA and PET, which are becoming ecologically less acceptable. There is a trend of development of agrotextile production from natural fibres such as jute, wool, kenaf and cellulose regenerates (only 10%). Agrotextile for weed suppression is one of the wide range of products in agriculture application. The conventional material for weed suppression is black PE foil which, characterized by exceptional durability and significant effects regarding to its application. Negative aspects connected to their usage are long lifespan, high possibility of leaving harmful residues in the soil and the product itself is not recyclable. Conversely, biobased agrotextiles reduce negative impact on environment where during and after use are completely decompose making them ecologically acceptable. A preliminary investigation of durability of various fabrics used for weed suppression (affected by weathering) and also those potentially applicable natural fabrics (taking into consideration the degradation time and efficiency) was conducted for the purpose of further extensive research. All the obtained results are important indicators for further research that will be conducted within the project "Development of biodegradable nonwoven agrotextiles from natural and renewable sources" (KK.01.2.1.02.0270). This Project is a collaborative project of the Croatian textile factory Renotex tt and the University of Zagreb Faculty of Textile Technology, financed by the European Regional Development Fund. The Project aim is to develop a biodegradable nonwoven agrotextile for weed suppression and promotion of plant growth that will reduce or eliminate the use of chemical pesticides and insecticides. After fabric application, it will be completely composted in accordance with the principles of "zero waste" philosophy providing organic food production. Additional project aim is to introduce a more environmentally friendly production process of cleaner technologies which will have a significant impact on environmental protection and CO_2 reduction. In general, plants are divided into annuals and perennials for which nonwoven agrotextiles are designed to compose considering time period of plant grow, maturation and fruiting. Nonwoven agrotextiles are produced by mechanical

process on card, bonded by needlepunch and/or thermal bonded technology in wide range of mass per unit area (up to 500 g m-2). Nonwoven fabrics are produced from natural raw materials (Polylactide, Polyglycol, Copolymer poly (D,L-lactide-co-) in ratio 50:50 and 85:50, Rayon, Viscose and Bamboo fibres) emphasizing the environmental acceptability with regard to complete degradability after use. During degradation, beside the ability to reduce or eliminate weed grow; it is considered that it will promote plant growth. The use of cellulose fibres and fibres from cellulose regenerates would continue the biological circulation of substances in the soil system (soil-plant) stimulating a plant growth as biological fertilizer. The result of the project is expected to be a product designed to maintain soil health, enhance growth glycolide and yield of plants without usage of pesticides and compostable after usage. This work has been supported by the European Union from the European Regional Development Fund under the project KK.01.2.1.02.0270 Development of biodegradable nonwoven agrotextiles from natural and renewable sources.

Keywords: Agrotextile, Nonwoven, Biodegradation, Natural Fibres.

POSTER SESSIONS

Id-1796

Biodegradabilty of Modacryl/Cotton Plied Yarns

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Abstract: Biodegradable fibre blends are composed of biodegradable fibres and fibres that are not. These blends are usually less expensive compared to pure biodegradable fibres. The presence of the biodegradable fibre makes the mixture suitable for partial biodegradation, making it an alternative to the use of fully biodegradable fibres that are more expensive. The concept of introducing materials of a specific degradation time primarily requires defining a period in which the material should perform the intended role (without significantly losing their properties). It should be selected so that the gradual deterioration of their properties is proportionate to the performance of the intended role. The goal of this research is to investigate the influence of plied yarn fineness and thus its structures, on the biodegradability period i.e. deterioration time. The plied yarns are produced by twisting together two single yarns of same fineness. Single yarns are spun in Z direction in following fineness: 20, 16.7, 14.3 and 12.5 tex. During plying, the yarns were twisted in S direction where fineness of plied yarns amount 40, 33.4, 28.6 and 25 tex. Each single yarn were spun with blend of 55% modacryl / 45% cotton fibres. The biodegradability of the plied yarns was investigated using soil burial tests under real conditions for a period of 25, 50 and 100 days. The influence of soil and atmospherics conditions on the plied yarns biodegradability was evaluated by measuring and comparing changes in fineness and tensile properties. By increasing the period of samples buried in the soil, breaking force and tenacity decrease, while fineness and breaking elongation increase. Obtained results are an obvious indicator of sample degradation. The trend of changes in yarn fineness (increase in fineness due to partial decomposition of plied yarns) after the total burying period is not visible. That is, the largest change in yarn fineness is visible for the coarsest and the finest yarn (by an average of 18.5%). This can be explained by the different yarn twist influence where twists provide a certain yarn compactness. For example, the plied yarn fineness of 14.3 tex has more twists (S800 m-1) than yarn of 20.0 tex (S670 m-1) and 12.5 tex (S760 m-1), which organize fibres more compactly, providing greater resistance to the soil and the atmosphere to penetrate within its structure. The smallest decrease in yarn finesses (by an average of 11.8%) is present with the 16.7 tex yarn. Comparing the results of plied yarns breaking force and elongation, it is

evident that the largest decrease of breaking force (higher decomposition) have coarser yarns. Larger degradation occurred due to less compactness of the yarn structures. Tenacity is continuing the trend of breaking force, i.e. the largest decrease in yarn tenacity is visible for coarser plied yarns. The result of the research clearly demonstrate the importance of yarn structure, as the basic two-dimensional semi-finished product intended for making knits and woven fabrics, when designing biodegradable textile products for different purposes. This work has been supported by the European Union from the European Regional Development Fund under the project KK.01.2.1.02.0270 Development of biodegradable nonwoven agrotextiles from natural and renewable sources.

Keywords: Biodegradability, Modacryl/Cotton plied yarn, Soil burial test, Yarn fineness.

POSTER SESSIONS

Id-1797

Influence of Carbon Yarn Arrangement on Fabric Electrical Conductivity

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Abstract: Conductive fabrics are textile materials, which in their construction partially or completely contain threads of electrically conductive yarn and consequently can conduct electricity. Conductive yarns contain conductive materials such as carbon, silver, stainless steel, nickel, copper, etc. and can be used as filaments, staple mixtures or electrically conductive threads obtained by mixing with conductive polymers, i.e., electrically conductive fillers such as carbon and metal particles. The application of electrically conductive fabrics is wide, e.g. for antistatic clothing preventing electrostatic discharge (for employees at gas stations and gas platforms), in medicine, space research, etc. In this paper, the influence of the presence (density) and position (arrangement) of conductive yarns, made of filament carbon bi-component yarn (Negastat), fineness 39 dtex, twisted with polyester staple single yarn, on the charge decay of the woven fabric was investigated. Seven fabric samples were woven in ripstop weave on a laboratory weaving machine. The base raw material for all samples were aramid warp and weft yarn. Conductive threads plied with bi-component carbon filament yarns were woven into the construction of the samples in different positions of the rib weave segments. Samples 1 to 4 contain carbon threads in rib weave segments of the weft. The carbon threads are arranged in various densities, while samples 5 to 7 contain carbon threads in warp and weft (grid form) in various densities. Tests of basic characteristics of fabrics and measurement of electrical charge decay were performed on all samples. The results of tested samples showed that the presence and position of carbon bi-component filaments affect the electric shielding factor. In general, a higher proportion of bi-component fibre per woven fabric unit area will give higher values of the shielding factor. Furthermore, samples containing carbon filaments in the warp and weft (samples 5 to 7) have a higher shielding effect compared to samples having carbon yarns only in the weft direction (samples 1 to 4). The reason for this is the grid shaped structure that allows a greater degree of freedom in the movement of electrons within the woven fabric.

This work has been supported by the European Union from the European Regional Development Fund under the project KK.01.2.1.02.0064 Development of multifunctional non-flammable fabric for dual use.

Keywords: Rip Stop, Conductive Yarn, Copper Fibre, Negastat, Protective Woven Fabric.

POSTER SESSIONS

Id-1799

Different Yarn Behaviours During the Abrasion Process

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Abstract: Yarn abrasion resistance is a significant property for the quality of the woven fabric production process. In the weaving process, the yarn passes through various metal elements on the loom, in a state of high tension and continuous cyclic stresses. The geometry of the staple yarn can be described as an elongated cylindrical shape of a very relief and rough surface conditioned by the number of twists and yarn hairiness (protruding fibre ends). Such structure, under conditions of high cyclic stresses, is subject to various deformations depending on the properties of the yarn itself. There are large number of various methods for determining the yarn abrasion resistance that are based solely on the number of cycles to yarn break. However, none of them provides insight into the structural changes that occur during the abrasion process, while the breakage has not yet occurred. Such changes remain unregistered by standard yarn abrasion resistance methods but have a large impact on the quality of the produced woven fabric. In this paper, the influence of yarns structural characteristics on their behaviour due to abrasion process was investigated. Seven yarn samples (four single and three plied yarns from a polyamide and cotton fibres blend, of fineness: 50, 38.5, 29.5, 20, 15.5x2, 14x2 and 10x2 tex) were tested. Fineness and twist number, as well as unevenness and hairiness were tested on all samples. All yarns are subjected to abrasion cycles on a yarn abrasion device according to standard FZ/T 01058-1999, „Reciprocating rubbing roller method “. Prior to abrasion was conducted and after 20, 50, 100, 500, 1000, 2000 and 3000 cycles, a microscopic image of five labelled yarns was taken for each sample. Later, the image analysis was conducted where the average diameter of each yarn sample was calculated. The number of cycles at the yarn break was also recorded and the basic statistical parameters were calculated. The results showed that single yarns behave completely differently from plied yarns when subjected to abrasion. In the case of single yarns, the velocity of diameter change is significant in relation to the plied ones. Furthermore, fineness significantly affects the velocity of diameter change (decrease), where the coarser yarn wears faster and consequently the diameter decreases faster. The reason for this may be a higher proportion of longer fibres and a higher number of twists in yarns of greater fineness compared to coarser ones. In the case of plied yarns, there is practically no change in

diameter with increasing abrasion cycles number. The behaviour of the plied yarns can be described as the apparent destruction of the structure due to abrasion, where the fibres are no longer parallel to each other but remain within the yarn where the relative diameter of the yarn does not change or is visually even increased. As for yarn breakage due to abrasion, coarser plied yarns withstand more abrasion cycles. As the fineness of the yarn increases and in a case of plied yarn, the abrasion resistance of yarn increases. This work has been supported by the European Union from the European Regional Development Fund under the project KK.01.2.1.02.0064 Development of multifunctional non-flammable fabric for dual use. **Keywords:** Yarn Abrasion, Staple Yarn, Polyamide Yarn, Cotton Yarn, Yarn Structure.

POSTER SESSIONS

Id-1801

Water Vapour Transmission of Thermal Protective Woven Fabrics

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Abstract: Water vapour permeability is a property of paramount importance for the production of woven fabrics for firefighting clothing. The porosity and the permeability of water vapour are influenced by fabric constructional and structural parameters, such as weave, warp and weft density, fabric thickness, yarn fineness, etc. Fabrics with a high degree of protection against high temperatures must have satisfactory comfort properties, in particular good breathability to ensure the transfer of metabolic heat and steam from sweating to the environment. By testing the resistance of the passage of water vapour through the materials, their breathability or wearing comfort can be defined. In this paper, the comfort of woven fabrics for protection against high temperatures depending on water vapour permeability and porosity of the structure was investigated. The influence of structural and construction parameters and material composition on the above properties was also investigated. Eight woven fabric samples were woven on a laboratory weaving machine. Samples were made in two different weaves (K2/2 and ripstop) and four different weft fineness and compositions from different proportions of polyamide, meta-aramid and viscose/cotton fibre. All samples were woven with the same aramid warp, fineness 14x2 tex in the same density and under the same weaving conditions. In addition to the basic characteristics of the samples, the water vapour transmission through the sample according to the ASTM E96 method was performed. The results showed that the material composition, structural and constructional characteristics of woven fabrics affect its water vapour transmission and thus the wearing comfort. In general, the more porous fabric structure, as in a case of samples in ripstop weave, has a higher rate of water vapour transmission compared to twill weave fabrics. Furthermore, the weft yarn fineness has a direct impact on the fabric porosity and thus on the rate of water vapour transmission which is higher in fabrics with a finer weft yarn. By determination of the samples warp and weft density, differences in values were found, and accordingly the fabric porosity was different from expected. This is especially noticeable with samples in the ripstop weave. This work has been fully supported by the Croatian Science Foundation under the project number IP-2018-01-3170

Keywords: Water Vapour Permeability, Protective Woven Fabrics, Thermal Protection, Structure Porosity, Fabric Comfort.

POSTER SESSIONS

Id-1810

New Design of Orthosis

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Abstract: Orthosis is a device used to immobilize a joint or fracture. It is recommended by orthopedic doctors in the case of bone and ligament disorders, having the role of stabilizing the joint/fracture, as well as reducing the pain in the respective segment, thus contributing to the healing of the injuries. With the help of 3D printing technology (also known as additive manufacturing), which allows the production of orthotics with adaptable dimensions and customized shapes, as well as the establishment of an ergonomic and cost-effective design, patients can wear orthotics throughout the day. Thus, very great progress can be achieved during rehabilitation therapy compared to the other available devices. Also, the reduction of the manufacturing time and costs are other advantages of the additive manufacturing technologies relevant in the further development and manufacture of orthotics. At the same time, 3D printing offers an increased degree of design complexity, and very complex forms can be created, which by traditional methods are not achievable. In addition, the 3D printing of hand orthosis allows them to be made in small series, adapted to the conditions of each patient. This approach saves materials, by reducing excessive and unnecessary material losses. The proposed models are made from biodegradable materials, easy to recycle. Our design provides an active interface, functionalized with substances efficient for skin and regeneration and antimicrobial activity. The new design also protects the skin during use, ensures a breathing/ventilation of the skin and accelerates the dermo-epidermal healing processes. Also, the active substance can have multiple action if the fracture is associated with a burn or damage of a different nature to the epithelial tissue. The orthosis has a good rigidity, ensured both by the material and by design. It is made of PLLA thermoplastic polymers, 3D printable. Authors acknowledge UEFISCDI, Romania, grants M-ERA.NET 74/2017 BIOMB and 5PTE/2020 BIOTEHKER.
Keywords: Orthosis, PLLA, Additive fabrication, Functional additions.

POSTER SESSIONS

Id-1815

New Intuitive Regularizating Approaches for Deconvolution Problems

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Abstract: We proposed a series of the nonstandard modifications of the toeplitz matrixes and the statistical regularizating approaches for deconvolution problems. We have shown their realization trend potentially to a significant improvement of the quality of results for signal (or image) deconvolution problems in the series of specific cases those are significant in some spectroscopic applications (x-ray fluorescence micro/nanoanalysis, photoelectronic spectroscopy). Especially it is valuable for problems with the specific restrictions of the spatial fields, the step of scanning, the requirement of the binding account of a-priory known information. As a result it may improve the results of works in exploring and controlling the distribution of the elemental and chemical composition of the selected fragments of samples of various origin (broadly speaking, material, geological, biological, cosmic, archeological, forensic samples). The work was carried out in the framework of the RFBR project no. 19-05-50046. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

Keywords: Deconvolution, Superresolution, Deblurring, Sub-Focus Microscopy, Micro-XRF.

POSTER SESSIONS

Id-1816

Investigation of the Morphology of Red Blood Cells in those who died from Hypothermia by Scanning Electron and Atomic Force Microscopy

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Abstract: General cooling and frostbite are some of the severe types of cold injury, often they lead to a high level of disability and death of the injured. Every year in the Republic of Sakha (Yakutia), more than two hundred people die and even more people become disabled. Currently, the problems of death and resuscitation of patients from general cooling at ultra-low temperatures (below -40°C) are not sufficiently studied in the world. To develop methods for restoring the body after general cooling at ultra-low temperatures, studies of fatal hypothermia at the molecular and cellular level are necessary by methods of medical physics, including medical biophysics. The aim of this study was to evaluate the morphology of red blood cells during fatal hypothermia at extremely low temperatures by atomic force and scanning electron microscopy. The subject of the study was blood smears of people who died from hypothermia and from a gunshot wound, using a high-resolution scanning electron microscope JSM-7800F ("Japanes Electron Optics Laboratory" - "JEOL", Japan) and an atomic force microscope SolverNext of the company" NT-MDT " (Russia). The red blood cells of a person who died from hypothermia at an extremely low temperature-42°C and from whom a blood smear was taken during the first day were characterized by minimal changes than the red blood cells of a person who died from a gunshot wound. The discocytic form of red blood cells was mostly preserved and an increase in the depth of the central concavity of red blood cells was found, which may be associated with an increase in the volume of red blood cells, while a large number of echinocytes and acanthocytes were observed in the deceased from a gunshot wound. It was

also found that even a slight difference in the temperature of the body areas during blood collection, for example, with a difference of 2.4°C, affects the ratio of different forms of red blood cells after complete thawing. The lower the temperature, the more degenerative forms of red blood cells become. After complete thawing of the corpse on the 4th day, all red blood cells (100%) had a different degree of dysmorphism, a flattened surface, an increase in diameter, heterogeneity and roughness of the plasma, indicating signs of hemolysis. Thus, the results of this study allowed us to determine significant differences in the morphology of red blood cells depending on the cause of death, which indicates the need for further study of the parameters of red blood cells to identify the possibility of restoring cells, their normal population and their functional properties, depending on the method of heating the deceased from hypothermia under certain temperature conditions.

Keywords: Medical physics, Red blood cells, Death from hypothermia, Atomic microscopy, Scanning electron microscopy.

POSTER SESSIONS

Id-1827

Morphological Characterization of Polydopamine Coated Surfaces

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Abstract: Polydopamine (PDA) is regarded nowadays as an almost universal surface modification agent due to its strong adhesion to virtually any substrate, on the one hand side, whereas on the other hand side, to its capacity to bind many types of functional molecules, including large biomolecules. Here, we report the results of a systematic Atomic Force Microscopy (AFM) study aimed at determining the morphology of the deposited PDA layers under different dopamine oxidation conditions. Specifically, the pH, oxidation agent, deposition times and mechanical postprocessing are varied and the PDA film thickness, rugosity and homogeneity are monitored. The obtained data will be correlated with the purpose of introducing a reliable methodology for quality control of the deposited PDA thin film, which is a necessary initial step in the perspective of the potential technological applications of the coated surfaces.

Keywords: Polydopamine thin films.

POSTER SESSIONS

Id-1828

Solid-State NMR as a Powerful Tool in Polydopamine Characterization

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Abstract: Inspired by the strong adhesion of mussels to any solid substrate, Messersmith has discovered in 2007 polydopamine (PDA) as a readily accessible synthetic analogue of the naturally occurring melanins, showing strong and universal adhesion ability to virtually any substrate. Despite the growing number of PDA applications reported each year, there are still fundamental challenges remained in the field, such as the formation and adhesion mechanisms as well as a widely accepted structural model. The amorphous character of PDA, and the high degree of disorder at all levels (monomers, oligomers, supramolecular aggregates), pose serious limitations upon the information content provided by the analytical techniques widely used for its investigations: mass spectrometry – mainly because this is a destructive technique, X Ray photoelectron spectroscopy, Fourier transform infrared spectroscopy – although non-destructive, they only offer global information, with no site-specificity. By contrast, solid-state NMR spectroscopy is non-destructive and offers a higher degree of chemical-site selectivity. Here we review the latest progresses in our ss-NMR investigations of polydopamine, focusing on the structural information they provide regarding the monomeric units and connectivity among them in the final material. It is also shown that sample engineering by isotopic labelling can bring new and valuable insights into this fascinating material.

Keywords: Polydopamine, Solid-state NMR.

POSTER SESSIONS

Id-1833

Solder Layer Influence on the Thermal Parameters of Insulated Gate Bipolar Transistors (IGBTs)

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Abstract: The effect of solder joint fabrication on the thermal properties of IGBTs soldered onto glass-epoxy substrate (FR4) was investigated. Glass-epoxy substrates with a thickness of 1.50 mm, covered with a 35 µm thick Cu layer, were used. A surface finish was prepared from a hot air leveling (HAL) Sn99Cu0.7Ag0.3 layer with a thickness of 1 ÷ 40 µm. IGBT transistors NGB8207BN were soldered with SACX0307 (Sn99Ag0.3Cu0.7) paste. The samples were soldered in different soldering ovens and at different temperature profiles. The thermal impedance $Z_{th}(t)$ and thermal resistance R_{th} of the samples were measured. Microstructural and voids analyses were performed. It was found that the differences for different samples reached 15% and 20% for $Z_{th}(t)$ and R_{th}, respectively. Although the ratio of the gas voids in the solder joints varied between 3% and 30%, no correlation between the void ratios and R_{th} increase was found. In the case of the different soldering technologies, the microstructure of the solder joint showed significant differences in the thickness of the intermetallic compounds (IMC) layer; these differences correlated well with the time above liquidus during the soldering process. The thermal parameters of IGBTs could be changed due to the increased thermal conductivity of the IMC layer as compared to the thermal conductivity of the solder bulk. Our research highlighted the importance of the soldering technology used and the thermal profile in the case of the assembly of IGBT components.

Keywords: Soldering technology, IGBT, Packaging, thermal parameters, Thermal pad, Thermal resistance.

POSTER SESSIONS

Id-1836

Using One Dimensional Convolutional Neural Networks for Classifying the Vibration of Process Pipework

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Abstract: Pipework in process facilities such as oil and gas or petrochemical plants is subjected to a variety of dynamic excitations. Such excitations may include flow-induced forces due to turbulence or at the locations of change of momentum, shaking due to imbalances of rotating machinery, gas pulsations closed branches and gas pulsations due to reciprocating machinery, etc. Since process pipework usually conveys hot/cooled fluids, they cannot be rigidly fixed and the design codes (e.g., ASME) dictate a degree of flexibility of process pipework. The ensuing vibrations from these dynamic loads (over time) may cause vibration-induced fatigue failures (VIF). It is in the operator's interest to quantify the risk of such vibrations as part of a risk-based inspection regime to ensure the optimal and safe operations of their plant. Ideally, the risk of VIF is quantified through measuring strain. However, measuring strain in process plants can be challenging for a variety of reasons: the installation of strain gauges requires paint removal and surface preparation; pipework is often hot or insulated; and the installation itself may be challenging physically if the pipework is excessively shaking. A popular alternative to strain measurement is measuring the vibration using widely available accelerometers and a single channel analyzer. The motive here is that the velocity of vibration is proportional to stress and thus, vibration levels can be used to as an indicated of the risk of VIF. Current vibration acceptance criteria use the root-mean-square of the velocity to classify pipework vibrations into three categories: OK, CONCERN and PROBLEM. In this paper, we use a multiheaded one dimensional (1D) convolutional neural networks (CNNs) to classify pipework vibrations. The impetus for using a multiheaded network is to enhance the feature extraction from the vibration signals and to make the network's architecture more flexible to the additional of new sensor information. Vibration and stress data are obtained from an inhouse experimental setup of a pipe that is mounted on a shaking table. We use the generated stress signals to pre-classify the vibration into the three categories mentioned earlier. We then use the vibration signals to train the 1D CNN. Preliminary results show that the proposed CNN can classify the vibration data

over 85% of the time. The developed approach has the potential to reduce the need to measure strain onsite and enhance integrity and inspection activities by detecting locations that could potentially experience fatigue earlier which would lead to reducing the risk of VIF and avoiding leaks of hydrocarbons or other fluids.

Keywords: Neural network, Vibration induced fatigue, Stress, Acceptance criteria.

POSTER SESSIONS

Id-1838

Mechanical Characteristics of Ultra-High Performance Steel FRC Made with Recycled Concrete Aggregates

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Abstract: Recycled concrete aggregates (RCA) is increasingly becoming a sustainable alternative to natural aggregate (NA) for concrete applications. This study, therefore, tests the mechanical characteristics of 6 ultra-high performance fiber reinforced concrete (UHPFRC) with different coarse aggregate types (NA, and RCA), steel fiber types (macro hooked-end, and micro straight), and volume fractions of steel fibers (0% and 1%). Tests were performed for the flowability and compressive and flexural tensile strengths. Test results showed that the flowability of UHPFRC was slightly affected by the coarse aggregate types. However, the flowability was decreased by 12% to 15% with steel fibers. The results also revealed that at a volume fraction of 0%, the aggregate type had little influence on the compressive strength, while the flexural strength was significantly influenced by the aggregate type. In addition, macro-fiber was shown to have no significant influence on the compressive strength, regardless of the coarse aggregate type. However, the use of micro-fibers increased the compressive strength by an average of 7%. Furthermore, UHPFRC with macro-fibers recorded the highest flexural strength, regardless of the coarse aggregate type.

Keywords: Recycled Concrete Aggregates, Ultra-High Performance Concrete, Fiber Reinforced Concrete, Mechanical Characteristic, Steel Fibers

POSTER SESSIONS

Id-1849

The Development of Manufacturing Technology of Refractory Products from Waste of Ferrochrome Production

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Abstract: Currently, the companies producing ferroalloys using electrothermal furnaces have accumulated a huge amount of intermediate products and wastes, including fine dust cyclone and bag gas cleaning, wet cakes filters, various slag and sludge. Recycling or returning these products to production is extremely difficult. They are stored in heaps in the open air, exposed to wind erosion, has a negative impact on the environment and the deteriorating environmental situation in the region. Chemical analysis of these products showed that they contain a significant number of oxides of magnesium, chromium, aluminum, silicon and other components useful from the point of view of refractory raw materials. In terms of their mineralogical and chemical composition, these wastes can act as raw materials for the production of magnesiochromite refractories. Calculations were conducted and studied various compositions of the refractory compositions containing ferrochromium production waste. A technology has been developed for the use of highly dispersed dusts (< 20 μm) by obtaining strong quasi-granules using various binders (sulfite-alcohol stillage, aqueous solutions of magnesium mineral salts, etc.). Quasigranules obtained by a special technology play the role of a granular component in the matrix of a refractory product. The estimation of the refractoriness of the compositions of the studied wastes was made according to their chemical and mineral composition using three-component phase diagrams: $MgO – Al_2O_3 – SiO_2$, $MgO – Cr_2O_3 – SiO_2$. The experiments confirmed the possibility of obtaining refractory products similar in mineral composition and physical and technical properties to forsterite refractories. The strength characteristics and refractoriness of non-fired and fired products have been determined 1580 - 1750 °C. It is shown that the main physico-chemical and mineral-phase significance in the development of masses and the production of refractory products is the chemical and phase compatibility of the components of dust, slag, cake and refractory scrap using technological methods: preparation and proper mixing of the charge, a compression pressure, a temperature mode of drying and heat treatment.

Keywords: Metallurgical Waste, Filter Cake, Slag and Dust.

POSTER SESSIONS

Id-1854

Experimental Investigation of the Machining Process of AISI 304 During Dry Metal Cutting Process Using Modern Nanocoated Cutting Tools.

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Abstract: By increasing of stainless steel wide application in the world and development of cutting tools materials and coatings, research and prediction of its wear and distribution of temperature fields became topical. Research of processing parameters is important, as well as it's impact on the final result. As stainless steel is stead and difficulty processed material and contains various alloy elements that in turning makes difficult processing and create significant inconveniences in chip formation process (it is necessary to break into pieces and), because these alloy elements increase flexibility of the steel, hardness, which in turning makes difficult processing by cutting. As a result we obtain flowing chips, which are not allowed in modern automated production of large series of parts, so it can be concluded that research of chip formation process is very topical. In turning process impact of various structures of stainless steel – martensitic, austenic were compared. Directly AISI 420 and AISI 304. Firstly tools with Duratomic nanocoated technology have been investigated, which are characterized by larger wear resistance in the previous rough turning (when removable metal amount exceeds the options of analogous type instrument), as well as in exact processing, when higher cutting speed and lower cutting depth are used, as well as cutting temperature increases significantly. Modern material systems for coatings on cutting tools, towards accomplishing clean manufacturing, i.e. without the use of a cutting fluid, are presented. They involve use of multilayer wear-resistant nanocoating architectures on cemented carbide tools by physical vapour deposition (PVD) process, namely, magnetron sputtering. By providing numerous (several layers in 2-12 μm) alternate nanolayers of hard and tough, hard and hard, or solid lubricating and tough materials, it is possible to take advantage of the unique properties of nanostructures, namely, higher hardness, higher strength, higher modulus, higher wear resistance, higher fracture toughness, higher chemical stability, and reduced friction than their counterparts where the coating layer thickness is in the micrometre range. Various features of these coatings are discussed from the point of view of their application in dry machining.In this research were estimated main elements of cutting process – chip formation process, temperature field distribution in cutting tool, as well

as wearing of cutting tool that significantly impacts on the roughness of processed surface and chip formation process, because of significant impact of alloy elements. The idea of mathematical analysis is, using various factors experiments, to receive a mathematical model of cutting process and to evaluate the accuracy of the experiments.

Keywords: Coatings, Tool, Machining, Metal cutting.

POSTER SESSIONS

Id-1856

Oxidation of CO and Benzene Over Metal Nanoparticles Loaded on Hierarchical ZSM-5 Zeolite

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Abstract: In order to obtain highly active catalytic materials for oxidation of carbon monoxide and volatile organic compounds (VOCs), monometallic platinum, copper and palladium catalysts have been prepared by using of two types of ZSM-5 zeolite as supports - parent ZSM-5 and treated with HF and NH_4F buffer solution. The catalysts, obtained by loading of platinum, palladium and copper on ZSM-5 zeolite treated with HF and NH_4F buffer solution are more active in the reaction of CO and benzene oxidation, compared with catalysts containing untreated zeolite. The presence of secondary mesoporosity plays a positive role in increasing the catalytic activity due to improved reagent diffusion. The only exception is copper catalysts in the reaction of CO oxidation, where more active is catalyst, based on untreated ZSM-5 zeolite. In this case the key role plays the oxidative state of copper species loaded on the ZSM-5 zeolites. In the case of benzene oxidation, H_2O and CO_2 are the only detectible reaction products in all studied samples. The samples are compared according to the temperature for 90 % reagent conversion or according to that one for maximum conversion in cases this value has not been reached. The following order of activity in the reaction of CO oxidation is established Pd-Tr > Pt-Tr > Cu-Par > Pt-Par > Pd-Par > Cu-Tr. The row of activity in the complete benzene oxidation is as follows: Pt-Tr > Cu-Tr > Pd-Tr > Pd-Par > Cu-Par > Pt-Par (85 %, 290 ˚C). The value in brackets for the last sample show the maximum conversion reached in the studied temperature interval 100-290 ˚C. The sample Pt-Par has the lowest redusibility.It is obvious that the preliminary treatment of the support has a crucial role on the catalytic activity of the samples investigated – the catalysts with treated support are more active. The effect is more pronounced in the reaction of benzene oxidation. The size of benzene molecules is higher than the size of CO molecules and the presence of secondary mesoporosity has bigger effect. The diffusion problems that would occur during the oxidation of benzene on a parent samples do not exist on the treated samples. Benzene molecules have improved access to the active catalytic sites. In CO oxidation, also the catalysts based on treated support are more active. The only exception are copper catalysts. The more active for CO oxidation is the catalyst with parent support CuPar than CuTr. Copper

can exist in different oxidation states such as Cu^{2+}, Cu^{1+} and Cu^{0}. These copper species can coexist together with different ratios depending on many factors such as preparation method and reduction process. These copper species have different CO oxidation activities. It is known that Cu^{1+} is very effective in CO oxidation compared to Cu^{2+}. This is with good agreement with our TPR results, which show preferable presence of Cu^{1+} in the sample CuPar than Cu^{2+}. This is the main reason for the higher activity of CuPar sample.

Keywords: ZSM-5 zeolite, Noble metals, Hierarchical materials, Catalysts, CO oxidation, Benzene oxidation.

POSTER SESSIONS

Id-1881

Synthesis of Narrowband Gap Binary Semiconductor for Enhancement of Thermoelectric Figure of Merit

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Abstract: PbTe is a typical intermediate-temperature range thermoelectric material, which has undergone extensive developments and achieved excellent high thermoelectric performance. In this perspective we have successfully synthesized PbTe-based thermoelectric materials through chemical route and electrodeposition method and manipulating charge and phonon transports, such as optimizing carrier density to tune Fermi level, tailoring band structure to enhance effective mass, and designing all-scale hierarchical architectures to suppress phonon propagation for the enhancement of thermoelectric properties of the synthesized material. PbTe was synthesized by chemical route method and by electrodeposition method with stainless steel and pure copper plate as working electrode. The synthesized material was characterized for different characterizations techniques like X- ray diffraction, Fourier infrared spectroscopy, cyclic voltammetry studies, Scanning electron microscopy, contact angle measurements, Raman spectroscopy for the physicochemical characterization of the material. Different thermoelectric parameters like thermo-emf, electrical conductivity and thermal conductivity are measured and power factor and the thermoelectric conversion efficiency of the synthesis material was determined.

Keywords: PbTe, Thermoelectric, Cyclic Voltammetry, Raman Spectroscopy etc.

POSTER SESSIONS

Id-1894

SMARTELECTRODES: Electrospark Alloying One of the Advanced Methods for Physical-chemical Processing of Metals at "TOPAZ"

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Abstract: According to the Food and Agricultural Organization (FAO), in order to bring the volume of agricultural production to a level that feeds the growing population of the Earth, it is necessary to increase investments significantly in the development and widespread introduction of new agricultural technologies and their mechanization. In many regions of the world, for economic reasons, there is an increasing demand for reconditioned machine assemblies as opposed to new ones. Therefore, modernization at the high technological level of aggregate repair enterprises for engines, diesel fuel equipment, hydraulic transmissions, turbochargers and other most complex units and assemblies is becoming a promising direction of development. Electro-spark alloying (ESA) in this field is in demand first of all.Application of this technology is especially effective in the repair of turbochargers and hydraulic units: distributors, pumps, hydrostatic transmissions, the resource of which becomes higher than new due to a change in the physico-mechanical properties of the working surfaces of the parts, including increased wear resistance factor. Coatings are applied on electrospark installations, both manual and automated. The technology of applying nanostructured coatings on the surface between turbine rotor shaft and bearing of turbochargers of tractors is carried out by electrospark processing. The test results of reconditioned and hardened parts showed a 2-fold increase of the resource of turbochargers. The technology for repairing hydrostatic transmissions of agricultural machinery by the restoration and hardening of worn parts by the method of electric spark alloying provides an increase of the resource of compounds by 1.5 times.Installations Topaz-ESA provide the ESA process with various technological methods by introducing additional energy release within the period of the main pulses that distinguishes them from most competitors in the world. The technology developed by Topaz allows: 1) to control the thermal conditions of the electrodes by means of the amplitude and duration of the main pulses of ESA; 2) Create pedestals in a pause; 3) To control the crystallization regimes of the liquid mass on the substrate by additional spark discharges; 4) Combine the ESA and electro-erosive smoothing depending on the requirements for roughness.

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Keywords: Electrospark Alloying, ESA Process, Controllable Spark Discharge.

POSTER SESSIONS

Id-1901

Azimuthally Asymmetric Gyrotron Cavities for Selective Excitation of Symmetric TE Modes

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Abstract: We develop an electrodynamic method based on azimuthally asymmetric cavities to provide selective excitation of symmetric TE waves in fundamental-harmonic gyrotrons. The presence of small azimuthal inhomogeneities in a cavity with a “close-to-circular” cross-section does not affect on excitation of the operating TE0,p mode, but increases the starting current of excitation of the parasitic TE2,p mode. This approach can ensure also mechanical adjustment of the frequency of the operating TE0,p mode. The work is supported by the Russian Science Foundation grant #20-72-10116.

Keywords: Gyrotron, Mode selection, Microwave, Sub-Terahertz sources.

POSTER SESSIONS

Id-1903

Gyrotron Complexes for Microwave Material Processing

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Abstract: Various technologies for microwave processing of materials require affordable radiation sources of moderate power of several hundred watts. In this case, important limitations are the requirements for minimizing X-ray radiation due to the high accelerating voltage, as well as the complexity, size, and cost of power supplies for gyrotron complexes. In this regard, the development of low-voltage gyrotron complexes based on shielded magnetic systems is topical, which is the subject of this work. This work was supported by the Russian State Assignment Program, IAP RAS project 0030-2019-0027 and by the Russian Foundation for Basic Research (project no. 21-58-53051)

Keywords: Technological gyrotron, Microwave processing, Low-voltage gyrotron

POSTER SESSIONS

Id-1905

Properties of $PbO-Bi_2O_3-Ga_2O_3$ Glasses Modified by Addition of Ag_2O and Sb_2O_3 to Form Ag Nanoparticles

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Abstract: We prepared a set of $PbO-Bi_2O_3-Ga_2O_3$ glasses modified by addition of Ag_2O and Sb_2O_3 in various ratios. The glasses were prepared by conventional melt-quenching method by melting in platinum crucibles at approximately 1000 °C. Annealing of glass samples cast in metal moulds was performed at the respective glass transition temperature T_g (around 310–320 °C). According to our hypothesis, the added modifiers should allow the formation of nanoparticles when a suitable temperature regime is applied to the annealed glass. The results of our experiments confirmed this assumption – the formation of Ag nanoparticles occurs at temperatures below T_g, significant formation occurs in the temperature interval of 260–280 °C. We report the properties of glasses before and after heat treatment, i.e. before and after formation of nanoparticles. The focus is on optical, electrical and dielectric properties. The formation of nanoparticles was confirmed by electron microscopy (scanning electron microscope, transmission electron microscope, electron diffraction). Due to their electro-optic properties (electro-optic coefficient of about $7.5–7.8\times10^{12}$ m/V^2), the investigated glasses appear to be suitable candidates for the use as electro-optic modulators.

Keywords: Heavy metal oxide glasses, Silver nanoparticles, Electro-optic effects.

POSTER SESSIONS

Id-1906

$PbCl_2 – Bi_2O_3 – TeO_2$ Glasses: Preparation and Physical Properties

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Abstract: Thermally stable glasses are formed in the ternary system and the glass forming area is adjacent to the TeO2 rich corner of the ternary diagram. The use of PbCl2 has two positive effects – firstly, the lead chloride extends the glass forming area and increases the thermal stability of the glasses in comparison to the system with PbO instead of PbCl2, secondly the presence of chlorine in the system protects the quartz glass crucible used for glass melting from the corrosive effects of the melt, thus protecting the melt from contamination by SiO2. On the other hand, lead chloride has definitely no positive effect on the resistance of the glass to water or humidity. However, glasses with higher TeO2 content (>60-70 cat.%) are not subject to moisture corrosion under normal conditions. The bismuth oxide has positive effects on the width of the transparency window and/or on the refraction index, among other things. The prepared glasses are yellow and are transparent approximately from 0.4 to 6.5 microns. Their refraction index largely exceeds 2.

Keywords: Tellurite glasses, Bismuth oxide, Infrared, Optical properties.

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