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Center of Excellence for the Synthesis, Processing and Characterization of Materials for use in Extreme Conditions “CEXTREME LAB” - Institute of Nuclear Sciences “Vinča”, University of Belgrade
Faculty of Mechanical Engineering, University of Belgrade

PROGRAMME AND THE BOOK OF ABSTRACTS

4th Conference of The Serbian Society for Ceramic Materials

June 14-16, 2017
Belgrade, Serbia
4CSCS-2017

Edited by:
Branko Matović
Zorica Branković
Dušan Bučevac
Vladimir V. Srdić

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WELCOME MESSAGE

On behalf of the organizers and organizing committee of the 4th Conference of the Serbian Society for Ceramic Materials (4CSCS-2017), I would like to extend my warmest welcome to all of you for attending the 4CSCS-2017. The conference is hosted and organized by the Serbian Society for Ceramic Materials, and co-organized by Institute for Multidisciplinary Research - University of Beograd, Institute of Physics - University of Beograd, Center of excellence for the synthesis, processing and characterization of materials for use in extreme conditions “CEXTREME LAB” - Institute of Nuclear Sciences Vinca, University of Belgrade and Faculty of Mechanical Engineering, University of Belgrade.

The goal of the Conference is to provide a platform for academic exchange among participants from universities, institutes, companies around the region in the field of ceramics research as well as to explore new direction for future development. 4CSCS-2017 aims to bring together leading academic scientists, researchers and research scholars to exchange and share their experiences and research results about all aspects of Ceramic Materials. It also provides the premier inter-multi-trans-disciplinary forum for researchers, practitioners and educators to present and discuss the most recent innovations, trends, and concerns, practical challenges encountered and the solutions adopted in the field of Ceramic Materials. We have received more tabout 100 abstracts submitted from 15 countries.

The Conference will feature two plenary lectures, 25 invited talks and more than 70, oral and poster presentations as well as exhibitions of some new ceramic materials and devices. 4CSCS-2017 includes Ceramic Powders, Characterization and Processing, High temperature Phenomena, Sintering, Microstructure Design and Mechanical Properties, Electro and Magnetic Ceramics, Ceramic Composites, Membranes and Multimaterials, Traditional Ceramics and Computing in Materials Science. Exhibitions from company sponsors will be held at the Conference as well.

We are grateful for the support from the Ministry of Education, Science and Technological Development of the Republic of Serbia. We would also like to express our sincere thanks to the symposia organizers, session chairs, presenters, exhibitors and all the Conference attendees for their efforts and enthusiastic support in this exciting time in Belgrade. I look forward to meeting you and interacting with you at Conference.

4SCSC-2017 President

Branko Matovic

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PL-1

DESIGN, PROCESSING AND APPICATION OF POLYMER-DERIVED SINGLE- AND MULTI-PHASE CERAMICS IN THE Si-X-C-N (X = Al, B AND/OR TRANSITION METALS) SYSTEM

David Ferber-Lopez, Diane Fonblanc, Abhijeet Lale, Marion Schmidt,
Antoine Viard, Samuel Bernard

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There is a trend toward more flexibility and an increased interest in “smart” and “adaptive” materials with the objective to meet most industrial specifications. Carbides and nitrides can be considered as such strategic materials. They attract increasing interest due to their properties targeted for future materials and technologies, especially their relatively high thermal robustness and chemical inertness, while bearing intrinsic multi-functionality by adding more elements to the conventional binary systems. Inherent difficulties to the traditional techniques for manufacturing such multiphasic materials can be overcome by the development of synthetic paths where chemistry of materials and ceramic science are combined rationally to process multi-scale complex solid state architectures. The *Polymer-Derived Ceramics* (PDCs) route offers new preparation opportunities in ceramic sciences. The molecular origin of preceramic polymers and the possibility to shape then pyrolyze them into “near net shape” advanced materials play a major role in the preparation of ceramics endowed with properties that reach far beyond those of existing materials. Here, we report the design of single- and multi-phase ceramics including Si_3N_4, SiCN, SiXCN (X = B, Al) and nanocomposites made of TiN nanocrystals dispersed in an amorphous phase of Si_3N_4. This presentation will be particularly focused on the polymer processing to generate mesoporous monoliths that can find application in energy domains such as hydrogen production.

PL-2

CALPHAD MODELLING APPLIED TO CERAMIC SYSTEMS

K.C. Hari Kumar

Department of Metallurgical & Materials Engineering, Indian Institute of Technology Madras, Chennai 600 036, India

It is widely recognised that phase diagram and thermochemical data are essential to answer many practical questions that arise in the development of materials and their processing. The CALPHAD method, a computer assisted calculation method, which offers a cost-effective and efficient alternative to conventional methods to obtain much needed phase diagram and thermochemical information in multicomponent systems. It is a combinatorial approach involving carefully selected experimental data, results from theoretical estimation techniques and Gibbs energy models. Result of such an exercise is a set of internally consistent Gibbs energy functions that describes the material system. Powerful computer programs in combination with reliable Gibbs energy functions stored in databases allow calculation of phase diagrams and thermochemical properties that suits one's need. Principles and advantages of the CALPHAD method are presented. Its application to material systems relevant to ceramics will be illustrated.

I-1

CHARACTERSITICS OF RED MUD AND/OR METAKAOLIN-BASED GEOPOLYMERS AS A FUNCTION OF MICROSTRUCTURE MODIFICATION BY Ca(OH)$_2$

Mira Vukčević[1], Ivana Bošković[1], Snežana Nenadović[2], Miljana Mirković[2], Marija Stojmenović[2], Vladimir Pavlović[3], Ljiljana Kljajević[2]

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[3]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, University of Belgrade, Serbia

One of the key issues in geopolymer synthesis is the low level of ductility. It can often lead to the limited application possibilities, so the objective is to obtain the enhanced ductility, as well as decreased cracking tendency by the microstructure modification. By introducing of inorganic modificator of microstructure calcium hydroxide (($Ca(OH)_2$), during the process of geopolymer synthesis the enhanced values of ductility and hardness can be obtained. Introduction of $Ca(OH)_2$, under the certain pH conditions, leads to the creation of isolated domains within the geopolymer matrix followed by the filling-the-pores process and decreasing the possibility of stress localization and cracking. The paper presents the influence of raw mixture, content of microstructure modificator, synthesis parameters (Si/Al, solid/liquid phase, pH, the conditions of alkali activation) as well as the conditions of post-synthesis thermal treatment and aging of geopolymers on the mechanical properties of the final product.

Research was performed on two types of raw mixture: the first one based on red mud-metakaolin-$Ca(OH)_2$ and the second one on metakaolin and $Ca(OH)_2$. The best raw mixture composition, S/L ratio as well as pH conditions were defined as well as the relation between the modificator's content and pH. Post-synthesis curing also play important role in obtaining of good-performing geopolymers. The aging time was between 21 and 28 days. Characteristics of geopolymers were defined by measuring of compressive strength, density, N_2-physisorption, electrical conductivity, as well as by SEM analysis. The presence of amorphous phase as well as inorganic domains was documented by using X-ray diffraction (XRD) and Fourier transform infra-red spectroscopy (FTIR).

Keywords: geopolymers, red mud, modification of microstructure, electrical conductivity

I-2

SYNTHESIS OF GADOLINIA NAMOMETRIC POWDERS

Branko Matovic

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University of Belgrade, Belgrade, Serbia

Nanometric-sized Eu doped gadolinia (Gd_2O_3) powders were synthesized by solid-state displacement reaction at room temperature and low temperature calcination. The crystal structure properties have been carried out using X-ray diffraction, which revealed that the room temperature product was gadolinium hydroxide, $Gd(OH)_3$ that upon calcining transforms to cubic Gd_2O_3 phase at 600 °C converting to monoclinic Gd_2O_3 phase between 1400 and 1600 °C.

Thermal stability as well as microstructural development was studied by thermal analysis (DSC-TG) and by field emission scanning electron microscopy (FE-SEM). High-density (96% of theoretical density) ceramic material was obtained after pressureless sintering at 1600 °C for 4 h in air. The luminescence measurements were performed at room temperature on the spectrofluorometric system, utilizing 500 W xenon lamp as excitation source. It is found that Eu doped gadolinia emits a strong visible light, implying its potential application in the field of luminescence devices.

I-3

BACTERIA AS SELF-HEALING AGENT, AN ALTERNATIVE TO RECOVER CEMENT MATERIALS

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Many bacterial microorganisms are developing metabolic activities with the production of urease enzyme which leads to the precipitation of calcium carbonate. The production of the crystal polymorphs of calcium carbonate depends on growing environments and bacterial strains. Microbial urease catalyzes the hydrolysis of urea and produces carbonate and ammonium. The precipitation depends on type of microorganism, concentration of dissolved inorganic carbon, pH values, concentration of calcium ions and presence of nucleation sites.

The present study investigates the potential of two bacterial common strains to be used for the biological production of calcium carbonate based minerals. The strains were grown in solid and liquid medium containing urea and Ca^{+2} ions. The microorganism ability of inducing $CaCO_3$ precipitation was evidenced with alizarin coloration test. Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD) analyses, and scanning electron microscopy (SEM) were performed in order to confirm the presence of calcium carbonate in the precipitate. Experimental data present promising results and further studies will be performed to implement on a larger scale this eco-friendly biological treatment.

Acknowledgments: The researches were financially supported by project PN-II-PT-PCCA-2013-4-1709/085/2014 (BIO-THERM) and PN-II-PT-PCCA-2013-4-1808/223/2014 (AWARE).

I-4

ELECTRONIC STRUCTURE CALCULATIONS IN SOLID STATE CHEMISTRY

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Electronic structure calculations based on density functional theory are becoming more and more important. Theoretical studies are widely used to explain experimental findings, and possibly predict results. In this talk, an overview of various topics will be given.

One set of examples are transition metal compounds where magnetic properties are in the center of interest. Computed properties are such as exchange couplings, or band structures in comparison with photoemission experiments [1].

Infrared and Raman spectra can nowadays be simulated and are in very good agreement with experimental data. Moreover, simulation can be used to identify peaks with little intensity and which are thus difficult to find in the experiment [2]. Also, questions about the space group can be addressed, such as whether a structure is centro-symmetric or not [3].

Finally, structure prediction based on *ab initio* simulations and using a global search will be presented [4]. This allows to predict new structures from scratch without any knowledge of the crystal unit cell. The only input required is the number of atoms per formula unit. Results for various systems including phases at external pressure are shown.

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I-5

CARBON-BASED MATERIALS FOR ENERGY CONVERSION APPLICATION - FIRST PRINCIPLES INSIGHTS

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Carbon-based materials have been found in the focus of research community due to numerous applications. Among these, one of the most important fields is related to energy conversion. Here carbon materials of different dimensionality as well as carbon-based composites are extensively used as electrocatalysts, active materials for charge/metal ion storage or as catalysts supports and current collectors. For these reasons it is of uttermost importance to understand the function of carbon-based materials in energy conversion devices at atomic level. In the present contribution we shall provide a comprehensive overview of recent theoretical results on reactivity of carbon-based materials using graphene as a model system. We shall address general reactivity trends and possible tuning of reactivity by doping and defect engineering. The insights in the electrocatalytic and the charge storage mechanisms of functionalized graphene will be provided. Finally, we shall critically address possible replacement of noble metal-based materials in electrochemical power sources with carbon-based ones, taking into account performance and prices of novel carbonaceous materials of reduced dimensionality.

I-6

EFFECTS OF BORON AND ALUMINUM ADDITIVES ON MICROSTRUCTURE OF POROUS SIC CERAMICS WITH IN-SITU GRAIN GROWTH

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Silicon carbide (SiC) ceramics have been expected to be an attractive material for high-temperature structural applications such as aerospace industries, nuclear applications and high-temperature gas turbine. Furthermore, porous SiC has been commercially used as the material for diesel particulate filter. Recently, porous ceramics have received great attention in many fields. The authors have proposed the surface functionalization of porous ceramics based on in-situ grain growth. In our previous studies, it was reported that large plate-like grain growth in porous SiC ceramics was promoted above the sintering temperature of 2000 °C by addition of aluminum, boron and carbon to β-SiC, and porous SiC ceramics with unique morphology was achieved. In this study, porous SiC ceramics with in-situ grain growth were fabricated with the addition of boron and aluminum, and the effects of boron and aluminum additives on the microstructure of the porous SiC ceramics were investigated.

I-7

NOVEL PRODUCTION ROUTES FOR POROUS BORON NITRIDE NANOSTRUCTURES AND CARBON FOAM-ALUMINIUM FLUORIDE NANOCOMPOSITES

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In recent years, much attention has been drawn towards nanostructured, nanoporous and nanocomposite materials since improved properties are expected. However, in most cases, the available physical and/or chemical methods of producing these systems may be considered rather complicated, difficult to reproduce as well as time consuming. Herein, two novel and simple methods of producing nanoporous boron nitride (h-BN) and carbon foam-aluminium fluoride (C-AlF_3) composite materials are presented. In the first approach, high-purity (> 99 wt.%) h-BN platelets, with 0.9 to 2 μm particle width and 30 to 90 nm particle thickness, were synthesized using H_3BO_3 and $CO(NH_2)_2$ as precursors followed by consecutive thermal treatments under inert and oxidized atmospheres. The h-BN material exhibits a large Brunauer-Emmet-Teller (BET) specific area (~213 m^2/g) combined with a significant (micropore specific area occupies 2/3 of the total) and narrow (average pore size of ~0.85 nm) microporosity. In the second method, a C-AlF3 nanocomposite was produced via direct flame ignition and combustion of a fluoropolymer mixed with nano-sized Al powder. The C-AlF_3 material exhibits an open carbon foam-like network with embedded cubic-like AlF_3 particles in the range of 100 to 500 nm. Extensive characterization work is presented to describe features related to the morphology, nanostructure, elemental composition/surface chemistry and porosity of both type of materials, while potential applications are also briefly discussed.

I-8

SYNTHESIS, CHARACTERIZATION AND EVALUATION OF PHOTOCATALYTIC PROPERTIES OF NANO-ZIRCONIA

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Nanoparticles of monoclinic white-zirconia were produced through precursor route by pyrolysing zirconium tetra n-butoxide at different temperatures ranging from 900–1400 °C in atmospheric ambience. Oxygen-deficient surface-defective black-zirconia with appropriate combination of crystal structures were produced by controlling the heat-treatment conditions and atmosphere. The produced powders were comprehensively characterized by various spectro-chemical & surface characterization techniques. Photocatalysis experiments in visible light indicated color change exemplifying degradation of the methylene blue dye for powders produced under reducing atmosphere which can be attributed to the creation of oxygen vacancies and surface defects. The band gap decreases due to the creation of new energy states near valance band and conduction band towards Fermi energy level. Interestingly, the experiments have also provided some new insights to the role of carbon in the photocatalytic activity.

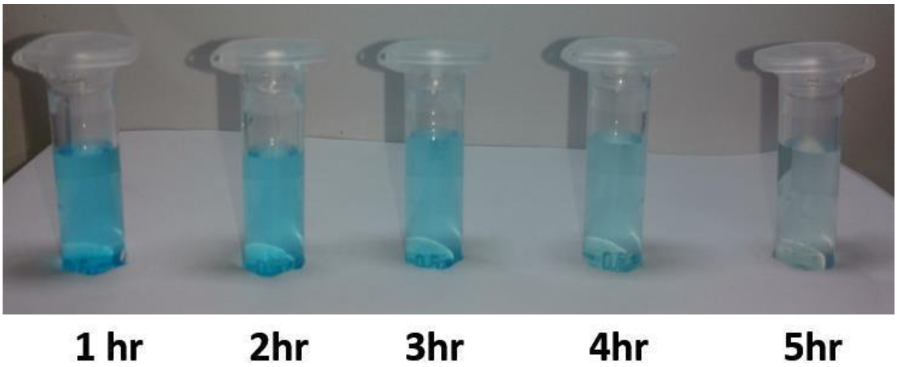

Figure 1. Degradation of methylene blue dye by nano-zirconia catalyst in visible light

I-9

LOW-TEMPERATURE SINTERING OF YAG:Ce FOR LASER PHOSPHOR PROJECTION

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One of the most frequently used strategies to generate white light is to combine highly efficient blue light emitting diode (LED) with yellow-emitting phosphor such as yttrium aluminum garnet (YAG) doped with Ce^{3+}. Therefore there is a constant effort to reduce the cost of blue-to-yellow conversion phosphors by reducing manufacture cost. Solid, transparent, YAG:Ce phosphor is normally fabricated by sintering powder compacts at ~1800 °C under vacuum in order to convert Ce^{4+} to Ce^{3+}. It was shown in this study that highly efficient YAG:Ce^{3+} phosphor can be made inexpensively by sintering at temperature below 1600 °C in air using simple muffle furnace. Photoluminescence of YAG:Ce^{3+} phosphor was improved by addition of small amount of SiC. Namely, SiC oxidizes during sintering crating SiO_2 and CO both of which increase the fraction of Ce^{3+} by reducing Ce^{4+} to Ce^{3+}. The effect of SiC amount on luminescence was studied. The role of SiO_2 and CO in reduction of Ce^{4+} to Ce^{3+} was discussed as well as the suitability of this simple and inexpensive technique for fabrication of phosphors for image projection. The solution to the lack of red component in whit light was also proposed.

I-10

FORMATION OF MULTIPHASE CERAMIC COMPOSITES BY REACTION OF NIOBIUM OR MOLYBDENUM WITH POLYSILAZANES

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Due to their extraordinary properties the interest in refractory metal based composites containing ultrahigh temperature stable carbide, nitride and silicide phases increased significantly in the last years. They are very interesting for structural components or matrix materials for high temperature (HT) or ultrahigh temperature (UHT) applications. Based on the high melting points of refractory metals itself as well as their carbides, nitrides and silicides processes like self-combustion high temperature synthesis (SHS), spark plasma sintering (SPS) or reactive hot pressing (RHP) are required to manufacture bulk composites. In comparison, polymer derived ceramics (PDC) technology is an alternative processing to simplify the manufacturing of ceramics at lower temperatures and to facilitate the shaping of complex geometries. During the transformation of the preceramic polymer into ceramics by pyrolysis the material shows an enhanced reactivity. The combination of preceramic polymers like polysilazanes with reactive refractory metals (e.g. Nb, Mo) should lead to UHT stable ceramic composites after pyrolysis composed of metal silicide, carbide and silicide phases. Additionally, this approach also allows for the processing of complex shaped geometries.

By using an organopolysilazane (OPSZ) and niobium powder as active filler with content variation from 40 to 70 vol% various, specially tailored multiphase Nb(C,N)/Nb_5Si_3 ceramic composites were designed after pyrolysis up to 1600 °C. X-ray analysis proved the formation of Nb_5Si_3, metastable Nb_5Si_4C and different Nb(C,N) phases depending on the starting OPSZ/Nb ratio and the pyrolysis conditions. After milling the resulting multiphase powders were densified by spark plasma sintering (SPS). The SPS approach led to highly dense samples at 1600 °C and an applied uniaxial pressure of 100 MPa. Furthermore, XRD measurements and EBSD analysis proofed that SPS is a feasible method to retain the original phase composition and grain size of the multiphase powders during sintering.

The use of molybdenum as active filler in combination with perhydropolysilazane (PHPS) led to the formation of Mo_5Si_3 particles within a Si_3N_4 matrix during pyrolysis at temperatures up to 1500 °C via solid-state reaction. To avoid pest oxidation of Mo_5Si_3 up to 700 °C in air the resulting ceramic composite was coated with PHPS to generate a protective SiO_2 layer before oxidation of Mo_5Si_3 starts. Oxidation experiments demonstrated the remarkably increased oxidation resistance up to 700 °C compared to the uncoated composite.

I-11

SUPPORTED CERAMIC MEMBRANES FOR ENERGY-RELATED GAS SEPARATION

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Ceramic membranes consist of a stand-alone or supported material with special transport properties, able to operate at elevated temperatures and pressure. Supported inorganic membranes hold the promise of highly effective separation and purification, and stable operation in harsh environments. However, compared to organic membranes, large-scale production of inorganic membranes requires improvements in reproducibility and cost processes.

This short presentation provides an overview on supported zeolite membranes being widely considered for gas separations. The supported zeolite Y membranes are fabricated by depositing a colloidal seed layer, followed by secondary growth. Membranes were made with two different secondary growth solutions: one without templating agent showing rapid growth, and the other with TMAOH template, showing slower growth. The separation characteristics of zeolite Y membranes for CO_2/N_2 separation were found to be extremely high with selectivities $\alpha_{CO_2,N_2} > 500$. Membranes had a thickness of 0.4…0.6 mm. The very high CO_2/N_2 selectivities in mixture separation are ascribed to sorption-induced size-exclusion at the window, possibly combined with diffusion correlation effects.

I-12

HYBRID ORGANIC-INORGANIC GEOPOLYMER FOAMS

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Porous materials are widely used in several applications including membranes, adsorption materials and catalysts. In the construction industry, porous materials find their application as insulating or soundproof panels or for structural lightweight components. Novel organic-inorganic geopolymer based foams have been obtained by reacting metakaolin and an aqueous alkalisilicate solution with mixtures of dialkylsiloxane oligomers or epoxy resins precursors. By using different amounts of Si^0 powder as in situ foaming agent, hybrid foams with densities ranging from 0.25 to 0.85 g/cm^3 have been successfully fabricated. Rheological behavior of the fresh mixtures has been evaluated, whereas the hardened specimens have been characterized by measuring thermal conductivity, fire resistance and mechanical strength. Further, microstructure of the specimens has been studied by optical and scanning electronic microscopy. The obtained foams are characterized by significant mechanical properties, good fire resistance and low thermal conductivity, lower than that of commonly used inorganic foamed materials with similar densities.

I-13

HIERARCHIC SELF-ASSEMBLY OF INORGANIC MESOCRYSTALS

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The growing need for renewable energy technologies has driven rapid development of novel hierarchic materials in the past few years. Most of these materials are produced by oriented-assembly of fully grown nanocrystal units into complex 3D superstructures that defy our conventional views on crystal growth by attachment of monomers. While diverse materials with promising properties have been synthesized with a great success, proper understanding of the driving force of this mesocrystal assembly has not evolved [1]. The main reason for this is lack of experimental evidence that would lead to a theoretical consensus on its nature.

Our study of mesocrystal assembly of rutile nanocrystals has given us a wealth of information to answer these questions. We report on first direct evidence of force fields that are active during oriented attachment of crystals, having a great potential to boost development of comprehensive theory on mesocrystal formation. We demonstrate that multilevel branched structures are in fact produced by self-assembly of primary rutile fibers on low-energy planes leading to lateral attachment and twinning. Attachment of nanocrystals is directed by an unidentified force field that transmits the crystallographic information and make self-replication possible. As precipitates are thermally agitated, their electromagnetic fields are coupled, and they are aligned parallel to their longer axis. Due to multiplicity of interactions particles are first attracted into a loosely associated state, however, as the distance between the fibers becomes shorter, by attraction, their crystallographic alignment along the lowest energy planes becomes dominant. Phase analysis of amorphous material enclosed in the pockets between imperfectly assembled rutile fibers showed harmonic ordering resembling that of the adjacent rutile structure. Through continuous condensation of ligands captured in the interparticle space the nanoparticles are fixed in accordance to their intrinsic electric field.

We present first experimental evidence that indicates a presence of electromagnettic force-fields conveying structural information through which oriented attachment of nanocrystals is possible. Main challenge of future studies will be resolving fundamental principles behind the mesocrystal assembly that would in effect provide key protocols for tailoring diverse crystalline architectures. The described mechanisms will open the prospects of exploiting electrostatic forces along with equilibrium crystal shapes to enforce self-sustained assembly of nanocrystals into desired crystalline architectures.

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I-14

LAYERED AND PARTICULATE SILICATE-POLYMER NANOCOMPOSITES FOR LIGHTWEIGHT HIGH STRENGTH APPLICATIONS

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The improvements of physical, chemical and thermomechanical properties of polymer composite materials has been a major research interest in the last few decades. Polymer nanocomposites represent a new class of materials alternative to conventional filled polymers. In this new class of material, nanosized inorganic filler (at least one dimension) are dispersed in polymer matrix offering tremendous improvement in performance properties of the polymer. Nanoscale materials have been the subject of research interest in recent years because of their unique properties as compared to the bulk counterparts and their potential applications in a wide variety of areas such as information storage, electronics, sensors, structural components, and catalysis etc.

The main challenge in fabrication of these polymer nanocomposites for structural applications is uniform dispersion of nanoparticles in the polymer matrix. However, good dispersion for nanoparticles in polymer composite materials is extremely difficult to achieve, since nanoparticles tend to aggregate together during fabrication. The degree with which the nanoparticles can be homogeneously dispersed in the polymer matrix would significantly influence the thermal, mechanical and optoelectronic properties of the material. It has used several techniques for dispersing nanoparticles. There is an ever-increasing demand for development of processing of polymer nanocomposites for advanced structural applications. In polymer composite fabrication, curing (polymerization) step is crucial and time-consuming process. This work is focused on polymeric matrix nanocomposites reinforced with organo-clays and particulate coal ash for lightweight and high strength applications devoted mainly for blast protection and mitigation of their effects

I-15

APLICATION OF METAL MATRIX COMPOSITE COATINGS IN THERMAL POWER PLANTS

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Erosive wear of coal-fired boilers components is recognized as the main cause of forced outages of power-generating plants. The erosive wear mechanism in boiler is almost entirely due to the presence of hard mineral matter in coals, since these materials that are present in the fly ash are harder than steels. The working environment in the gas duct of power plant boilers has sufficient oxygen content in a gas flow which together with fly ash contributes to combined erosion-corrosion process and exerts detrimental effects on the integrity of boiler tubing system. Over the years, considerable research efforts are being devoted towards finding a way to reduce or minimize these deleterious effects. There are several methods to protect boilers components from erosive wear due to solid particle impingement and one of them is by applying a protective coating. In this paper characterization of coatings applied on plain carbon and heat resistant steels were carried out. Coatings consists of carbides (tungsten and chromium carbide) in metall matrix are deposited by different techniques such as plasma transferred arc method (PTA), electric arc techniques and oxy-acetylene flame thermal spray process.

I-16

STRUCTURAL DESIGN OF OXIDE BASED FUNCTIONAL MATERIALS INSPIRED BY NATURE

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Nanostructured biominerals produced by living organisms are tailored by nature to fulfill their structural and functional requirements. They have attracted strong attention in material science during the past decades. In fact, their excellent mechanical performance, as reflected by a unique combination of high strength and fracture resistance, has inspired numerous researchers to transfer the underlying structural design to functional materials.

In this talk, I will summarize our recent contributions to the field of bioinspired material synthesis. Our major aim was to improve the mechanical properties of oxide- based functional materials by mimicking the structure of biomaterials. To this end, we have developed a novel synthesis approach to nanostructured composite films whose an alternating layer architecture combines a soft, organic component with a hard, inorganic material (e.g., TiO_2, ZnO) [1]. In addition, we have thoroughly investigated various types of paper-like materials with nacre-like architecture such as V_2O_5/GO, SnO_2/GO and $LiMnPO_4$/GO nanocomposites [2,3]. All these papers with thicknesses of a few micrometres have a well-ordered layer structure, are mechanically stable and after reduction of the graphene oxide (GO) also electrically conductive. Moreover, the investigation of their electrochemical properties has shown them to be promising candidates for energy storage and energy conversation applications. Complementary to the dense vanadia papers, we have very recently succeeded in assembling the V_2O_5 nanofibres into highly porous scaffolds by ice-templating of aqueous nanofibre suspensions. This synthetic material represents the first known successful attempt to mimic the structure of natural cuttlebone with its regularly stacked cavities and evenly distributed pillars, although at much smaller dimensions. Damping behavior of such scaffolds outperforms that of polyurethane foams.

Our results demonstrate that bioinspired structural design provides access to mechanically stable oxide-based materials whose other functional properties are well maintained or even improved. This renders such materials especially attractive for applications that require a long-term mechanical stability.

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I-17

STATE OF THE ART OF NEUTRON ACTIVATION ANALYSIS AT THE REACTOR IBR-2 OF FLNP JINR

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$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ (LSGM) based porous/dense structures were optimized for infiltration of different metal catalysts. Porous anodic substrates with an open porosity larger than 65% were fabricated by using LSGM commercial powders By using with two different types of porogens: micrometric carbon and polymethilmetacrilate (PMMA). The anodes were pre-sintered at 1250 °C for 2 hours to get enough mechanical strength to be used as substrates for spin-coating deposition of micrometric layers of electrolyte. Micrometric dense layers of LSGM of thickness ranging from 10 to 25 micron were obtained depositing various spun layers and then co-sintered at 1450 °C for 6 h. $La_{0.8}Sr_{0.2}Fe_{0.8}Co_{0.2}O_{3-\delta}$ was used as cathode and deposited by using a screen-printing oil and firing at 900 °C. A solution of metal (Ni, Co, Cu and their 1:1 mixtures) salts was used for infiltration, dried and heated at 350 °C for 30 min. Multiple infiltrations were necessary to get a metal catalyst amount of 25 wt.% that is the required value to get performing electrocatalytic performance. The reduction behavior of the different catalysts was examined by H_2-TPR techniques. Ex-situ catalyst activity measurement was used for the initial catalyst screening. The catalytic activity for CH_4 and CO_2 conversion followed the order Ni~Ni-Co>Co>Ni-Cu>>Co-Cu. The catalysts selectivity of different catalysts for the dry reforming reaction increased with temperature reaching a value of ~ 0.9, close to the thermodynamic value, both for Ni and Ni-Co catalysts. Stability tests were also performed on Ni and Ni-Co impregnated powders, both methane and carbon dioxide conversions were stable in Ni-Co without sign of conversion decrease, showing thus promising performance for the internal reforming of bio-gas in LSGM-based SOFCs.

The electrochemical measurements were performed on infiltrated cells with the same amount of Ni and Ni-Co in the temperature range between 650 and 750 °C. Measurements were performed both in H_2 and CH_4 and results compared. The maximum power density at 750 °C in 100 cm^3min^{-1} of H_2 was 813 mw/cm^2 and 446 mw/cm^2 in 60 cm^3min^{-1} of CH_4 and 40 cm^3min^{-1} of CO_2 for Ni infiltrated cell (electrolyte thickness 13–15 μm) confirming the results of the catalytic investigation on the corresponding infiltrated LSGM powders. The catalytic activity of Ni-Co infiltrated anodes show catalytic activity comparable to that of Ni infiltrated anodes. From the electrochemical impedance measurements at OCV and at 0.5 V of Ni and Ni-Co infiltrated cells, both ohmic and polarization resistances increase in time so a further investigation on the cell stability is in progress.

I-18

DEVELOPMENT OF SOLID ELECTROLYTE CERAMIC SENSORS FOR OXYGEN AND HYDROGEN MONITORING IN FAST REACTORS AND FUSION REACTORS

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The development of solid electrolyte oxygen sensor is one of the critical issues for the development of lead (Pb) and lead-bismuth (Pb-Bi) cooled fast reactors. The online monitoring of hydrogen isotopes (H, D and T) by proton conducting ceramic sensors is key technology for the development of liquid metal type breeder blanket systems of fusion reactors. The performance of the solid electrolyte sensors based on Y_2O_3 stabilized ZrO_2, CaO stabilized ZrO_2 and $CaZrO_3$-based ceramics has been studied.

The oxygen sensor based on YSZ with liquid reference (Bi_2O_3 doped Bi) for flowing Pb-Bi condition was developed. Figure 1a shows the schematic drawing of the sensor structure. The oxygen sensors were installed in the forced convection type Pb-Bi loop. The oxygen concentration in the flowing Pb-Bi was evaluated from the electro motive force and the Nernst equation. The stable output was obtained for 2000 hours continuously. The sensor with the reference material of Fe_3O_4/Fe mixed powders was developed, and the excellent performance with shorter response time was newly obtained.

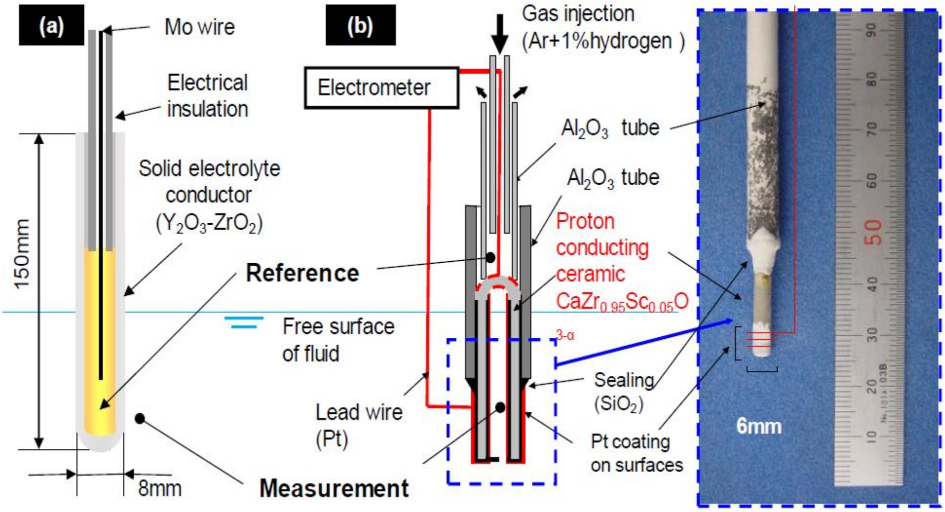

Figure 1. Schematic drawing of: a) oxygen sensor and b) hydrogen sensor

The hydrogen sensor based on $CaZrO_3$ was developed for the measurement of hydrogen isotopes in the liquid breeder blanket system of fusion reactors. The liquid breeders are liquid lithium (Li) metal, liquid Pb-17Li alloy and molten salts LiF-BeF_2 (Flibe) and LiF-NaF-KF (Flinak). These fluids are corrosive and reductive for the solid electrolyte ceramics. Then, the material and the structure of the sensors were improved especially for the application to the fusion reactors as shown in Fig. 1b. The thermodynamic stability of the sensor material is important in the corrosive condition. The solid electrolyte of Sc doped $CaZrO_3$ was used as the sensor material due to its excellent thermodynamic stability. The cap type structure of the sensor was designed to protect the sensor material from the corrosion by the direct contact with the melts. The membrane type electrode was also developed to protect the sensor material. The hydrogen concentration in the molten salt Flinak was successfully measured.

In the presentation, the technological development of the solid electrolyte sensors and the chemical characteristics of the high-temperature melts obtained by the sensors are reviewed, and the further challenges in the field of ceramics sensors and ceramics coatings for the development of the innovative nuclear reactors are introduced.

I-19

SYNTHESIS AND PROCESSING OF p-TYPE $Ca_3Co_4O_9$ CERAMICS FOR MICROSTRUCTURAL ENHANCEMENT OF THE THERMOELECTRIC CHARACTERISTICS

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The Peltier effect is already widely used in cooling devices made from classic thermoelectric (TE) alloys. The exploitation of another characteristic of TE materials, the Seebeck effect, nowadays represents one of the key technological challenges, as modules made from n- and p-type TE materials provide the only viable possibility for harvesting waste heat by its direct conversion into electricity. Waste heat represents almost 70% of all primary produced energy, and therefore its exploitation could be an important pillar of energy sustainability. The best TE materials, metallic alloys, already have the required thermoelectric characteristics, which are usually expressed by the figure of merit ZT, having ZT values close to 2. However, they are thermally unstable in air at temperatures above 300 °C and made from expensive and toxic elements. Their limitations bring forward the potential advantages of the oxide TE materials at higher temperatures. However, they could be realized only after a significant improvement to their TE characteristics, which are for polycrystalline ceramics much too low, with ZT values mostly well below 1.

In recent decades the n-type In_2O_3-doped ZnO ceramics and the p-type $Ca_3Co_4O_9$-based ceramics were shown to be promising thermoelectric materials. The $Ca_3Co_4O_9$ phase has a distinct plate-like morphology of the grains and is characterized by a complex misfit structure composed of CoO_2 layers with free charge carriers for the enhanced electrical conductivity along the ab planes, and Ca_2CoO_3 layers, weakly connected to each other, which enhances the phonon scattering along the c-axis for a reduced thermal conductivity. The morphological anisotropy of the grains with an anisotropy of the physical properties indicates that the microstructure can have a significant role in the enhancement of the TE characteristics of polycrystalline ceramics. The synthesis, processing and microstructure development, which markedly influence the structure, the microstructure and, consequently, the TE characteristics of TE ceramics will be presented and discussed. Microstructure optimization resulted in an increase of ZT from typically obtained values of about 0.1 to the highest ZT reported for the undoped $Ca_3Co_4O_9$ ceramics of 0.31 at 627 °C.

I-20

THE OVERVIEW OF BARIUM TITANATE PROPERTIES AND APPLICATION OPPORTUNITIES

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Barium titanate (BT) is a ferroelectric material with a perovskite structure important in the field of electronics. Due to high flexiblity of its crystal lattice it has the capabilty to host ions with different oxidation state and careful selection of dopants could enable tailoring of barium titanate structure and electrical properties.

Barium titanate doped with La, Sb, Sm, Nb and Mn will be presented in the light of structural changes and their influence on electrical properties modification. Doping with La, Sb and Sm in very low concentrations induces symmetry change from tatragonal to pseudo-cubic. La, Sb, Nb and Sm are proven to be grain growth inhibitors, with the different effect on obtained ceramics density. Dielectric permittivity value was significantly changed depending on dopant kind and concentration. Partial substitution of Ba or Ti ions by some of this dopants induced the movement of phase transition peaks to the lower temperatures and caused the formation of diffuse phase transition. In this way, the application of barium titanate can be widened from capacitors to PTCR sensors, gas and humidity sensors, etc.

In the recent years, there is a growing interest for multiferroic materials with barium titanate as a main component. When being mixed with ferrites in the multiferroic composites the electrical properties of barium titanate are being compromised. Dielectric permittivity starts to decrease in comparison with pure BT ferroelectric material. Using of doped barium titanate as a part of the multiferroic material could enhance the overall dielectric permittivity of barium titanate and therefore the dielectric properties of the multiferroic material. Mixing route was used for the preparation of $BaTiO_3$-$NiFe_2O_4$, $BaTiO_3$-$NiZnFe_2O_4$, Ba(Sb)TiO_3-$NiFe_2O_4$ composite materials. Magnetic and electrical properties of multiferroic materials have shown the dilution effect due to existence of both, ferroelectric and ferrite phases in the same material.

I-21

TAILORING THE CATHODE NANOSTRUCTURE TO ACHIEVE HIGH POWER OUTPUT FOR SOLID OXIDE FUEL CELLS OPERATING AT 600 °C

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Solid oxide fuel cells (SOFCs) are an efficient and environmental-friendly alternative to combustion engines for supplying power. However, their high operating temperatures and cost hampers their broad use and causes long-term stability problems. A step forward towards reducing the SOFC working temperature at 600 °C or below can be the use of high temperature proton conductor (HTPC) oxides as electrolytes, due to their lower activation energy for proton conduction (0.3–0.6 eV), with respect to oxygen-ion conducting electrolytes. Moreover, essential for the development of low temperature SOFCs is the role of the cathode material and its microstructure. This is due to the fact that since oxygen reduction reaction kinetics is sluggish due to thermally activated processes, polarization losses increase significantly with reducing the temperature.

We have recently made significant progresses in the development of chemically-stable HTPC electrolytes and cathode materials associated, by using Y-doped barium zirconate (BZY). However, the power output obtained were not satisfactory, showing the need of improving the catode/electrolyte interface. We report here that nanostructuring the cathode materials using inkjet impregnation, we were able to obtain large power output both using chemically stable proton conducting and oxygen-ion conducting electrolytes. In fact, outstanding results were obtained at 600 °C using $La_{0.8}Sr_{0.2}MnO_{3-\delta}$ (LSM), the standard cathode material for high-temperature SOFCs, which was supposed not to be used at low temperatures due to its low oxygen-ion diffusivity and conductivity at 600 °C. Reducing LSM particle size to the nanometer scale revealed the feasibility of using the chemically stable LSM even at 600 °C with large power outputs

I-22

CHARGED DEFECTS AND DOMAIN WALLS IN $Pb(Zr,Ti)O_3$ AND $BiFeO_3$ CERAMICS

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Configuration and dynamics of ferroelectric and ferroelastic domain walls are major contributors to the global dielectric, mechanical and piezoelectric properties of ferroelectric ceramics. Both can be controlled by engineering microstructure, grain boundaries and charged point defects; at the same time, presence of domain walls may affect distribution and character of charged point defects inside the grains. In addition, significant strain gradients may develop around domain walls that in turn also affect distribution of point defects. After a brief general overview of the problem, we discuss in this presentation recent results of macroscopic properties investigations, DFT calculations, and PFM and HRTEM studies of pure and doped $Pb(Zr,Ti)O_3$ (PZT) and $BiFeO_3$. We show evidence of strong interaction of point defects with domain walls and discuss how this interaction affects local and macroscopic properties of examined materials.

I-23

VORTEX PINNING AND CONNECTIVITY IN NOVEL SUPERCONDUCTORS

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Main results of extensive study [1] of the influence of magnetic nanoadditives (MN) on electromagnetic properties of high quality MgB_2/Fe wires are reported and compared with the effects of nanomagnetic nanoadditives (NN) in bulk MgB_2 as well as with impurity and irradiation effects in ceramic HT_c tapes. In order to shed more light on the efficacy of MN in enhancing vortex pinning (thus J_c, B_{irr}) in MgB_2 we studied 80 wires doped with different amounts and types of MNs. Both coated (carbon, silica or dextrin shell) and uncoated MN were used in order to asses the effects of co-doping and interparticle interaction. The effect of the shape of MN (sphere, rod) and the synthesis temperature were studied, too. The magnetic state of MNs, both as-prepared and inside the wire was deduced from magnetization studies. Transport and magnetic measurements were used in order to determine connectivity, characteristic fields (B_{irr}, B_{c2}) and J_c of all wires. In heavily MN doped wires the enhanced pair breaking and reduced connectivity overcome the benefit of enhanced vortex pinning at MNs and grain boundaries. This is similar to effect of impurities and irradiation in ceramic HT_c tapes. However, light doping ($\leq$ 3wt.%) enhances J_c and/or B_{irr} for almost all types of MN, and indicates contribution of magnetic pinning. In spite of low content of MNs the enhancement of J_c is comparable to that for best NN (e.g. SiC [2]). In both MN and NN doped MgB_2 clear matching effects in vortex pinning appear. These effects cause the maximum enhancement of B_{irr} at elevated temperatures, but some enhancement of B_{irr} persist to the lowest temperatures. Similar matching effects are also observed in irradiated HT_c tapes, but there enhancement of B_{irr} is limited to vicinity of matching field only [3]. The advantage of enhanced B_{irr} at all temperatures in doped MgB_2 wires is practicaly annulled by poor connectivity in porous in-situ prepared wires. Methods to reduce porosity in MgB_2 wires and HT_c tapes are proposed.

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I-24

HIGH CONDUCTIVITY OF ZnO CERAMICS AND ITS ENHANCED THERMOELECTRIC PROPERTIES

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ZnO is a promising thermoelectric materialfor high-temperature application, but the strong correlation betweenthe electrical and thermal transport properties limited the simultaneous optimization to achieve superior thermoelectric performance. In this work, defect engineering was proposed to solve this problem. The results revealed that increased solid solution of trivalent dopant, Al^{3+}, has been successfully achieved to increase the carrier concentration. Meanwhile, by depleting the native acceptor defects at grain boundaries, the Schottky barrier disappeared and led to a huge increase ofhall mobility. The increased carrier concentration and hall mobility gave rise toa maximum electric conductivity (σ_{310K}) of 1.9×10^{5} Sm^{-1}, showing a metallic-like behavior. Owing to the ultrahighσ, a maximum power factor (P_{980K}) of 8.2×10^{-4} $Wm^{-1}K^{-2}$ was obtained. Moreover, by introducing large amounts of lattice defects inthe grains, the lattice thermal conductivity was simultaneously lowered to compensate the increased electronic thermal conductivity that accompanied with the high electric conductivity. Therefore, the multiple-doped ZnO polycrystalline materials with defect engineering of both grains and grain boundaries successfully increased the electrical conductivity and decreased κ_L in a relatively independent way which provided a new and effective route to optimize the performance of ZnO-based thermoelectric materials.

I-25

IMPROVED PROPERTIES OF DOPED $BaCe_{0.9}Y_{0.1}O_{3-\delta}$ AS A PROTON CONDUCTING ELECTROLYTE FOR IT-SOFC

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The proton conductivity is an exclusive property of mixed oxides with perovskite structure and large unit cell volume, such as $BaCeO_3$ or $SrCeO_3$. Doping with aliovalent cations (Y^{3+}) that replace Ce^{4+} induces formation of point defects (oxygen vacancies), which in wet or hydrogen containing atmosphere produce proton defects highly mobile at elevated temperatures. $BaCe_{0.9}Y_{0.1}O_{3-\delta}$ (BCY) is one of the best proton conducting electrolyte at temperatures between 500 and 700 ºC, which allows its application in intermediate-temperature solid oxide fuel cells (IT-SOFC). Yet, one of the main drawbacks of this material is its instability in CO_2-rich atmospheres. Since BCY is basic in character, it normally reacts with CO_2 to form $BaCO_3$ and yttria doped ceria. Both products exhibit no proton conductivity, thus limiting application of BCY in IT-SOFCs where CO_2 appears as a product of electrochemical performance. However, the stability of BCY can be improved by doping with cations that may raise the acidic character of the material, such as Nb^{5+}, Ta^{5+} or In^{3+}. Introduction of Nb^{5+} and Ta^{5+} will reduce the amount of point defects and consequently decrease the proton conductivity. This relation has been known as trade-off effect. Nevertheless, if their molar concentration exceed no more than 5% it is possible to obtain functional electrolytes with satisfying stability and conductivity. On the other hand, trivalent In^{3+} can completely replace Y^{3+} since it can both serve as a point defect source and increase acidity of the crystal lattice. Accordingly, it can be introduced in much larger amounts than Nb^{5+} or Ta^{5+}.

In this study $BaCe_{0.9-x}Nb_xY_{0.1}O_{3-\delta}$ (where x = 0.01, 0.03 and 0.05) and $BaCe_{1-x}In_xO_{3-\delta}$ (where x = 0.15, 0.20 and 0.25) powders were synthesized by the method of autocombustion, while $BaCe_{0.9-x}Ta_xY_{0.1}O_{3-\delta}$ (where x = 0.01, 0.03 and 0.05) powders were prepared by the classical solid state route. Much higher specific surface areas were observed for the samples synthesized by the autocombustion method. In the case of the samples doped with Nb and Ta, the dense electrolytes were formed after sintering at 1550 ºC for 5 h in air. Temperature of 1300 °C was enough to complete sintering of the samples doped with In after 5 h in air, which was another advantage of In as a dopant. The conductivities determined by impedance measurements in temperature range of 550–700 °C in wet hydrogen showed a decreasing trend with increase of Nb and Ta content, while it was the opposite in the case of In. Interestingly, the total conductivity of $BaCe_{0.85}Nb_{0.05}Y_{0.1}O_{3-\delta}$, $BaCe_{0.85}Ta_{0.05}Y_{0.1}O_{3-\delta}$ and $BaCe_{0.75}In_{0.25}O_{3-\delta}$ reached around 5×10^{-3} S/cm in wet hydrogen atmosphere at 700 °C. After exposure in 100 % CO_2

atmosphere at 700 °C for 5 h, the samples were investigated by X-ray analysis. It was found that even 15 % In could completely supress degradation of the electrolyte, while the highest concentrations of Nb and Ta (5%) were necessary to secure sufficient stability in CO_2.

O-1

SYNTHESIS AND CHARACTERIZATION OF ZINC DOPED COBALT FERRITE NANOPARTICLES

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In the last two decades spinel ferrites nanoparticles have been one of the most versatile system due to their potential applications in a wide variety of fields such as data storage, catalysis, environment, and especially biomedicine. Among them, cobalt ferrite ($CoFe_2O_4$, CFO) is material with the large magnetocrystalline anisotropy and high magnetization; also it shows good chemical and thermal stability and good mechanical properties.

In the present work, a set of zinc doped CFO nanoparticles with different amounts of zinc ions ($Co_{1-x}Zn_xFe_2O_4$; x=0, 0.05, 0.1, 0.3 and 0.5) but with the same particles size, particles size distribution and capping agent were prepared by solvothermal synthesis method. The obtained samples were characterized by X-ray powder diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR) and superconducting quantum interference device (SQUID). The XRD patterns show the common Bragg peaks typical of a cubic spinel structure (PDF card 22-1086) for all the samples. No other phases are detected. TEM analysis confirms the presence of sphere-like particles with equal mean diameter for all the samples ($<D_{TEM}>$ = 5 nm). The FT-IR analysis confirms the presence of oleic acid on the surface of the nanoparticles and revealed that oleic acid forms covalent bidentate with metal ions on the particle surface. Preliminary magnetization measurements has been done on all the samples. Field dependence of magnetization recorded at low temperature 5 K show an hysteretic behavior with increase of coercive field with decrease of zinc content (Hc(CFO)=1.13 T; H_C(CoZn_x_0.3)=0.81 T).

Temperature dependence of magnetization, recorded by Zero Field Cooled and Field Cooled protocols, indicates that all the samples are superparamagnetic at room temperature. M_{ZFC} show a maximum for all the samples, with T_{max} decreasing with the increasing of Zn content.

O-2

DEPENDENCE OF LUMINESCENCE PROPERTIES OF Y_2MoO_6:Eu^{3+} ON TEMPERATURE

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Light emitting diodes (LEDs) are a widely used solid-state lighting source; they are used in display backlighting, medical services, general illumination and communications. For generating the white light, blue LED chips with red/green/blue/orange/yellow phosphors are used. Widely investigated are red phosphors that can transform the cold blue light to the warm white light. Red phosphors consist of activator doped with some rare earth elements at a proper position on the host lattice. One of the phosphors extensively studied is Y_2MoO_6 doped with Eu^{3+}. The advantage of Eu^{3+} as a dopant is that it shows narrow emission band at 590–630 nm with central emission band at around 611 nm when it is in non-centrosymmetric site; it also shows sharp excitation peak around 400 nm. The characteristic spectra are due to intraconfigurational 4f –4f transitions.

In this study we report an experimental investigation of the Eu^{3+} ion-doped Y_2MoO_6 powders prepared with the new method, by means of the self-propagating method and then annealed at different temperatures (600–1400 °C) for 4 h. The synthesized powders were examined by X-ray diffraction (XRD), scanning electron microscopy (SEM) and luminescence emission and excitation spectra. The XRD showed that all products are single phase and that at 600 °C they have very low crystallinity which is confirmed with the very broad emission band in PLE spectra. However, already at 800 °C, both XRD and emission spectra show ordering of the structure, and increase in luminescence intensity and the appearance of narrow emission lines. Increasing of annealing temperature leads to ordering of MoO_5 and YO_8:Eu^{3+} units and reducing the defects number. In the excitation spectrum broad absorption line at 324 nm to 425 nm is result of electron charge transfer (CT) from MoO_6^{6-} to Eu^{3+}.

O-3

INFLUENCE OF SYNTHESIS CONDITIONS ON MORPHOLOGICAL FEATURES OF SBA-15

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Mesoporous SBA-15 materials, of high specific surface area, (~700 $m^2\ g^{-1}$), were synthesized by using block copolymer Pluronic P123 as a template and tetraethoxysilane as a silica source. The obtained materials were characterized by X-ray diffraction, scanning electron microscopy (SEM), energy dispersive X-ray (EDS) analysis, and atomic force microscopy (AFM). It was found that small modifications of synthesis conditions influenced morphological features of the synthesized SBA-15 samples. The SEM analysis has shown that the SBA-15 synthesized at a lower temperature and a longer time of reaction (80 °C, 48 h) provided elongated rod-shaped grains about 1μm long. The other sample synthesized at a higher temperature and a shorter time of reaction (100 °C, 24 h) has rounded grains and grains of regular spherical shape with diameters up to 2 μm. The EDS analysis confirmed that the particles of both synthesized samples were of SiO_2 content. In addition, the AFM analysis has shown different surface morphologies of the materials synthesized under various conditions.

O-4

NANOSCALE-TO-BULK: SIZE-DEPENDENT CRYSTALLINITY OF CERAMIC OXIDES

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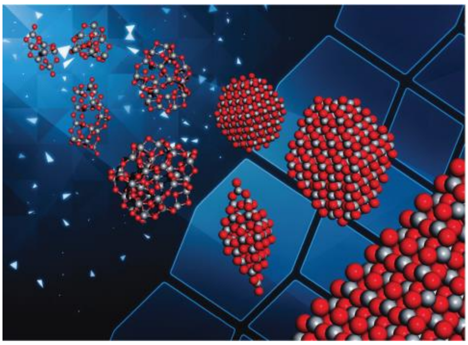
Naturally abundant and inherently a reactive electronegative element, oxygen chemically bonds with almost all other atoms to produce a corresponding oxide. Numerous ceramic oxide materials have had a massive technological impact in fields as diverse as catalysis, abrasives, absorbents, photovoltaics, and electronics. Key to this success is the wide range of chemical and physical properties exhibited

by oxide materials combined with their intrinsic stability. The properties of ceramic oxides can be enhanced and even augmented with new features by reducing their size down to the nanoscale. In purely length-scale terms, the nanoscale may be taken to be the size range between 1 and 100 nanometres. From a phenomenological perspective the start of the nanoscale is often the scale at which a material begins to display specific, non-bulk-like properties upon sample size reduction. Such nanomaterials, having at least one dimension intermediate between those of extended bulk-like systems and molecules, are attracting a great deal of attention due to their tremendous importance for emerging nanotechnologies.

Here, we present an overview of work in our group investigating when non-bulk-like ceramic oxide nanoclusters start to display properties (e.g. structure, band gap) more characteristic of the corresponding macroscopic material with increasing size. We approach this problem using oxide structures derived from both bottom-up global optimization and top-down bulk cuts and focus on the size-dependent onset of crystallinity. In this way we attempt to discern the nanoscale-to-bulk crossover size range for these important materials. We show examples from a range of systems including: silicon oxides (SiO_x), cerium oxides (Ce_xO_y), titania (TiO_2), zinc oxide (ZnO), magnesium oxide (MgO) to highlight the differences and similarities between the size dependent behaviour of various nanooxides [1-5].



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O-5

STRUCTURE PREDICTION OF ALUMINIUM NITRIDE MODIFICATIONS USING DATA MINING

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Aluminum nitride (AlN) is an interesting semiconductor ceramic material with high melting point, high thermal conductivity, high electrical resistivity and high thermal shock resistance. A wide range of AlN application makes it a good candidate for energy landscape exploration in more details. In order to find structure candidates for the AlN system we have performed data mining based explorations of the compounds with the general formula *AX* within the ICSD database. We have found 89 structure candidates and for each of them a local minimization on the *ab initio* level has been performed. We have used the first-principles method within the Hartree-Fock (HF), density-functional theory (DFT) and hybrid (B3LYP) approximation. The calculations were carried out with the *ab initio* program CRYSTAL14 using a linear combination of atomic orbitals (LCAO).

Furthermore, an in depth study of AlN at various pressures is presented, e.g. novel high pressure modifications and their respective transition routes have been predicted. In this way, we provide scientific answers to open questions on AlN behavior at extreme conditions of pressure and/or temperature, as well as new possibilities of technological applications of this very important semiconducting material.

O-6

THEORETICAL STUDY ON TITANOSILICATES MIXING: FROM NANOSCALE TO BULK

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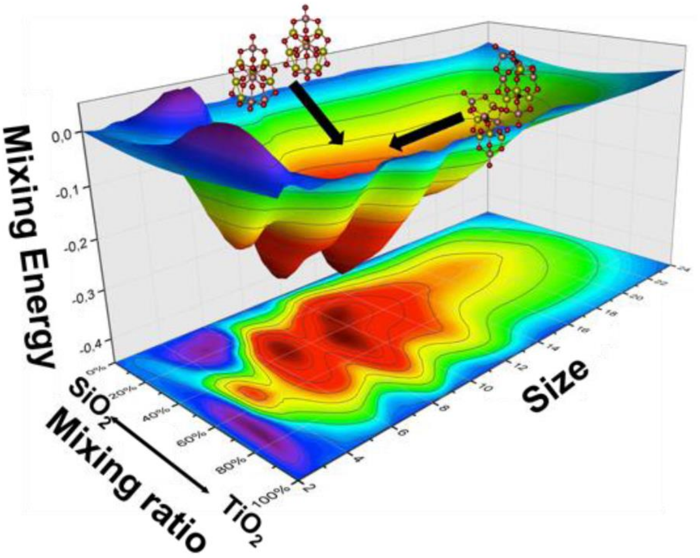
Materials based on mixing titania (TiO_2) and silica (SiO_2), titanosilicates, represent an important class of materials widely studied and used for many applications such as an industrial redox catalysts, solar cells, self cleaning systems, selective molecular sieves, materials for removing water pollutants and photocatalysts for many reactions.

Of a particular interest are ceramic frameworks of the $A_2TiSi_6O_{15}$ (A: K, Rb, Cs) type studied for potential applications in storing radioactive elements such as ^{137}Cs nuclear waste[1]. Another interesting application is the use of titanosilicate microcrystals immobilized on ceramic surfaces for buildings depollution materials by combining photo-catalytic properties of titanosilicates with high mechanical strength, with the thermal and chemical stability of the ceramic materials[2]. TS-1 (titanosilicate 1), maybe one of the most famous titanosilicate, patented in 1983, is an important industrial catalyst for oxidation of organic molecules[3]. The active site of this catalyst is a non-photoactive 4-coordinate Ti centre incorporated into a porous zeolite SiO_2 framework.

It is relatively difficult to synthesize homogeneous $Ti_xSi_{(1-x)}O_2$ mixed oxides material due to their tendency to self-aggregate and separate into two phases. So far, the homogeneous mixing in crystalline systems seems to be only possible by the inclusion a very small percentage of TiO_2 in a silica framework. Such bulk phase titanosilicates are metastable (energetically unstable but kinetically stable) with respect to the separate pure polymorphs (quartz and rutile). At the nanoscale, however, the mixing of these two materials is energetically favorable as we show in this work and our aim is to understand the main factors playing a role in this mixing favorability.

We first analyzed mixed $(TiO_2)_N(SiO_2)_M$ clusters and their relative stability with respect the pure (i.e. non-mixed) oxide clusters and then we calculated the associated mixing energy and how it depends on the system size (ranging from 2 to 24 N+M units) for different $(TiO_2)_N(SiO_2)_M$ mixing ratios. The Monte Carlo Basin-hopping global optimization algorithm was used in order to find reasonable low energy structures for each cluster type. A new interatomic potential has also been developed for our mixed systems to make the global optimizations computationally efficient. A selection of low energy isomers is subsequently refined at a DFT level of theory. Our results point to a number of important factors which determine how favorable the $(TiO_2)_N(SiO_2)_M$ mixing is. We hope to use these atomic scale insights to design new cluster-assembled titanosilicate materials, which, depending on the clusters employed, could be optimized for a range of applications.



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O-7

ENERGY LANDSCAPE INVESTIGATIONS OF COBALT MOLYBDATE AND CONNECTION TO THE EXPERIMENT

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Cobalt molybdate ($CoMoO_4$) is an important technological material used as catalysts in many chemical and petrochemical processes such as cracking, dehydrogenation, hydrogenation, and hydrodesulfurization (HDS), and especially important in mobile communication systems and high quality microwave dielectric ceramics. $CoMoO_4$ appears in three polymorphic modifications: α, β, and γ (HP). The α-$CoMoO_4$ modification crystallizes in the monoclinic space group *C2/m*, No.12, as well as β-$CoMoO_4$ phase but, clearly distinguished form α-phase by tetrahedral coordination of Mo^{6+} atoms. The γ-$CoMoO_4$ appears under high pressures (HP) and crystallizes in monoclinic space group *P2/c*, No.13, with $NiWO_4$ structure type.

The global search for structure candidates in the $CoMoO_4$ system was performed using a global optimization procedure, in order to identify local minima on the energy landscape of the system. The method consisted of many long simulated annealing runs with local stochastic quenches using empirical two-body potential. The local minimizations are included, in order to gain an overview over the range of possible metastable structures in the system. As a result we have obtained ten additional structure candidates, beside experimentally known phases of cobalt molybdate. In the next stage, these structures were locally optimized on *ab initio* level using DFT and hybrid functionals. Finally, our refined calculated structures were compared to the synthesized cobalt molybdate and results of XRD and DTA analysis.

O-8

V_2O_5 NANOFIBER SCAFFOLDS - A CONCEPT TO GENERATE DAMPING CERAMICS

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Ceramics stand out due to their thermal, chemical and mechanical stability, making them widely applicable in today's technologies. However, the hard and stiff nature of ceramics can easily lead to brittle fracturing when exposed to mechanical shock or vibrations, thus negatively affecting the lifetime of the ceramics' technical applications. A typical approach to enhance the fracture toughness is to combine the ceramic with a soft and ductile component, which serves as shock absorber. Even though the mechanical performance is improved in this way, the presence of a second component could shield the functionality of the ceramic, reducing their performance.

Here we report an alternative concept to generate a shock and vibration resistant functional all-ceramic material, using V_2O_5 as model system. This concept includes the synthesis of hydrated V_2O_5 nanofibers and their assembly into a filigree microstructure followed by a thermal post-treatment. The nanosized V_2O_5 building blocks exhibit a high aspect ratio, enabling the ceramic nanofibers' unusual mechanical flexibility. This flexibility is transferred to the macroscopic level by their filigree assembly. The assembly was achieved *via* ice-templating of aqueous nanofiber solutions, yielding highly porous (up to 99.8 %) scaffolds that mimic the structure of cuttlebone - a biomaterial, which unites high porosity with excellent mechanical stability. Subsequent annealing the scaffolds at 350 °C removes the residual water and preserves the identity of the nanofibers, likewise preserving the filigree microstructure. The resulting scaffolds feature a macroscopic elastic deformation of 3 %, which is exceptional among other all-ceramic materials. Moreover, this elasticity enables the investigation of the scaffolds' dynamic mechanical performance. Compression and frequency dependent damping tests revealed a high damping capacity with a loss factor $\tan\delta$ of up to 0.45, which outperforms conventional polyurethane foams ($\tan\delta \sim 0.14$).

This concept could be transferred to other fiber-shaped ceramic nanomaterials, allowing to generate various shock and vibration resistant functional materials.

1. A. Knöller, T. Runčevski, R.E. Dinnebier, J. Bill, Z. Burghard, *Sci. Rep.*, **7** (2017) 42951

O-9

M13 BACTERIOPHAGES AS VERSATILE BIO-TEMPLATES FOR FUNCTIONAL CERAMIC COMPOSITE MATERIALS

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Bio-templates are organic molecules, which have defined biochemical functionalities for the specific interaction with inorganic materials. Viruses like the filamentous M13 bacteriophage (phage) provide a uniform structure that can be used as template for the deposition of inorganic materials in order to generate nanostructured hybrid materials (e.g. nanowires). By genetical engineering, the protein surface can be modified to present specific peptide sequences controlling the organic/inorganic interface. The aim of this work was to create functional ceramic composite materials for applications like transparent electrodes, piezoelectric generators, semiconductors and battery systems. Based on the tailored organic/inorganic interfaces as well as structural mimicking of natural materials, mechanically resistant and multifunctional materials were created. Thereby model systems like nacre (shell of the red abalone) or sponge spicules (backbone of deep-sea sponges) well known for their outstanding mechanical performance served as structural inspiration.

O-10

NANOSIZED TITANIA PHOTOCATALYSTS OBTAINED BY SIMPLE CHEMICAL METHOD

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In this work we present sol-gel synthetic method designed to produce high surface area titania (TiO_2) particles for the photocatalytic degradation of waste water pollutants. Method involves usage of titanium(IV)-isopropoxide, polysaccharide chitosan, and thiourea or urea for N-doping purpose. Thorough characterization of the obtained powders was conducted using several instrumental techniques (FE-

SEM, XRD, BET and UV-VIS-NIR spectroscopy) which revealed the presence of sub-10 nm particles, and confirmed pure or predominant presence of anatase crystallographic phase, higher surface area than in commercial referent samples, and slightly enhanced absorption in the visible portion of the spectrum. The photocatalytic degradation of textile azo dye (Reactive Orange 16) under UV-enriched light source was investigated (230 mW cm^{-2}, 20 °C), showing very high adsorption capability of the powders, and superior photocatalytic behaviour compared to referent samples

O-11

ZnO NANORODS GROWN BY VAPOUR-LIQUID-SOLID METHOD

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ZnO nanorods were grown by vapour - liquid - solid method (VLS), on the silicon monocrystal substrate, of the (1 0 0) preferential orientation. A thin layer of gold, 5 – 10 nm thick was deposited on the silicon substrate. Deposition of ZnO was performed in the home made VLS deposition system, by heating ZnO powder up to temperature of 1350 °C degrees, while Ar was used as a carrier gas. The deposition process lasted for 2 hours. The samples were analyzed by scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). ZnO nanorods of the regular hexagonal structure were formed, up to 1μm in length, and ranging from 60 nm to 900 nm in diameter. The radius of the nanorods depends on a distance of substrate from the source material i.e. on the quantity and gradient of the evaporated material.

O-12

SPIDER SILK-AN EXTRAORDINARY CANDIDATE FOR SYNTHESIS OF NOVEL BIOPOLYMERS

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Spider silk (SS) has been well known by its extraordinary mechanical properties paired with biocompatibility and possibility of transformation into a various material forms. In this work SS was used as a template for synthesis of two novel biomaterials: SS-calcite composite and SS coated with europium doped ceria nanoparticles. SS-calcite composite was synthesized by simple method using biomineralization approach. The biomineralization process was observed during five days and it was found that two days of treatment were sufficient to obtain pure rhombic-shaped calcite crystals homogeneously dispersed trough 3D spider mesh. With increasing the incubation time, the number and size of crystals increased. SS coated with Eu doped nanoceria was easily obtained by time and cost effective precipitation synthesis procedure. The SS fibers were homogeneously coated with Eu doped CeO_2 nanoparticles with average nanoparticle size of 3 nm due to a great affinity of ceria to oxygen rich functional groups of SS proteins. Eu^{3+} was introduced as an activator ion in ceria crystal lattice and luminescent properties of the obtained composite were investigated by excitation spectra. These two novel composites were characterized with following methods: FESEM, XRD, FTIR, EDS, TEM and SAED.

O-13

RESEARCH POSSIBILITIES IN FRANK LABORATORY OF NEURTON PHYSICS AT JOINT INSTITUTE FOR NUCLEAR RESEARCH

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The high flux pulsed reactor IBR-2 in Frank Laboratory of Neutron Physics at Joint Institute for Nuclear Research (FLNP JINR) in Dubna, Russia is one of the most powerful neutron sources in Eastern Europe. From 2006 to 2010 the reactor and partly its spectrometers were modernized. The produced neutrons are now available for the world-wide scientific community for research purposes. The mean power of 2MW provides an average thermal neutron flux at the surface of the moderator of ~ 10^{13} n/cm^2/s and a maximum flux of ~ 10^{16} n/cm^2/s in burst.

A more detailed description of the parameters of the modernized IBR-2 reactor, current status and prospects for the development of its instrumentation, as well as the principles of the user program of the FLNP JINR and information for users are given.

O-14

ENHANCED LOCAL PIEZOELECRTIC RESPONSE IN Mn-DOPED $(K_{0.5}Na_{0.5})_{0.99}Sr_{0.01}NbO_3$ FILMS

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The interest for the lead-free materials rapidly increased after 2003, when the legislation against the use of lead-based piezoelectric materials in electronics had passed. Among the numerous lead-free materials, special attention was paid to some compositions of potassium sodium niobate solid solutions, $K_{0.5}Na_{0.5}NbO_3$ (KNN) obtained by a partial replacement of A- and B- site atoms from the perovskite KNN crystal lattice with dopants, which in the form of ceramic showed excellent piezoelectric and ferroelectric properties. Driven by the miniaturization and integration into sensors and energy harvesters, great efforts have been also made in processing of high quality KNN thin films.

In this contribution, the effects of the A-site doping of KNN films with Sr (KNN-xSr) on the microstructure and electrical properties were investigated for the first time. For that purpose, liquid precursors of $(K_{0.5}Na_{0.5})_{1-x}Sr_xNbO_3$ (KNN-xSr, x = 0, 0.005, 0.01) thin-films, were prepared from potassium and sodium acetates, niobium ethoxide and an appropriate amount of strontium nitrate in 2-methoxyethanol solvent with 5 mol% of potassium acetate excess. The approximately 250 nm thick KNN-xSr thin films on $Pt(111)/TiO_x/SiO_2/Si$ substrates were obtained through repeated spin-coating and pyrolysis steps, followed by the rapid thermal annealing at 650 °C.

All KNN films crystallized in pure perovskite structure with (100) preferential orientation, which became more pronounced in doped films, as confirmed by the Lotgering factor. The addition of 1 mole% Sr dopant, however, effectively reduced the leakage current density to $4.2 \cdot 10^{-8}$ A/cm^2 at the electric field of 100 kV/cm and contributed to the well-saturated ferroelectric hysteresis loop of the film. The major drawback of this film was in the low piezoelectric response (a few pm/V measured by piezoresponse force microscopy) and inability to switch ferroelectric polarization by electric field, which can be related to the defects, such as oxygen vacancies. To overcome the problem, an improved synthesis of the KNN-1Sr films with 1 mole% Mn was introduced. The reasons for decrease in the leakage current density and improvement of piezoelectric response will be discussed.

O-15

DESIGN OF DOPED BARIUM TITANATE THIN FILMS BASED VARACTOR AND GOLD ELECTRODES FOR MEASUREMENT OF TUNABLE PROPERTIES

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One of the main components in microwave tunable devices is variable capacitor, commonly known as varactor. Varactors can be used for fabrication of tunable phase shifter, delay lines, filters, etc. Ferroelectric materials in thin film form are recognized as good potential candidate for that purpose. Barium titanate based materials, where one part of Ba^{2+} and Ti^{4+} ions are replaced by Sr^{2+} and Zr^{4+}, have huge potential in this area. Involvement of strontium and zirconium in structure of barium titanate, have significant influence on ferroelectric behavior of material and approach to paraelectric state. Aim of this work was preparation of barium titanate based thin films and design of top electrodes in order to build required device architecture suitable for dielectric measurements at GHz frequencies. First step was preparation $Ba_{1-x}Sr_xTiO_3$ and $BaZr_xTi_{1-x}TiO_3$ (x = 0.1, 0.2, 0.3, 0.4) thin films by chemical solution deposition on platinized silicon substrates. Obtained thin films were thermal treated at temperatures up to 1000 °C. Influence of Sr^{2+} and Zr^{4+} concentration as well as sintering temperature on structure and functional properties of thin films were examined by XRD, Raman spectroscopy, dielectric measurement, etc. According to results, samples with structure closest to paraelectric state were selected for further investigation. Due the complicated setup for tunable measurement, electrodes with clearly defined dimensions and shapes were prepared by combination of different techniques such as sputtering, inkjet printing, laser, etc. This work represents challenges during the preparation samples for tunable measurements; from synthesis of materials to the electrode preparation in order to obtain representative architectures for future measurements.

O-16

SYNTHESIS AND CHARACTERISAZATION OF DOUBLE FERRITE NANOCOMPOSITES

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Co-precipitation and hydrothermal synthesis were used for preparation of different ferrite nanoparticles, such as nickel ferrite, zinc ferrite and iron oxides. Those oxides were combined in different manner in order to investigate the possibility to obtain the core/shell structure. The phase evolution, morphology, coercivity and magnetization of the nanocomposites were examined by X-ray diffraction, electron diffraction pattern, transmission electron microscope, and vibrating sample magnetometer. Spinel structure was confirmed by X-ray and Raman measurements. Magnetic measurements indicated on superparamagnetic to ferromagnetic behavior at room temperature of the prepared nanoparticles. Results suggest that the magnetic properties of one ferrite could be modified by coating it with another. Using of $ZnFe_2O_4$ as a shell with different thickness may be used to tune the magnetic parameters of ferrites based on nickel and iron for the desired application.

P-1

RADIOLOGICAL AND PHYSICOCHEMICAL PROPERTIES OF RED MUD BASED GEOPOLYMERS

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The aim of this work was the characterization of red mud as industrial waste generated by the Bayer process in the aluminum industry. Significant amount of generated by-product may cause environmental problems if appropriate treatment is not carried out. The chemical and mineralogical compositions and natural radioactivity of red mud and geopolymer (GP) were analyzed. The radiological hazard orginated from ^{238}U, ^{232}Th, ^{40}K in the samples was assesed throught the absorbet dose rate (*D*) and the annual effective dose rate (*E*), calculated in accordance with the UNSCEAR 2000 report. Physicochemical characterization of all samples was conducted using X-ray diffraction (XRD) and Fourier transform infra-red spectroscopy (FTIR). The presented research dealt with the possibility of application of red mud as a pigment or as raw material for use in the construction material industry. Obtained results are presented in this paper.

Keywords: geopolymer, natural radioactivity, red mud, raw materials.

P-2

SYNTHESIS, CHARACTERIZATION AND APPLICATION OF PURE AND DOPED CALCIUM PHOSPHATE MATERIALS

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To prepare pure and Mg, Sr and Na hydroxyapatite type materials (CaP, MgCaP and CaSrNaP) modified solution precipitation method was used. In order to achive a more soluble and cost effective synthesis modified method was consisted of nitrate substitution by acetate solution. The synthesized samples were calcinated firstly at 400 °C, and than densified at 1000 °C in air for 3 h. Obtained samples were characterized using X-ray diffraction (XRD), Fourier transform infrared (FTIR) and scanning electron microscopy (SEM-EDS) analysis. To investigate potential application of densified multi-doped CaP materials as solid electrolytes for intermediate temperature solid oxide fuel cells the complex impedance method was used. For $CaSrNaP_{1000}$ sample the highest conductivity was found at 700 °C (1.90×10^{-3} $\Omega^{-1}cm^{-1}$), for the corresponding activation energies of conductivity amounted to 0.31 eV in the temperature range 500–700 °C.

P-3

TRANSFORMATION OF Cs-LTA TYPE OF ZEOLITE TO POLLUCITE PHASE USING HOT PRESSING METHOD

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Cesium aluminosilicate phases are of the great interest as possible hosts for Cs immobilization in radioactive waste management. Cs-exchanged form of Na, Ca-LTA type of zeolite (Cs-LTA) was prepared by standard procedure of ion exchange. In order to obtain pollucite this Cs-LTA zeolite was pressurless sintered and hot pressed at certain temperatures. XRD analyses were used to study structural changes of Cs-LTA before and after thermal treatments. Pressurless sintered sample recrystallized into pollucite phase after heat treatment at 1000 °C (3 h) (PLS1000) and hot pressed sample at 750 °C (3 h) using pressure of 35 MPa (HP750), indicating reduced temperature of 250 degrees. HP750 has higher density than PLS1000 which leads to higher value of compressive strength. The HP750 showed better resistance to Cs leaching than the PLS1000. Obtained results of HP750 sample indicate that these ceramic forms, based on pollucite phase, are promising for the permanent immobilization of Cs radionuclides.

P-4

SYNTHESIS AND PHOTOCATALYTIC ACTIVITY OF N-DOPED TiO_2/CARBON COMPOSITES

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N-doped TiO_2/carbon composites (N-TiO_2/HTC) were synthesized by hydrothermal carbonization using glucose, titanium isopropoxide and melamine, as a carbon, titanium and nitrogen precursors, respectively. In order to achieve good photocatalytic activity, different material samples were obtained by varying the amount of melamine. Characterization of obtained composites was performed by thermogravimetric analysis, scanning electron microscopy, X-ray diffraction, UV-Vis diffuse reflectance spectroscopy and Fourier transform infrared spectroscopy. The photocatalytic activity of N-TiO_2/HTC composites was examined via photocatalytic degradation of methylene blue (MB) under UV and visible light, and compared to the photocatalytic activity of undoped TiO_2/HTC and commercial TiO_2. Variation of melamine amount, added in the precursor solution, induced slight structural and morphological changes in N-TiO_2/HTC composites. Although minor, these changes caused different adsorption and photocatalytic characteristics of obtained composites. It was found that the lowest addition of melamine raises the adsorption capacity of composite material. Also, the increase in melamine concentration in precursor solution increases the photocatalytic activity of N-doped composites under both, UV and visible irradiation.

P-5

THE INFLUENCE OF ALKALI ACTIVATION ON THE PROCESS OF POLYMERIZATION OF GEOPOLYMERS

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Geopolymers represent an innovative class of ceramic materials that are characterized by advanced technological features, such as low energy consumption of production for construction purposes. In this paper, the synthesis of inorganic polymer (geopolymer) using metakaolin as a precursor is presented. Metakaolin as aluminosilicate solid raw material is the dehydroxylation product of the industrial mineral kaolin in the temperature range 650–900 °C. The thermal dehydroxylation process of kaolin increases its solubility in alkaline media, making metakaolin an excellent raw material for production of inorganic polymers through the geopolymerization process. The kaolin used in this experiment is high quality clay obtained from Rudovci, Lazarevac, Serbia. Metakaolin (MK) was prepared by calcining kaolinite at 750 °C for 3 h. The alkaline solution was prepared from sodium silicate (volume ratio $Na_2SiO_3/NaOH = 1.6$) and NaOH (analytical grade) of different concentration (2, 4, 6, 8 M). The reference geopolymer (GP) was formed from metakaolin and the alkaline activator solution, which were mixed for 10 min and then left at room temperature for one day. Finally, the mixture was kept in a sample drying oven for 2 days at 60 °C. The influence of alkali activation, i.e. different concentration of NaOH as a component of alkali activator mixture on the process of geopolymerization of metakaolin is investigated. Also, process of aging time of geopolymer samples at 7th, 14th, 21st and 28th days is followed by some analytical methods (XRD, FTIR). The structure of metakaolin and metakaolin based geopolymers and their physicochemical properties were studied using X-ray diffraction (XRD), Fourier transformation infrared spectroscopy (FTIR), particle size distribution (PSD) and scanning electron microscopy (SEM).

Keywords: geopolymerization, metakaolin, alkali activator, aging time, XRD

P-6

FLEXIBLE V_2O_5-BASED SCROLLS – MIMICKING THE STRUCTURE OF THE SPONGE SPICULE

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By mimicking the structure of biomaterials, the mechanical performance of synthetic ceramics can be drastically improved. The sponge spicule is one intriguing example of highly flexible bio-ceramic rods, in particular under bending stress. This property is assured by its hierarchically organized structure in the form of cylindrically arranged lamellas, which are glued together by an organic matrix. Achieving such mechanical flexibility by mimicking the spicule's unique structure is challenging, as it requires the complex assembly of the nanostructured building blocks at multiple hierarchical levels.

In this scope, we have established a new fabrication approach, which allowed to closely mimic the 3D structure of the sponge spicule in the form of scrolls. It is based on precisely controlled removing of a micrometer thin film from a substrate by a razor blade, which is in contact with the substrate under a specifically determined angle. The model system was chosen to be a highly ordered V_2O_5 nanofiber-based thin film, which can be obtained *via* a facile self-assembly process [1]. Owing to its intrinsic mechanical flexibility, the thin films can be rolled-up into scrolls. Scanning electron microscopy (SEM) of the scrolls revealed an uniform cylindrical organized structure with a scale-like surface morphology. The diameter of such scrolls is in the micrometer range, while they are several millimeters in length. 3-point bending experiments were performed in order to determine the fracture strength and failure mechanisms under bending stress. It was observed that the scrolls exhibit a stepwise fracturing mechanism, comparable to that of sponge spicules, which resulted in an enhanced fracture resistance.

The novel way to fabricate such 3D spicule-like materials, starting from a 2D thin film, opens new pathways in the synthesis of bioinspired, nanostructured and multifunctional materials in the form of micrometer-sized rods.

1. Z. Burghard, A. Leineweber, P.A. van Aken, T. Dufaux, M. Burghard, J. Bill, *Adv. Mater.*, **25** (2013) 2468.

P-7

HIGH-PERFORMANCE rGO-SnO_2 FLEXIBLE ELECTRODES

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The fast evolution of nowadays technologies in the field of portable and bendable devices requires the development of novel storage systems for electrical energy. Flexible paper-like electrodes are considered as promising candidates for lithium-ion batteries (LIBs), as they unite high electrochemical storage capacity and mechanical stability. Conventionally, the inorganic storage material is mixed with binder and a conductive agent and then deposited onto a flexible substrate. However, this method reduces the overall capacity due to the significant amount of additives in the system. Furthermore, this fabrication procedure is very complex and time consuming, thus making it comparably expensive.

Here we propose an alternative route to fabricate free-standing flexible paper-like electrodes, which are absolutely binder-free. Our type of electrode is composed of high capacity SnO_2 nanoparticles embedded into a highly flexible and electrically conductive matrix made from reduced graphene oxide (rGO). In principle, its synthesis route involves three major steps: The synthesis of the precursor building blocks (SnO_x nanoparticles and graphene oxide (GO) nanosheets), their co-assembling into a hierarchically arranged microstructure and finally the thermal treatment. Along this line, a specific combination of process parameters is decisive to achieve the desired high capacity battery performance. It was found the optimum SnO_x to GO weight ratio to be 1 : 2, which results in uniformly distributed SnO_x nanoparticles between the GO nanosheets, maximizing the interfacial area between the both components. Subsequent annealing at 500 °C under argon atmosphere allows simultaneously reducing the GO and oxidizing the SnO_x to SnO_2 *via* a direct oxygen transfer between them. The redox reaction not only led to a drastic increase in the electrical conductivity of the rGO matrix, but also to a recrystallization of the SnO_2 nanoparticles directly onto the rGO sheets. This templating effect ensures a good connection between the different building blocks, enabling to reach capacity values of over 80% of the theoretical maximum at an increased charging rate.

These findings qualify this three-step synthesis route to be transferred to other electrochemically active systems, which require mechanical stability coupled with high storage capacity.

P-8

HYDROGEN STORAGE AND SELECTIVE GAS SEPARATION PERFORMANCE OF A NANOPOROUS CARBON CLOTH-LIKE MATERIAL

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Nanoporous carbon-based materials have attracted significant research focus over the last years towards physical adsorption, storage and selective separation of energy-dense gases and mixtures thereof due to their low densities, excellent thermochemical stability, large surface areas and pore volumes, as well as tunable pore sizes. However, these materials are usually produced as loose and fine powders, thus raising issues regarding their safe handling and processing, as well as creating major obstacles towards their practical implementation in commercial-scale systems for stationary and mobile applications. Herein, an oxygen-functionalized carbon material was produced in a flexible and non-fragile cloth-like form via carbonization and CO_2 activation of a low-cost cellulose-based polymeric fabric. The activated carbon cloth (ACC) exhibited a high specific area (~1200 m^2/g) and pore volume (~0.5 cm^3/g) combined with dominant (more than 98 % micropore surface area/volume) and narrow (average pore size of ~0.7 nm) ultra-micropore features. The ACC material was studied for a set of energy-related applications, including H_2 storage based on cryo-adsorption and separation of energy-dense CO_2/CH_4 mixtures using selective adsorption. Fully reversible H_2 uptake capacities in excess of 3.1 wt.% at 77 K and 72 bar were recorded along with a significant heat/enthalpy of adsorption value of up to 8.4 kJ/mol calculated for low surface coverage. By incorporating low-pressure adsorption data in the Ideal Adsorbed Solution Theory model, the ACC was predicted to selectively adsorb up to 5 times more CO_2 than CH_4 in ambient conditions, thus representing an appealing adsorbent for the purification of such gaseous mixtures. The enhanced performance in both cases seems to be attributed to the mean ultra-micropore size of the ACC material and not only to the available specific area and/or pore volume.

P-9

$BiFeO_3$ PEROVSKITES: THEORETICAL AND EXPERIMENTAL INVESTIGATIONS

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Bismuth ferrite ($BiFeO_3$) is one of the most studied multiferroic system. $BiFeO_3$ has been synthesized by controlled hydrothermal process, where the particles of small sizes and with high purity were obtained. Structural analysis showed that non-annealed powder can be perfectly fitted to rhombohedral space group *R3c* as α-$BiFeO_3$ phase. In addition, a structure prediction has been performed and 11 additional $BiFeO_3$ modifications have been proposed. In the next phase, an *ab initio* optimization of predicted structures has been performed and the structure of the γ-phase has been elucidated.

In addition, electronic and magnetic properties of $BiFeO_3$ were investigated using combination of experimental and theoretical methods. Theoretical studies were performed using a full potential linearized augmented plane-waves plus local orbital (FP(L)APW+lo) method, based on density functional theory (DFT). HRTEM analysis confirmed existence of twin stacking faults, which are responsible for enhanced magnetic properties. EPR measurements suggested existence of electrons trapped by vacancies or defects, while magnetic behavior of synthesized material was investigated by SQUID.

P-10

HYDROPHOBICITY CONTROL OF ALKALI ACTIVATED ALUMINO-SILICATE MATERIALS-GEOPOLYMERS

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Geopolymer technology is progressively overcoming the challenges associated to its commercialization with the increase of several practical applications. Permeability or waterproof property is a very important parameter for geopolymers as it indicates the degree of reaction and long-term durability. Protecting the surface of geopolymer is essential for improving its durability under certain exposure conditions. Contact angle measurement as reliable indicator of hydrophobicity was determined for synthesized geopolymers using water and ethylene - glycol as reference liquids. Geopolymers were synthesized from various precursors: kaolin, bentonite and diatomite and were subjected to a physicochemical characterization (X ray diffraction - XRD, Fourier transform infrared spectroscopy- FTIR and Scanning electron microscopy - SEM-EDS). All geopolymer matrix materials have shown different behavior during the characterization, which is a consequence of reaction route during synthesis process. FTIR analysis revealed alumino-silicate binding modes from precursor via meta-phase up to final geopolymer. Vibrational line shifts were observed for Al–O, Si–O and O–H groups during the polymerization for all three samples. Contact angle measurement revealed that the contact angle values for ethylene-glycol in some geopolymer samples are three times higher compared to water. These measurements have also confirmed that the geopolymers synthesized from kaolin are the most porous, which can be explained by the smallest Si/Al ratio.

Keywords: geopolymers, hydrophobicity/hydrophilicity, contact angle measurement, free surface energy

P-11

ELECTRONIC PROPERTIES INVESTIGATION OF $CaMnO_3$ DOPED WITH Gd USING THEORETICAL AND EXPERIMENTAL METHODS

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$CaMnO_3$-based ceramics doped with gadolinium has become a matter of great scientific interest, because of their physical, electronic and magnetic properties, and many intriguing phenomena, such as colossal magnetoresistance (CMR) involving potential applications in magnetic memory devices and sensors. Electronic properties of $CaMnO_3$ doped with different amount of gadolinium were investigated using combination of experimental and theoretical methods. Spectroscopic Ellipsometry has been used to study electronic properties and band gap variation as function of Gd doping (up to 20% Gd). Furthermore, for each of the structure candidates, a local optimization on the *ab initio* level using density-functional theory (DFT), hybrid (B3LYP) and the Hartree–Fock (HF) method was performed.

P-12

CHARACTERIZATION OF IRON IN THE HYDROTHERMAL DICKITE FROM JEDLINA ZDROJ (NOWA RUDA, LOWER SILESIA, POLAND)

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In recent years, considerable attention has been given to the genesis of dickite in sedimentary conditions. One way to obtain an objective evaluation of the nature of a

solution during the formation (precipitation) of hydrothermal dickite is to examine components that undoubtedly were introduced into its lattice by this solution. Such a component is, for certain, iron (Fe).

Characterization for Fe was made on a representative sample of dickite-rich hydrothermal clay from Jedlina Zdroj. The mineralogy of the sample is comparatively simple, dickite being the principal component (>95 wt.% of the total sample), with lesser amounts of goethite and barite. Geochemical fractionation and inductively coupled plasma-optical emission spectrometry indicated that most of the Fe (*ca*. 97 wt.% of the total metal) resides in the dickite. Electron spin resonance showed that some of the Fe in the dickite structure is in the form of Fe^{3+}. A substantial proportion of these ions (as well as Fe) in the dickite matrix were probably contained in the original hydrothermal dickite-forming solution. From the geochemistry of Fe^{3+}, it was deduced that the oxidation potential (*Eh*) and pH of the solution during the formation of dickite from the Jedlina Zdroj were approximately 0.45–0.95 V (highly oxygenated) and 0–4 (highly acidic), respectively.

P-13

NOVEL SYNTHESIS ROUTE FOR OBTAINING HIGHLY EFFICIENT Ag_3PO_4 PHOTOCATALYST NANOSPHERES

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Novel synthesis route based on nanoemulsion technique was applied for fast and simple synthesis of Ag_3PO_4 at room temperature. X-ray powder diffraction analysis and Raman spectroscopy reviled that synthesized powder was single-phase. Using scanning electron microscopy analysis, it was found that the synthesized Ag_3PO_4 particles were near-spherical shape with an average diameter of 50 nm. Specific surface area of obtained powder was measured by Brunauer-Emmet-Teller (BET) method. Finally, Ag_3PO_4 product was used as photocatalyst for the photodegradation of crystal violet in aqueous solution. The degradation results show complete degradation with short irradiation time. The recyclability and stability of the photocatalyst were also evaluated by cycle test experiments.

P-14

MOSSBAUER SPECTRA OF SOL-GEL IRON SUBSTITUTED MULLITE

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The oxidation state of the introduced iron cation, its position and concentration in mullite lattice was studied by Mossbauer spectroscopy supplemented by X-ray diffractometry and Rietveld refinements. The sol-gel amorphous powders were synthesized using ethanol-water solutions of TEOS, Al(III) nitrate, Fe(III) nitrate and urea, which composition correspond to Fe-doped 3 : 2 mullite ($3Al_2O_3{\cdot}2SiO_2$) powders. After heat treatment at 1300 and 1550 °C, the distribution of iron in the sample with 15 wt.% of Fe_2O_3 was examined. The iron quantity attains a saturation level for a content of Fe_2O_3 between 12 wt.% and 15 wt.% depending on the heating temperature. At 1550 °C, magnetite (Fe_3O_4) and hematite phase (Fe_2O_3) are identified besides mullite. Fe atoms are essentially in octahedral sites replacing Al^{3+} ion, which favors an increase of the *c* parameter of the orthorhombic cell as previously reported.

P-15

ZnO NANOPOWDERS OBTAINED BY THERMOLYSIS OF ZINC BENZENEDICARBOXYLATE COMPLEXES WITH 2,2'-DIPYRIDYLAMINE

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Coordination chemistry provides the know-how for the synthesis of the precursor compounds with variable composition and structures, while the thermal induced changes may control the crystalline structure, phase composition, morphology, size, texture, and other properties of their pyrolytic products [1]. In terms of coordination chemistry and thermal analysis, our research has been focused on the synthesis of mixed ligand complexes [2] that can be used as precursors for obtaining diverse (compositional and structural) oxides, depending on their thermoreactivity.

The main goal of this approach was the reduction of the temperature at which the oxides are formed (up to 600–700 °C) comparative to the standard ceramic methods. The effect of the different atmospheres (dynamic air or N_2) on the thermal decomposition of Zn benzenedicarboxylate complexes with 2,2'-dipyridylamine was investigated. The formation of ZnO nanopowders was identified using XRPD and FESEM techniques. The influence of the adopted architecture of ternary metal complexes used as templates for ZnO nanopowders was discussed. The thermal decomposition kinetics of precursors was studied under non-isothermal conditions. In addition, the antibacterial activity of obtained ZnO nanopowders was also analyzed.

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P-16

QUANTUM MECHANICAL INVESTIGATIONS OF ELECTRONIC PROPERTIES OF BARIUM SULFIDE UNDER EXTREME CONDITIONS

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Barium chalcogenides BaX (X = S, Se and Te) are currently under extensive research due to their potential technological applications in microelectronics, light-emitting diodes (LEDs), laser diodes (LDs), and magneto-optical devices. Barium sulfide (BaS) is an important precursor to other barium compounds with applications from ceramics and flame retardants to luminous paints and additives, and recent research shows potential technological applications in opto-electrical devices. In this study we have performed *ab inito* modeling of barium sulfide under pressure, using various quantum mechanical methods: Hartree-Fock approximation (HF), *Density Functional Theory* (DFT) with Local-Density Approximations (LDA) and Generalised Gradient Approximation (GGA), and hybrid (Becke, three-parameter, Lee-Yang-Parr, B3LYP) functional. We investigate the electronic properties of experimentally known structures, as well as novel predicted modifications of BaS, and our calculations were in very good agreement with previous experimental and theoretical observations, where such data were available.

P-17

STRUCTURE AND CHARACTERIZATION OF (x)$Ni_{0.7}Zn_{0.3}Fe_2O_4$ – (1-x)$BaTiO_3$ COMPOSITES

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Multiferroic composites with formula $Ni_{0.7}Zn_{0.3}Fe_2O_4$ - $BaTiO_3$ (x = 0.1, 0.3, 0.5, 0.7, 0.9) were prepared by mixing chemically obtained NZF and BT powders in the planetary mill for 24 h. $NiZnFe_2O_4$ (NZF) powder was prepared by auto-combustion method starting from nickel, zinc and iron nitrates. Barium titanate (BT) powder was prepared with the same method. The optimization of sintering process was performed. One series of powders were pressed and sintered at 1170 °C, while the others were sintered at 1120 °C. X-ray measurements confirmed the presence of NZF, BT phases and the traces of barium ferrite phase. The microstructures of the ceramics show (Fig. 1.) the formation of grains with different shape and size. The formation of polygonal (NZF grains), rounded (BT grains) and plate like grains (barium ferrite phase) was noticed. The magnetic analyses showed that in the composites due to existence of ferroelectric phase a dilution effect appears.

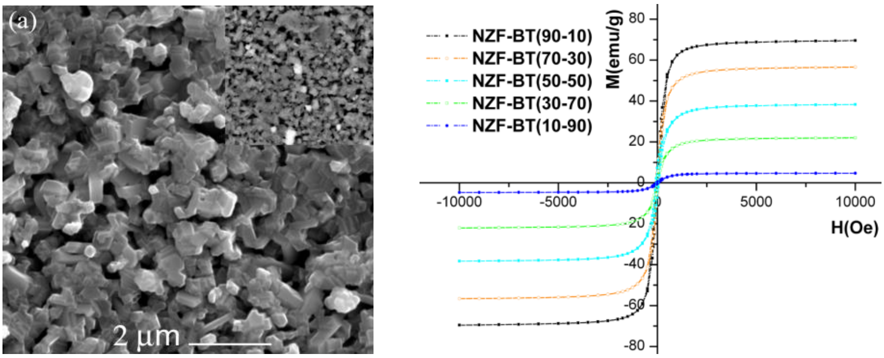

Figure 1. SEM images of NZF-BT (90-10) and magnetic measurements for all samples

P-18

THE INFLUENCE OF DREDGE WASTE AND EFFLUENT TREATMENT PLANTS SLUDGE ON THE PORTLAND CEMENT CLINKER MANUFACTURE

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Alternative materials such as industrial wastes and by-products can be easily and economically utilized as raw material in Portland cement clinker manufacture. These materials are generated in abundance as a result of growing worldwide industrialization. Two types of wastes from mining industry were used as secondary raw material in a concentration ranging from 1.4 to 3.5%. CEM I cements were obtained from these clinkers and compressive strength was determined. The chemical and mineralogical compositions of the wastes and raw meals were determined. The influence of homogeneous raw mixes containing different concentrations of wastes on all steps of burning in a laboratory furnace to form a Portland cement clinker was investigated. It was noticed in the case of mining wastes an improved burnability and no apparent deterioration in clinker quality.

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P-19

HIGHLY CONDUCTIVE V-DOPED δ-Bi_2O_3 WITH 3×3×3 SUPERSTRUCTURE

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Due to the increasing demands for new highly efficient and environmentally friendly energy conversion technologies, the oxide ion conductors applicable in solid oxide fuel cells (SOFCs) have widely been investigated. The high temperature

δ-Bi_2O_3 phase has been proposed as a good candidate for electrolyte in SOFCs because it is the fastest known ionic conductor.

In this study, the possibility to stabilize O^{2-} ion conductors related to the δ-Bi_2O_3 polymorph in $Bi_{12}V_xO_{18+5x/2}$ (x = 0.5–1) system was investigated. Six starting mixtures of α-Bi_2O_3 and V_2O_5 were dry homogenized in an agate mortar, heat treated at 1000 °C for 1 h and then slowly furnace cooled. The samples were characterized by XRD, TEM/SAED, optical microscopy, DTA and EIS techniques.

Based on XRD and TEM/SAED, if $x \geq 0.6$ the high-temperature reaction between α-Bi_2O_3 and V_2O_5 resulted in formation of microcrystalline single-phase specimens containing the phase based on δ-Bi_2O_3. The obtained phases showed main diffraction peaks corresponding to the cubic δ-Bi_2O_3 (space group *Fm*-3*m* and $a \approx 5.6$ Å). However, the detected weak reflections indicate that the true unit cell is the 3×3×3 supercell with $a \approx 16.6$ Å. An expected decrease of the unit cell parameters with the dopant amount was found as the consequence of smaller dopant ionic radius $\{r_i(V^{5+}) = 0.54$ Å and $r_i(Bi^{3+}) = 1.03$ Å in the six-coordinated environment [1]$\}$. In the case of $Bi_{12}V_{0.5}O_{19.25}$, traces of α-Bi_2O_3 were also found.

The XRD data of $Bi_{12}V_{0.7}O_{19.75}$ were used for the Rietveld refinement giving $Bi_{102}V_6O_{168}$ as the composition of the 3×3×3 supercell. The octahedrally coordinated V^{5+} ions fully occupy 4*a* Wyckoff position, *i.e.* the corners and face centers of cubic supercell, and partially occupy 32*f*. The Bi^{3+} ions are placed at the rest of 32*f* and at 24*e* and 48*h* with full occupation. At the 32*f* site, the cations are surrounded by five oxide ions making a square pyramid. At the 24*e* site, the Bi^{3+} ions with four oxide ions form a square pyramid with the cation at the apex. The coordination of Bi^{3+} at the 48*h* is square planar.

Cyclic DTA curves showed that the following 3×3×3 → γ-Bi_2O_3 → δ-Bi_2O_3 → Bi_2O_3(l) consecutive phase transitions occur on heating. On cooling, δ-Bi_2O_3 crystallizes from the melts and remains stable to about 530 °C. At this temperature, an order-disorder transition takes place, *i.e.* δ-Bi_2O_3 → 3×3×3.

The sintered disk-shaped pellets were characterized by EIS at temperatures between 760 and 820 °C. The sample with $x = 0.6$ demonstrates one of the highest known conductivity among the published O^{2-} ion conductors, *i.e.* 0.66 S cm^{-1} at 760 °C with the lowest activation energy of 0.21(1) eV.

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P-20

TUNGSTEN BASED SILICIDES: FROM QUANTUM MECHANICS TO ACTUAL SYNTHESIS

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Transition metal silicides attracted great attention due to its potential applications in integrated circuits based on silicon. W-Si system is one of the most important refractory metal–silicon systems due to their applications in integrated circuits.

W-Si phase diagram has been calculated and individual phases have been investigated using the first-principles calculations within the Hartree-Fock (HF), density-functional theory (DFT) and hybrid (B3LYP) approximations. The calculations were carried out with the CRYSTAL14 program based on linear combination of atomic orbitals (LCAO).

Two different phases of tungsten silicides - tungsten disilicide (WSi_2) and pentatungsten trisilicide (W_5Si_3) were synthesized by simple thermal treatment at 1450 °C for 4 h in an argon atmosphere. These optimal synthesis conditions were obtained by preceded variation of temperatures and times of heating. The variations of these parameters enabled us to observe phase evolution of tungsten silicides determined by the XRD analysis.

P-21

CORRELATION BETWEEN STRUCTURE AND ELECTRICAL CHARACTERISTICS IN SAMARIUM DOPED BARIUM TITANATE SYSTEMS

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Conventional solid-state method was used to prepare powders of barium titanate (BT) doped with different concentration of Sm. Influence of Sm addition on the structure modification, grain growth inhibition and microstructure development was studied. Dielectric properties of doped samples were significantly modified. With doping, a diffuse kind of ferro-para phase transition was induced, phase transition positions were moved and dielectric permittivity values were lowered. On the other hand, Sm doping affected the decrease of dielectric losses. The impedance complex plane plots showed a one single semicircular arc, indicating grain contribution as a main effect on the total conduction of the doped materials. On the other hand, different electro-active regions in the modulus plane plots were distinguish. The comparison between impedance and modulus scaling behavior presented the localized movement of charge carriers. P-E hysteresis loops have shown the dilution of ferroelectric properties with Sm doping.

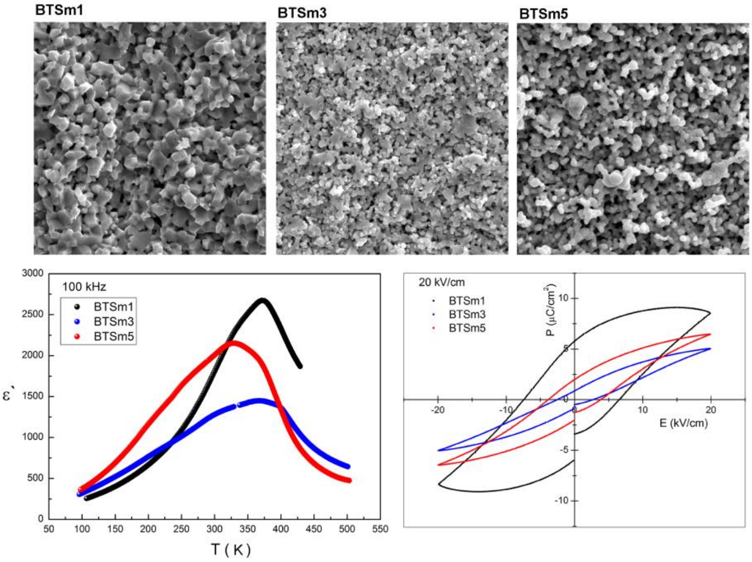

Figure 1. SEM, dielectric and ferroelectric properties of Sm doped barium titanate ceramics

P-22

INCREASE OF THE BREAKDOWN FIELD IN $BiFeO_3$ NANOPOWDERS WITH Ho DOPING

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$Bi_{1-x}Ho_xFeO_3$ (x = 0, 0.05, 0.07, 0.10, 0.12, and 0.15) nanopowders were synthesized by sol-gel method. The structural, vibrational, ferroelectric and dielectric properties of $Bi_{1-x}Ho_xFeO_3$ samples at room temperature were examined by X–ray diffraction (XRD), Raman spectroscopy, ferroelectric and dielectric measurements. Higher content of Ho dopant (x = 0.10, 0.12, and 0.15) induced partial phase transformation from rhombohedral to orthorhombic phase, confirmed from XRD and Raman spectroscopy, where the content of orthorhombic phase is about 69% in 15% Ho-doped sample.

The appearance of orthorhombic phase substantially influences the electrical properties of $Bi_{1-x}Ho_xFeO_3$ nanopowders. We have found that only 15% Ho-doped sample withstands strong applied fields (up to 100 kV/cm) at lower frequencies without breakdown. Analyzing the frequency dependence of permittivity, applying UDR and Cole-Cole models, we obtained that dc conductivity significantly decreases with higher Ho content, reaching the lowest value for 15% Ho doped sample. The dielectric loss values were reduced and low for 12% and 15 % doped samples. These results imply that the appearance of orthorhombic structure suppresses the conductive properties of $BiFeO_3$ nanopowders.

P-23

PZT-NICKEL FERRITE AND PZT-COBALT FERRITE COMPARATIVE STUDY: STRUCTURE, DIELECTRIC, FERROELECTRIC AND MAGNETIC PROPERTIES OF COMPOSITE CERAMICS

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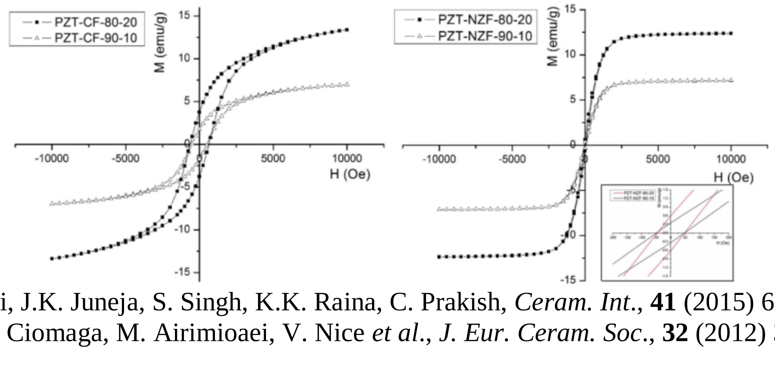
Multiferroic (MF) materials with simultaneous magnetic and electric long range order and occasionally, mutual magnetoelectric (ME) coupling, have recently attracted considerable interest. These compounds present opportunities for potential applications in information storage, the emerging field of spintronics, sensors, and multistate memory devices [1]. The ME phenomenon is observed in both single-phase as well as composite materials. The challenge in preparing such materials is to find equilibrium ferroelectric and magnetic structures preserving both properties close to the room temperature [2].

The individual phases ($Ni_{0.7}Zn_{0.3}Fe_2O_4$, $CoFe_2O_4$ and $PbZr_{0.52}Ti_{0.48}O_3$) were prepared by citrate-nitrate combustion reaction method. Composites were prepared by mixing and homogenizing PZT and NZF/CF powders in a planetary ball mill in the ratio: (x) PZT + (1-x) CF/NZF (x = 0.8 and 0.9). XRD diagrams of a sintered composite confirm the presence of only two phases, ferroelectric PZT phase and ferrite phase. SEM analysis revealed a uniform grain arrangement of both phases. Similar values of saturation magnetization (Ms) for both types of composites were observed. Ms increases with increasing magnetic phase, as it was expected. Significantly higher values of coercive field (H_C) can be seen in the composite with a cobalt-ferrite, which belongs to the group of hard ferrite unlike NZF which is soft ferrite and characterized by low values of coercive field. The ferroelectric properties of all ceramic composites were also studied.



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P-24

MECHANICAL AND COUPLED MECHANICAL-ULTRASONIC ACTIVATION OF HIGH BREAKDOWN FIELD ZnO VARISTORS

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Increasing of varistors breakdown field value is desirable for applications in current technologies. Using the nanoprecursors with the lowest possible degree of agglomeration and their activation pretreatments are usual ways for obtaining high breakdown field varistors with small grain size. Basic varistor mixture was prepared by the addition of previously synthesized Co/Mn-doped ZnO into the solution of bismuth and antimony salts, $Bi(NO_3)_3 \cdot 5H_2O$ and $Sb(CH_3COO)_3$. The suspension was evaporated and obtained powder was calcined at 530 °C. The final varistor powder consisted of Co/Mn-doped ZnO, Bi_2O_3 and Sb_2O_3 in the 70 : 25 : 5 mass ratio. The powder mixture was dry milled and the mechanically activated powder, named ZBS_{slnM}, was pressed into pellets and sintered at 770, 800 and 850 °C. The effects of mechanical activation manifested by very small average grain size in the range of 0.47–0.58 μm and consequently by very high breakdown field values in the range from 3400 to 6400 V mm^{-1}. The main disadvantage of the applied activation process was high agglomeration of precursor powder mixture, which reflected on current-voltage characteristics with two non-linear regions. In order to decrease agglomeration, wet milling with ammonium carbonate water solution as dispersing agent was applied on the basic powder mixture and the obtained wet milled powder was named ZBS_{slnMAK}. The powder was pressed into pellets and sintered at the same temperatures as ZBS_{slnM}. Powder subjected to wet milling was more activated for sintering that resulted in increased average grain size (0.60–0.90 μm) and decreased breakdown field values (2500–2050 V mm^{-1}). Also, lower agglomeration degree of ZBS_{slnMAK} powder partially helped to reduce anomalous voltage-current characteristics. Final step for decreasing agglomeration and increasing breakdown field values was ultrasonic activation in ethanol of the ZBS_{slnMAK} powder with subsequent addition of ammonium carbonate in 0–10 mass % during the activation process. Varistors prepared from these powders, named $ZBS_{slnMAK0}$ to $ZBS_{slnMAK10}$, were sintered at 850 °C. The optimal amount of added ammonium carbonate was 4 mass %. Varistor $ZBS_{slnMAK4}$ had uniform microstructure, density of 94 %, very small average grain size of only 0.45 μm and excellent electrical characteristics: extremely high breakdown field of 3420 V mm^{-1}, nonlinear coefficients of 28 and 51, and acceptable low leakage current of 40 μA cm^{-2}.

P-25

COMPARISION OF ANALYTICAL AND NUMERICAL RESULTS OF ALUMINA CERAMIC MATERIALS BEHAVIOR UNDER THE BRAZILIAN DISK TEST

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Alumina ceramics are widely used materials in the engineering ceramics where low density, high temperature properties and high hardness are required, but alumina disadvantages are brittleness, low thermal shock resistance and low fracture toughness. This is an ideal material to test the accordance of the numerical simulation results of the crack initiation and growth to the obtained experimental results. The samples are cylinder of dimensions 30×9 mm and they were subjected to Brazilian test method in order to obtain tensile strength and elastic modulus. The finite element model was developed to calculate the stress distribution using the approximation directed by the experimental setup. ABAQUS is a finite element program which was used for solving the numerical model. The results of obtained calculated fracture surface were compared to the observed surface of the real specimen and this was used to evaluate the quality of mathematical modeling.

Keywords: ceramics, mechanical properties, Brazilian test, numerical modeling

P-26

IMPLEMENTATION OF IMAGE ANALYSIS ON COMPARISON OF CAVITATION EROSION DEGRADATION OF MULITE AND CIRCON SAMPLES BASED

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Mulilte and zircon are widely used for different applications for refractory materials. In this paper their behavior in conditions of the cavitation erosion was investigated. Cavitation erosion testing was applied using standard the ultrasonic vibratory cavitation set up with stationary specimen. Weight loss as well as image analysis were used for comparison of the different samples to the effects of cavitation. In this paper image analysis was implemented for monitoring degradation level during testing, as well as number of formed pits during testing, and their characterization (average diameter and area). Obtained results were discussed in order to compare and analyze resistance of the different materials (mullite and zircon) to the cavitation erosion, as well as used methodology.

Keywords: mullite, zircon, cavitation erosion, image analysis, level of degradation

P-27

PHOTODEGRADATION OF ORGANIC DYE USING $BiFeO_3$ PARTICLES SYNTHESIZED BY ULTRASOUND ROUTE

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$BiFeO_3$ precursor powder was synthesized by ultrasound asissted sol–gel route at relatively low temperature, starting from Bi-nitrate, Fe-nitrate, and ethylene glycol. Structural, optical, and photocatalytic properties of the obtained powder were investigated. X-ray diffraction analysis confirmed that thermal treatment of precursor powder at 500 °C led to formation of pure phase $BiFeO_3$. The determined band gap was 2.20 eV, indicating its potential application as visible-light-response photocatalyst. The powder is used for photocatalytic degradation of typical organic azo dye Mordant Blue 9 in concentration of 50 mg/l. Measurements were performed for different times of irradiation and *p*H of the dye solution. Changes in UV-Vis absorption spectra revealed the decolorization and decomposition of organic dye during the photodegradation process. Photodegradation products were analyzied by HPLC technique, and mechanism of photocatalytic degradation of organic dye was proposed.

P-28

THE EFFECT OF GADOLINIUM SUBSTITUTION ON THE STRUCTURAL, FERROELECTRIC AND MAGNETIC PROPERTIES OF BISMUTH FERRITE CERAMICS

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$Bi_{1-x}Gd_xFeO_3$ (x = 0.01; 0.05; 0.075; 0.09; 0.10; 0.20; 0.30) powders were synthesized by hydro-evaporation method. The optimization of sintering conditions indicated that temperature of 870 °C and time of 2 hours (after pressing at 9 t/cm^2) provided the densest ceramics samples (up to 88 % of theoretical density) and the lowest amount of secondary phases (≤ 5.5 wt.%). The increase of gadolinium content resulted in polar-to-nonpolar ($R3c \rightarrow Pnma$) structural phase transition at about x = 0.10, which was reflected on deterioration of ferroelectric property. Structural analysis indicated decrease of unit cell volume with the increase of x, but the (Bi,Gd)–Fe distance did not exhibit regularity in change. The bismuth ferrite ceramics samples doped with x = 0.075 and x = 0.09 of gadolinium showed the greatest lattice distortion along the [111] axis. These samples also exhibited larger values of remnant electric polarization and less leakage processes than the pure bismuth ferrite ceramics samples. Magnetic behavior of $Bi_{1-x}Gd_xFeO_3$ samples revealed that the weak ferromagnetic moment strengthened with increase of the gadolinium content.

P-29

INFLUENCE OF DOPING ION VALENCE AND SIZE ON PROPERTIES OF $BiFeO_3$ MATERIALS

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Bismuth ferrite ($BiFeO_3$) is one of the most promising single multiferroic materials, and for sure the most studied one. It expresses specific magnetic and electric properties well above the room temperature. However, the nature of its properties is still arguable. In this study, an attempt to reveal some of the peculiarities of $BiFeO_3$ by introducing metal ions of various valences and sizes in the places of Bi^{3+} and Fe^{3+} ions. Powders with 5 mol% of doping metals were synthesized by auto-combustion method using glycine as a fuel. The powders and ceramic samples prepared from them were characterized. At this level, doping ions make significant change in structure, phase composition, rate of the solid state reaction, microstructure, conductivity, electrical polarization and magnetization. Potential mechanisms of their influence on different properties are discussed.

P-30

MICROSTRUCTURE OF SOME CLINKERS THROUGH THEIR FRACTAL DIMENSION

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Multivariate Analysis on a complex database has been performed, aiming to reveal correlations *composition-processing conditions-microstructure*. Database was made of cement clinker chemical analysis, information extracted from image analysis of clinker micrographs and process parameters recorded on the clinkering plant were the clinkers were obtained. Clinkers were burned in different conditions in industrial environments (19 clinkers) and in laboratory (7 clinkers). Image analysis of each clinker has been made by computing *Shape Parameters, Fractal*

Dimension and a parameter derived from *Shannon Entropy*, called the *Uniformity Degree*. Analysis has been made with a heuristic approach in mind. The procedure given here can be used on any material, on optical microscopy or SEM images, with very few adjustments.

P-31

ELECTROCHEMICAL BEHAVIOUR OF SERPENTINITE AND FORSTERITE IN FERRI/FERRO CYANIDE BENCHMARK REDOX SYSTEM

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Serpentinite rock collected near Kopaonik Mountain in Serbia is considered as a multiphase assemblage mostly consisting of mineral lizardite. Forsterite has been obtained by chemical-thermal treatment of grounded sample of serpentinite. Electrochemical features of these two materials were investigated by using modified carbon paste electrode (CPE) which included mixing analytes, graphite powder and parafin oil as a binder and packing the mixture in a Teflon holder. Morphological and structural characteristics of the samples were analyzed by SEM and XRD techniques which revealed presence of certain crystal phases and agregates of irregular shapes sized from 10 to 40 µm. Cyclic voltammetry was employed to study their electrochemical characteristics. The peak current height and peak-to-peak separation showed that the electrochemical reaction is quasi-reversible. Kinetic parameters were derived from Tafel analysis. Calculated kinetic parameters indicated prominent electrocatalytic effect of the minerals for ferri/ferro cyanide redox reaction in aqueous solution

P-32

B-SITE DOPING AS A STRATEGY FOR TAILORING $BiFeO_3$ PROPERTIES

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Ferroelectric, magnetic and structural properties of $BiFe_{1-x}Nb_xO_3$ (x = 0.002, 0.005 and 0.01) ceramics were investigated in order to study the influence of B-site doping of multiferroic $BiFeO_3$. It is known that pure $BiFeO_3$ exhibits G-type of antiferromagnetism below Néel temperature (T_N = 370 °C) and spontaneous polarization along one of the eight pseudo-cubic [111] axes below Curie temperature (T_C = 826–845 °C). However, poor ferroelectric (high electrical conductivity) and weak ferromagnetism of pure $BiFeO_3$ can be enhanced by doping. In this study, Nb^{5+} was introduced to replace Fe^{3+} (B-site doping) since it could disturb the nearly antiparallel spin ordering of the adjacent Fe^{3+} ions responsible for cycloidal (spiral) spin structure. On the other hand, the pentivalent Nb cations will reduce the amount of oxygen vacancies and consequently reduce the electrical conductivity. It was shown that 1 % Nb drastically changed the magnetic properties compared with pure $BiFeO_3$: while the remnant magnetization at 300 K reaches only 0.0042 emu/g at applied magnetic fields up to 50 000 Oe, the coercive magnetic field as high as ~7460 Oe classifies $BiFe_{0.99}Nb_{0.01}O_3$ as hard magnetic material. With lower Nb content the magnetic properties moved up towards the properties of pure $BiFeO_3$. Relatively inferior ferroelectric properties showed the sample with 0.2 % Nb, since its hysteresis loops deformed at electrical fields higher than 40 kV/cm. At the highest applied electrical field (70 kV/cm) only the sample with 1 % Nb showed a stable ferroelectric response with hysteresis periods up to 1000 ms, with the highest remnant electrical polarization of 0.5 $\mu C/cm^2$ and the coercive electrical field of 22.2 kV/cm. Thus, it was shown that by carefully selected dopant it was possible to improve both magnetic and ferroelectric properties of $BiFeO_3$.

P-33

DFT SCREENING OF DOPANTS TRIGGERING THE FORMATION OF BASAL-PLANE INVERSION BOUNDARIES IN ZnO

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The central task of this study was to construct possible structural variants of atomic models of head-to-head inversion boundaries (IBs) in zinc oxide (ZnO) and investigate their stability by density functional theory (DFT) computations. We constructed models for diverse metal oxide dopants that have been reported in the literature. These include Sb_2O_3, SnO_2, Fe_2O_3 and In_2O_3. Using different crystallographic operations on wurtzite ZnO structure, such as, translation and polarity inversion, we prepared 6 different IB models with either octahedral or trigonal prismatic interstice at IB plane containing the dopant. Basically, 3 different types of head-to-head IB with octahedral coordination of cations at IB-plane are obtained: (i) IB with αβαβ|α|γβγβ stacking of cation sublattice, as observed with Sb doping, (ii) IB with αβαβ|α|γαγα, as observed with In, Fe, and Sn doping, and (iii) IB with αβαβ|γ|αβαβ, that has not yet been observed experimentally. In addition, we will also include dopants with known IB structure Mn_2O_3, TiO_2 and SiO_2 for which IB structure has not yet been determined. For each dopant all structural variants will be considered by the first principles studies, summing up to 42 structural IB models to be optimized. IB models were generated by CrystalMaker software in such a manner that IB-plane is placed at the centre of the super-cell along it’s A-axis that is parallel with the ZnO polar c-axis. IB stacking and polarity inversion disrupts the lattice periodicity along the super-cell A-axis direction, whereas the structure remains periodic along the B- and C-axes. We’ve considered two strategies for solving the problem of A-axis non-periodicity. In the first strategy we considered the slab system, where only 2D periodicity is taken into account, whereas in the second we made an attempt to handle 3D periodicity by adding hydrogen atoms to the super-cell terminations along the non-periodic A-axis to compensate for the artificial tail-to-tail inversion. In both case charge neutrality and lattice continuity has been considered. First principles methods within the frame of density-functional theory (DFT) will be used for ab-initio calculations of static properties and screening of dopants. To test the relaxation span due to the presence of dopants and inversion we prepared super-cells with increasing widths along the A-axis, containing from 3 to 19 Zn–O layers on both sides of the IB. We are expecting that after certain number of layers stabilization energy will not change significantly, which will serve as a reference width for super-cells for DFT computations. Initial calculations will be performed first to determine the stability of the systems, after which the full scale computations will be performed.

P-34

STRUCTURES OF TRIMETALLIC $Ag_lAu_mPt_n$ (l+m+n=13, 19, 33 and 38) CLUSTERS

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Using the basin-hopping method, an exhaustive global search of the potential energy surface of trimetallic Ag-Au-Pt clusters was performed through multiple explorations for sampling a broad region of the PES. The Gupta potential is utilized to model the interatomic interactions of the ternary configurations. A menagerie of geometries is found, which are catalogued into structural families according to geometrical considerations. Structural families contain a fixed number of Pt atoms while the Ag and Au atoms loading varies accordingly to keep constant the cluster sizes. Optimal structures stability trend is observed thus obtaining the optimal composition for each cluster size. Chemical ordering shows a size-dependent behavior and a structural phase transition from mixed to segregated structures is unambiguosly manifested at 38-atom cluster sizes.

P-35

ENHANCEMENT OF THERMOELECTRIC PROPERTIES INDUCED BY Cu SUBSTITUTION IN $NaCo_2O_4$

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In this work polycrystalline samples of $NaCo_{2-x}Cu_xO_4$ (x = 0, 0.01, 0.03, 0.05) were obtained from the powder precursors synthesized in two different ways: 1) by a mechanochemically assisted solid-state reaction method (MASSR) and 2) a citric acid complex method (CAC). Ceramic samples were prepared by pressing into disc-shaped pellets and subsequently sintered at 880 °C in inert argon atmosphere. The electrical resistivity (ρ), the thermal conductivity (κ) and the Seebeck coefficient (S) were measured simultaneously in the temperature range from 330 K to 830 K, and the effect of small concentrations of the dopant and syntheses procedures on the thermoelectric properties was observed. According to the temperature dependence of ρ, all MASSR samples showed metal-insulator transition. The values of κ were lower for undoped samples in both syntheses. S increased with temperature and it was higher in all Cu doped samples, reaching 145 μV/K at 830 K for the sample with 3 mol% of Cu prepared by the CAC method. High thermopower is the consequence of the strong electron correlation, present in this type of compounds. The CAC samples showed higher ZT compared with the MASSR samples of the same composition. The highest figure of merit ($ZT = 0.056$) was obtained for the sample with 5 mol% of Cu prepared by the CAC method, and it was 1.5 times higher than the highest value obtained for the MASSR sample (ZT (NCO3-MASSR) = 0.036). This result confirmed that, beside the dopant concentration, synthesis procedure considerably affected the thermoelectric properties of $NaCo_2O_4$.

P-36

SINTERING BEHAVIOR AND MECHANICAL PROPERTIES OF SINTERED CATISIO$_5$ (SPHENE)

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Sphene based ceramics ($CaTiSiO_5$), apart from being considered as a host material for radioactive nuclear waste, the material also finds use in the field of biomedical engineering. XRD and DTA analysis provides phase identifications during thermal treatment. Mechanical stability of sphene (hardness, Young's modulus and fracture toughness) were determined from indentation experiments. The microstructure revealed the presence of densely packed grains in the sintered body. $CaTiSiO_5$ possess good thermal expansion coefficient, high hardness and lower elastic modulus and with these characteristic can be candidate for biomedical applications.

P-37

PHOTOELECTROCHEMICAL WATER SPLITTING POTENTIAL OF $ZnFe_2O_4$ THICK FILMS

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Starting hematite (Fe_2O_3) and zinc oxide (ZnO) nanopowders were homogenized in the in a planetary ball mill in stainless steel bowls with stainless steel balls for 15 min and calcined in air at 900 °C for 2 h to form zinc ferrite, $ZnFe_2O_4$. Thick film paste was made by mixing the homogenized starting oxide powder mixture with ethyl cellulose as a binder, α- terpinol as a dispersant and the combination of acetic acid and distilled water as adhesion agents. The paste was screen-printed on conductive FTO substrate and in several layers to change the

thickness of film. Photoanodes coated with $ZnFe_2O_4$ paste were gradually heated to prevent cracks and to avoid degradation of FTO. Structural, morphological and optical studies have been carried out using X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM) and UV-VIS spectroscopy. The photo-electrochemical behavior of $ZnFe_2O_4$ screen printed thick films was examined under UV light illumination in 1 M NaOH electrolyte.

P-38

PHOTOELECTROCHEMICAL WATER SPLITTING BEHAVIOR OF NANOSTRUCTURED Fe_2TiO_5 THICK FILMS PREPARED BY A SOLID STATE REACTION

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Starting hematite (Fe_2O_3) and anatase (TiO_2) nanopowders were homogenized in the 55:45 wt.% in a planetary ball mill in stainless steel bowls with stainless steel balls for 15 min and calcined in air at 900 °C for 2 h to form pseudobrookite, Fe_2TiO_5. Thick film paste was made by mixing the homogenized starting oxide powder mixture with a ethyl cellulose as a binder, α- terpinol as a dispersant and the combination of acetic acid and distilled water as adhesion agents. A layer of paste was screen-printed on conductive FTO substrate and repeated for several times to change the thickness of film. The photoanodes coated with Fe_2TiO_5 pastes were gradually heated to prevent cracks and to avoid degradation of FTO. Structural, morphological and optical studies have been carried out using X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM) and UV-VIS spectroscopy. The photo-electrochemical behavior of Fe_2TiO_5 screen printed thick films was examined under UV light illumination in 1 M NaOH electrolyte

P-39

INFLUENCE OF ALUMINA NANOPARTICLES AS REINFORCEMENT ON MECHANICAL PROPERTIES OF ACRYLOID COPOLYMERS

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Copolymer materials of acryloide type are often used in processes of conservation and restoration of sculptures and archaeological artefacts, as they have proven to give good results in conservation practice. However, acryloids by themselves do not have enough strength to satisfy more demanding conservation interventions. For such cases, alumina nanoparticles reinforced composite materials with acryloid polymer matrix ware made. Usage of iron modified alumina nanoparticles as reinforcement significantly influences mechanical properties of composite materials with polymer matrix. The reinforcement was used in three different ratios of 5%, 10% and 15%. Obtained composite materials were tested using micro Vickers method for determining micro hardness. The results showed significant improvement of micro hardness of 7, 8.2 and 9.3 times comapred to polymer matrix without any filler, for reinforcement ratios of 5%, 10% and 15%, respectively.

P-40

STRUCTURAL, ELECTRICAL AND MAGNETIC PROPERTIES OF MECHANICALLY ACTIVATED MANGANESE AND ZINC FERRITE

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Starting hematite (Fe_2O_3), zinc oxide (ZnO) and manganese carbonate ($MnCO_3$) powders were homogenized in a planetary ball mill in stainless steel bowls with stainless steel balls for 15 min, calcined in air at 1000 °C for 2 h, milled in a planetary ball mill for 30 minutes, followed by 4 h in an aghate mill, sieved through a 325 mesh to form four starting powders: $MnFe_2O_4$, $ZnFe_2O_4$, $Mn_{0.5}Zn_{0.5}Fe_2O_4$ and a two-phase mixture of zinc and manganese ferrite. Structural properties of the obtained powders were analyzed using XRD, SEM and EDS. Electrical properties of disk shaped samples were measured at room temperature on an impedance analyzer in the frequency range 100 to 40 MHz, enabling determination and comparison of dielectric permittivity and complex impedance. Complex relative permeability of toroid shaped samples was measured on an impedance analyzer in the frequency range from 1 MHz to 500 MHz.

P-41

INFLUENCE OF Cu-Zn SUBSTITUTION ON MAGNETIC BEHAVIOUR OF MULTIFERROIC CuO

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Magnetic behaviour of $Cu_{(1-x)}Zn_xO$, x=0, 0.0125, 0.025, was investigated in order to study the influence of substitution of Cu with Zn on magnetic properties. Copper(II) oxide attracted attention of the scientific community because it exhibits ferroelectricity driven by magnetic order at temperature as high as 230 K [1]. It was shown that disorder in the form of impurities can stabilize the ferroelectric phase [2]. In pure CuO the multiferroic phase is present above the first order phase transition at T_{N1} = 213 K and exists up to the subsequent first order phase transition T_{N2} = 230 K [1,2]. Pyroelectric measurements showed that the multiferroic temperature window widen with doping [2].

Motivated with this, we performed syntheses of undoped and Zn-doped CuO powders by pyrolytical method. Precursors $Cu(CH_3COO)_2 \cdot H_2O$, $NaHCO_3$ and $Zn(CH_3COO)_2 \cdot 2H_2O$ were homogenized in agate mortar and the mixtures were subjected to thermal treatment on 180 °C during 2 h and 200 °C during 16 h. XRD analysis showed that the rinsed and dried powders were single-phase CuO. Obtained powders consisted of very small sized nanocrystalline particles in the range of 10–15 nm, that was confirmed by TEM analysis.

Measurements of magnetization of the pelleted samples were performed using the MPMS SQUID magnetometer in the sweep temperature mode in order to collect the changes of magnetization very densely. With careful analysis we observed the two phase transition temperatures in accordance with previous results, even though the samples are not the monocrystals, but are in the ceramic polycrystalline form. From the magnetic measurements we confirmed that the Cu-Zn substitution successfully influences the temperatures of the phase transitions and enlarges the temperature window between those transitions. Therefore, doping can enhance multiferroic properties of CuO what makes it very interesting for future investigations [3].

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MATERIALS AND CONCEPT OF PLASMA SPRAYING

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In order to extend service life of equipment and machine parts, or to increase resistance of mechanical parts exposed to severe conditions, different coatings are applied. There are numerous options in the process of providing a coating to mechanical components in order to protect them. Being versatile, and providing for an array of different materials makes plasma spraying a very popular process, although it is not the best choice for others. Materials in the form of powder commonly used in the process are oxides (TiO_2, ZrO_2, $ZrSiO_4$, Cr_2O_3, Y_2O_3, their mixtures, etc.), carbides, borides, nitrides and cermets (WC–Co and Cr_3C_2–NiCr is the most widely applied one). In the process of plasma spraying, plasma is generated within the plasma torch via an electric arc. Depending on the material being coated or substrates and their different properties, a large number of different process parameters can be adapted to suit the specific need. The plasma spraying process can be implemented as: 1) atmospheric plasma spraying, where the plasma jet exits the torch into the atmospheric environment; 2) controlled atmosphere plasma spraying, where the jet is exiting into a chamber providing the controlled atmosphere (Ar); 3) low pressure plasma spraying or vacuum plasma spraying, where the jet is exiting the torch into a low pressure chamber at vacuum conditions; 4) plasma spraying physical vapor deposition as hybrid process.

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DISTRIBUTION OF ACTIVATION ENERGY COUNTERPARTS DURING ISOTHERMAL THERMO-ANALYTICAL MEASUREMENTS OF MECHANICALLY ACTIVATED INDIUM TIN OXIDE (ITO) POWDERS

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Isothermal decomposition process of chemically transformed indium tin oxide (ITO) powders into indium (III) hydroxide powders was investigated. Only

mechanically activated powders were studied. Specific “model-fitting” and the isoconversional (“model-free”) kinetic methods, together with DAEM (distributed activation energy model) approach have been applied in order to determine the real kinetic triplet for the process under investigation. The DAEM has shown that decomposition process of mechanically activated sample can be described with first-order kinetic model, with a single symmetrical density distribution function of activation energy counterparts (the pseudo Voigt type 1 density distribution). It was established that the obtained low values of the pre-exponential factors (*A*) indicate a predominantly surface reactions. Results presented in this work, can contribute towards about testing the thermal stability and kinetics of decomposition of mechanically treated powders which are applicable within transparent conducting oxide (TCO) area. Indium tin oxide (ITO) used as TCO sputtering targets actually belong to ceramic suppliers to the equipment sector.

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AN ASSESSMENT OF GROSS ALPHA AND BETA ACTIVITY IN KAOLIN

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Materials used in industry usually contain naturally occurring radioactive materials (NORM) at different activity concentrations. The natural radioactivity concentrations of industrial raw minerals depend on their mineralogy and geochemistry. Raw material kaolin is clay (known as China clay) composed essentially of the mineral kaolinite, a hydrous aluminum silicate formed by the decomposition of minerals such as feldspar. It is a naturally occurring weathered product characterized by its white color that may be changed by impurities. Kaolin is widely used in paper industry, ceramics, refractory bricks, white cement, extiles, rubber, medical industries, and special types of plastics. This paper presents screening method for determination of gross alpha and beta activity in kaolin as raw material. Equipment used for this determination was α/β low level proportional counter Thermo Eberline FHT 770 T.

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INFLUENCE OF La, Yb AND Gd SUBSTITUTION ON MAGNETIC BEHAVIOUR OF BULK $BiFeO_3$

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Bismuth ferrite, $BiFeO_3$ is perovskite multiferroic often studied because of its high ferroelectric and magnetic ordering temperatures, 1100 K and 630 K, respectively. Despite its room temperature multiferroicity, pure $BiFeO_3$ is of limited technological importance, especially in bulk ceramic form, due to the antiferromagnetic state with very low net magnetic moment. Doping of $BiFeO_3$ could disturb the antiferromagnetic order and induce magnetically ordered state with considerable magnetization coming from the uncompensated or canted spins. Therefore, magnetic behaviour of $BiFeO_3$ doped with the heavy rare earth elements such as La, Yb and Gd, was investigated.

Compounds of $BiFeO_3$ in which 10% of Bi atoms are substituted with La, Yb and Gd were prepared using the hydro-evaporation synthesis. Magnetization of polycrystalline samples in powder form was investigated in a broad temperature range of 2–900 K. Splitting between the zero field cooled (ZFC) and field cooled (FC) magnetization curves indicate development of the weak ferromagnetism below the Néel temperature of around 610–640 K which is dependent on the composition. Magnetic hysteresis loops measured at the low temperature (5 K), room temperature, and high temperatures, just under and above transition temperature, also suggest the weak ferromagnetic behavior with relatively high coercive field.

Complete magnetic results in full temperature range (2–900 K) clearly indicate enhancement of the weak ferromagnetism after performed substitution with rare earth elements La, Yb and Gd in bulk $BiFeO_3$ ceramic.

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Sb_2S_3 BASED HYBRID SOLAR CELLS AT LOW LIGHTS WITH CHITOSAN AND PEG AS A SOLID HOLDER OF ELECTROLYTE

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Here in this paper, we present a low-cost hybrid solar cell made of ITO / composite p-doped Sb_2S_3+P3HT+PANI+TiO_2 / amorphous Sb_2S_3+P3HT+PANI+TiO_2 / n-doped Sb_2S_3+P3HT+PANI+TiO_2 / solid holder / aluminium as a counter electrode. Layers were deposit by spraying technique and had a thickness of a 1μm. A completely new solid carrier was a blend consisted of chitosan (low MW), polyethylene glycol and electrolyte (0.5M KI + 0.05M I_2). X-ray diffraction (XRD) was recorded in order to confirm amorphous nature of the blend. Information about the surface appearance and roughness of solid carrier dry and soaked in the electrolyte was given by atomic force microscope (AFM). The solar cell was investigated at very low light (5% of sun), low light (35% of sun) and at Standard test conditions (1 sun). It is observed that solar cell showed the highest efficiency of around 23% at 5% of sun. At higher intensities the efficiency for the cell was around 3% at 35% of sun and only 0.75% at intensity of 1 sun.

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INVESTIGATION OF THE Mo DISTRIBUTION THROUGH THE LARGE Β-PHASE GRAINS AND ITS INFLUENCE ON ELASTIC MODULUS OF Ti-12Mo ALLOY BY NANOINDENTATION TEST

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In this study, β-phase Ti-12 mass% Mo alloy was fabricated by using crucible levitation melting (CLM) technique. Examination of ingots before and after deformation was done by nanoindentation, X-ray diffraction (XRD) and scanning electron microscopy (SEM) equipped with energy dispersive spectroscopy (EDS) and electron backscatter diffraction (EBSD). Obtained results show that Mo segregation and grain orientation has great influence on Young's modulus. Crystal orientation maps (after nanoindentation test) reveal that β-grains (~60 μm in size) with orientation closer to {111} plain demonstrate the higher values of Young's modulus. Effects of grain boundaries and elemental distribution of Mo through the grains in Ti-12Mo alloy on its mechanical properties were also analyzed. Non-deformed grains showed higher and more uniform values of Young's modulus compering to deformed grains.Regions with lower Mo content showed higher values of hardness and Young's modulus as a consequence of higher content of ω-phase.

Keywords: Ti-beta alloy, nanoindentation, SEM, EBSD, Young's modulus

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INVESTIGATION OF DIFFERENT SINTERING CONDITIONS ON MECHNAICAL PROPERTIES OF NANOSTRUCTURED BIOCERAMICS

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In the present work, the sintering behaviour of hydroxyapatite (HA) particles prepared via the wet precipitation method was investigated. Green samples were prepared by uniaxial pressing at different pressure and sintered in air and vacuum at different temperature. The sintered bodies were studied in terms of the phase stability, Vickers hardness, fracture toughness and grain size. The results showed that mechanical properties of sintered samples were governed by both the bulk density and sintering atmosphere. HAp samples sintered in vacuum exhibited higher hardness and fracture toughness compare to sample sintered in air. This is induced by increase of density and decrease of average grain size from 80 to 30 nm for HA sintered in the air and vacuum. Translucency was observed at the samples sintered in vacuum as a consequence of decrease on grain size and reduced porosity.

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APPLICATION OF PRINCIPAL COMPONENT ANALYSIS TO INVESTIGATE THE MORPHOLOGY DAMAGE CAUSED BY CAVITATION

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The aim of this study was to exam the influence of cavitation erosion process to the morphology of defects caused on the surface of alumina based materials. The samples without fibers and samples with addition of 2 wt.% of the ceramic fibers were pressed at the pressure of the 36 MPa. The samples were exposed to cavitation erosion through time, while the damages that occurred were followed in the predefined time intervals and the surface of the samples was scanned after each interval in order to take a digitalized picture suitable for further analysis. The digitalized surface images were analyzed using software for image analysis in order to define the morphological characteristics of the damages. Principal component analysis was applied to explore the appearance of the particular morphological characteristics depending on the behavior of the materials during cavitation erosion. The time characteristics of the difference in the morphology parameters of the samples without and with ceramic fibers are presented. It was concluded that the addition of the ceramic fibers becomes important after long time of cavitation erosion, while during short time periods the samples were damaged in the similar way.

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COMBINED MAGNETIC AND STRUCTURAL CHARACTERIZATION OF HIDROTHERMAL BISMUTH FERRITE ($BiFeO_3$) NANOPARTICLES

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Bismuth ferrite ($BiFeO_3$) was synthesized by hydrothermal method. The crystal and magnetic structures of $BiFeO_3$ have been studied by means of X-ray diffraction and neutron powder diffraction at ambient temperature. Microstructure were analyzed by scanning electron microscopy. Quantitative phase analysis by the Rietveld method was conducted and crystallite sizes of 27 nm were determined from the XRD line broadening. The magnetic structure of $BiFeO_3$ is described by the G-type antiferromagnetic order with magnetic peak located at 4.6 Å and a noticeable magnetic contribution to a reflection located at 2.4 Å in the diffraction pattern. The values of the ordered magnetic moment of Fe ions μ_{Fe}=3.8(1) μB, obtained at ambient conditions, are consistent with those determined early

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NZF-BT COMPOSITES: A PHOTOLUMINESCENCE APPROACH

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Photoluminescence (PL) analysis provide us important information about the structure of materials, however the PL behavior of (x)$Ni_{0.7}Zn_{0.3}Fe_2O_4$-(1-x)$BaTiO_3$ ((x)NZF-(1-x)BT) multiferroic composites is not very well know. Based on this, (x)NZF-(1-x)BT powders whit different ratio of NZF/BT (x= 0.1, 0.3, 0.5, 0.7, 0.9) were synthesized by auto-combustion method. After that, the PL property of the composites was explored through measurements carried out using as excitation source a krypton laser with wavelength of 350 nm. The presence of PL emission suggests that the structures of the materials are medium range disordered. Oxygen vacancies (anion vacancies), metal vacancies (cation vacancy) and lattice distortion are responsible by PL emission due to formation of structural defects which are essential to promote the electronic transitions inside band gap. Emission at low energy (green/yellow/red) occurs due to deep defects which modify the Fermi level generating intermediary levels near the conduction band. On the other hand, PL emission at high energy region (violet/ blue) is originated by the presence of shallow defects which generate states next to the valence band. In the present work, all samples showed a broad band emission centered around 450 nm (Figure 1), being a region characteristic of contribution of shallow defects for photoluminescence emission. In addition, the PL broad band emission is an evidence of structural disorder in the lattice of materials which promotes the formation of numerous states within the band gap.

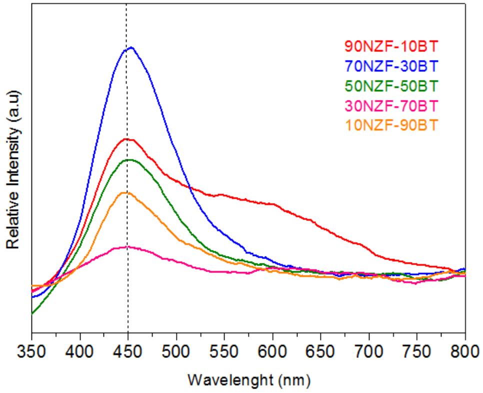

Figure 1. Photoluminescence spectra of (x)NZF-(1-x)BT multiferroic composites

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CHARACTERISATION OF CALCIUM ALUMINATE PHASES IN CEMENTS BY ^{27}AL-MAS-NMR SPECTROSCOPY

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Solid-state nuclear magnetic resonance (NMR) spectroscopy is a useful analytical technique for amorphous systems, since it is sensitive only to the local environment of the observed nuclide. Here, the application of ^{27}Al-NMR under magic-angle-spinning (MAS) conditions for characterisation of calcium aluminate phases in cements will be shown. The importance of the NMR parameters chemical shift and quadrupolar coupling for identification of cement phases will be discussed. As an illustrative example, a NMR study of the mayenite phase (C12A7) will be presented, which was carried out in collaboration with the Matovic group in Belgrade. For different synthesis and densification protocols, the presence or absence of various phases could be tracked by ^{27}Al-MAS-NMR. Application of NMR may hence give useful information, which can be difficult to obtain by standard PXRD analysis.

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PREPARATION OF $YMnO_3$ CERAMIC MATERIAL FROM CHEMICALLY PREPARED POWDERS

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The aim of this work was the preparation of ceramic samples of yttrium-manganite ($YMnO_3$), well-known and one of the most studied multiferroic materials.

Starting $YMnO_3$ powders were prepared by polymeric precursor method from the solution containing yttrium nitrate, manganese acetate, citric acid and ethylene glycol. Prepared powders were calcined at 900 °C for 10 h, and afterwards uniaxially pressed into pellets and sintered at 1300 °C and 1400 °C for 5 h. Detailed analysis of ceramic samples was performed by means of XRD analysis, electron microscopy, magnetic measurements and characterization of ferroelectric properties.

The XRD analysis showed that sintering at 1300 °C results in the formation of ceramic material containing hexagonal $YMnO_3$ as a major phase and Mn_3O_4 as a secondary phase. The presence of ferrimagnetic Mn_3O_4 strongly affected the magnetic properties of the prepared ceramic samples. Rising the sintering temperature to 1400 °C resulted in the preparation of pure hexagonal $YMnO_3$. Low temperature magnetization curve showed linear dependence of magnetization on applied magnetic field which is a sure sign of antiferromagnetic order in the sample. This ceramic material has high density (96 %), but also contains inter and intragranular cracks characteristic for $YMnO_3$. Sintered samples exhibit lossy ferroelectric behaviour with remanent polarization of 0.21 $\mu C/cm^2$ and coercive field of 6.0 kV/cm.

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NANOLAYERED CrAlN/TiSiN COATING DESIGNED FOR TRIBOLOGICAL APPLICATION

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Ceramic thin coatings have been widely applied on surfaces of manufacturing tools and mechanical components to increase their lifetime, reduce energy losses due to friction, reduce environmental pollution, and to decrease downtimes necessary for replacement of defective tools.

Nitride TiAlN and CrAlN coatings are among the most studied and most applied tribological ceramic coatings. Both coatings are characterized by high hardness of around 30 GPa, high oxidation resistance and thermal stability up to around 900 °C, which are key factors making ceramic coatings perfect candidates for protection of manufacturing tools.

Nowadays nanocomposite and nanolayered coatings receive the greatest attention. The mostly studied tribological coating, TiSiN, consists of TiN crystallites surrounded by amorphous Si_3N_4 tissue. TiSiN coatings are characterized by superhardness (> 40 GPa), high oxidation resistance and thermal stability up to 1100 °C. Nanolayered coatings consist of few nm thin layers of alternatively deposited different materials, and exhibit properties superior to consisting material.

In this research nanocomposite and nanolayered design were combined to produce novel nanolayered CrAlN/TiSiN coating. Industrial magnetron sputtering unit with two CrAl and two TiSi targets was used for coating preparation. Scanning electron microscopy (SEM), conventional and high resolution transmission microscopy (TEM and HR TEM), and X-ray diffraction (XRD) were applied for microstructural analysis. Chemical and phase composition were assessed by X-ray photoelectron spectroscopy (XPS). Mechanical properties were determined by instrumented nanoindentation technique.

XRD and XPS analysis revealed that CrAlN/TiSiN coating consists of fcc-$Cr_{1-X}Al_XN$, fcc-TiN and SiN_X phases. Formation of Cr_2N and AlN phases with hexagonal lattice was not observed. TEM analysis revealed fine grained microstructure with grain width of ≈ 10 nm, and length ≈ 100 nm. Presence of such a structure resulted in high hardness of 34 GPa, and high toughness, which are of great importance for tribological application.

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ELECTRICAL PROPERTIES OF $BaSn_{(1-x)}Sb_xO_3$ CERAMICS MATERIALS

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$BaSnO_3$ is a perovskite oxide widely used as dielectric ceramic material, thermally stable capacitor in electronic industry and chemical humidity sensor. It is also an electrical insulator (band gap ~ 3.1 eV), which becomes an n-type conductor by doping.

The aim of this work was to prepare $BaSn_{(1-x)}Sb_xO_3$ (BSSO) by mechanochemically assisted solid-state synthesis, starting from $BaCO_3$, SnO_2 and Sb_2O_3 as precursors. The concentration of Sb in BSSO was varied from 0.04 to 0.1. All starting mixtures were homogenized and activated in a planetary ball mill with isopropanol as a solvent. As-prepared powders were dried and calcined at 900 °C for 4 h. After calcination, powders were uniaxially pressed into pellets and sintered at temperature of 1200 °C for 3 h. Phase composition and microstructure of perovskite BSSO were identified by X-ray diffraction (XRD) and scanning electron microscopy (SEM), respectively. The influence of Sb doping on electrical characteristics of ceramic material was determined by measuring the current-voltage characteristics for all samples at room temperature in air. The band gap values for BSSO calculated using Kubelka-Munk transformation and Tauc linearization of the obtained diffuse reflectance spectra, confirmed conductive behavior of preparedceramic samples.

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MORPHOLOGY EVOLUTION OF ZnO FILMS INFLUENCED BY DOPANTS UNDER HYDROTHERMAL CONDITIONS

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Hydrothermal (HT) syntheses are one of the solution-based techniques that are commonly employed to grow zinc oxide (ZnO), either as loose crystals or as films on different substrates. ZnO is attractive for numerous applications and among them, due to its transparency for visible light and capability to transport electric charge, are various optoelectronic devices. It was shown that specially engineered ZnO crystals can readily replace indium-tin-oxide (ITO) film, which still dominates the field of transparent electrodes.

A common process, to prepare ZnO film on substrate, involves; (i) the nuclei deposition on the substrate (seed-layer preparation) and (ii) the subsequent growth, into thicker film under HT conditions. Crystal growth of ZnO seeds, which are randomly oriented, follows the Spatially Confined Oriented Growth (SCOG) mechanism and results in a (0001)-oriented ZnO film on amorphous substrate. We have shown that ideal pre-deposited seed-layer should have as small as possible ZnO grains, densely packed and homogeneously deposited all over the substrate. Pure ZnO film grown from such fine-grained and compact seed-layer, is highly oriented, smooth and dense and it has a high transparency (82%) and a good conductivity (few 100 Ωsq^{-1}).

To improve the film's electrical and optical properties, we doped ZnO films with aluminum (Al) and gallium (Ga). Firstly, 1.00 M zinc acetate solution was spin-coated onto 2 cm x 2 cm glass substrates and calcined at 360 °C in air. Secondly, resulted ZnO seed-layer was exposed to hydrothermal conditions, where dopants in the form of aluminum nitrate (from 2 to 4 at.% of Al) and gallium nitrate (from 2 to 4 at.% of Ga) were added to 24 ml of aqueous solution containing 0.20 g of zinc nitrate and 0.05 g of sodium citrate. Solution's pH (10.8) was controlled by addition of ammonia while the autoclave was kept at 90 °C from 2 to 24 hours.

The transparencies of synthesized films were measured by UV-Vis-NIR absorption spectroscopy and the electrical characteristics were determined using 4-point current-voltage measurement at room temperature. To define the thickness and porosity of films scanning electron microscopy (SEM) was used and orientation of ZnO grains in films was investigated by x-ray diffraction (XRD). On the basis of the obtained results, supported also by transmission electron microscopy (TEM), crystal growth mechanism was proposed.

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