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Institute for Multidisciplinary Research - University of Belgrade
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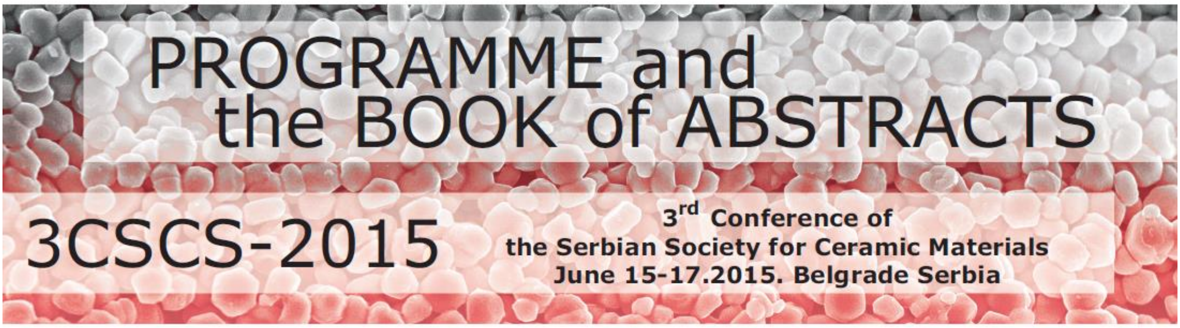

PROGRAMME and the BOOK of ABSTRACTS

3CSCS-2015

3rd Conference of
the Serbian Society for Ceramic Materials
June 15-17.2015. Belgrade Serbia

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

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SPECIAL THANKS TO

Република Србија
МИНИСТАРСТВО ПРОСВЕТЕ,
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WELCOME MESSAGE

On behalf of the organizers and organizing committee of the 3rd Conference of the Serbian Society for Ceramic Materials (3CSCS-2015), I would like to extend my warmest welcome to all of you for attending the 3CSCS-2015. The conference is hosted and organized by the Serbian Society for Ceramic Materials, and co-organized by Academy of Engineering Sciences of Serbia, Institute for Multidisciplinary Research - University of Beograd, Institute of Physics - University of Beograd, Vinca Institute for Nuclear Sciences - University of Beograd.

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. 3CSCS-2015 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 than 100 abstracts submitted from 16 countries.

The Conference will feature four plenary lectures, 25 invited talks and more than 80 oral and poster presentations as well as exhibitions of some new ceramic materials and devices. 3CSCS-2015 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.

3CSCS-2015 President

Branko Matovic

Content

PROGRAMME

PLENARY LETURES

INVITED LETURES

ORAL PRESENTATIONS

POSTER PRESENTATIONS

PROGRAMME

Day 1. Monday - June 15, 2015

07.30 – 08.30 h, Registration

08.30 – 09.00 h, Opening ceremony and Welcome addresses

09.00 – 09.30 h, Cocktail

Session 1: Electro and magnetic ceramics

Chair: Biljana Stojanović, Victor Fruth

09.30 – 10.00 h, Plenary lecture, PL-1
D. Damjanovic, *MORPHOTROPIC PHASE BOUNDARY SYSTEMS: CONCEPT, MATERIALS AND APPLICATIONS*

10.20 – 10.40 h, Invited lecture, I-1
S. Bernik, M. Košir, N. Daneu, A. Rečnik, E. Guilmeau, M. Čeh, *STRUCTURAL AND MICROSTRUCTURAL CHALLENGES FOR THE ENHANCED THERMOELECTRIC PERFORMANCE OF ZnO-BASED CERAMICS*

10.20 – 10.40 h, Invited lecture, I-2
T. Rojac, J. Walker, M. Makarovic, E. Khomyakova, H. Ursic, A. Bencan, B. Malic, D. Damjanovic, *PROCESSING AND CONDUCTIVITY ISSUES IN* $BiFeO_3$*-BASED PIEZOELECTRIC CERAMICS*

10.40 – 10.55 h, O-1
A. Radojković, S. Savić, N. Jović, J. Ćirković, Z. Branković, G. Branković, *Eu DOPED BARIUM CERIUM OXIDE AS A PROMISING ELECTROLYTE FOR INTERMEDIATE TEMPERATURE SOFCs*

10.55 – 11.10 h, O-2
D. Luković Golić, A. Radojković, J. Ćirković, N. Tasić, D. Pajić, G. Branković, Z. Marinković Stanojević, Z. Branković, *STRUCTURAL, FERROELECTRIC AND MAGNETIC PROPERTIES OF* $BiFeO_3$ *SYNTHESIZED BY HYDRO-EVAPORATION AND SONOCHEMICALLY ASSISTED HYDROTHERMAL METHODS*

11.10 – 11.25 h, O-3
D. Tripkovic, J. Vukmirovic, B. Bajac, J. Stanojev, N. Samardzic, E. Djurdjic, S. Rakic, G. Stojanovic, V.V. Srdic, *ELECTRICAL AND STRUCTURAL CHARACTERIZATION OF INKJET SHAPED PASSIVE COMPONENTS BASED ON BARIUM TITANATE AND Ni-Zn FERRITE CERAMICS*

11.25 – 11.45 h, Coffee break

Session 1: Electro and magnetic ceramics

Chair: Vladimir V. Srdic, Slavko Bernik

11.45 – 12.05 h, Invited lecture, I-3
V. Stamenković, *MATERIALS WITH TAILORED PROPERTIES FOR ELECTROCHEMICAL SYSTEMS*

12.05 – 12.25 h, Invited lecture, I-4
P. Gao, A. Bolon, E. Lara-Curzio, Z. Brankovic, G. Brankovic, M. Radovic, *ON ANELASTIC AND DIELECTRIC RELAXATION IN DOPED CERIA AND ZIRCONIA CERAMICS*

12.25 – 12.40 h, O-4
V. Fruth, M. Cernea, I. Atkinson, J. Pandele, E. Tenea, E. Volceanov, F. Craciun, C. Galassi, M. Dinescu, M. Zaharescu**,** *MULTIFERROIC PROPERTIES OF (Nd,Fe)-DOPED* $PbTi(Mn)O_3$ *PEROVSKITE CERAMICS*

12.40 – 12.55 h, O-5
S. Pršić, S.M. Savić, Z. Branković, S. Vrtnik, S. Bernik, G. Branković**,** *THERMOELECTRIC PROPERTIES OF Cu- DOPED SODIUM COBALTITE CERAMICS*

12.55 – 13.10 h, O-6
N. Ilić, B. Stojadinović, A. Džunuzović, J. Bobić, N. Tasić, L. Curecheriu, Z. Dohčević-Mitrović, B. Stojanović**,** *IMPROVED ELECTRICAL AND MAGNETIC PROPERTIES IN Y DOPED* $BiFeO_3$ *CERAMICS*

13.10 – 13.25 h, O-7
N. Tasić**,** Z. Marinković Stanojević, Z. Branković, M. Podlogar, M. Gilić, A. Matković, G. Branković, *NANO-ANATASE* TiO_2 *FILMS PREPARED BY HYDROTHERMAL SYNTHESIS AND THEIR PHOTOVOLTAIC PERFORMANCE*

13.25 – 13.40 h, O-8
R. Rudež, S. Bernik**,** *THE EFFECT OF* Bi_2O_3 *AND* Sb_2O_3 *ON THE MICROSTRUCTURE AND ELECTRICAL PROPERTIES OF THE THICK-FILM VARISTORS*

13.40 – 14.40 h, Lunch break

14.10 – 15.10 h, Poster Session 1
Sessions: *Electro and Magnetic Ceramics* & *Ceramic Composites, Membranes and Multimaterials*

Session 2: Ceramic Composites, Membranes and Multimaterials

Chair: Ravi Kumar, Tadej Rojac

15.10 – 15.30 h, Invited lecture, I-5
E. Traversa, *CERIUM OXIDE NANOPARTICLES FOR ANTIOXIDANT THERAPY PERSPECTIVES*

15.30 – 15.50 h, Invited lecture, I-6
D. Makovec, *SYNTHESIS OF MAGNETIC AND MULTIFUNCTIONAL NANOCOMPOSITES BASED ON THE COLLOIDAL PROCESSING OF NANOPARTICLES*

15.50 – 16.10 h, Invited lecture, I-7
C.E. Ciomaga, L. Padurariu, L. Mitoseriu, *FERROELECTRIC-FERRITE/CNT CERAMIC COMPOSITES: SYNTHESIS, FUNCTIONAL PROPERTIES AND MODELING*

16.10 – 16.30 h, Invited lecture, I-8
Z. Burghard, *NANOSTRUCTURED OXIDE BASED THIN FILMS AND PAPERS TAILORED BY NATURE ADAPTED NANOSCALE DESIGN*

16.30 – 16.45 h, O-9
J. Stanojev, B. Bajac, D. Tripkovic, J. Vukmirovic, M. Ivanov, R. Grigalaitis, J. Banys, V.V. Srdic, *STRUCTURAL CHARACTERIZATION AND DIELECTRIC PROPERTIES OF* $BaTiO_3/NiFe_2O_4$ *MULTILAYER THIN FILMS*

Day 2. Tuesday - June 16, 2015

Session 3: Computing in Materials Science

Chair: Tahir Cagin, Dejan Zagorac

09.00 – 09.30 h, Plenary lecture, PL-2
J. Christian Schön, *NANOMATERIALS: WHAT DO THEIR ENERGY LANDSCAPES TELL US?*

09.30 – 09.50 h, Invited lecture, I-9
T. Cagin, *THERMO-ELECTRO-MECHANICAL COUPLING IN PIEZOELECTRIC MATERILAS: MOLECULAR THEORIES AND ATOMISTIC SIMULATIONS*

09.50 – 10.10 h, Invited lecture, I-10
S. Woodley, M. Farrow, R. Catlow, S. Shevlin, J. Buckeridge, M. Watkins, T. Lazauskas, A. Sokol, *STRUCTURE PREDICTION OF CRYSTALLINE NANO-COMPOSITES: A BOTTOM UP APPROACH*

10.10 – 10.30 h, Invited lecture, I-11
D. Zagorac, J. Zagorac, M. Rosić, B. Matović, *THEORETICAL INVESTIGATIONS OF BaS, AlN AND BN SYSTEM ON ab initio LEVEL*

10.30 – 10.45 h, O-10
S. Neelamraju, *ATOMISTIC MODELING OF THE LOW-TEMPERATURE ATOM-BEAM DEPOSITION OF MAGNESIUM FLUORIDE*

10.45 – 11.10 h, Coffee break

Session 4: Ceramic Powders, Characterization and Processing

Chair: Biljana Babić, Katsumi Yoshida

11.10 – 11.30 h, Invited lecture, I-12
A. Gajović, M. Plodinec, A. Šantić, D. Iveković, J. Macan, T. Haramina, M. Čeh, M. Willinger, *TITANIA BASED NANOSTRUCTURES FOR VARIOUS APPLICATIONS*

11.30 – 11.50 h, Invited lecture, I-13
T. Bräuniger, *CHARACTERISATION OF CERAMIC SYSTEMS BY SOLID-STATE NMR SPECTROSCOPY*

11.50 – 12.05 h, O-11
A. Dapčević, D. Poleti, J. Rogan, A. Radojković, G. Branković, *HIGHLY CONDUCTIVE LANTHANOIDE STABILIZED* δ-Bi_2O_3 *PHASES*

12.05 – 12.20 h, O-12
I. Stijepović, M. Milanović, V.V. Srdić, *SURFACE MODIFICATION OF ZINC FERRITE NANOPARTICLES AND THEIR PROPERTIES*

12.20 – 12.35 h, O-13
J.P. Cusu, C. Stan, C. Munteanu, D. Culita, I. Atkinson, V. Parvulescu, V. Fruth, *SYNTHESIS AND CHARACTERIZATION OF* CeO_2- SiO_2 *MESOPOROUS MATERIALS FOR PHOTOCATALYTIC OXIDATION OF* CH_4

12.35 – 12.50 h, O-14
I. Atkinson, J.P. Cusu, V. Parvulescu, M. Filip, M. Voicescu, D. Culita, C. Munteanu, V. Fruth, *MESOPOROUS NITROGEN DOPED* $SrTiO_3$ *OBTAINED BY DIFFERENT METHODS*

12.50 – 13.05 h, O-15
A. Mrkonjić, *BRUKER INSTRUMENTS FOR MATERIAL RESEARCH - NEW DETECTORS AND TECHNICAL SOLUTIONS FOR XRD*

13.05 – 14.05 h, Lunch break

13.35 – 14.35 h, Poster Session 2
Sessions: *Computing in Materials Science* & *Ceramic Powders, Characterization and Processing*

Session 4: Ceramic Powders, Characterization and Processing

Chair: Miladin Radovic, Eniko Volceanov

14.35 – 14.55 h, Invited lecture, I-14
M. Prekajski, M. Miljević, B. Todorović, A. Matković, M. Marinković-Cicović, J. Luković, B. Matović, *SYNTHESIS OF NANOSPHERES CARBONATED STRONTIUM HYDROXYAPATITE THROUGH A SIMPLE NANOEMULSION METHOD*

14.55 – 15.10 h, O-16
C. Stan, J. P. Cusu, I. Atkinson, C. Munteanu, D. Culita, A. Rusu, V. Fruth, *MESOPOROUS BIOACTIVE* $SrO\text{-}SiO_2$ *GLASSES AS DRUG DELIVERY*

15.10 – 15.25 h, O-17
L. Predoana, D.C. Nastac, I. Atkinson, J. Pandele, C. Munteanu, V. Fruth, *INCORPORATION OF Sn IN TRICALCIUM SILICATE AND DICALCIUM SILICATE*

15.25 – 15.40 h, O-18
N. Stanković, A. Rečnik, N. Daneu, *ILMENITE SINGLE CRYSTAL TRANSFORMATION TO RUTILE AND HEMATITE INDUCED BY HEATING IN AIR ATMOSPHERE*

15.40 – 15.55 h, O-19
B. Matovic, *PREPARATION AND CHARACTERIZATION OF NANOCRYSTALLINE Mg DOPED CERIA POWDERS*

Day 3. Wednesday – June 17, 2015

Session 5: High Temperature Phenomena, Sintering, Microstructure Design and Mechanical Properties

Chair: Branko Matović, Javier Garay

09.00 – 09.30 h, Plenary lecture, PL-3
N.K. Kostoglou, C. Rebholz, *THERMAL STABILITY OF DIFFERENT HEXAGONAL BORON NITRIDE (h-BN) NANOSTRUCTURES*

09.30 – 10.00 h, Plenary lecture, PL-4
P.M. Vilarinho, *TO BE OR NOT TO BE POROUS? Open questions on the role of porosity in ferroelectric thin films*

10.00 – 10.20 h, Invited lecture, I-15
C.-A. Wang, *FABRICATION, STRUCTURE CONTROL AND FUNCTIONAL CHARACTERISTICS OF POROUS CERAMICS*

10.20 – 10.40 h, Invited lecture, I-16
E. Di Bartolomeo, I. Luisetto, F. Basoli, F. Zurlo, S. Licoccia, *INFILTRATED* $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ *BASED FUEL CELLS FOR BIOGAS FEEDING*

10.40 – 10.55 h, O-20
R. Benitez, G. Proust, I. Karaman, M. Radovic, *HYSTERETIC STRESS-STRAIN BEHAVIOR OF* Ti_2AlC

10.55 – 11.10 h, O-21
M. Presečnik, S. Bernik, *MICROSTRUCTURAL AND THERMOELECTRIC CHARACTERISTICS OF* WO_3*-DOPED* $Ca_3Co_4O_9$

11.10 – 11.30 h, Coffee break

Session 5: High Temperature Phenomena, Sintering, Microstructure Design and Mechanical Properties

Chair: Andreja Gajović, Elisabetta Di Bartolomeo

11.30 – 11.50 h, Invited lecture, I-17
R. Kumar, *SYNTHESIS, CHARACTERIZATION AND PHOTOCATALYTIC PROPERTIES OF TITANIA/ZIRCONIA-SILICON OXYCARBONITRIDE NANOCOMPOSITES*

11.50 – 12.10 h, Invited lecture, I-18
K. Yoshida, C.-C. See, S. Yokoyama, M. Takahashi, T.Yano, *DEVELOPMENT OF POROUS SiC CERAMICS BASED ON IN-SITU GRAIN GROWTH*

12.10 – 12.30 h, Invited lecture, I-19
J.E. Garay, *PROCESSING AND PERFORMANCE OF TRANSPARENT CERAMICS FOR LIGHT EMISSION AND LIGHT MANIPULATION*

12.30 – 12.45 h, O-22
E. Khomyakova, J. Pavlič, J. Walker, M. Makarovič, T. Rojac, B. Malič, A. Benčan, $BiFeO_3$ *THICK FILMS ON DIFFERENT SUBSTRATES*

12.45 – 13.00 h, O-23
J. Pantić, M. Milošević, J. Luković, M. Prekajski, M. Mirković, B. Matović, *PHASE EVOLUTION OF SPHENE* ($CaTiSiO_5$) *DURING ANNEALING*

13.00 – 13.15 h, O-24
D. Bučevac, V. Krstić, A. Kocjan, T. Kosmač, *EFFECT OF* Y_2O_3 *PARTITIONING ON AGEING OF* Y_2O_3*-STABILIZED TETRAGONAL* ZrO_2 *DENTAL CERAMICS*

13.15 – 14.30 h, Lunch break

14.00 – 15.00 h, Poster Session 3
Sessions: *High Temperature Phenomena, Sintering, Microstructure Design and Mechanical Properties* & *Traditional Ceramics*

Session 6: Traditional Ceramics

Chair: Tatjana Volkov-Husović, Maja Gajić-Kvaščev

15.00 – 15.20 h, Invited lecture, I-20
M. Komljenović, V. Nikolić, N. Marjanović, Z. Baščarević, *ALKALI ACTIVATED MATERIALS: CRUCIAL FACTORS AFFECTING THE STRENGTH*

15.20 – 15.40 h, Invited lecture, I-21
M. Gajić-Kvaščev, *PATTERN RECOGNITION TECHNIQUES AS SUPPORT FOR ARCHAEOMETRIC STUDY OF CERAMIC ARTEFACTS*

15.40 – 16.00 h, Invited lecture, I-22
M. Grujić-Brojčin, M. Šćepanović, *THE APPLICATION OF RAMAN SPECTROSCOPY IN THE ANALYSIS OF ANCIENT CERAMICS*

16.00 – 16.20 h, Invited lecture, I-23
Z. Baščarević, V. Nikolić, N. Marjanović, L. Petrašinović-Stojkanović, Z. Miladinović, M. Ršumović, M. Komljenović, *DURABILITY OF ALKALI ACTIVATED MATERIALS*

16.20 – 16.40 h, Invited lecture, I-24
M. Vlahović, S. Martinović, T. Volkov-Husović, *NON-DESTRUCTIVE EVALUATION OF SULFUR-POLYMER COMPOSITE BEHAVIOR UNDER INDUCED DESTRUCTION INFLUENCE*

16.40 – 17.00 h, Invited lecture, I-25
S. Martinovic, Z. Stevic. Vlahovic, T. Volkov-Husovic, *BEHAVIOR OF LOW CEMENT CASTABLE IN EXTREME CONDITIONS: THERMAL SHOCK, CAVITATION EROSION, LOW LEVEL LASER ACTION*

PL-1

MORPHOTROPIC PHASE BOUNDARY SYSTEMS: CONCEPT, MATERIALS AND APPLICATIONS

Dragan Damjanovic

Swiss Federal Institute of Technology in Lausanne – EPFL, Lausanne, Switzerland

The morphotropic phase boundary (MPB) is arguably the most important and the least understood phenomenon in piezoelectric materials. In its narrow and the most often used sense, the term describes a region / boundary in a phase diagram of a solid solution where two phases meet and where electro-mechanical properties are maximized. Lately, however, the term has been used to describe coexistence of two crystal phases of the same composition and electric field induced phase transitions in single phases. Those broader definitions will be discussed but the term MPB will be used in its narrow sense.

Several mechanisms have been proposed as origin of the high properties at MPB: facilitated switching of domain walls and thus an easy poling of ceramic materials; coexistence of two phases separated by a low energy barrier; hierarchical domain wall structure; and, most recently, the facilitated polarization rotation via monoclinic phases which were recently discovered in several ferroelectric solid solutions. The presentation will give an overview of these interpretations and will discuss in detail the polarization rotation mechanism – what does it mean, how does it explain large properties, is it the only mechanism of the properties enhancement in solid solutions, is monoclinic phase essential for large properties? It will be shown that the underlying origin of the properties enhancement in the vicinity of the MPB is the flattening (isotropy) of the free energy profile. In this sense, the polarization rotation is just a special case and other paths in the energy profile may exist for easy, “non-rotational”, polarization change. Examples of such cases, such as polarization extension/contraction will be given. Other mechanisms (e.g., those related to domain wall motion) that operate in the material may be particularly enhanced in the vicinity of MPB.

While a free energy isotropy is a necessary condition for properties enhancement at MPB, some very recent studies indicate that other mechanisms, such as elastic softening of the material, must also be present to achieve a large piezoelectric response.

PL-2

NANOMATERIALS: WHAT DO THEIR ENERGY LANDSCAPES TELL US?

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The drive to develop new materials with well-specified properties lies behind the creation of a new class of materials, the so-called nanomaterials. They bridge the gap between classical multi-crystalline, crystalline and amorphous materials investigated in solid state chemistry and materials science, and the molecules of various sizes who are studied in the fields of organic and inorganic molecular chemistry. The combination of small size with (partly) regular extended structure and a relatively large surface-to-volume ratio leads to the existence of many modifications of a nano-object for the same overall composition. This structural plethora allows us to tune the physical and chemical properties of the nanomaterial to a much larger degree than possible in macroscopic materials. On the other hand, it is considerably more difficult to analyze the atomic arrangements of these nano-particles, and thus theoretical tools are needed to determine or even predict the (possible) structures present in the chemical system. Furthermore, the stability of a given modification of a nano-particle is usually considerably lower than the one of a bulk modification due to the fewer number of atoms in the system and the large free surface that allows for fast re-arrangements of the atoms in the system. Both the investigation of the wide range of possible structures in the system and the analysis of their stability rely on the study of the energy landscape of the system: the determination of the minima on the landscape and the generalized barriers separating them. Furthermore, the possible design of nanomaterials e.g. via atom by atom or atom cluster by atom cluster assembly or via the decoration of clusters by molecules, relies on information about the properties of the corresponding energy landscape.

In this presentation, we introduce the basic concepts of energy landscapes, and show applications of energy landscapes to nanomaterials, ranging from the study of clusters over molecules and surfaces to periodic systems.

PL-3

THERMAL STABILITY OF DIFFERENT HEXAGONAL BORON NITRIDE (h-BN) NANOSTRUCTURES

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Boron nitride (BN) is a quite versatile inorganic compound used for a wide range of industrial applications due to a combination of unique characteristics, including high oxidation resistance, large thermal conductivity, good electrical insulation, chemical inertness, excellent lubricity, non-toxicity and environmental friendliness. Even though BN is well-known for a variety of crystalline structures, its hexagonal polymorph (i.e. h-BN) is the most stable one exhibiting a structure similar to graphite. In recent years, much attention has been drawn towards nanoscale h-BN, since improved properties (e.g. mechanical strength) are expected. In this study, an extensive series of hexagonal BN nanostructures with different structural properties were investigated for their high-temperature resistance and oxidation behavior up to 1500 °C under air-flow conditions. Both commercially available (e.g. nanoplatelets, nanotubes) and laboratory synthesized (e.g. nanosheets, nanofibers) h-BN materials were systematically evaluated for their high-temperature properties through thermal gravimetric analysis (TGA) in combination with differential scanning calorimetry (DSC). Additional characterization techniques were employed, including nitrogen adsorption/desorption at 77 K, X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy in order to investigate thoroughly their texture/porosity, structure, surface chemistry, morphology and elemental composition, respectively. The experimental results revealed which of the tested nanomaterials demonstrated the best high-temperature performance/resistance and allowed the correlation of oxidation behavior with specific structural features (e.g. crystallinity, specific surface area, particle shape).

PL-4

TO BE OR NOT TO BE POROUS?
Open questions on the role of porosity in ferroelectric thin films

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How does porosity affect the electrical response of ferroelectrics at the nanoscale? Responding to this question is the main topic of this talk.

The progress of microelectronics has been associated with device miniaturization. And although it is recognized that, as the transistor size approaches tens of nanometers, the end of planar CMOS transistor scaling is near, there is not yet an alternative.On this background the Road Map for Semiconductor Industry (ITRS) suggests since 2011 alternative technologies, designated as More than Moore. Scaling that traditionally meant reducing feature-size, currently encompasses wider concepts such as adding functionalities to the device. Within this context, the introduction of porosity at the nanoscale in functional materials (such as ferroelectrics) might be a way, in particular if pores will be functionalized, of creating opportunities to achieve new functionalities and devices. A primary example is a multifunctional composite structure, in which a porous matrix with a narrow pore size distribution is available for further incorporation of a material with a different functional property than the matrix.

In this talk I will present our systematic work carried out on the fabrication and characterization of nanoporous ferroelectric structures. I will describe the preparation of barium titanate ($BaTiO_3$) and lead titanate ($PbTiO_3$) nanoporous thin films and theirpiezo and ferroelectric response at the nanoscale. This will be followed by the discussion onthe role of porosity on the microstructure development and phase evolution. The relations between nanoporosity and the electrical properties at the nanoscale will be established.

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I-1

STRUCTURAL AND MICROSTRUCTURAL CHALLENGES FOR THE ENHANCED THERMOELECTRIC PERFORMANCE OF ZnO-BASED CERAMICS

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In recent years, thermoelectric (TE) materials have received significant attention because of the possibility to convert waste heat directly into electricity using modules from p- and n-type TE materials. For good TE characteristics, typically expressed by the dimensionless figure of merit (ZT), a reasonably good electrical conductivity, a high Seebeck coefficient and a low thermal conductivity of the material are required, which demands an intricate optimization of contradicting parameters. Conventional TE materials are based on alloys that are expensive can be toxic and have a problem with high-temperature stability in air, so oxide TE materials are increasingly being investigated. Oxide-based TE materials have many advantages, especially their high-temperature stability and the use of mainly non-toxic materials.

ZnO doped with In_2O_3 is a very promising n-type thermoelectric ceramic with a series of homologous $(ZnO)_k{\cdot}In_2O_3$ phases, having a complex structure, resulting from multiple planar defects of InO_2^- octahedral layers acting as inversion boundaries (IBs) with a head-to-head configuration and zigzag-patterned (Zn/In)O slabs in between with a tail-to-tail polarity configuration of the IBs. Multiple In-occupied defects form a framework for the electron conduction and also result in phonon scattering for reduced thermal conductivity, which offers an interesting platform for tailoring the TE properties.

The formation of the $(ZnO)_k{\cdot}In_2O_3$ homologues with the influence on the microstructure development and thermoelectric characteristics will be presented with respect to the amount of added In_2O_3, the sintering temperature and the processing (conventional, spark plasma and microwave sintering). Furthermore, the addition of Al as a standard dopant in highly conductive ZnO to the ZnO-In_2O_3 ceramics was studied with respect to the effects on the main charge-carrier paths. Tailoring the thermoelectric characteristics of In_2O_3-doped ZnO ceramics will be discussed in terms of the samples' composition, microstructure, structure and charge-carrier concentration determined by the Hall measurements.

I-2

PROCESSING AND CONDUCTIVITY ISSUES IN $BiFeO_3$-BASED PIEZOELECTRIC CERAMICS

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For more than ten years, bismuth ferrite ($BiFeO_3$) has been the most studied perovskite material. Owing to its high ferroelectric-paraelectric transition temperature (T_C~825 °C), the initial interest in this prototypic multiferroic material has been recently extended to the field of high-temperature piezoelectric ceramics. Despite the vast interest, however, there are still two main issues that need to be addressed before the full functional potential of $BiFeO_3$ and related materials can be unveiled; these are i) complicated processing and ii) high electrical conductivity. In this contribution, we address in detail the two issues, focusing on $BiFeO_3$ and a number of $BiFeO_3$-based solid solutions, including those with $SmFeO_3$ and $SrTiO_3$.

The problem of the secondary phases, $Bi_{25}FeO_{39}$ and $Bi_2Fe_4O_9$, which appear during the synthesis of $BiFeO_3$ powder and usually persist in the ceramics, has been known for almost 40 years [1]. Only recently, however, the complex origins of the formation and stabilization of the non-perovskite phases have been revealed and involve an interplay between thermodynamic stability of the perovskite phase, presence of impurities in the powders and formation of intermediate Bi-rich phases with low melting temperature (<800°C) [2]. These thermodynamic and kinetic aspects associated with the processing will be discussed through case studies on $BiFeO_3$, $BiFeO_3$-$SmFeO_3$ and $BiFeO_3$-$SrTiO_3$ systems.

While several experimental and theoretical studies have confirmed the p-type conducting behavior of $BiFeO_3$ ceramics, little is known on the role of the local electrical conductivity, e.g., of the role of the conductivity of the domain walls on the macroscopic electromechanical properties of $BiFeO_3$. We will present evidence of spontaneously formed conductive domain walls in polycrystalline $BiFeO_3$ using a combination of scanning electron microscopy (SEM), electron backscattered diffraction (EBSD), atomic- and piezo-response force microscopy (AFM, PFM), and Cs-probe corrected transmission electron microscopy (TEM) analyses. The coupling between the local conductivity at the domain walls and the macroscopic piezoelectric response of $BiFeO_3$ will be discussed in terms of the dynamics of the conductive walls under applied electric and stress fields.

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I-3

MATERIALS WITH TAILORED PROPERTIES FOR ELECTROCHEMICAL SYSTEMS

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Research aimed towards fundamental understanding of processes that are relevant to electrochemical energy conversion and storage will be presented. Atomic scale insight at the topmost surface layer is essential to understand and control properties of materials that are employed at electrified interfaces. Well-defined materials have been in focus of research that is executed in ultra-high vacuum and electrochemical environments. Materials-by-design approach has been used to establish guiding principles in rational design and synthesis of materials for electrochemical systems such as batteries, fuel cells and electrolyzers.

The following topics will be discussed: 1) approach towards well-defined systems; 2) formation of the electrified solid-liquid interfaces; 3) ex-situ and in-situ characterizations; 4) design and synthesis of tailored materials with advanced properties for electrochemical systems.

I-4

ON ANELASTIC AND DIELECTRIC RELAXATION IN DOPED CERIA AND ZIRCONIA CERAMICS

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Doped cerias and zirconias with high ionic conductivities are currently essential electrolyte material for solid oxide fuel cells (SOFCs). In this paper, we report on the temperature dependent elastic properties of doped CeO_2 and ZrO_2. The elastic moduli and mechanical damping were studied using Resonant Ultrasound Spectroscopy (RUS), Dynamic Mechanical Analysis (DMA) and Cyclic Compression Testing. It was found that although elastic moduli decrease almost linearly with temperature, mechanical damping (loss coefficient) Q^{-1} shows frequency dependent maximum at different temperatures for different doped cerias. In zirconias, elastic moduli change with temperature in non-linear manner with large frequency dependent peaks Q^{-1} at different temperatures. The change of elastic moduli and strong mechanical damping are related to the either reversible phase transformations or to the stress induced anelastic relaxation due to hopping of the oxygen vacancies in dopant-vacancy defect complexes and local ordering of oxygen vacancies. In addition, stress dependent hysteresis stress-strain loops were observed in the temperature range showing high mechanical damping. Activation energy determined for anelastic relaxation of oxygen vacancy – dopant dipoles using mechanical spectroscopy methods were found to be a strong function of dopant radius and equal to activation energy for dielectric relaxation of those dipoles. Coupling between anelastic and dielectric relaxation in this class of doped oxides with fluorite structure is discussed in more details in this paper.

I-5

CERIUM OXIDE NANOPARTICLES FOR ANTIOXIDANT THERAPY PERSPECTIVES

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Nanotechnology is offering unprecedented tools to medicine over the last few years. The extensive use of nanoparticles for therapy and/or diagnostics has unveiled a new generation of nano-biomaterials for medical applications. The general trend is now towards the development of bioactive rather than bio-inert materials, with materials directly triggering or participating to cellular reaction pathways. Nanostructured oxides play also an important role in this scenario, and not only as inert materials as one would expect. Recently, cerium oxide nanoparticles (nanoceria) have been reported to show outstanding biomedical activity, acting as well tolerated anti-age and anti-inflammatory agents [1]. The search for reliable and effective antioxidant therapy is a focus of current pharmacological research, since many serious diseases imply oxidative stress. Potential pharmacological applications of nanoceria are proposed due to redox changes in the Ce oxidation state (Ce^{4+}/Ce^{3+}) that trigger the abatement of intracellular reactive oxygen species (ROS), hindering the oxidative stress cytotoxic effects [2]. However, the understanding of the nanoceria biological antioxidant mechanisms is at an early stage and controversial results are reported in the literature.

This talk will summarize our recent studies on the antioxidant effects of nanoceria. It was found that nanoceria reduce the oxidative status and the extent of damage-induced apoptosis, in various cellular systems, including cardiac progenitor cells, subjected to various oxidative stresses [3,4].

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I-6

SYNTHESIS OF MAGNETIC AND MULTIFUNCTIONAL NANOCOMPOSITES BASED ON THE COLLOIDAL PROCESSING OF NANOPARTICLES

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Nanocomposites are multicomponent solid materials where at least one of the phases has at least one of its dimensions in the nano range. Because of this nanostructure, these materials frequently display unique properties. Such nanocomposites can be synthesised in different forms, i.e., bulk, films or (nano)particles, using the colloidal processing of nanoparticles in suspensions.

In the presentation, the synthesis of composite nanoparticles and some bulk nanocomposites will be discussed. First, the basic principles of the synthesis will be presented on model systems of nanoparticles, followed by some practical examples of the synthesis of magnetic and multifunctional nanocomposites, mainly those combining magnetic nanoparticles with nanoparticles or layers of other functional materials.

The composite nanoparticles can be synthesized by assembling two or more nanoparticles of different materials into a single nanoparticle. Different attractive interactions acting between the nanoparticles in the aqueous suspension can be applied for their controlled heteroaggregation. The interactions were studied on model suspensions of smaller carboxyl-functionalized maghemite nanoparticles (15 nm in size) and larger (80 nm) amino-functionalized silica nanoparticles. Electrostatic interactions between two types of nanoparticles displaying an opposite surface charge will be directly compared with the chemical interactions originating from the covalent bonding between the molecules at the surfaces of the nanoparticles.

Another method that can be used for the synthesis of composite nanoparticles is based on coating the core nanoparticles made of one material with a shell made of another material. The principles will be discussed in the case of coating silica-core nanoparticles with a magnetic shell of maghemite. The shell is formed by heterogeneous nucleation of the initial product of Fe^{3+}/Fe^{2+} co-precipitation at the surfaces of the core nanoparticles. The method, which is based on close control of the supersaturation during the co-precipitation, was also applied for the synthesis of bi-magnetic, sandwich-type nanoparticles combining hard-magnetic hexaferrite core nanoplatelets with a soft-magnetic maghemite shell. Due to direct magnetic coupling, the energy product of the nanocomposite is greatly increased compared to that of the core nanoparticles.

The synthesis of bulk nanocomposites will also be presented with a focus on nanocomposites containing a high concentration of (magnetic) nanoparticles dispersed in a polymer matrix.

I-7

FERROELECTRIC-FERRITE/CNT CERAMIC COMPOSITES: SYNTHESIS, FUNCTIONAL PROPERTIES AND MODELING

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The composite properties are determined by the number, type and volume ratio of the phases, as well as by the individual properties, degree of interconnectivity and interface properties. Combination of two phases, such as a combination of magnetostrictive and ferroelectric (thus, piezoelectric) phases, can yield a desirable magnetoelectric (ME) property, in spite the individual components do not show it. In order to realize composites with radically new properties (for example the transition dielectric-conductor) and exceptional characteristics in comparison to those of the individual components, the investigation of functional properties and the understanding of the intrinsic/extrinsic contribution to the properties are presently of high interest.

In the present work, we have investigated the structural, microstructural and functional properties of the two types of composite systems: (i) Co and/or Ni ferrite - $(1\text{-}x)\mathrm{Pb(Zr,Ti)O_3}$ pure and Nb-doped with different composition of ferrite (x=2÷70wt%) magnetoelectric composites prepared in situ by sol-gel method [1,2], and (ii) the ferroelectric ($\mathrm{Pb(Zr_{0.47}Ti_{0.53})O_3}$ -PZT) with multi-walled carbon nanotubes (MWCNTs) composites prepared by spark plasma sintering. The ferroelectric results on the ferroelectric-CNTs investigated system were correlated with the microstructure investigations, and explained or confirmed that the intragranular pores plays a dominant role on the ferroelectric properties. Calculations by finite element modeling demonstrated that by addition of 1-D conductive fillers with compositions below the percolation limits to porous microstructures, the major role in changing the electrical properties via local field modification is related to the induced porosity rather than to the influence of the small amounts of MWCNTs survived after sintering and post-annealing treatment. In case of the ferroelectric-ferrite ceramic composites, the experimental dielectric data on composites were compared with theoretical models (the effective field models (EMA) and finite element approach (FEM)) in order to describe the effective dielectric properties of the composite with contrasting permittivity's and to understand the role of microstructural characteristics on the dielectric response of the composite ceramics in a broad filling factor range [3].

I-8

NANOSTRUCTURED OXIDE BASED THIN FILMS AND PAPERS TAILORED BY NATURE ADAPTED NANOSCALE DESIGN

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The extraordinary combination of strength and toughness of biomaterials, as implemented by nature's highly sophisticated structural design principles, has inspired the synthesis of advanced ceramic based nanocomposites. In this manner, novel materials with unique mechanical properties and sophisticated functionality are expected to become accessible. However, despite ongoing efforts to understand the assembly mechanisms that are operative in biomaterial formation, the transfer of their structural organization to synthetic materials, still remains a major challenge.

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 thin films and paper-like hybrid materials. To this end, we have developed a novel synthesis approach to nanostructured composite films whose an alternating layer architecture combines a soft, organic component (polyelectrolyte (PE)) with a robust, inorganic material (e.g., TiO_2, ZnO). The mechanical performance of these multilayered films, as determined by micro/nanoindentation tests, turned out to be notably enhanced in comparison to the pure oxide films. This is reflected by an appreciable enhancement of fracture toughness, combined with a moderate increase in hardness and preservation of the Young's modulus of the major component. Moreover, by controlling the thickness of the organic component, we were able to obtain films that closely mimic the detailed microscopic structure of nacre, including the presence of mineral bridges. As another intriguing observation, the hardness, Young‘s modulus and fracture toughness of the films assumed a maximum for the inorganic/organic layer thickness ratio of 10:1, in close correspondence to natural nacre.

Furthermore, by closely mimicking the structure of biominerals, we succeeded in the fabrication of highly flexible ceramic paper. Such freestanding films with a thickness of several μm were obtained via self-assembly of vanadia (V_2O_5) nanofibers from aqueous solution at room temperature. The transparent, orange-colored paper can be easily bent into harmonica-like three-dimensional structures, or rolled-up into spiral-like cylinders or narrow tubes with diameters as small as 1 mm. This property arises from the fact that, similar to its natural counterparts, a stiff inorganic component in the form of single-crystalline oxide nanofibers is combined with a hydrogen-bonded water network between them as soft component. Finally, in addition to its excellent mechanical properties, the vanadia nanofiber paper is electrically conductive without requiring any additional processing steps, which opens up tremendous technologically relevant applications in the fast growing fields of flexible energy storage, artificial muscles, and sensors.

I-9

THERMO-ELECTRO-MECHANICAL COUPLING IN PIEZOELECTRIC MATERILAS: MOLECULAR THEORIES AND ATOMISTIC SIMULATIONS

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To provide the molecular basis in determining the electromechanical coupling coefficients at elevated temperatures and under varying mechanical or electrical loading conditions require refinement of molecular dynamics (MD) simulation methods to accurately describe piezoelectricity akin to quantum mechanics. The currently available density functional theory (DFT) based techniques properly simulate this coupling at ground state conditions and without including the thermal effects and advance forms are being developed to include the applied electric field. Of course, DFT is a fully quantum description of the system and can only reasonably simulate systems with hundreds of atoms, thus precluding the simulation of any reasonable nanostructure that would appear in a device. However, the development of an accurate MD method would allow the simulation of hundreds of thousand of atoms, allowing a multitude of nanostructures with varied compositions and thermodynamic conditions to be studied. The development of such a technique is not straightforward, as the interactions that define the coupling greatly depend on the density of electrons in the material. For instance, the ferroelectric perovskite barium titanate ($BaTiO_3$) has four phases with drastically different electron distributions and spontaneous polarizations in each. In order for a simulation technique to adequately describe piezoelectric and ferroelectric response to stimuli, the electron density must be coupled to structural variations.

As the electronic structure plays a dominant role in the materials of interest for various devices, it is important that an MD method retain an accurate description of the electron distribution. Accordingly, we propose an extended Hamiltonian formalism that, in addition to the 3N degrees of freedom for atomic motion, can include degrees of freedom for charge transfer or distribution. The general form of the Hamiltonian is:

$$H = K_{ATOM} + K_{EXT} + U_{ATOM} + U_{EXT}$$

where K denotes the kinetic energy and U denotes the potential energy of the atoms (ATOM) and extended degrees of freedom (EXT). The choice of the extended variables is dependent upon the system of interest. For ferroelectric and piezoelectric materials, the extended variables would govern the charge transfer inherent in these systems. This formalism provides the unification of the atomic and electronic properties into a single Hamiltonian, allowing the simultaneous solution of the total dynamic behavior of the system.

In ferroelectric and piezoelectric systems, the charge interactions are of singular importance; so the additional energy terms in the above Hamiltonian take the following form:

$$U_{EXT} = \sum_{ij} q_i q_j f(r_{ij}) + \sum_{i} U_{SELF}(q_i) - \lambda(\sum_{i} q_i - 0); K_{EXT} = \sum_{i} \frac{\pi_i^2}{2m_i}$$

In this Hamiltonian, each atom is given a charge density with a total charge, q. The interaction of the charge distribution with all other atoms is given by the first term in U_{EXT}. Each atom is also given a measure of how adding additional electrons would increase the atomic energy, U_{SELF}. Each charge is then given a conjugate momentum variable, U_{EXT}, and is allowed to dynamically evolve under the constraint that total charge must be conserved, the third term of U_{EXT}. In essence, this method includes valuable aspects of DFT, a charge density that is responsive to atomic structure, into an MD framework, and is necessary to describe the ferroelectric and piezoelectric effects accurately.

There are many issues in piezoelectric and ferroelectric device materials that can be addressed using this Hamiltonian formalism. For ferroelectric devices, like nonvolatile memories and switches for devices, it is important to have a large polarization material associated with a low coercive field, allowing the polarization state of the material to be switch with a minimum power consumption. With an appropriate simulation method, investigation of possible polar nanostructures or alloys that are switched with less power would save time and clarify the physics of the atomic interactions that cannot be directly determined from experiment. The development of new materials with better piezo-response for more efficient energy harvesting devices will likely involve the exploitation of what is known as the flexoelectric effect. In short, whereas the piezoelectric coefficient couples to the strain, the flexoelectric coefficient couples to the strain gradient. This effect characterizes the electronic response of a material to a large irregular deformation. The optimum exploitation of this effect involves analysis of the inherent strain characteristics of nanostructures. The large surface to volume ratio in such structured materials always results in a strain that can alter the piezoelectric coefficient of the material and lead to a large effective piezoelectric-response.

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I-10

STRUCTURE PREDICTION OF CRYSTALLINE NANO-COMPOSITES: A BOTTOM UP APPROACH

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The search for novel materials with open flexible architectures, which are accessible to external chemical species while retaining their physical properties, is one of the most fundamental challenges in contemporary materials science. The development of new robust nanoporous materials that are stable at high temperatures promises to be of great relevance for energy and environmental applications, e.g. for CO_2 capture or hydrogen storage. New composite materials and *ceramics* have already been prepared for a number of carbon based and wide-gap semiconductor compounds. In this set of compounds, there is growing interest in silicon carbide, which naturally exhibits polymorphism and polytypism under ambient conditions, and therefore could be a good candidate as an advanced functional and environmentally friendly light-weight material in energy, electronics and bio applications. Of particular interest are microporous, and mesoporous, pure and *composite SiC materials*, which exhibit chemical stability and mechanical strength along with relatively narrow pore size distributions, as well as their composites. Such structures could be utilised as membranes in gas separation under high pressure and temperature. While the macroscopic properties of these novel materials have been the focus of attention, only limited data could be obtained concerning their local structure not least due to the limitations of current characterisation techniques applied to nanostructured and disordered systems. Thus, it would be of benefit to find or synthesise new periodic SiC materials, which could be used as models in future industrial applications.

In this presentation I will give an insight into the methods we employ to predict the atomic structures of nanoclusters, and how these nanoclusters are then used as secondary building units in the construction of composite frameworks. The automation of the former procedure has been achieved by the development of our in-house software, KLMC. KLMC includes global optimization routines, as well as routines for book keeping, creation, extracting and running of input/output files of external software used for the calculation of energy, atomic forces and physical properties. Published atomic structure predictions for nanoclusters are uploaded into the WASP@N database. The atomic and electronic properties of materials, both nanoclusters and composites frameworks, for a number of examples obtained using this approach will be discussed. Time permitting I will also demonstrate the capabilities of WASP@N.

I-11

THEORETICAL INVESTIGATIONS OF BaS, AlN AND BN SYSTEM ON *ab initio* LEVEL

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In this work we present three binary systems: barium sulfide (BaS), aluminium nitride (AlN) and boron nitride (BN); since they are important industrial materials and wide gap semiconducting compounds. The BaS is an important precursor to other barium compounds with applications from flame retardants to luminous paints and additives. Under normal conditions BaS crystallizes in the NaCl type of structure, with space group *Fm-3m* (SG number 225) and a wide band gap of a ~3.9eV. With the increase of pressure BaS compound undergoes a structural phase transition to CsC1 type modification with space group *Pm-3m* (no. 221).

The AlN is important industrial material with applications from opto-electronics, microchips and LED, to military and steel industry, while BN has applications from electronics, paint and abrasives, to lubricants, cements and ceramics. The AlN exhibits wurtzite type of modification (w-AlN) at equilibrium with space group $P6_3mc$ (no. 186) and a wide band gap of a ~6.03 eV, while BN crystallize in graphite type of structure (also known as hexagonal BN or *h*-BN), with space group $P6_3/mmc$ (no. 194) and also a wide band gap of a ~5.02 eV. The sphalerite modification (space group *F-43m*, no. 216) is known to exist in both systems at high pressures, and wurtzite type of structure has also been observed as a high pressure phase in the BN system.

Each of the investigated compounds was optimized on *ab initio* level using Hartree-Fock, DFT-LDA and hybrid B3LYP functional. Focus of our research was on theoretical investigations of properties of the materials; e.g. in BaS system we have focused on the electronic and vibrational properties, while in AlN and BN system we have focused on structural and electronic properties. Our results were in good agreement with previous experimental and theoretical observations in BaS, AlN and BN system, and we have shown several additional theoretical models.

I-12

TITANIA BASED NANOSTRUCTURES FOR VARIOUS APPLICATIONS

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Titania based nanostructures have been extensively investigated materials because of their promising physical and chemical properties, such as a high specific surface area, the low costs of synthesis, a high photo-activity and environmental stability. Titanate ($H_2Ti_3O_7$) nanotubes (TiNT) exhibit some distinct advantages as high density of surface OH-groups that enable surface modifications, and ion-exchange. Different surface modification of TiNT and TiO_2 nanotubes (TiO2NT) array with the aim to manipulate with the nanotubes properties toward various applications will be presented.

TiNTs were synthesized by hydrothermal method, while TiO2NT arrays were prepared by anodization of titanium plates. In case of nanotubes decorated by the silver particles the photo-reduction of $AgNO_3$ under UV light were used. Pure and Ag-decorated nanotubes were further modified by heat treatment in hidrogen. TiNT were surface-modified with (3-aminopropyl)trimethoxy silane (APTMS) and imbuilt in the epoxy matrix as nanofiller. For preparation of $BaTiO_3/TiO_2$ nanotubes heterostructure (BTO/TiO2NT), TiO2NT arrays were hydrothermally treated. The structural characterization was done using TEM, XRD and Raman spectroscopy. The band gaps and the photo-catalytic activity were studied using UV–ViS-NIR spectroscopy. Polymer nanocomposites were studied by dynamic mechanical analysis, while the persistent photoconductivity in BTO/TiO2NT was studied by impedance spectroscopy.

We found that high temperature hydrogenation of pure and Ag decorated nanotubes is essential to increase the absorption of light in the visible and near-IR regions. Both hydrogenated and Ag decorated sample had higher photo-degradation impact on model organic compounds (wastewater) as a consequence of the increased absorption of visible light and the synergetic effects of the surface plasmon resonance of Ag nanoparticles and oxygen vacancies.

APTMS-modified TiNTs have proven to be promising nanofiller for reinforcement of epoxy-based nanocomposites since addition of the nanotubes significantly increased the glass transition temperature and the modulus in the rubbery state of the polymer.

The BTO/TiO2NT heterostructures exhibited a giant persistent photoconductivity effect that was six orders of magnitude higher than the dark conductivity, followed by a slow relaxation for 3 h.

I-13

CHARACTERISATION OF CERAMIC SYSTEMS BY SOLID-STATE NMR SPECTROSCOPY

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Because of the amorphous nature of ceramic systems, the information that can be gained from scattering methods such as powder X-ray diffraction (PXRD) is very limited. A useful analytical technique for amorphous systems is solid-state nuclear magnetic resonance (NMR) spectroscopy, since it is sensitive only to the local environment of the observed nuclide. We will discuss the general principles of solid-state NMR and its merits to study ceramic systems. As an illustrative example, a NMR study of a series of β'-SiAlON ceramics will be presented. β'-SiAlONs are formed by the extensive solid solution of Al and O in β-Si_3N_4, described by the general formula $Si_{6-z}Al_zO_zN_{8-z}$ ($0 \leq z \leq 4$). In particular, state-of-the-art ^{27}Al MAS-NMR is shown to be a very effective characterization technique for ceramic samples of the SiAlON type, giving useful information which complements the standard PXRD analysis.

I-14

SYNTHESIS OF NANOSPHERES CARBONATED STRONTIUM HYDROXYAPATITE THROUGH A SIMPLE NANOEMULSION METHOD

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Carbonated strontium hydroxyapatite (CSrHAp) was synthesized at room temperature by applying nanoemulsion technique. X-ray powder diffraction analysis accompanied with Rietveld refinement reviled that synthesized powder were singlephase hydroxyapatite. Fourier transform infrared (FTIR) spectroscopy showed that the CSrHAp was A-type substitution. The carbonate amount substituting the hydroxide group in the synthesized apatite was estimated, from the corresponding CO_2 weight loss in the range 600–1100 ºC. According to this empirical formula of as synthesized CHAp is $Sr_{10}(PO_4)_6(OH)_{0.60}(CO_3)_{0.70}$ This results were confirmed by the Rietveld refinement analysis. Scanning electron microscopy revealed that the synthesized CSrHAp particles were spherical in shape and that their sizes were in the nanometer range. Nanoemulsion strategy procedure provides a simple pathway to obtain singlephase CSrHAp.

I-15

FABRICATION, STRUCTURE CONTROL AND FUNCTIONAL CHARACTERISTICS OF POROUS CERAMICS

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Porous ceramics have been widely used for filtration, separation, heat insulation, sound adsorption, catalyst support, bioceramics and so on due to their special properties including high porosity, high specific surface area, lightweight, refractory, erosion-resistant, heat-insulation and other good properties. The properties of porous ceramics depend on the characteristics of the composition and structure including porosity, pore configuration, pore size and distribution.

In this presentation, I will report some progress on porous ceramics in my group. Some novel processing techniques, including modified gelcasting, freeze-casting, fiber reinforcing, aerogel impregnation, hydrothermal and so on, have been developed to design and control the specific porous structure, therefore, some specific properties including ultra-high porosity, ultra-lightweight, high strength, low thermal conductivity and other physical and chemical properties can be achieved for some potential applications. Some progress in application research on porous ceramics will also be introduced for lithium battery, supercapacitors, acoustic transducers and catalyst.

I-16

INFILTRATED $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ BASED FUEL CELLS FOR BIOGAS FEEDING

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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 hours. $La_{0.8}Sr_{0.2}Fe_{0.8}Co_{0.2}O_{3-\delta}$ 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 minutes. Multiple infiltrations were necessary to get a metal catalyst amount of 25wt% 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 values 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-17

SYNTHESIS, CHARACTERIZATION AND PHOTOCATALYTIC PROPERTIES OF TITANIA/ZIRCONIA-SILICON OXYCARBONITRIDE NANOCOMPOSITES

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Silica modified titanium dioxide has been synthesized by various methods such as chemical vapor deposition and sol–gel methods for possible photocatalytic applications. However, in all these approaches, there have been glitches such as agglomeration, large crystal grain during the transformation of titania/zirconia from amorphous to anatase phase. The *ex situ* inclusion of titania into a matrix also involves similar problems as mentioned above.

Silicon oxycarbonitrides (SiOCN) are a class of materials known for its excellent mechanical, chemical and thermal stability. Recently, the lotus type SiOCN ceramic was shown to exhibit excellent thermal and mechanical stability. However, incorporation of titania/zirconia in to the aforementioned matrix shows very high potential of these materials for photocatalytic applications in visible and UV range. Insitu crystallization of titania/zirconia in these materials is also expected to possess high photocatalytic activity. The incorporation of nitrogen in titania has also proved to increase the photocatalytic effect. Most importantly, the incorporation of nano-titania/zirconia into a more mechanically stable amorphous SiOCN matrix has not been studied till date.

In this work, we have *in situ* crystallized titania/zirconia in an amorphous SiOCN matrix through a polymer precursor derived ceramic (PDC) route. The PDC route was chosen because of its easiness to control the composition of the final material in the atomic scale and the ease of producing near net shaped materials. The structural characterization of the above synthesized material was done using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Spectroscopic techniques such as FTIR and CHN analyzer were used to analyze the spectro-chemical composition of the nanocomposite. The phase evolution and the crystallite size were investigated with the aid of XRD and Scherrer's equation respectively. In addition to this, a porous monolith of SiOCN-TiO_2/ZrO_2 nanocomposite was produced using spark plasma sintering (SPS) and casting route. The SPS as well as cast compacts were subjected to mechanical characterization techniques such as nano-indentation, micro- and macro indentation techniques to evaluate their mechanical stability. The photocatalytic activitiy of these materials were investigated both in the visible and UV range. The properties (structural, mechanical and as well as photocatalytic activity) of SiOCN/TiO_2 are compared with nitrogen-free SiOC-TiO_2/ZrO_2nanocomposites.

I-18

DEVELOPMENT OF POROUS SiC CERAMICS BASED ON IN-SITU GRAIN GROWTH

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Silicon carbide (SiC) is one of the key materials for structural applications such as aerospace industries, nuclear and fusion power reactors, and high-temperature gas turbine because it shows excellent heat resistance, corrosion resistance, high-temperature mechanical properties and low activation after the neutron irradiation. Furthermore, porous SiC ceramics have been commercially used as the material for diesel particulate filter (DPF). Recently, porous ceramics have received great attention in various fields. Present authors have proposed the surface functionalization of porous ceramics based on in-situ grain growth defined as the grain growth on the sintered surface such as the surface of pore walls and frameworks in porous ceramics.

In this study, porous SiC ceramics were fabricated based on in-situ grain growth and their microstructures were investigated. In addition, the effects of SiC particle size and sintering additives on their microstructures were also investigated.

I-19

PROCESSING AND PERFORMANCE OF TRANSPARENT CERAMICS FOR LIGHT EMISSION AND LIGHT MANIPULATION

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It is well known that microstructure can significantly affect the optical properties of polycrystalline ceramics. For example, holding the grain and pore sizes to length scales less than the wavelength of light can be significantly increase transparency. Recently, the versatile material processing technique of current activated pressure assisted densification (CAPAD), often called Spark Plasma

Sintering (SPS) has been gaining momentum as a tool for producing optical ceramics. The primary reason is that CAPAD is especially effective in overcoming the grain growth challenge. Additionally, there is now evidence that the technique is capable of producing non-equilibrium ceramics, i.e. materials that cannot be made using conventional sintering. After an overview of our processing techniques, we will present results from ongoing work on tailoring the optical properties of oxide and nitride ceramics. We will discuss results showing improved visible light transmittance and luminescence. We will also discuss how these materials perform in optical devices such as optical diodes and amplitude modulators.

I-20

ALKALI ACTIVATED MATERIALS: CRUCIAL FACTORS AFFECTING THE STRENGTH

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Alkali activated materials (AAM) are produced by a chemical reaction between solid raw materials and alkaline solution. The strength, as the most important mechanical property, is commonly used as a basic measure of usability of different raw materials in the production of AAM.

Raw materials differ markedly in physical, chemical and mineralogical properties. Most common types of raw materials used for AAM production are calcined materials, such as metallurgical slags, thermally activated (calcined) clays, and fly ashes based on the coal combustion. Calcined materials are mostly amorphous since the calcination process activates materials by changing their crystalline structure into amorphous one. Non-calcined raw materials, such as kaolinite, mine tailings and naturally occurring minerals, are also used.

During the alkali activation process, the vitreous phase of raw materials dissolves, forming calciumsilicate or aluminosilicate gel afterwards. This reaction depends on a whole series of parameters such as: raw materials particle size distribution, amount and chemical composition of vitreous phase, as well as the activator type, concentration, and pH of the activator solution. Conditions of the reaction of alkali activation, such as temperature, time and relative humidity, also have a great impact on the microstructure development, and thereafter on the strength of AAM.

I-21

PATTERN RECOGNITION TECHNIQUES AS SUPPORT FOR ARCHAEOMETRIC STUDY OF CERAMIC ARTEFACTS

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It can be assumed that the modeling wet raw clays into different shapes was a very early human activity, known since about 30,000 BC. Once produced, ceramics are almost indestructible and stabile through the time. Because of the fact that it can be found in large quantities at the majority of archaeological sites, the study of ceramic artefacts can bring to light answers to a variety of questions.

How, when, and where was the artefact produced are the three basic questions that need to be answered during examination of ceramics artefacts. In the chain from excavating ceramic artefacts assemblages, through materials analysis to interpretation, physical and chemistry scientific methods supported by the pattern recognition techniques play an important role. Their application to the study of ceramic artefacts contributes to the reconstruction of their life cycles (from production through distribution to use) and supports interpretations of these reconstructed life cycles in archaeological context. A variety of analytical techniques have been used up today to provide information on ceramic properties necessary for reconstruction of the production technology. Based on the results of pattern recognition techniques treatment of the analytical results conclusions about the distribution or provenance studies, the use of ceramic vessels and subsequent interpretation of the ceramic life cycle can be derived.

Despite numerous techniques employed to characterize ceramic atrefacts, only few pattern recognition techniques has been commonly used for the interpretation of analytical results. Among them, cluster and principal component analysis together with discriminant analysis are the most often used. What can we expect as the result of the analysis by pattern recognition techniques? Which analysis is the most suitable to be performed? What can influence the choice and the use of the particular technique? These are only some of the questions concerning the use of pattern recognition techniques in archaeometric researches. In this paper some answers to the previously asked questions will be provided through the examples of the analysis of the ceramic artefacts using different combinations of analytical and pattern recognition techniques performed in Chemical Dynamic Laboratory of Vinca Iinstitute of Nuclear Sciences and partner institutions.

I-22

THE APPLICATION OF RAMAN SPECTROSCOPY IN THE ANALYSIS OF ANCIENT CERAMICS

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The potential of Raman spectroscopy as non-destructive technique for the characterization of ancient ceramics has been demonstrated. The analysis of the results obtained by Raman scattering measurements of ancient artefacts may reveal a lot of information captured in the microstructure of ceramics bodies. Namely, Raman spectrum, as unique signature, is specific to the technology applied to a given mixture of starting materials and to the process of pottery production.

Micro-Raman spectroscopy is here applied for the study of several classes of ancient ceramic artifacts showing different features and technological background. The analyzed shards of ancient pottery originate from two archaeological sites: the site of Kale-Krševica (South Serbia) and the site of the palace of Masud III in Ghazni (Afganistan). Spectroscopic data were collected on different spots of the groundmass and inclusions of each sample, to investigate the composition of the pottery. Especially, the Raman scattering measurements were performed at the surface of painted ceramics in order to analyze existing pigments.

The results of Raman scattering measurements have shown that the ceramic body of analyzed potteries is composed from materials typical for ancient ceramics: quartz, feldspars and hematite. Additionally, Micro-Raman spectroscopy has allowed the estimation of the maximum firing temperature of some analyzed ceramics due to the presence of low- and high-temperature polymorphs of titania, anatase and rutile, that can be easily differentiated on the basis of their Raman spectra. Micro-Raman spectroscopy has also been helpful to investigate the nature of the pigments found in the ceramic body, as well as to identify the pigments used to paint the surfaces (for instance, it has been shown that red color was obtained from hematite, whereas dark pigment was produced from amorphous carbon).

The results of the application of micro-Raman spectroscopy in the analysis of ancient ceramics presented here suggest that this method could have a key role in revealing the mineral composition and technological aspects of pottery production. Despite the fact that Raman scattering efficiency is often low in the case of clay components and that photolumescence is commonly associated with pottery samples, Raman scattering, should be considered as valuable technique in the study of these artefacts.

I-23

DURABILITY OF ALKALI ACTIVATED MATERIALS

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In the last decade, great scientific attention has been devoted to alkali activated materials, including geopolymers and other related materials. These materials are seen as promising alternative binders, with a possibility to reduce CO_2 emission associated with production of traditionally used Portland cement. Alkali activated materials are produced by reaction of solid silicate and/or aluminosilicate precursors with alkaline solution. Possibility to use waste materials, such as fly ash and blast furnace slag, as raw materials for alkali activated materials production is the second advantage of these alternative binders. However, wider commercial adoption of alkali activated materials is somewhat hindered by the lack of data on long-term properties and durability. In this work, we will give an overview of the results obtained when alkali activated materials are subjected to different aggressive environments.

I-24

NON-DESTRUCTIVE EVALUATION OF SULFUR-POLYMER COMPOSITE BEHAVIOR UNDER INDUCED DESTRUCTION INFLUENCE

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In order to avoid undesirable effects, caused by interactions between the material and environment, changes in properties of materials during their exploitation periods have to be determined. In this research, the induced destruction methodology was applied for evaluation of material behavior. The methodology is based on the usage of agents in increased concentrations that can lead to destruction of the material (cause changes in physical, chemical and mechanical properties) as fast as possible. Sulfur-polymer composite was exposed to the influence of hydrochloric acid, which was chosen as an induced destruction agent. The analysis of sulfur-polymer composite behavior required methods capable of quantifying the material microstructural characteristics. Since sulfur-polymer composite is inhomogeneous material, evaluation of its properties, as well as the effect of external influence on its microstructure, was investigated using non-destructive methodologies. Image analysis and ultrasonic measurements were applied to quantify the material destruction on the surface and in the bulk. Morphological and structural changes in the inner structure of sulfur-polymer composite were inspected by scanning electron microscopy (SEM). According to the obtained results, used methodologies present a powerful tool for the characterization of phenomena occurring in the specimens during the investigation.

I-25

BEHAVIOR OF LOW CEMENT CASTABLE IN EXTREME CONDITIONS: THERMAL SHOCK, CAVITATION EROSION, LOW LEVEL LASER ACTION

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The goal of this study was to use the quantitative analysis of surface and bulk degradation of low cement castable. Alumina based low cement castable (LCC) was synthetized, cured, and then sintered at 1600 °C with the dwell time of 3 h. Prepared samples were subjected to the influence of following extreme conditions: thermal shock, cavitation, and low level laser (LLL). Water quench test as a form of thermal shock was applied as experimental method for thermal stability testing according standard laboratory procedure. Surface degradation of the samples subjected to thermal shock was determined by image analysis using Image Pro Plus Program. Degradation inside of the samples was monitored by ultrasonic pulse velocity. Cavitation damage of alumina based refractory specimen was performed using the modified vibratory cavitation set up. Mass loss during the cavitation was measured while the Image Pro Plus Program was applied for surface analysis. Continuous wave low level laser beam was applied for monitoring of thermal properties and sensitivity of ceramics. Degradation level of the samples was characterized by affected surface area and depth of pit using Image Pro Plus Program and mechanical comparator Orion, respectively. Samples showed dominant degradation inside the sample unlike the surface degradation during the thermal shock, so explosive breakage is possible. Excellent resistance of material exposed to the cavitation erosion is evident as well. A minimal level of degradation was observed for the material exposed to the low level laser. Based on the results it can be concluded that investigated material can be successfully used in applied extreme conditions.

O-1

Eu DOPED BARIUM CERIUM OXIDE AS A PROMISING ELECTROLYTE FOR INTERMEDIATE TEMPERATURE SOFCs

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$BaCe_{0.9}Eu_{0.1}O_{2.95}$ (BCE) powder was synthesized by citric-nitric autocombustion method. According to Rietveld analysis, BCE also possesses slightly larger unit cell volume than mostly investigated $BaCe_{0.9}Y_{0.1}O_{2.95}$ (BCY), which allows higher proton mobility through the perovskite lattice. Sinterability of $BaCeO_3$ is enhanced by doping with Eu since dense electrolyte microstructure with 1–2 μm grains can be obtained at temperatures below 1500 ºC. Conductivity measurements revealed separate bulk and grain boundary contributions to the total electrolyte conductivity below 200 ºC. The grain boundary conductivity was one order of magnitude higher than the bulk conductivity, indicating the blocking effect of the grain boundaries to the mobility of charge carriers. As this effect ceased with temperature, it was possible to determine only total conductivities above 500 ºC. Conductivity of BCE in a wet hydrogen atmosphere at 600 ºC reached 1.2×10^{-2} S/cm, which can be considered as one of the highest conductivities among $BaCeO_3$ based proton conductors. Thus, doping of $BaCeO_3$ with europium offers multiple improvements that can eventually lead to decrease in operating temperature of SOFCs based on this type of proton conducting electrolyte

O-2

STRUCTURAL, FERROELECTRIC AND MAGNETIC PROPERTIES OF $BiFeO_3$ SYNTHESIZED BY HYDRO-EVAPORATION AND SONOCHEMICALLY ASSISTED HYDROTHERMAL METHODS

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Multiferroic bismuth ferrite ($BiFeO_3$) powders were synthesized using hydro-evaporation (HE) and sonochemically assisted hydrothermal (HT) method to investigate how different synthesis methods affect the properties of the powders and sintered samples. The structural and microstructural analyses revealed that all the samples contain secondary phases, $Bi_{25}FeO_{40}$ and $Bi_2Fe_4O_9$, but their contribution depends on conditions of thermal treatment (calcination and sintering). The densest (88% and 95 % of theoretical density for HE and HT sample, respectively) ceramics were obtained after pressing of powders at 9 t/cm^2 followed by sintering at 820 °C for 2 h. Ferroelectric properties of sintered samples were correlated with grain size and density, while the presence of charge defects indicated distortion of crystal lattice. Magnetic measurements of M(H) for both sintered samples showed small deviation from linearity. The sample sintered from HT powder exhibited greater remnant electric polarization as well as greater value of magnetization as a function of temperature. Also, after cooling in magnetic field this sample indicated the asymmetric magnetic hysteresis loop (exchange bias effect). Although both samples showed weak electric ($P_r \leq 1$ μC/cm^2) and magnetic polarization ($M \leq 0.01$ emu/g) at room temperature, ceramics obtained from HT powder was overall superior with respect to multiferroic properties.

O-3

ELECTRICAL AND STRUCTURAL CHARACTERIZATION OF INKJET SHAPED PASSIVE COMPONENTS BASED ON BARIUM TITANATE AND Ni-Zn FERRITE CERAMICS

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Barium titanate and Ni-Zn ferrite ceramics have been widely used for fabrication of passive electronic components such as capacitors and inductors. Nowadays, great significance has been given to 2D structures, namely thin and thick films of electronic and magnetic materials. However, as the trend towards miniaturization goes further, problems with deposition and shaping of such structures becomes more pronounced. Inkjet technique is a novel approach for materials deposition which allows moldless shaping without post-processing and can be digitally controlled. Nevertheless, inkjet printing requires specific ink properties in the terms of viscosity, surface tension, particle size and stability. Inks were synthesized by sol-gel route using barium carbonate, titanium butoxide, and Ni-, Zn-Fe-nitrates as precursors. In order to obtain printable and stable inks, effect of concentration and additives on rheology of the prepared inks was extensively examined. Thin films of material (less than 1 µm) were deposited by inkjet printing on silicon substrate and calcinated. Dimensional precision and uniformity were examined using optical and SEM microscopy, while phase composition was confirmed by XRD and Raman spectroscopy. In order to evaluate applicability, appropriate electrical properties were examined as well.

O-4

MULTIFERROIC PROPERTIES OF (Nd,Fe)-DOPED PbTi(Mn)O_3 PEROVSKITE CERAMICS

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Multiferroics with magnetoelectric properties have recently become the focus of intensive research due to coexistence of magnetic and electric ordering parameters. We propose to explore different (Pb,R,Fe)TiO_3 compositions with the nominal formula $(Pb_{1-3x/2-y}R_xFe_y)TiO_3$, by varying the type of rare earth R-ion and the amount of R and Fe ions, with the aim to improve their properties. In this study powders and ceramics with nominal formula $(Pb^{2+}_{1-3x/2-y}Nb^{3+}_{x}Fe^{2+}_{y})(Ti^{4+}_{0.98}Mn^{4+}_{0.02})O_3$ were prepared by solid state reaction method and conventional ceramic processing. The values of *x* and *y* were: x = 0.08 and, y= 0; 0.01, 0.02, 0.03, 0.04 and 0.05. Microstructural and compositional analyses of these doped ceramics havebeen carried out using X-ray diffractometer (XRD), scanning electron microscope (SEM-EDX) and wavelength dispersive X-ray fluorescence (WDXRF) spectroscopy method. Thelmal behaviour of the materials was evaluated by DSC and dilatometry measurements. Dielectric and impedance spectroscopy and megnetic measurements evaluated the coresponding properties as a function of compositions.

Thetragonality of the unite cell decreased with the increasing content in iron ion and minor deviation from nominal compositions can be noticed. The dielectric loss tangent tan δ is strongly dependent on frequency. It increases towards low frequency and high temperature range, indicating a contribution from the hopping conductivity.

O-5

THERMOELECTRIC PROPERTIES OF Cu- DOPED SODIUM COBALTITE CERAMICS

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Layered cobalt oxide materials have lately been the subject of considerable fundamental and practical interest as potential candidates for thermoelectric application. The polycrystalline samples of $NaCo_{2-x}Cu_xO_4$ (x = 0, 0.01, 0.03, 0.05) were obtained by mechanochemically assisted solid-state reaction method (MASSR) and the citric acid complex method (CAC). Ceramic samples were prepared by pressing into disc-shaped pellets and subsequently sintered at 880 °C for 20 h in inert argon atmosphere. The electrical resistivity (ρ), the thermal conductivity (κ) and the Seebeck coefficient (S) were measured and observed in two temperature regions: low (from 0 to 300 K) and high (from 300 K to 800 K), and the effect of small concentrations of the dopant on the thermoelectric properties was observed. The values of κ were lower in higher temperature region, and almost independent of Cu concentration. S was positive above 25 K, and higher for Cu-doped samples, reaching the highest values for both syntheses for samples with x = 0.03(~145 μV/K at 873 K for CAC sample). The highest figure of merit (ZT) at room temperature (0.022) was obtained for x = 0.01 while at high temperature region ZT were 0.050 and 0.034 for CAC and MASSR samples, respectively. ZT values for all samples were higher than in undoped samples, confirming that even small concentration of Cu significantly influences the thermoelectric properties of $NaCo_2O_4$. It was found that the samples synthesized by CAC method possess better thermoelectric properties, confirming the fact that this type of synthesis enables obtaining fine, homogeneous precursor powders with fine microstructures and small grains which presents prerequisite for obtaining material with good thermoelectric performances.

O-6

IMPROVED ELECTRICAL AND MAGNETIC PROPERTIES IN Y DOPED $BiFeO_3$ CERAMICS

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Bismuth ferrite ($BiFeO_3$) is considered one of the most promising single phase multiferroic materials thanks to the fact it exhibits ferroelectric and antiferromagnetic properties in the same time in very wide range of temperatures (up to 370 °C). Difficulties in obtaining pure $BiFeO_3$ phase and dense ceramics, together with occurrence of leakage currents have prevented application of $BiFeO_3$. Substitution of Bi^{3+} or Fe^{3+} ions with some transition metal or rare earth ions can improve both electrical and magnetic properties by reducing leakage currents and introducing weak ferromagnetism through structural changes.

Y doped bismuth ferrite, $Bi_{1-x}Y_xFeO_3$, was synthesized by auto-combustion method using urea as a fuel. Precursor powders were annealed, pressed and sintered. Powders and ceramic samples were characterized by XRD, SEM, Raman, impedance spectroscopy, ferroelectric and magnetic measurements.

X-ray diffractograms and Raman spectra showed no presence of secondary phases. SEM images indicated lowering of grain size with higher concentration of Y^{3+}. Electrical resistance is highly improved even at 1 % of Y, while 10 % of Y was necessary to break spiral spin structure, leading to weak ferromagnetism.

O-7

NANO-ANATASE TiO_2 FILMS PREPARED BY HYDROTHERMAL SYNTHESIS AND THEIR PHOTOVOLTAIC PERFORMANCE

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Dye-sensitized solar cells (DSSCs) are considered to be a promising alternative to conventional solid state photovoltaic devices, due to wide availability and low-cost of its key component, titanium dioxide (TiO_2). The heart of a typical DSSC is the photoactive electrode, consisting of TiO_2 layer, onto which is adsorbed a monolayer of photosensitive dye. The crucial demands for highly efficient photoactive electrode are good overall porosity, large internal surface area, good pores and particles connectivity, absence of the cracks, and decent adhesion.

We propose a new method for preparation of porous nanostructured layers, consisting of pure nano-anatase TiO_2 particles, which satisfy above listed demands. The method includes the sol–gel processing of titanium(IV) isopropoxide with EDTA–Na_2 and Triton X–100, and hydrothermal treatment of as prepared gels. The final product of the autoclaving was turned into paste, and deposited onto FTO substrates using doctor blade technique. The films were calcined at 500°C, and treated with $TiCl_4$ in order to increase the number of surface binding sites for dye molecules.

The mesoporosity and uniformity of the structure was confirmed on the SEM and FE-SEM images. The primary particles exhibited rice-like shape, barely exceeding 25 nm in length, according to TEM high resolution images. The presence of anatase crystallographic phase was confirmed by XRD pattern, SAED pattern, and Raman spectrum. Desirable high transparency of the films in the visible region (40-65%) was observed in the optical UV-VIS-NIR spectrum.

Furthermore, we have fabricated DSSCs using as prepared films and commercially available dye (N719) and electrolyte. For the photovoltaic measurements, the fabricated cells were illuminated with 300W halogen bulb at 100 $mW\cdot cm^{-2}$ and their current density–voltage characteristics were registered. The cells exhibited extraordinary short-current density response, up to 18 $mA\ cm^{-2}$, for the cell area of 0.219 cm^2. The registered open-circuit voltages are in the region of 0.70-0.75 V, while the values of output power maximum have reached 5.6 $mW\ cm^{-2}$.

O-8

THE EFFECT OF Bi_2O_3 AND Sb_2O_3 ON THE MICROSTRUCTURE AND ELECTRICAL PROPERTIES OF THE THICK-FILM VARISTORS

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ZnO based varistors are very efficient as surge and voltage protectors due to their highly non-linear current-voltage response, which is closely related to their microstructure composed of a highly conducted ZnO grains and a Bi_2O_3 rich grain boundaries. The voltage, at which grain boundary becomes highly conductive and current start to flow, is referred to as the break-down voltage and is ideally about 3V. The break-down voltage of the varistor is the sum of the break down voltages of the grain boundaries between the two electrodes and depends on the ZnO grain size and the thickness of the varistor. In order to control the grain growth dopants such as Bi_2O_3 and Sb_2O_3 are added. During firing, usually at temperature in range of 1100 °C and 1300 °C, the complex microstructure of the varistor ceramics develops, which results in specific electrical characteristics.

For the overvoltage protection of the low voltage devices, such as microelectronics circuit boards and hybrid circuits, thick-film varistors made by screen printing open up another possibility for the integration. The possible advantages of screen printing are miniaturization, the faster and easier production of complex structures and lower production cost. However, the successful realization of the thick-film varistor is omitted to a large vaporization of Bi_2O_3 due to the high surface-area-to-volume at firing temperature typical for varistor ceramics. These instruct lower sintering temperatures, below 1000 °C, and usually lower sintering times; however, such heat treatment can cause poor densification and microstructure development of the thick film.

Our present work was focused on the influence of the Bi_2O_3 content and Sb-to-Bi ratio (Sb/Bi) on a microstructure development and consequently electrical properties of the thick-film varistors fired at 900 °C for 15 minutes, the firing conditions typically used in hybrid circuit technology. The Bi_2O_3 is required to get electrically active grain boundaries. On the other hand the Sb/Bi ratio influences the temperature of the Bi_2O_3-rich liquid phase formation and hence sintering, grain growth, microstructure development and current-voltage (*I-U*) characteristics with breakdown voltage V_N of the varistor ceramics. We varied the Bi-content from 0.4 to 0.8 mol. % and Sb/Bi ratio from 0.25 to 1.25. All the films had a homogenous microstructure, a uniformly distributed Bi_2O_3-rich phase and a well-established contact between the varistor ceramics and the electrode. This could be attributed to the fact that we used screen-printing paste optimized for high solids load of 70 wt. %. The nominal breakdown voltage and the nonlinear coefficient *α* varied with Bi_2O_3 contend and the Sb/Bi ratio. The influence of the composition on the sintering, microstructure development and current-voltage (*I-U)* characteristics of the thick film varistors will be presented and discussed.

O-9

STRUCTURAL CHARACTERIZATION AND DIELECTRIC PROPERTIES OF $BaTiO_3/NiFe_2O_4$ MULTILAYER THIN FILMS

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Recently, nanostructured ceramic materials have found application in processing microelectronic components. A lot of attention has been given to research in the field of multiferroic ceramic materials, especially thin films, which posses both ferroelectric and ferromagnetic behavior. Multiferroics are widely investigated due to their potential application in many microelectronic devices. In this research, multiferroic multilayer thin films were obtained from $BaTiO_3$ as ferroelectric component and $NiFe_2O_4$ as ferromagnetic component. $BaTiO_3/NiFe_2O_4$ multilayer thin films were prepared by sol-gel method and deposited on $Pt/TiO_2/SiO_2$ substrate by spin coating process, where layers were deposited in alternating order. Phase composition of synthesized multiferroics was investigated by X-ray diffraction and Raman spectroscopy. Microstructure of multilayer thin films was investigated by scanning electron microscopy. Dielectric properties were examined on LCR device, in wide range of frequencies and temperatures. Results have shown that dielectric constant of the multilayer films increases as the thickness of $BaTiO_3$ layers increases. The value of dielectric loss (tan δ) for all films was relatively low which is very important for the application.

O-10

ATOMISTIC MODELING OF THE LOW-TEMPERATURE ATOM-BEAM DEPOSITION OF MAGNESIUM FLUORIDE

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We model the deposition and growth of MgF_2 on a sapphire substrate as it occurs in a low-temperature atom-beam-deposition experiment. In the experiment, an (X-ray) amorphous film of MgF_2 is obtained at low temperatures of 170–180 K, and upon heating, this transforms to the expected rutile phase via the $CaCl_2$-type structure. We confirm this from our simulations and propose a mechanism for this transformation. The growth process is analyzed as a function of the synthesis parameters, which include the substrate temperature, deposition rate of clusters, and types of clusters deposited. Upon annealing an initially amorphous deposit, we observe the formation of two competing nanocrystalline modifications during this process, which exhibit the $CaCl_2$ and CdI_2 structure types, respectively. We argue that this joint growth of the two nanocrystalline polymorphs stabilizes the kinetically unstable $CaCl_2$-type structure on the macroscopic level long enough to be observed in the experiment.

O-11

HIGHLY CONDUCTIVE LANTHANOIDE STABILIZED δ-Bi_2O_3 PHASES

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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 aim is to find a suitable electrolyte with the ionic conductivity high enough at intermediate temperatures in order to reduce the operating temperature of SOFCs. 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_2O_3–Tm_2O_3 and Bi_2O_3–Lu_2O_3 systems was investigated. Six starting mixtures with the following compositions $(Bi_{1-x}Tm_x)_2O_3$, x = 0.11, 0.14 and 0.20, and $(Bi_{1-y}Lu_y)_2O_3$, y = 0.15, 0.20 and 0.25, were dry homogenized in an agate mortar, heat treated at 750 °C for 3 h and then slowly furnace cooled. The samples were characterized by XRD, TEM/SAED, SEM, DTA and SEI techniques.

Based on XRD and TEM/SAED, the targeted cubic δ-Bi_2O_3 single-phase samples (space group $Fm\bar{3}m$) were successfully obtained within all six systems. The unit cell parameter of both Tm- and Lu-doped δ-Bi_2O_3 decreases as dopant content increases. By comparing Tm- and Lu-doped δ-Bi_2O_3 phases mutually, an expected increase of the unit cell parameters with larger ionic radii of dopant was found [$r_i(Tm^{3+})$ = 0.88 Å, and $r_i(Lu^{3+})$ = 0.86 Å in the octahedral environment[1]].

Electrochemical impedance of δ-Bi_2O_3 phases was measured between 300 and 800 °C. At temperatures 550 – 800 °C the conductivities are of the same order of magnitude (0.1 – 0.4 S cm^{-1}), but with lowering temperature they rapidly decrease resulting in two activation energies. This is due to the changes in conductivity mechanism which will be discussed.According to the cyclic DTA curves, no phase transitions were observed in the following samples: $(Bi_{0.8}Tm_{0.2})_2O_3$, $(Bi_{0.8}Lu_{0.2})_2O_3$ and $(Bi_{0.75}Lu_{0.25})_2O_3$, indicating that these δ-Bi_2O_3 phases are stable within the whole investigated interval, *i.e.*, from room temperature to 985 °C. This means that the application of these electrolyte materials could result not only in the significant enhancement of IT-SOFC electrochemical performance, but also in their good structural stability over long time service in a wide temperature range.

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O-12

SURFACE MODIFICATION OF ZINC FERRITE NANOPARTICLES AND THEIR PROPERTIES

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Zinc ferrite nanoparticles obtained by co-precipitation method have particle size of about 5 nm but the powder is usually highly agglomerated. In this work, surface modification of zinc ferrite particles is investigated, both during and after the synthesis, using citric acid (CA), poly-ethylene-glycol (PEG), poly-vinyl-alcohol (PVA) and tetra-methyl-ammonium-hydroxide (TMAOH). Zeta-potential of the synthesized particles is measured in order to determine their colloidal stability and choose the most appropriate surface modifier. Influence of the modifier on the structure and morphology of the powders is elucidated by means of XRD, FT-IR and SEM measurements.

O-13

SYNTHESIS AND CHARACTERIZATION OF CeO_2- SiO_2 MESOPOROUS MATERIALS FOR PHOTOCATALYTIC OXIDATION OF CH_4

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Ceria plays multiple roles in various catalyst systems. A series of mesoporous CeO_2 particles with Ce/Si molar ratio ranging from 0.01, 0.05, 0.1, 0.2 to 0.4 are synthesized using a sol–gel method involving Pluronic P123 as template , tetraethylorthosilicate as silica source and hexahydrated cerium nitrate as precursor under acid condition. The chemical and structural characterization of the obtained materials was realized by X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), specific surface measurements, pore size distribution, catalytic properties of CeO_2-SiO_2 material and thermal analysis and FTIR spectroscopy. Characterization revealed that all samples possess ordered hexagonal mesoporous structure and possess high surface area 500-600 m^2/g, large pore volume and uniformpore size estimated to be 0.1 cm^3/g respectively 5nm, based on the N_2 sorption isotherms.

The increase of cerium content increase the cristalinity range of samples was confirmed by XRD, TEM analysis showed that all glass particles hadwell-ordered mesoporous channel structures. For Ce doped samples the mesopority is favorised by a low content in dopant. At higher dopant content, CeO_2 nanoparticles were formed. Catalytic properties of CeO_2/SiO_2 samples were tested in complete oxidation of CH_4 in air between 200 and 550^oC. A significant effect of ceria on catalytic activity was evidenced as conversion of methane increases with ceria content, which means the obtained materials are active in complete oxidation of methane in air.

O-14

MESOPOROUS NITROGEN DOPED $SrTiO_3$ OBTAINED BY DIFFERENT METHODS

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Nitrogen (N)-doped $SrTiO_3$ ($SrTiO_{3-x}N_y$) photocatalysts were synthesized by a hydrothermal method and also by an evaporation induced self-assembling (EISA) method with the aid of the structure directing agent. Nonmetal-doping represents effective strategy to realize visible-light response, N-doped $SrTiO_3$ exhibiting excellent photoreactivity and stability under visible-light irradiation. The obtained photocatalysts were characterized by means of X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), UV-vis spectroscopy Brunauer–Emmett–Teller (BET) surface area and pore size analyzer. The photocatalytic activity of the $SrTiO_{3-x}N_y$ was evaluated by photodegradation of methyl orange (MO) dye under the visible light irradiation. The results demonstrated that the N doping amount had an important effect on the photocatalytic activity of the catalysts.

O-15

BRUKER INSTRUMENTS FOR MATERIAL RESEARCH - NEW DETECTORS AND TECHNICAL SOLUTIONS FOR XRD

Ante Mrkonjić

Bruker, Austria

O-16

MESOPOROUS BIOACTIVE SrO-SiO$_2$ GLASSES AS DRUG DELIVERY

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The features like ordered pore network, high pore volume and large surface area make mesoporous materials excellent candidates for controlled drug delivery systems.

The aim of this study was to incorporate Sr^{2+} into mesoporous SiO$_2$ in order to develop a bioactive mesoporous material with an improved drug delivery profile.

A series of mesoporous SrO-SiO$_2$ species with two different chemical compositions were prepared by a template-induced self-assembling method. As SiO$_2$ source, tetraethylortosilicate (TEOS) was used in the presence of Pluronic 123 (Triblock copolymers based on poly(ethylene glycol)-poly(propylene glycol)-poly(ethylene glycol)) template agent. The chemical and structural characterization of the obtained materials was realized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, thermal analysis, infra-red spectroscopy, specific surface measurements, pore size distribution and Raman and FTIR spectroscopy.

One described the effects of Sr cations on mesoporous structure and its suitable properties for drug delivery applications. The release profile of bioactive Sr^{2+} ions and a model drug – dexamethasone (DEX) can be controlled by altering the Sr content in mesoporous glass samples.

O-17

INCORPORATION OF Sn IN TRICALCIUM SILICATE AND DICALCIUM SILICATE

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The paper deals with the study of tricalcium silicate and dicalcium silicate as solid solutions with SnO_2. This research was required, from the industrial perspective, to study the feasibility of the replacement of raw materials for cement production with alternative materials containing trace amount of tin like, fly ash, refuse derived fuels or plastics. The effect of tin oxide on the formation of solid solutions with tricalcium silicate and dicalcium silicate was also investigated from the threshold limits perspective, in order to prevent deleterious effects if Sn content increase in cement. Two references of pure tricalcium silicate and dicalcium silicate were synthesized for this study and used for preparation of solid solutions with tin oxide. Thus, five samples were obtained by mixing pure tricalcium silicate with increased content of tin oxide from 0.6 up to 14 wt. %. Similarly, five samples of pure dicalcium silicate mixed with increasing amounts of tin oxide from 0.9 up to 18 wt % were obtained. Results derived from X-ray diffraction analysis revealed that tin oxide addition led to gradual structural changes, until a second phase was formed. This second phase was identified as Ca_2SnO_4 and starts to form at 1.6 wt % SnO_2, in the case of tricalcium silicate solid solutions. The second phase formed in the case of dicalcium silicate solid solutions was $CaSnO_3$, which starts to form at 2.1 wt % SnO_2. Moreover, increasing tin content considerably affects the morphology of tricalcium silicate and dicalcium silicate, crystals becoming more rounded and larger. Remarkable configuration of elongated crystals that present a twisting tendency was observed.

O-18

ILMENITE SINGLE CRYSTAL TRANSFORMATION TO RUTILE AND HEMATITE INDUCED BY HEATING IN AIR ATMOSPHERE

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In the last few decades, the demand for titania (TiO_2) is increasing and therefore industrial processes are being developed for its production from different sources. One of the most abundant sources of titanium in nature is ilmenite ($FeTiO_3$) and it used for the production of TiO_2 by acid leaching. In order to obtain a more TiO_2-rich slag it is important that the starting ilmenite is chemically homogeneous and this is achieved by pre-treatment of ilmenite. One of the most efficient pre-processes is oxidetion in controlled atmosphere where iron is oxidized from ferrous to ferric state [1].

Most of the previous studies on ilmenite oxidation were conducted on powders, where the mechanism of transformation is difficult to observe. In our study we used an oriented single crystal of ilmenite in order to observe the transformation in different orientations down to the atomic level. The single crystal was cut into 2.5 mm cubes, which were heated in a tube furnace in air atmosphere at temperatures between 600 and 1200°C for different periods of time (5 min - 100 h). The samples were analyzed by X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM, TEM).

According to the results of XRD analyses, rutile and hematite are the products of low-temperature (700-800°C) oxidation, while the high-temperature mixed Fe-Ti oxide pseudobrookite (Fe_2TiO_5) starts to form at 900°C. Microstructural observations by SEM revealed that transformation of the single crystal starts at the surface and propagates into the interior. Kinetics of the transformation is faster at higher temperatures. The effects of low temperature oxidation observed within the recrystallisation zone are (*i*) formation of a surface hematite (Fe_2O_3) layer, (*ii*) exsolution of rutile lamellae and (*iii*) the formation of cracks. Thickness of the hematite layer and the width of the recrystallisation zone are increasing with the temperature and time, which is in accordance with results of previous investigations on powdered ilmenite [2,3]. TEM analyses of the samples prepared from the recrystallisation front revealed that the formation of rutile from the starting ilmenite is indirect and involves the formation of a transient crystallographic shear TiO_2 phase.

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O-19

PREPARATION AND CHARACTERIZATION OF NANOCRYSTALLINE Mg DOPED CERIA POWDERS

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Nanostructured solid solution $Ce_{1-x}Mg_xO_{2-\sigma}$ samples ($0 \geq x \leq 0.5$) were synthesized by a self-propagating room temperature synthesis (SPRT). XRD and Raman spectroscopy at room temperature were used to study the Mg solubility in ceria lattice. Results show that all obtained powders are solid solutions with a fluorite-type crystal structure with average crystallite size of about 5 nm. Thermal stability of these solid solutions with different concentration of Mg cation was investigated at various temperatures up to 1500 °C. Thermal treated samples were characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM). It was revealed that all samples with higher magnesium concentration are unstable during thermal treatment resulting in Mg leaving the structure of ceria and formation of periclase (MgO) secondary phase. The densification process was studied by constant heating rate dilatometry, and microstructural development by scanning electron microscopy. The relative density as a function of temperature for different Mg contents is investigated.

O-20

HYSTERETIC STRESS-STRAIN BEHAVIOR OF Ti_2AlC

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Ti_2AlC belongs to a new class of materials referred to as MAX phases. The term “MAX phases” was coined in the late 1990s and applies to a family of 60+ ternary carbides and nitrides that common chemical formula: Mn+1AXn —where n = 1, 2, or 3, where M is an early transition metal, A is an A-group element and X is carbon and/or nitrogen. Their unique combination of metallic and ceramic properties makes them ideal candidates for high temperature applications. These properties include: high stiffness, high strength, low density, high electrical conductivity, high thermal conductivity, oxidation resistance, high creep strength, and thermal shock resistant. Moreover, although the MAX phases are quite stiff, they respond to cyclic loading, whether compression or tension, with spontaneous, fully reversible, strain rate independent hysteretic stress-strain loops. Although the hysteretic behavior of MAX phases is well known, the underlying mechanism responsible for this behavior is still a subject of debate. In this study, high purity Ti_2AlC with fine and coarse microstructures was exposed to cyclic compressive loading and complemented with Resonant Ultrasound Spectroscopy (RUS). Four regions with distinct underlying hysteretic mechanisms were identified. The regions are bound by the maximum applied stress, whose magnitude is grain size dependent. The later findings cannot be overestimated, because they show that neither of three currently proposed models can be single-handed implemented to describe mechanical behavior of the MAX phases over the entire range of stresses, but instead the three and more are needed to fully describe the hysteretic behavior.

O-21

MICROSTRUCTURAL AND THERMOELECTRIC CHARACTERISTICS OF WO_3-DOPED $Ca_3Co_4O_9$

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Thermoelectric (TE) materials are converting thermal energy directly into electrical and vice versa. Good thermoelectric materials require a large thermo power (S) for generating a large thermal voltage, a low electrical resistivity (ρ) for minimizing the Joule heating and a low thermal conductivity (κ) for retaining the heat at the junctions, all in order to obtain a high figure of merit Z in accordance to the equation $Z=S^2/\rho\kappa$. The misfit layered cobalt oxide $Ca_3Co_4O_9$ composed of distorted triple rock salt layers of Ca_2CoO_3 and hexagonal CdJ_2-type layers of CoO_2 received considerable attention due to a large figure of merit obtained in the single crystal material [1]. There have been many studies how to improve TE properties of the polycrystalline $Ca_3Co_4O_9$ ceramics, either with various processing methods (SPS, Hot pressing) or by incorporating of various dopants, such as Cu, La, Ir, Pt and also W. According to some authors doping on the Co-site can affect the band structure and transport mechanism, whereas doping the Ca-site has less influence on physical properties. The W is a high-valence and heavy element and its successful doping to the Co-site could possibly diminish thermal conductivity, improve a power factor and hence positively affected the TE properties of the $Ca_3Co_4O_9$.

In this work a series of samples with composition $Ca_3Co_{4-x}W_xO_9$ (x=0, 0.02, 0.05, 0.1, 0.2) were made using classical ceramic procedure with sintering at 900 °C four times for 20 hours with intermediate grinding. The phase composition and the microstructure of the samples were analyzed after each step of sintering using x-ray diffraction analysis (XRD), scanning electron microscopy (SEM) and energy-dispersive x-ray spectroscopy (EDXS). The density of the samples was also determined. Thermoelectric characteristics were measured using the Z-meter in the temperature range from room temperature to about 630 °C. The WO_3-doped samples had lower thermal conductivity than un-doped ones; however, the relation between amount of the W substituted for Co and the thermal conductivity was not observed. With increased W-doping for $x > 0.05$ the electrical resistivity and the Seebeck coefficient increased. The highest electrical conductivity at 630 °C had the samples for x= 0.05. The sample for x= 0.1, sintered at 900 °C only once showed the highest ZT of 0.065 at 600 °C, also higher than the un-doped sample with ZT 0.04.

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O-22

$BiFeO_3$ THICK FILMS ON DIFFERENT SUBSTRATES

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$BiFeO_3$ (BFO) is a promising material for integration in multilayered electronic devices, due to its high T_C (~830°C [1]) and ability to exhibit both ferroelectric and antiferromagnetic ordering at room temperature. However, the processing issues associated with BFO [2] have made its integration rather challenging. In addition, interactions between a thick film and a substrate, such as chemical reactions, thermal stresses and constrained sintering [3], influence the microstructure and consequently, the final functional properties of the film. Therefore, in order to prepare high phase purity BFO thick films, both annealing conditions and the substrate material must be carefully selected.

In this work, we report on the influence of different substrates (electroded alumina and metal foils) on the structure, microstructure and phase composition of BFO thick films.

The films were prepared by the screen-printing method. The powders for pastes were prepared from a homogenized mixture of ultrapure Bi_2O_3 and Fe_2O_3 with and without additional calcination, thus two sintering paths, i.e. conventional sintering of BFO and reactive sintering of a Bi_2O_3-Fe_2O_3 mixture, were investigated. Each powder was mixed with an organic vehicle and printed on different substrates (Pt/Al_2O_3, Au/Al_2O_3, Ag/Al_2O_3 and Pt, Au, Ag foils). The as-printed films were annealed at temperatures from 750°C to 820°C for 4 hours. The phase compositions and microstructures of the BFO thick films were characterized by X-ray diffraction analysis and scanning electron microscopy.

Interface reactions between BFO and (Ag or Au)/Al_2O_3 substrate, which led to the formation of secondary phases, associated with the presence of Cu, Si and Al impurities in the electrodes are discussed. The BFO thick film phase purity was significantly improved when Ag paste with higher purity was used, while BFO thick films on pure Ag, Au and Pt metal foils exhibited only a very small amount (~1 wt%) of secondary phases. However, the porosity was markedly influenced by the choice of the substrate material, with films on Ag or Ag/Al_2O_3 and Au or Au/Al_2O_3 exhibiting a higher density than those on Pt or Pt/Al_2O_3. This is discussed together with the influence of the substrate material on the BFO phase composition and its structure.

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O-23

PHASE EVOLUTION OF SPHENE ($CaTiSiO_5$) DURING ANNEALING

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Sphene ($CaTiSiO_5$) has been prepared from a powder mixture of $CaCO_3$, TiO_2 and SiO_2 using vibro-milling for homogenization and activation of the precursors. The mechanochemical process initially yielded amorphous powders, which crystallized by thermal treatment yielding a sphene ceramic. The evolution of the phase composition during thermal treatment was investigated by X-ray powder diffraction (XRPD) and thermal analyses (DTA-TGA). Sintering behavior of the synthesized sphene powder was followed by hot stage microscopy. An exothermic peak was observed in the DTA curve at 857 °C which could be associated to the sphene crystallization. The formation of sphene at 900 °C was confirmed also by XRPD, where it was observed to be the major crystalline phase.

O-24

EFFECT OF Y_2O_3 PARTITIONING ON AGEING OF Y_2O_3-STABILIZED TETRAGONAL ZrO_2 DENTAL CERAMICS

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Y_2O_3-stabilized tetragonal zirconia polycrystal (Y-TZP) is becoming a prevalent biomaterial in dentistry owing to its excellent tissue compatibility and mechanical properties. However, under certain conditions, such as a humid environment and elevated temperature, Y-TZP suffers from slow, spontaneous tetragonal-to-monoclinic transformation which is followed by microcracking and degradation of mechanical properties. This process, called low temperature ageing, takes place even at temperature as low as the human body temperature and is considered as a serious issue for safe application of Y-TZP as biomaterial. It is known that the ageing is strongly affected by the grain size and the amount of Y_2O_3 stabilizer in Y-TZP. In this study, the effect of amount of stabilizer on ageing of Y-TZP was distinguished from the effect of grain size. Sintering of 3 mol% Y_2O_3-doped TZP powder compacts under different sintering conditions resulted in samples having the same mean grain size but different content of Y_2O_3 in tetragonal ZrO_2. The change of Y_2O_3 content in tetragonal ZrO_2 was the result of Y_2O_3 partitioning between tetragonal ZrO_2 and cubic ZrO_2 which is normally present at high sintering temperature and can accommodate large amount of Y_2O_3. It was found that prolonged sintering at 1350-1450 ^{o}C increases the volume fraction of cubic ZrO_2 and therefore reduces the amount of Y_2O_3 in tetragonal ZrO_2. The accelerated ageing of these samples was directly related to the reduction of Y_2O_3 content in tetragonal ZrO_2.

P-1

INSECTICIDE EFFECT OF ALUMINA POWDERS AGAINST BEAN WEEVILS

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Alumina powders synthesized by combustion method were applied on uninfested grains of bean to examine their insecticide effect against bean weevil (*Acanthoscelides obtectus*). Effects of pH value (6, 8 and 10) of the precursor solution, as well as citric/nitric molar ratio (0.5, 0.8 and 1.2) on the powder properties were observed. XRD analysis of the samples calcined at 1200 ºC for 1 h showed only the presence of α–Al_2O_3 phase. SEM analysis revealed difference between the samples in respect to particle size, which varied from nano- and submicron size to characteristic rectangular particles of several µm and larger. The powder obtained from the solution with the pH value of 10 had the highest content of submicron and nanosized particles. Mortality rate of both male and female insects after seven days of exposure was the highest right for this sample, indicating that the particle size has the greatest influence on insecticide properties of alumina powders. Thus, by increasing the pH of the precursor solution it is possible to prevent higher degree of particles agglomeration. The lowest insecticide efficiency of the powder synthesized at pH = 6 can be prescribed to a weak chelating effect of the citric acid that allowed higher coarsening rate of the particles. When it comes to citric/nitric molar ratio at pH = 8, it had no significant effect on mortality rates, which were higher for male insects in general, while a slight efficiency trend was observed towards fuel lean region, i.e. when the ratio was ≤ 0.8.

P-2

SYNTHESIS AND CHARACTERIZATION OF SEPIOLITE-SUPPORTED NANO ZERO-VALENT IRON

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Nano zero-valent iron (NZVI) has been demonstrated to be an effective material for removal or decomposition of many contaminants in water. However, the NZVI particles tend to agglomerate due to the high surface energy and intrinsic magnetic interactions. In addition, the NZVI particles are easily oxidized, thus reducing their reactivity and stability. Numerous studies have attempted to resolve this problem by fixing NZVI with various materials, increasing their stability and reducing aggregation during practical applications. In this research, natural mineral sepiolite was used as a support for NZVI in order to prepare adsorbents for the removal of chromium (VI) from polluted waters. The sepiolite-NZVI composites were synthesized by the sodium borohydride reduction method, at different sepiolite/NZVI ratio. The obtained composites were characterized using X-ray diffraction, Fourier transform infrared spectroscopy, scanning electron microscope with element analysis, the specific surface area and the point of zero charge determination. It was shown that the adsorption capacity for chromium (VI) was strongly dependent on the quantity of NZVI in the composites.

P-3

EFFECT OF POLYETHYLENE GLYCOL ADDITION ON THE PROPERTIES OF HYDROTHERMALLY SYNTHESIZED MAGNETITE POWDERS

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The application of magnetic materials for the removal of various polutants in the water treatment processes increases, since the magnetic separation produces less contaminants then other methods. The adsorption capacity of magnetic materials mostly depends on their specific surface area.

Magnetite powders were successfully produced using polymer supported hydrothermal tehnique, *in-situ* approach. The powder precursors used were ferrous sulphate ($FeSO_4 \cdot 7H_2O$), sodium thiosulfate ($Na_2S_2O_3 \cdot 5H_2O$) and sodium hydroxide (NaOH). The synthesis was performed in the presssure reactor, heated at 150 °C for 24 h, without and with assistance of polyethylene glycol (PEG) of different molecular weights (400 and 20000). The PEG to water volume ratios of 1:3 and 3:1 were applied.

The crystal structure, morphology, specific surface area (Sp) and types of chemical bonds of synthesized powders were investigated by X-ray diffraction, scanning electron microscopy, BET analysis and FTIR spectroscopy.

The existence of considerable magnetic moment for all samples at room temperature was confirmed by measuring saturation magnetization. A significant increase in the Sp values of nanopowders was obtained by using PEG:water ratio of 3:1. Removal of phosphates ions was probed, showing the promissing results.

P-4

INFLUENCE OF THE SOLVENT TYPE ON THE PROPERTIES AND PHOTOCATALYTIC ACTIVITY OF TITANIA POWDERS SYNTHESIZED BY A NONHYDROLYTIC SOL-GEL PROCESS

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The mesoporous nanocrystalline titania powders of a narrow particle and a pore size distribution have been produced by a nonhydrolytic sol–gel process coupled with solvothermal treatment, starting from titanium(IV)-chloride, titanium(IV)-isopropoxide and carbon-tetrachloride as a solvent. The obtained powders showed a high photocatalytic activity under UV light irradiation. In order to avoid carbon-tetrachloride, which is regarded as highly toxic, the other aprotic solvents of the similar boiling point, chloroform and cyclohexane, were used for the synthesis in this research. The gels obtained after solvothermal treatment were calcinated at 350, 400 and 500 ºC for 3 h to obtain the crystalline titania. The X-ray diffraction analysis showed that anatase was the only crystal phase in all cases. The crystal sizes increased with the calcination temperature and were similar for the samples obtained with different solvents. The textural properties, specific surface area and pore volume, changed with the calcination temperature in the same way as for the samples obtained with different solvents. The SEM studies showed that all powders consisted of spherical particles, that aggregated to form larger spherical particles. The photocatalytic activity of the powders was tested by measuring the degradation of the azo dye CI Reactive orange 16 under UV light irradiation. The results indicated that powders obtained at lower temperatures had higher adsorption capacity for the dye. However, the gels calcination at 500 ºC provided higher photocatalytic activity. The powders obtained with different solvents and calcinated at the same temperatures had approximately the same photocatalytic activity.

P-5

SYNTHESIS OF MAGNETIC SEPIOLITE NANOCOMPOSITES FOR THE REMOVAL OF HEAVY METAL IONS FROM AQUEOUS SOLUTIONS

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Magnetic nanoparticles have drawn much attention over the past years because they possess different physical properties with respect to bulk materials with the same composition. However, the strong tendency of nanoparticles to coalesce, their chemical instability against oxidation, and the health problems related to the production and manipulation of nanoparticles have hindered their application on a large scale. In order to overcome these problems, the magnetic nanoparticles can be synthesized in the presence of a support that provides the stabilization of the magnetic nanoparticles on the surface of carrier. In this research, a natural mineral sepiolite was used as the support for magnetic particles in order to prepare the adsorbents for the removal of heavy metal ions from polluted waters. The magnetite was synthesized by chemical co-precipitation technique, using NaOH or ammonia. The composites were characterized by X-ray diffraction, Fourier transform infrared spectroscopy, scanning electron microscope, and the specific surface area and the point of zero charge determination. The results showed that the adsorption capacities of the obtained adsorbents were dependent on the type of the base used for precipitation. In both cases, the adsorption capacity was higher than the capacity of the pure sepiolite and the pure magnetite.

P-6

SYNTHESIS, CHARACTERIZATION AND APPLICATION OF NANOSTRUCTURED IRON-DOPED TITANIA

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Titanium dioxide nanopowders, doped with different amounts of Fe^{3+} ions, were synthesized by acid-catalyzed sol-gel method in a non-aqueous medium. The obtained nanopowders were characterized by scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and Ultraviolet-visible spectroscopy (UV/Vis). The degradation kinetics of crystal violet dye is used to test the photocatalytic capability. The activities of samples increase with increasing the amount of doped iron. Results are correlated with previous investigations of structure and morphology of doped TiO_2 samples.

P-7

PHOTOCATALYTIC DEGRADATION OF TEXTILE DYE WITH HYDROTHERMALLY MODIFIED NANOANATASE

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The environmental friendly materials based on titanium oxides are often chosen for the industrial application due to their extraordinary characteristics (biological and chemical stability, good photocatalitic activity, wide band gap and cost-effectiveness). On the other hand, the hydrothermal process in alkaline solutions became a very important treatment in the production of titania and titanate nanostructures. The aim of this work was to investigate how different conditions of hydrothermal treatment could modify the structural, microstructural and photocatalytic properties of starting nanoanatase.

Nanoanatase powder was hydrothermally treated with NaOH solution (c = 5 mol/dm) at different temperatures (T = 110, 135 and 160 °C) and durations (t = 6, 12 and 18 h). The obtained samples were washed out with distilled water, centrifuged and dried. Nine specimens are prepared and labeled as $A_{T\text{–}t}$, where T is temperature of the treatment and t is duration of the treatment. The nanocrystalline samples were characterized by XRD, TEM/SAED and FESEM techniques. The photocatalytic activity was tested on the Reactive Orange 16 (RO16) textile azo dye.

The XRD analysis showed that the hydrothermal treatment caused the formation of a secondary phase ($H_2Ti_2O_5 \cdot H_2O$, PDF 47–0124) besides anatase. This is due to the reaction between anatase and NaOH. The increase of temperature and/or time increases the amount of secondary phase. For example, the specimen $A_{110\text{–}6}$ contains about 12 wt.% of $H_2Ti_2O_5 \cdot H_2O$, while the content of this phase amounts about 37 wt.% in $A_{135\text{–}12}$. The average crystallite size of all samples was smaller than 20 nm. This was comfirmed by TEM. The FESEM revealed soft agglomerates created from nanoparticles.

The photocatalytic experiments showed that the presence of secondary phase decreases the photocatalytic activity. For example, $A_{110\text{–}6}$ decolorized 35 % of the RO16 dye within 90 minutes, while $A_{135\text{–}12}$ degraded only 15% of the same dye in the same time interval.

P-8

THE REMOVAL OF HEAVY METAL CATIONS (Pb, Cu) BY LINDE TYPE-A ZEOLITE

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In this work, the adsorption behavior of LTA type of zeolite with respect to Cu^{2+} and Pb^{2+} has been studied in order to consider its application for metal removal from wastewaters. The batch method was employed, using metal concentrations in solution ranging from 10 to 200 mg/l. The degree of metal adsorption was evaluated analyzing the Cu(II), Pb(II) contaminated samples by using AAS (Aanalyst 700/Perkin-Elmer). The phase composition of the LTA zeolite was determined by x-ray diffraction (XRD) analysis. The microstructure and morphology of the powders were analyzed using Scanning Electron Microscopy (SEM). The results show high degree impact of immobilization efficiency for both ions. LTA type of zeolite possesses better selectivity for Pb ions than that for Cu ions.

P-9

BST CERAMICS OBTAINED BY HYDROTHERMALLY ASSISTED COMPLEX POLYMERIZATION METHOD

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Barium strontium titanate powder $Ba_{0.8}Sr_{0.2}TiO_3$ (BST) has been obtained by hydrothermal treatment of precursor solution containing titanium citrate, previously prepared by complex polymerization method, and barium and strontium acetates. The powders were calcined at 700 °C, pressed into pellets and further sintered at 1280 °C for a various sintering times (from 1 to 32 h), and structural parameters, phase composition, dielectric and ferroelectric properties were investigated. Rietveld refinement analysis of BST ceramics showed that predominant phase was tetragonal BST with monoclinic $Ba_6Ti_{17}O_{40}$ (B6T17) as a secondary phase. Phase contents determined by Rietveld refinement match well with the results of energy dispersive X-ray analysis and ICP analysis. SEM micrographs of sintered samples revealed the abnormal grain growth where elongated twinned grains of BST grow in a matrix of smaller B6T17 grains. Dielectric and ferroelectric properties of BST ceramics have been correlated with density of sintered compacts, phase composition, structural parameters and microstructure. The sample sintered for 16 h showed the highest density (93% ρt), as well as the highest value of dielectric constant (~2300) and remanent polarization – Pr (2 $\mu C/cm^2$) among investigated samples.

P-10

CRYSTAL GROWTH OF ZnO FROM AQUEOUS SOLUTIONS AT LOW TEMPERATURES

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The research in material science is lately focused in the direction where not only the size but also the shape of the crystal is being controlled. The main reason behind the interest is the fact that material completely changes its properties when the dimension at one region of a crystal for example, approaches nano. Because of the high environmental standards and a low cost in production, the most attractive syntheses appear to be the one performed in toxic free aqueous medium. In this study such syntheses from zinc nitrate and sodium hydroxide were performed.

We showed how different precipitates can be formed regarding the Zn^{2+}/OH^- ion ratio. The suspension prepared from solutions with Zn^{2+}/OH^- ratio 0.10 was composed of ZnO nanocrystals agglomerated into platelets. At higher ratio of 0.5, precipitant resulted in a flower-like ZnO but had also bipyramidal $Zn(OH)_2$ crystals present. When the ratio of Zn^{2+}/OH^- was increased to 2.5 only bipyramidal $Zn(OH)_2$ were observed and at an even higher ratio of 5, only platelets of $Zn_5(OH)_8(NO_3)_2(H_2O)_2$ were found. We showed that precipitated ZnO crystals when hydrothermal treated at mild conditions does not change the composition or the morphology. Platelets and flower-like ZnO crystals remained the same. On the other hand, hydrothermal treatment of $Zn(OH)_2$ and $Zn_5(OH)_8(NO_3)_2(H_2O)_2$ powders resulted in phase change and a variety of different morphologies. At different HT conditions such as temperature, time, and addition of growth controlling agent we prepared ZnO crystals in a form of platelets, flowers, rods, bow-ties, etc. The used processes are technologically attractive; therefore we also considered the possibility of scaling up.

P-11

HEXAGONAL Os B_2: MECHOCHEMICAL SYNTHESIS, SPARK PLASMA SINTERING, STRUCTURE AND MECHANICAL PROPERTIES

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Hexagonal OsB_2 has been synthesized for the first time by mechanochemistry. [1-3] High energy ball milling was used to introduce high shear and normal impact forces on raw Os and B materials, which resulted in mechanochemical reactions forming hexagonal OsB_2. X-ray diffraction indicated that OsB_2 starts to form after 2.5 hours of milling, and the reaction reaches equilibrium after 18 hours of milling. No phase transformation was observed after OsB_2 powder was annealed at 1050 °C *in vacuo* for 6 days. The lattice parameters of the hexagonal OsB_2 are a=2.916 Å and c=7.376 Å, with P63/mmc space group according to the refinement of the powder XRD pattern. TEM results have confirmed the appearance of hexagonal OsB_2 phase. The synthesized hexagonal OsB_2 powder was sintered with spark plasma sintering at 1500 °C and 50 MPa for 5 minutes. The sintered OsB_2 contains ~80 wt.% of hexagonal and ~20 wt.% orthorhombic phases. It has a density of 9.46 g/cm^3 and porosity of 26.9%. Hardness and Young's modulus were measured to be 31 ± 9 GPa and 574 ± 112 GPa, respectively by nanoindentation.

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P-12

OPTIMIZATION OF SINTERING CONDITIONS OF MECHANOCEMICALLY SYNTHESIZED YTTRIUM MANGANITE

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Yttrium manganite, $YMnO_3$ (YMO), has been a subject of scientific investigation for decades because of its multiferroic character which can lead to many potential applications. Unlike other rare earth manganites ($REMnO_3$), this material can crystallize in two different structures – hexagonal (h-YMO) and orthorhombic (o-YMO). The first one is stable under normal conditions and the latter is the metastable one, but both of them are multiferroic.

Various methods are used for the preparation of $YMnO_3$: chemical methods, solid state sintering, mechanochemical synthesis etc. In this paper, YMO powders were mechanochemically synthesized from Y_2O_3 and Mn_2O_3 milled for different periods of time. In order to prepare pure h-YMO ceramic samples the sintering conditions were investigated. Powders were pressed into pellets and sintered in the temperature range from 900°C – 1400°C for different periods of time. Complete structural and microstructural characterization with magnetic measurements was performed, and results compared with available literature data. XRD analyses show that sintering temperature of 900°C results in the preparation of mixture of h- and o-YMO. Rising the temperature above 1000°C increases the density of the samples, but it also changes the phase composition of ceramic samples. Hexagonal YMO is the major phase, but at higher temperatures, some quantity of orthorhombic YMn_2O_5 and even Mn_3O_4 appear in some samples. These results are in accordance with the results of magnetic measurements. After the optimization of experimental conditions we can conclude that pure hexagonal yttrium manganite can be obtained by two-step sintering at temperatures of 900°C and 1100°C.

P-13

MECHANICAL PROPERTIES OF MICROWAVE SINTERED HYDROXYLAPATITE (HAP)

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In biology and medicine different types of calcium phosphates materials (CaP) play a very significant role. They can be found in a human body as one of the crystalline components of human enamel, dentine, and bones. Calcium phosphate ceramics based on hydroxyapatite due to his chemical composition, excellent biocompatibility, bioactivity and osteoconduction can be used as reparation material in maxillofacial, dental and orthopedic surgery. Hydroxylapatite (HAP) $Ca_5(PO_4)_3OH$ was synthesized by a simple precipitation method. Phase composition of the obtained powder was analyzed by X-ray powder diffraction (XRD), and the morphology of grains was recorded by Scanning electron microscopy (SEM). The HAP powder were compacted by uniaxial pressing at 78 MPa and then by cold isostatic pressing (CIP) at 250 MPa, for microwave sintering. The effect of microwave sintering conditions on the microstructure, phase composition and mechanical properties of synthesized hydroxylapatite (HAP) material was investigated. Nanoindentation and modulus mapping were performed. The micro hardness, toughness and Young’s module was investigated.

P-14

EFFICIENT PHOTOCATALYTIC DEGRADATION OF AZO-DYE RO16 BY PURE AND Eu-DOPED $Pr(OH)_3$ NANOSTRUCTURES

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Mixed nanorods/nanopowders of pure $Pr(OH)_3$ and doped with Eu^{3+} (1, 3, and 5 mol %) were synthesized by microwave-assisted hydrothermal method. The oxides Pr_6O_{11} and Eu_2O_3 were dissolved in aqueous HNO_3 and used as the precursors.

Structural properties of synthesized nanomaterials were analyzed by X-ray diffraction (XRD) spectroscopy. The influence of Eu^{3+} content on structural and morphological characteristics of nanorods/nanopowders was also investigated by Raman spectroscopy and Field Emission Scanning Electron Microscopy (FESEM).

Synthesized nanostructures were tested for photocatalytic degradation of azo-dye Reactive Orange 16 since azo-dyes belong to the most toxic ones among various types of dyes. Eu-doped $Pr(OH)_3$ nanostructures showed very good photocatalytic performances, higher than pure $Pr(OH)_3$.

P-15

PREPARATION OF CARBONACEOUS MICROSPHERES BY HYDROTHERMAL TREATMENT OF FRUCTOSE WITH PHOSPHORIC ACID AND DIAMETER SIZE COMPARISON

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Carbonaceous microspheres have been prepared by hydrothermal treatment of fructose. Parameters such as concentration of carbohydrate, reaction time, treatment temperature and concentration of phosphoric acid have been changed. Obtained

spherical carbonaceous particles maintained their spherical morphology with phosphoric acid concentration under 70%. Sample with 85% phosphoric acid did not give spherical shape of the particles. Comparison of the diameters of the prepared carbonaceous microspheres shows that particle sizes of the material were in the range of 0.6-7.0 µm, depending on reaction conditions. In this work it was shown that diameter of the carbonaceous microspheres can be easily modulated by the change of the reaction conditions, as a function of application needs.

P-16

ELECTRICAL PROPERTIES OF OXYAPATITE $La_{9.33}(SiO_4)_6O_2$

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Lanthanum silicates with the apatite-type structure are the potential new ionic conductors with the high and anisotropic conductivity based on the migration of interstitial oxide ions. In this study $La_{9.33}(SiO_4)_6O_2$ oxyapatite was synthesized from ethanol-water solution of lanthanum nitrate hexahydrate, tetraethyl orthosilicate (TEOS) and glycine by sol-gel combustion method. Single phase powder of crystallized La-apatite with composition $La_{9.33}(SiO_4)_6O_2$ was obtained during the combustion of the gel produced from the solution with the molar ratio of TEOS to H_2O equal 1:20 and the molar ratio of glicine to nitrate ions of 0.56. $La_{9.33}(SiO_4)_6O_2$ powder was uniaxialy pressed and sintered at 1550 °C for 4 h. Relative density of sintered material was 81%. Powder and sintered sample were characterized by X-ray diffraction and scanning electron microscopy. The electrical properties were measured by complex impedance method performed in air atmosphere, in the temperature range 500–700 °C. The obtained values of total ionic conductivity of $4.18\times10^{-3}\ \Omega^{-1}cm^{-1}$at 700 °C and activation energy of 0.37 eV indicate that lanthanum silicates with apatite structure produced by sol-gel combustion method are convenient as new solid ionic conductors.

P-17

SYNTHESIS AND CHARACTERIZATION OF CARBON CRYOGEL/CeO_2 COMPOSITE AND ITS APPLICATION IN ARSENIC (III) ADSORPTION FROM AQUEOUS SOLUTIONS

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Adsorption of As(III) ions from aqueous solutions was studied on resorcinol-formaldehyde (RF) carbon cryogel/CeO_2 composite. The obtained material was characterized using following methods: nitrogen adsorption-desorption measurements, field emission scanning electron microscopy (FESEM), temperature programmed desorption (TPD) and Raman spectroscopy. Also, isoelectric point (IEP) and point of zero charge (PZC) were determined. Dose and kinetic studies were conducted and adsorption of As(III) on CC/CeO_2 was investigated as a function of arsenic concentration and solution pH. The adsorption mechanism of As(III) ions was discussed in view of arsenic speciation and adsorbent PZC.

P-18

PREPARATION AND CHARACTERIZATION OF ACTIVE CARBON FROM BIOWASTE PLANE TREE FRUIT USING H_3PO_4

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Hydrothermal carbonization is used to obtain active carbon from plane tree fruit. Phosphoric acid (H_3PO_4) is used as the activating agent in the preparation. The influences of the chemical agent on the structure of the obtained active carbon material were examined. It was noticed that mentioned process parameter pH value of starting solution affected the structure and characteristics of obtained active carbon material. The pH value of the phosphoric solution was changed in the range of 0.5 to 6. Value of the specific surface areas of treated sample are increased by lowering the pH value. Characterization of obtained active carbon material was

carried out by nitrogen adsorption-desorption isotherms, X ray diffraction (XRD) and scanning electron microscopy (SEM). Functional surface groups were determinated by fourier transform infrared spectroscopy (FTIR).

P-19

INFLUENCE OF DISODIUM ETHYLENEDIAMINE-TETRAACETATE ON THE MORPHOLOGY OF HYDROTHERMALLY SYNTHESIZED UNDOPED AND COPPER-DOPED CALCIUM DEFICIENT HYDROXYAPATITE

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Calcium deficient hydroxyapatite (CDHAp) powders, undoped and doped with Cu^{2+}, were synthesized by a hydrothermal method at 160 °C. Doping was performed with initial solution concentration of 0.4 mol % according to the formula [Cu / (Cu + Ca)] * 100 and on a constant atomic ratio (Ca + Cu) / P = 1.50. In these syntheses the disodium ethylenediaminetetraacetate dihydrate (Na_2EDTA) and urea were added. Na_2EDTA acted as a nucleating agent while urea decomposed during synthesis and changed the pH for precipitation of the product. In order to investigate the influence of the amounts of Na_2EDTA on morphology of powders, Ca / Na_2EDTA molar ratio was 1, 4, 6 and 8. Analyses of all powders, undoped and doped, were performed by field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS) and Fourier transform infrared spectroscopy (FTIR). These analyses confirmed that the amount of Na_2EDTA in the initial solution has significant influence on the particle size and morphology of synthesized powders.

P-20

SYNTHESIS AND CHARACTERIZATION OF POROUS CERAMIC MONOLITHS BASED ON DIATOMITE

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Porous silica ceramics were obtained at a low forming pressure and a low sintering temperature by using diatomaceous earth as a silica source and boric acid as an inexpensive additive. The starting raw material, diatomite from surface coal mine Kolubara, Serbia, was purified from organic and inorganic impurities by using heat and chemical treatment. Boric acid was used as binding and sintering aid up to 2 wt%. Powder was compacted by using different pressures of 40, 60 and 80 MPa. The pressed samples were sintered at 850, 1000, 1150, and 1300 ºC for 4 h in air. Mercury intrusion porosimetry shows that median pore size diameters are in the macroporous range (porous size more than 50 nm), i.e. from 0.2 to 4 µm in the samples sintered at 1150 and 1300 ºC. X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), and mercury porosimetry measurements were employed to characterize the phases, functional groups, and microstructure of the obtained ceramics.

P-21

IMPROVEMENT IN THE MECHANICAL PROPERTIES OF MICROWAVE AND CONVENTIONALLY SINTERED HAP BASED BIOCERAMICS BY ADDITION OF YTTRIA-STABILIZED ZrO_2

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Bioceramic materials based on hydroxyapatite (HAP, $Ca_{10}(PO_4)_6(OH)_2$) are often used to substitute damaged parts of the human skeleton in dental, maxillofacial and orthopedic practice. The implants fabricated by HAP based bioceramics often have low fracture toughness especially in wet environments as would be found in physiological conditions. The aim of this investigation was to improve the mechanical properties, especially fracture toughness of microwave and conventionally sintered hydroxyapatite bioceramic materials by addition of yttria-stabilized ZrO_2 (YSZ). Nano-sized stoichiometric HAP powder was synthesized by modified precipitation method based on the chemical interaction between calcium hydroxide and phosphoric acid, and YSZ, composed of nano-sized particles and spherical particles of micron dimensions, was processed by plasma technique. The composite suspension was obtained by mixing of 20 wt% of YSZ and 80 wt% of HAP under ultrasound treatment and further composite powder was spray-dried. The powders were uniaxially pressed at 100 MPa and isostatically pressed at 400 MPa. The green samples were sintered by single- and two-step microwave technique and the conventional single-step method, in the temperature range of 1200–1300 ºC. The powders and sintered bioceramic compacts was characterized by FESEM, XRD, EDS and by measuring of density, hardness and fracture toughness. It was showed that the present of YSZ powder of bimodal particle size distribution (nano-sized particles with an average size of 0.95 nm and spherical particles of micron dimensions with an average size of 1.7 µm) in HAP matrix significantly affect the density, microstructure, grain size, hardness and fracture toughness of processed bioceramics. It was concluded that incorporated nano-sized particles and micron-sized spherical particles of yttria-stabilized ZrO_2 by two different mechanisms had the effect on the fracture toughness improvement of processed bioceramics. The maximum value of fracture toughness (1.88 $MPam^{1/2}$) was measured in the case of isostatically pressed and further conventionally sintered samples at 1200 ºC for 2 h, which was certainly higher value compared to HAP bioceramic materials without stabilized ZrO_2 particles. Bioceramics with also high value of fracture toughness (in

the range of 1.58 - 1.82 MPam$^{1/2}$), but with slightly lower hardness compared to conventionally processed samples was obtained by microwave sintering in single- and two-step at certainly lower temperatures.

P-22

ENHANCED ANTI-DELIQUESCENT PROPERTY AND ULTRALOW THERMAL CONDUCTIVITY OF MAGNETOPLUMBITE-TYPE $\mathbf{LnMeA_{11}O_{19}}$ VIA A PANOSCOPIC APPROACH

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Magnetoplumbite-type $LaMgAl_{11}O_{19}$ ceramics have been proposed as one of promising candidates for the next generation thermal barrier coatings (TBCs) duo to its low thermal conductivity. However, $LaMgAl_{11}O_{19}$ showed poor water-resistance with significant weight loss at elevated temperatures in water containing atmosphere. Here we reported the primary cause for the poor water-resistance of magnetoplumbite-type $LaMgAl_{11}O_{19}$ ceramic and proposed an effective approach to improve its anti-deliquescent property by completely substituting divalent alkaline earth ions Mg^{2+} with Zn^{2+}. Further more, La-Zn sites co-substituted $LaZnAl_{11}O_{19}$ ceramics with nano-platelet-like microstructures were synthesized through citric acid sol-incorporated alumina aerogels. The mechanism behind the lowered thermal conductivity was due to the panoscopic approach, which providing all-scale hierarchical architectures of phonon scattering mechanisms. The excellent anti-moisture performance and ultralow thermal conductivity qualify the $LaZnAl_{11}O_{19}$ based-bulk ceramics as a kind of promising candidates for advanced thermal barrier coatings.

P-23

SINTERING AND CHARACTERIZATION OF TUNGSTEN CARBIDE WITH TUNGSTEN SILICIDES AS SINTERING ADDITIVES

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Tungsten carbide (WC) is interstitial carbide, with properties characteristic for both ceramic and metal materials, such as high melting point, very high hardness, low friction coefficients, low reactivity, high oxidation resistance, and good thermal and electrical conductivity. Those properties make him appropriate material for usage in hard metal industry. High temperatures, above 1600 °C, are required to sinter pure WC. In this research tungsten silicides (W_5Si_3 and WSi_2) were used as sintering additives, in a different percentage (5, 7.5, and 10 %). The mixtures of commercial WC and home made additives were spark plasma sintered. Phase analysis of the material was conducted using X-ray diffraction. The experimental determination of density was done using Archimedes method. Nanoindentation tests were applied to determine hardness, toughness and Young's modulus of material. Surface was observed using atomic force microscopy (AFM). The microstructural observation was performed by scanning electron microscopy (SEM). Cavitation resistance was observed with a cavitation erosion test. Characterization was done on all materials, and results were compared.

P-24

CHARACTERIZATION OF METAKAOLIN BASED GEOPOLYMERS

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Geopolymerization is a very promising innovative technology that can transform between the other raw materials useless industrial solid wastes of aluminosilicate composition into useful products competitive with many known construction materials. A variety of industrial minerals as kaolinite and feldspar and industrial solid residues or wastes such as fly ashes, metallurgical slags, and mine wastes have been used for the synthesis of geopolymers. Geopolymerization includes a chemical heterogeneous reaction between aluminosilicate compounds and alkali silicate solutions under strong basic conditions and mild temperatures, which leads to the creation of polymeric Si–O–Al and Si–O–Si frameworks. The hardening of geopolymers is based on polycondensation reactions of alkali (Na or K) oligo-(sialatesiloxo) precursors that have been formed from the dissolution of active silicates and/or aluminosilicate solid raw materials in alkali (Na or K) hydroxide solutions. Due to they have very good physicochemical and mechanical properties, geopolymers can be used in a broad field of applications and especially in the construction sector.

This paper examined the characterizations of the metakaolin and metakaolin based geopolymers and materials were obtained in process of heating geopolymers in air conditions at 600 and 900^oC (GP600 and GP900, respectively). Metakaolin was made by thermally treating raw kaoline originated from Serbia at 750^oC in air conditions. The geopolymer was made by condensing a mixture of metakaolin and alkali solution at room temperature, curring two days at 50^oC. The structure and properties of the metakaolin and metakaolin based geopolymers were studied by X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) spectroscopy.

Microstructure/chemical analysis of the obtained materials in process of heating geopolymers in air conditions at 600 and 900^oC was done using scanning electron microscope (SEM/EDS). Phase identification was carried out by XRD analysis. Also, the density all of the samples were measured by the Archimedes' principle (water displacement). Mechanical properties such as compressive strength and Vickers hardness of the geopolymers are presented and mean value reaches 24.6 MPa and 26.2 MPa respectively while Vickers hardness of GP600 material is 168.6 MPa.

P-25

MECHANICAL PROPRETIES OF POROUS CERAMIC MONOLITHS BASED ON DIATOMITE

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Diatomite from surface coal mine Kolubara, Serbia, was used as a silica source. Firstly, diatomite was purified from organic and inorganic impurities by the heat and chemical treatments. Secondly, boric acid was used as a sintering aid up to 2 wt%. So, after using different pressures of 40, 60, and 80 MPa, the compacted samples were sintered at 850, 1000, 1150, and 1300 ºC for 4 h in air. A relatively high porosity in the range of 60-70% is obtained for the samples pressed at the applied pressures and sintered at 1000 ºC. The relations between mechanical properties like Young modulus, Poisson ratio, and compressive strength versus content of boric acid in the investigated samples were studied and discussed. Young modulus increases with lowering porosity in the samples sintered at 1300 ^{o}C, while Young modulus of the samples sintered at 1150 ^{o}C are assumed to be almost linear function of the forming pressure. Compressive strength of the observed samples is higher for the samples sintered at 1300 ^{o}C in comparison with the samples sintered at 1150 ^{o}C.

P-26

STRUCTURAL AND ELECTRONIC PROPERTIES OF PSEUDOBROOKITE

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Starting powders of TiO_2 (anatase) and Fe_2O_3 (hematite) were mixed in the molar ratio 1:1. Pseudobrookite powder was obtained by a combined milling/calcination procedure. Particle size distribution was analyzed on a laser

particle size analyzer and correlated with XRD and SEM analysis. The band gap was determined using UV/Vis spectroscopy. Green samples were sintered in a dilatometer and at 1000°C for 2h in air. Thermal diffusivity was determined from photoacoustic measurements. Electrical conductivity measurements were performed. The aim was to obtain pseudobrookite with properties suitable for polymer paste for thick films to be applied as gas sensors.

P-27

SAFE TRAPPING OF Cs RADIONUCLIDES IN THERMALLY TREATED MATRIX OF NATURAL ZEOLITE-CLINOPTILOLITE

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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 natural zeolite-clinoptilolite was prepared by standard procedure. Powder and cold pressed powder of Cs-exchanged clinoptilolite samples were heated at 1200 ^{0}C and compared. After thermal treatment, both Cs-exchanged clinoptilolite samples (non-sintered and sintered) showed satisfactory Cs ions retention during leaching test. Obtained results indicate that these cesium aluminosilicate ceramic forms are promising for the permanent immobilization of Cs radionuclides.

P-28

THE ANALYSIS OF KEY PARAMETERS FOR THE PRODUCTION OF GLASS-CERAMICS FROM FINAL FLOTATION WASTE

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The manufacturing processes of non-ferrous metals and their alloys, particularly the flotation enrichment and metallurgical processing, generate waste materials that cause environmental pollution. Flotation waste dumps and slag from smelters covers large areas of land and presents the permanent sources of pollution of soil, water and air. According to the fact that those are materials of ferro silicate composition, examining a possibility of their use as a row material is of great significance.

The paper presents the analysis of some important parameters for the control of technological process of glass-ceramics production from final flotation waist from in RTB Bor Company, Serbia. We found that it is possible to control the kinetics of sintering by controlling the particle size distribution of final flotation waist, or heating regime or both. That provides a solid basis for the determination the optimal results in the production of glass-ceramics.

Key words: Kinetics of sintering, Final flotation waste, Heating regimes, Particle size distribution, Glass-ceramics

P-29

TWO STEP SINTERING OF THE $ZnTiO_3$ NANOPOWDER

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Metastabile nanopowder $ZnTiO_3$ pressed into cylindrical compacts at 200 MPa was submitted to conventional heating with isothermal holding at 931°C for 10 minutes, 25 minutes and 40 minutes. Same compacts were heated with two-step sintering schedule with maximal 912°C and isothermal holding at 896oC, for approximately the same holding times as with isothermal. Shrinkage during heating was monitored with dilatometric device, while microstructure was determined with atomic force microscopy. XRD patterns were collected for the most prominent samples. Sintered specimens microstructure showed differences introduced during last sintering stage by two heating schedules.

P-30

TAILORING THE MICROSTRUCTURE OF Mn-Zn FERRITE TO ELECTRONIC PROPERTIES

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Commercial Mn-Zn ferrite powder was milled in a planetary ball mill for 30-240 minutes. Particle size distribution in the milled powders was analyzed using a laser particle size analyzer and correlated with XRD and SEM analysis of the milled powders. Green disc and torroid samples were sintered in air in the temperature interval 800 -1300°C for 2 hours. SEM/EDS, AFM/MFM analysis of the sintered samples and measurements of their electrical properties such as DC resistance up to 500 MHz enabled establishment of a correlation between the microstructure and properties in the high-frequency range.

P-31

HOLLOW NANO-GRAINED CERAMICS WITH ULTRALOW THERMAL CONDUCTIVITY AND HIGH MECHANICAL STRENGTH

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The desire for materials with ultralow thermal conductivity for energy conservation and thermal protection/insulation has greatly motivated research and development recently. Despite significant progress made to date, the synthesis of bulk materials with ultralow thermal conductivity and high mechanical strength is still a challenging task. Herein, we propose a new concept of hollow nano-grained materials to solve this problem, where pores are isolated within individual nano-sized grains to lower thermal conductivity and to retain structural integrity for high mechanical strength. We have proved the concept with hollow-grained $La_2Zr_2O_7$ ceramic. We demonstrate that the material exhibits exceptionally low thermal conductivity (0.016 $Wm^{-1}K^{-1}$), which is the lowest value that has ever been reported for bulk materials and even lower than that of air, as well as ultrahigh strength (251.3 MPa) and excellent thermal stability (up to 1400 ^oC). The unique behavior of the material has been compared with theoretical models to elaborate the effect of structural parameters. The results open up a new possibility to design and develop new high performance super-insulating material systems.

P-32

SPIDER SILK BASED MATERIALS

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During the evolution, insects and in particular spiders have developed silk spinning skills which lead to formation of fibers with a different purpose such as pray capture, egg case formation, dragline and sticky silk formation, etc. Spider silk is well known by its excellent mechanical properties, its strength and toughness, but also high elasticity. Because of that, spider cobweb and its remarkable performances is competing with the best materials made by men. Carbonization of crude cobweb and embedding metal in structure of cobweb before carbonization can result in creation of new materials which mechanical properties have been examined. This material has a great potential for being used in medical application, tissue engineering, drug delivery, filters for water purification and much more.

P-33

THE INFLUENCE OF TEMPERATURE ON MICROSTRUCTURE OF MULLITE SINTERED AT HIGH PRESURE

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The effect of sintering temperature on microstructure and density of the sintered mullite samples during the high pressure sintering process was investigated. High pressure sintering is one of the effective methods for producing fully dense bulk ceramics products enhancing densification and limiting grain growth. Synthesized mullite precursor powder was calcinated at 1200 °C for 4 h in order to obtain crystalline mullite powder that was confirmed by XRPD analysis. To determine the optimum sintering temperature for obtaining fully dense mullite samples crystalline mullite powder was compacted at 4.0 GPa in the temperature range 1100-1500 °C with step of 100 °C for 60 s. The measured densities of sintered samples rise with increasing the sintering temperature due to recrystallization of mullite particles. The particles of the starting powder are agglomerated while the microstructure of sintered samples reveals needle-like grains. The needles become elongated with increasing the temperature of sintering process and reach the grain length about 5 μm at 1400 and 1500 °C whereas the grains at 1500 °C are wider.

P-34

COMPARATIVE STUDY OF STRUCTURAL AND ELECTRICAL PROPERTIES OF Pr(Ce)-DOPED BiFeO$_3$ CERAMICS BY AUTO-COMBUSTION METHOD

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Polycrystalline ceramics of pure and Pr(Ce) doped BiFeO$_3$ (Bi$_{1-x}$Pr(Ce)$_x$FeO$_3$, x=0.03, 0.05 and 0.1) were synthesized by auto–combustion method using urea as fuel. The structural, vibrational, morphological, dielectric and ferroelectric properties of Bi$_{1-x}$Pr(Ce)$_x$FeO$_3$ polycrystalline ceramics at room temperature were examined by X–ray diffraction (XRD), Raman spectroscopy, Scanning electron microscopy and dielectric and ferroelectric measurements. The XRD and SEM measurements showed that the crystallite (particle) size of doped samples decreased. XRD and Raman measurements revealed the structural phase transition from rhombohedral to orthorhombic (pseudotetragonal) phase in the samples doped with 10% of Pr(Ce).

The pristine BiFeO$_3$ exhibited non-saturated P-E loop, typical for conductive BiFeO$_3$. The room-temperature P-E loop study of doped samples showed that partial substitution of Bi^{3+} ions with Pr$^{3+(4+)}$ and Ce$^{3+(4+)}$ ions reduced the concentration of oxygen vacancies and leakage current of BiFeO$_3$, although the saturation and remnant polarization in doped samples were lower than in pristine BiFeO$_3$. The saturation polarization increased (decreased) with Pr(Ce) doping. Up to 10% of Pr(Ce) substitution, significant reduction of dielectric loss and low-frequency dielectric constant dispersion was noticed. The structural transition influenced the ferroelectric and dielectric properties of Pr(Ce) doped BiFeO$_3$.

P-35

TAILORING THE DIELECTRIC PROPERTIES OF SPINEL FERRITE (MFe_2O_4) CERAMICS BY INCORPORATING DIFFERENT CATIONS (M = Mn, Mg, and Zn) IN THE STRUCTURE

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Spinel ferrite (MFe_2O_4; M = Mn, Mg, and Zn) ceramics with mean crystallite sizes in the nm–range were successfully prepared by a conventional sintering of powders, synthesized by using soft mechanochemical route. The structural studies have been made by using the X–ray diffraction, transmission microscopy, and Raman spectroscopy, which confirmed the presence of single cubic spinel phase in MFe_2O_4 and their nanostructured nature. In the frequency range of 10^2 Hz to 10^6 Hz, the dielectric properties were examined at and above ambient temperature. The results revealed that the dielectric constant of prepared ferrites is significantly influenced by the incorporated different cation in the spinel structure. Further, the dielectric constant and loss tangent of all ferrite samples decrease with increase in frequency, while these parameters increase with increasing temperature. Such dielectric behavior is explained by using the mechanism of polarization process, which is correlated to hopping of charge between Fe^{2+} and Fe^{3+} ions at octahedral sites.

P-36

ELECTRICAL AND MAGNETIC PROPERTIES OF MULTIFERROIC $Bi_5FeTi_3O_{15}$ AND $Bi_{4.25}La_{0.75}Ti_3FeO_{15}$ CERAMICS

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Multifferioc materials exhibiting ferroelectric and magnetic orders simultaneously have attracted a lot of interest in recent years due to their special phenomena and potential applications in multifunctional devices [1]. One of the most frequently investigated single-phase multiferroic materials is perovskite $BiFeO_3$ (BFO) but it shows weak ferromagnetics at room temperature due to its canted spin structure. Among the compounds, $Bi_5FeTi_3O_{15}$ (BFT) ceramics can be regarded as a model of the Aurivillius type of ferroelectromagnetics.

BFT was prepared by solid state reaction methods from the constituting high purity oxides (Fe_2O_3, Bi_2O_3, TiO_2 and La_2O_3). XRD data confirm the formation of single-phase Aurivillius compounds while SEM micrographs shows a evident decrease of grain size of La modified ceramics in comparison with pure BFT. Dielectric properties were investigated in a wide range of temperatures (300-1000 K) and frequencies (1 Hz – 1 MHz). The conductivity of sintered samples was studied, suggesting decreasing of conductivity of La modified ceramics in comparison with pure BFT. Ferroelectric and ferromagnetic measurements of both samples were also performed.

1. Nicola A. Hill, *J. Phys. Chem. B*, **104** (2000) 6694

P-37

MAGNETIC AND ELECTRICAL PROPERTIES OF SINGLE PHASE MULTIFERROIC $BiFeO_3$

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Single-phase BFO perovskite crystallites have been prepared from bismuth and iron nitrates by using the hydrothermal method assisted by KOH. Optimum conditions for the synthesis of single-phase $BiFeO_3$ ceramics were obtained. It was found that KOH as a mineralizer played an important role in the formation of $BiFeO_3$ nanoparticles. We have reported the structural, microscopic, magnetization and dielectric properties of $BiFeO_3$ ceramics. The microstructure, morphology and chemical analysis of the powders were analyzed using Scanning Electron Microscopy (SEM) combined with X-ray microanalysis (by Energy Dispersive Spectrometer – EDS) and transmission electron microscopy (TEM). The phase composition of obtained samples was determined by X-ray diffraction (XRD) analysis. It revealed that synthesized material crystallize in space group $R3c$ with cell parameters $a = b = 5.5780(10)$ Å and $c = 13,863(3)$ Å. ^{57}Fe Mössbauer spectroscopy was performed in order to provide information on Fe cation arrangement in the $BiFeO_3$ phase. The magnetic behavior of synthesized material is done by means of SQUID device.

P-38

ULTRASONIC PRETREATMENT OF NANOPRECURSORS – INFLUENCE ON ELECTRICAL CHARACTERISTICS OF HIGH VOLTAGE ZnO VARISTORS

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Application of nanopowders for varistors preparation provides possibilities for enhancement of electrical characteristics. Mixture of nanoprecursors: Co/Mn doped ZnO, Bi_2O_3 and Sb_2O_3 was prepared in 70:25:5 mass ratio, respectively. Additives Bi_2O_3 and Sb_2O_3 were introduced into previously synthesized Co/Mn doped ZnO through the solution of $Bi(NO_3)_3x5H_2O$ and $Sb(CH_3COO)_3$ salts and subsequent calcination. Ultrasonic pretreatment was performed on ethanolic powder dispersion for a period of 10 min. Series of pellets of pretreated and untreated powder were pressed and sintered at 770 °C, 850 °C, 900 °C, 950 °C and 1000 °C for 1 hour. XDR analysis of sintered varistors showed the presence of ZnO, γ- or β-Bi_2O_3 and $Zn_2Bi_3Sb_3O_{14}$-type pyrochlore, whereas the appearance of β-Bi_3SbO_7 was noticed in samples sintered at 770 °C. Densities of obtained varistors were in the range of 71–88% of the theoretical value. Significant increase of the breakdown field values was observed with the samples prepared from ultrasonically pretreated precursors, together with the decrease of the mean ZnO grain size. The most pronounced effect was established comparing the samples sintered at 900 °C, with the decrease of the mean grain size of 20% and the increase of the breakdown field of 41%. It was concluded that ultrasonic pretreatment was effective not only for the reduction of the grain size, but also for more uniform phase distribution in varistors ceramics, which resulted in increased number of electrically active grain boundaries. Both factors at the same time contributed to the improvement of the breakdown field values.

P-39

ELECTRICAL PROPERTIES OF $Ca_{1-x}Gd_xMnO_3$ ($x = 0.05–0.20$) NANOPOWDERS

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Nanosized powders with composition $Ca_{1-x}Gd_xMnO_3$ ($x = 0.05–0.20$) were successfully synthesized by modified glycine nitrate procedure (MGNP). Sintering of the green bodies was carried out by conventional sintering (CS) method at 1400 ºC in an air atmosphere. A single–phase crystalline form was evidenced by X–ray diffractometry for all sintered samples. SEM analysis confirmed that the sintered samples displayed a dense microstructure, low porosity, with the mean grain size in the range of 1–2 μm. The electrical conductivity of Gd^{3+} doped sintered samples $CaMnO_3$ in function of temperature was measured by complex impedance method, in the temperature range 300–700 ºC. The corresponding activation energies of conductivity, measured in the investigated temperature range, were also discussed.

P-40

ELECTRICAL PROPERTIES OF BARIUM TITANATE CO-DOPED WITH Nb AND Mn

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A modified Pechini process was used to prepare nanopowders of barium titanate (BT) co-doped with niobium and manganese. Prepared BT compositions were (1) BT doped with 0.4 mol% Nb and 0.1 mol% Mn (BT1); (2) 0.4 mol% Nb and 0.05 mol% Mn (BT2) and (3) 0.8 mol% Nb and 0.01 mol% Mn (BT3). The XRD results of sintered samples showed the formation of barium titanate tetragonal crystal structure. Microstructure was consisted of polygonal grains but the differences in the grain size, homogeneity and porosity between the doped ceramics were noticed. The addition of dopants influenced the grain size and microstructure development. The dielectric measurements of all ceramics showed the behavior of classical ferroelectric material. In comparison with pure barium titanate, structural transition of all co-doped ceramics are shifted to lower temperatures. The real permittivity value increase in all co-doped ceramics in the whole frequency range, reaching much higher values then in pure barium titanate ceramics obtained by polymeric precursors method. The analysis of impedance spectrum at higher temperatures showed the presence of both, grain interior and grain boundary effects.

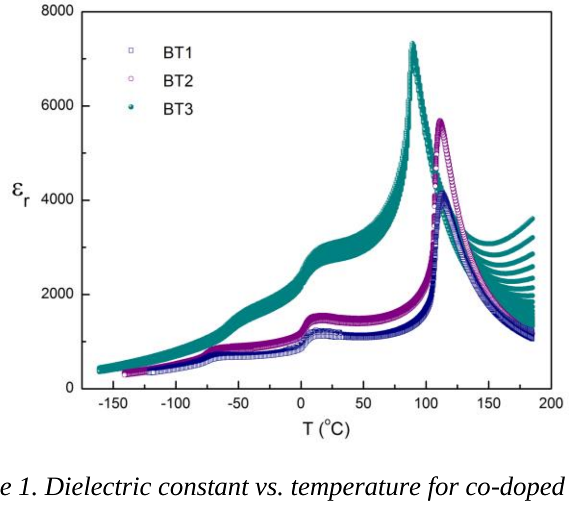

Figure 1. Dielectric constant vs. temperature for co-doped BT ceramics

P-41

ELECTRONIC PROPERTIES OF PSEUDOBROOKITE NANOSTRUCTURED THICK FILMS

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Thick film pastes were formed using TiO_2 (anatase) and Fe_2O_3 (hematite) nanopowder in different weight ratios, organic vehicle and glass fritt. Two types of test matrices (sandwich and interdigitated) were screen printed on alumina substrate using conductive PdAg paste and sintered at 850°C/10 minutes in a conveyor furnace. The sandwich thickness and interdigitated electrode spacing were varied. UI characteristics were measured enabling determination of the voltage threshold typical for oxide semiconductors. Measurements of DC resistance vs. temperature enabled determination of the exponential factor B from NTC behavior.

P-42

MAGNETIC PROPERTIES OF NICKEL MANGANITE OBTAINED BY A COMPLEX POLYMERIZATION METHOD

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Spinel materials based on Mn and Ni has been intensively studied over the past years due to their excellent semiconductor properties. Nickel manganite as NTC thermistor is widely used today in different industrial sectors. Here we report the complex polymerization method (CPM) for producing nickel manganite fine particles with a homogeneous distribution of constituent cations in the crystal lattice

that ensures formation of dense monophased ceramic with the novel magnetic properties after been sintered in oxygen and air atmosphere. Phase composition of the synthesized materials was examined by XRPD, while the morphology of the powder and microstructure of ceramic were investigated using FESEM and SEM analyses, respectively. The magnetic properties of the samples have been studied by measuring the temperature and field dependence of magnetization.

Magnetic measurements of M(T) reveal rather complex magnetic properties and multiple magnetic phase transitions. In the case of air atmosphere we found three magnetic phase transitions with transition temperatures at T_{M1}=35 K, T_{M2}=101 K and T_{M3}=120 K. T_{M1} maximum is strongly dependent on the strength of the applied magnetic field (T_{M1} decreases with increasing applied field) whereas the T_{M3} is field independent The values of the coercivity, remanent magnetization and saturation magnetization at 100 K are: H_C = 184 Oe, Mr = 1.92 emu/g and M_S = 7.88 emu/g, respectively. The measured values at 5 K are H_C = 1035 Oe, Mr = 7.70 emu/g and M_S = 14.47 emu/g. Moreover, hysteresis properties measured after cooling of the sample in magnetic field show exchange bias effect with an exchange bias field $|H_{EB|}$=196 Oe.

For the sample synthetized in oxygen atmosphere, the magnetization dependence of temperature M(T) and AC susceptibility data obtained from SQUID measurements clearly demonstrates that quadruple magnetic phase transitions can be readily detected at T_{M1}~115 K, T_{M2}~105 K, T_{M3}~38 K and T_{M4}~7 K. These findings suggest the novel magnetic transition for nickel manganite at low temperature T_{M4}. The temperatures of observed maximums in χ'(T) and χ''(T) parts of susceptibility are frequency independent, whereas the height of the peaks decreases with increasing frequency. The fact that T_{M4} does not shift with the increase of the frequency led us to the conclusion that there are no spin-glass/surface effect and/or blocking temperature/finite size effect connected to the $NiMn_2O_4$ ceramic. Therefore, the low-temperature peak T_{M4} in AC susceptibility is associated with ferromagnetic-like and antiferromagnetic-like magnetic transition in the interfacial FM/AFM internal structure. The exchange bias effect was found in a field cooled hysteresis loops at 5 K. The field cooling of the sample was under a magnetic field of 100 Oe and 10 kOe whereas the determined exchange bias fields were $|H_{EB}|$=129 Oe and 182 Oe, respectively. The analysis of the results and comparison with literature data allowed us to conjecture that the mixed oxidation states of Mn ions and ferromagnetic and antiferromagnetic sublattice orders tailor these interesting magnetic properties.

P-43

SYNTHESIS AND CHARACTERIZATION OF COBALT FERRITE NANOSPHERES

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In the last twenty years cobalt ferrite nanoparticles (CFO NPs) have been attracting considerable attention because of their high coercivity, moderate saturation magnetization, large magnetocrystalline anisotropy, large magnetostrictive coefficient, chemical stability and mechanical hardness. Due to these properties the CFO NPs can be used in optics, electronics, ferrofluids, biomedicine, recording media, etc.

In the present work the CFO nanospheres were prepared in high yield via one-step and template free solvothermal method. The obtained samples were characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and vibrating sample magnetometry (VSM). The XRD results confirmed the cubic spinel structure of CFO. The SEM revealed that the diameters of CFO nanospheres are in the range of 100-300 nm, each being composed of smaller CFO nanoparticles (7-8 nm) as observed by TEM. The VSM investigations of CFO nanospheres showed ferrimagnetic character with the maximum saturation magnetization, remanent magnetization and coercivity of 75 emu/g, 23 emu/g and 677 Oe, respectively. Due to high saturation magnetization the obtained CFO nanospheres can potentially be used for magnetic removal of heavy metals in wastewater.

P-44

CONTROL OF PORE SIZE AND WALL THICKNESS AND THEIR EFFECTS ON PIEZOELECTRIC COEFFICIENT OF 3-1 TYPE POROUS PZT CERAMICS BY FREEZE-CASTING PROCESS

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3-1 type porous lead zirconate titanate (PZT) ceramics with unidirectionally aligned pore channels have been prepared by freeze-casting process of PZT/tert-butyl alcohol (TBA) slurry. By adjusting the freezing temperature of -10, -25, -40, -60, -78 and -100 °C and the solid content of slurry of 15, 20, 25, 30, 35 and 40 vol%, different pore size and ceramic wall thickness were obtained and their effects on piezoelectric coefficient (d_{33}) of the PZT ceramics were studied. The results show that the freezing temperature significantly influences microstructure such as pore size and wall thickness of the porous ceramics, while the solid content of slurry makes a great difference on the porosity. With the same solid content of slurry, both the pore size and wall thickness decrease with decreasing freezing temperature. Within a certain freezing temperature range, thinner wall thickness and smaller pore size are both conducive to the piezoelectric properties. When the freezing temperature is fixed, the porosity linearly decreases as the solid content increases, resulting in enhanced piezoelectric coefficient regardless of microstructure variations.

P-45

SYNTHESIS AND CHARACTERIZATION OF BULK $(Cr_{1-x}Mn_x)_2AlC$ (0<x<0.2) MAX PHASE SOLID SOLUTIONS

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A novel magnetic $(Cr_{1-x}Mn_x)_2AlC$ ceramic (where x is varied between 0 and 0.2) belonging to the family of the MAX phases, was successfully fabricated in bulk by substitution of Cr with Mn on the M site through Spark Plasma Sintering of Cr, Mn, Al and Cr_3C_2 powders. EDS and EBSD studies showed that solubility of Mn in Cr_2AlC reaches maximum value of 16 at.%. Addition of more than 16 at.% of Mn resulted in the formation of large amount of different secondary phases. Results of XRD analysis showed that c-lattice parameter decreases linearly while a-lattice parameter remains almost constant with addition of Mn. Magnetic measurement on bulk $(Cr_{1-x}Mn_x)_2AlC$ (0<x<0.2) indicated that magnetic behavior of these solid solutions changed from paramagnetic Cr_2AlC to a weak ferri-magnetic response by addition of Mn on the M site. According to TEM and EDX analysis, $(Cr_{1-x}Mn_x)_2AlC$ has a typical nano-laminated structure for MAX phase with nonuniform distribution of Mn on the M site. These results reviled existence of Mn-rich and Mn-poor region formed by Mn incorporated into Cr_2AlC MAX phase, with the size of approximately 10 nm. The existence of those regions with nonuniform distribution of Mn is believed to be the reason for complex magnetic response that was observed in in $(Cr_{1-x}Mn_x)_2AlC$. Effect of substitution of Cr with Mn on the magnetic properties of $(Cr_{1-x}Mn_x)_2AlC$ is discussed in more details in this paper.

P-46

THE EFFECT OF VOLUME FRACTION OF YAG ON MECHANICAL PROPERTIES OF Al_2O_3/YAG COMPOSITE

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Mechanical properties of Al_2O_3 were improved by addition of 7-28 vol% of yttrium aluminium garnet ($Y_3Al_5O_{12}$) commonly called YAG. Al_2O_3/YAG composite was fabricated by sintering a mixture of previously prepared YAG powder and commercially available Al_2O_3 powder at 1550 °C for different sintering time. YAG powder was obtained by calcination of YAG precursor powder synthesised by aluminium nitrate-yttrium nitrate glycine reaction. Characterization of YAG powder was performed by DTA analysis, X-ray diffraction and BET technique. Mechanical properties such as fracture toughness, fracture strength and hardness were measured. It was found that the presence of YAG suppresses densification of the composite. Therefore longer sintering time than that for pure alumina was needed to achieve sufficiently high density. YAG grains not only inhibited the growth of Al_2O_3 grains but also interacted with the crack tip which increased fracture toughness of the composite comparing to monolithic Al_2O_3. No considerable decrease in hardness was measured.

P-47

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

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$NiZnFe_2O_4$ (NZF) powder was prepared by auto-combustion method starting from nickel, zinc and iron nitrates. Thermal treatment was performed at 1000 °C for 1 h after which the nickel ferrite powder was formed. Barium titanate (BT) powder was prepared with same method using titanyl nitrate and barium nitrate as a starting reagents. Multiferroic composites with formula $BaTiO_3$– $Ni_{(1-x)}Zn_xFe_2O_4$ (x = 0.3, 0.5, 0.7) were prepared by mixing chemically obtained NZF and BT powders in the planetary mill for 24 h. Powders were pressed and sintered at 1170 °C for 4 h. Samples were characterized by XRD, Raman, SEM, IR. Magnetic and electrical measurements were also carried out. X-ray and Raman measurements confirmed the presence of NZF, BT phases and the traces of barium ferrite phase. The microstructure of the ceramics shows (Fig. 1.) the formation of polygonal (NZF grains), rounded (BT grains) and plate like grains (barium ferrite phase). The impedance analyses of multifferoic composites at 200 °C have shown the contribution of both, grain and grain boundary resistivity.

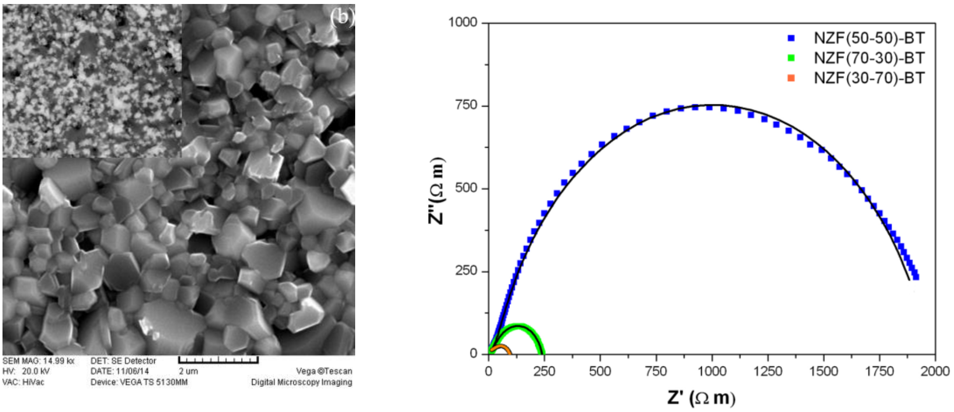

Figure 1. SEM images of NZF(50-50)-BT and impedance measurements

P-48

THE EFFECT OF “AMORPHOUS KAOLIN” ON PROPERTIES OF CEMENT-BASED COMPOSITES

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Although pozzolanic materials are used successfully in many countries, nowadays the goal of many studies is to manufacture new pozzolans for making high strength composites. In that sense, influence of different cement replacement level with the amorphous kaolin, obtained by mechanochemical treatment, in the cement-based composites was investigated. The cement-based composites, made with amorphous kaolin and addition of hydrated lime, water glass, standardized quartz sand and superplasticizer, were exposed to autoclaving curing. The obtained result of the compressive strength 91.2MPa, in composite with cement replacement level of 50% of amorphous kaolin, is slightly higher than those obtained on control sample. It was concluded that amorphous kaolin can be classified as advanced material, which use in cement-based composites have numerous technical and ecological advantages.

P-49

GRAPHENE OXIDE-REINFORCED VANADIA PAPER WITH AN EXTRAORDINARY COMBINATION OF STRENGTH AND FLEXIBILITY

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Vanadia (V_2O_5) is a promising material for advanced Li-ion battery electrodes. However, its small diffusion coefficient for Li-ions and low electrical conductivity have limited the realization of high performance vanadia-based electrodes so far. As a major step forward, we have recently developed vanadia nanofiber-based papers exhibiting a large surface area and shorter diffusion paths for Li-ions. Here, we

report further improvement of this paper through incorporation of graphene oxide sheets (GO) during the self-assembly of vanadia fibers in aqueous solution. Incorporation of GO yields composite papers with better mechanical performance compared to the single-component papers. Another outstanding property of the paper is pronounced macroscopic flexibility combined with high stiffness. We demonstrate that the excellent mechanical performance arises from a hydrogen bond network between the two components. Thermal reduction of the GO to graphene by thermal annealing in vacuum furthermore increases the electrical conductivity.

P-50

INVESTIGATION OF THIN TITANIUM OXIDE LAYERS ON THE SURFACE OF TITANIUM IMPLANTS

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Biological properties of titanium and its alloys can be enhanced by formation of thin oxide layers on their surface. In this research, the titanium substrate was etched with NaOH and subsequently thermally treated at various temperatures between 300 and 800 °C. Methods of X ray diffraction, Fourier transformed infrared spectroscopy and Auger electron spectroscopy were used to get insight into the chemical changes and changes of Ti oxidation states and consequent phase analysis, along the depth of the titanium oxide coatings. Secondary Electron Imaging showed very interesting nanotopology of all samples, consisting of very thin nano-designed walls between mutually interconnected pores. This structure seems to be promising for further deposition of hydroxyapatite coating and also as a suitable scaffold for cell adhesion and proliferation.

P-51

MODIFIED SERPENTINITE AS AN ACTIVE MATERIAL FOR WATER PURIFICATION: ADSORPTION-SORPTION AND ELECTROCHEMICAL CHARACTERISTICS

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Serpentinite is a rock which consists predominantly of one or more serpentine group minerals: antigorite, chrysotile, and lizardite. Besides traditional applications, large serpentinite reserves have the potential for being used also in more sophisticated non-traditional fields. This study aimed to examine modified serpentinite adsorption-sorption characteristics towards Cd^{2+} and anionic textile dyes (Procion red MX-5B, Procion orange and Ramazol black) in aqueous solutions as well as its potential application for the purification of real water systems. All adsorption experiments were carried out in batch conditions by varying initial parameters, such as contact time, mass of adsorbent, pH etc. Based on the obtained results, modified serpentinite has proven to be efficient, cost-effective adsorbent whose specific application should be purification of drinking and other types of waters. Its electrochemical characteristics were examined by using cyclic voltammetry of potassium ferrocyanide ($K_4Fe(CN)_6$), a redox model compound. Due to its specific structure, surface groups, morphology and non-stoichiometric composition, modified serpentinite exhibited prominent electrocatalytic activity. SEM and XRD experimental techniques were employed to study the surface morphology and structural properties of active material.

P-52

PAPER-LIKE SnO_2 NANOHYBRID ELECTRODES REINFORCED BY GRAPHENE OXIDE FOR BATTERY APPLICATIONS

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The high energy storage capacity of tin oxide (SnO_2) renders it a promising electrode material in Li-ion batteries. However, its brittleness and low electrical conductivity limits such applications. This necessitates suitable strategies to deal with the large volume changes that occur during lithium ion intercalation, as well as to ensure a fast electron transport within the electrode.

We address these two main hurdles by fabricating a nanostructured paper-like composite wherein SnO_2 nanostructures are combined with graphene oxide (GO). In this hybrid material, the SnO_2 nanostructures serve as lithium storage units, while the GO sheets function as charge transport elements. As one advantage, the large surface area of the SnO_2 nanoparticles leads to short diffusion paths for Li ions. Moreover, the high mechanical flexibility of graphene oxide is well suited to accommodate the volume change of SnO_2 nanostructures occurring upon Li insertion.

We have combined both, thin SnO_2 nanoplatelets and nanofibers with graphene oxide sheets by a solution-based self-assembly process at room temperature. Thus obtained nanostructured paper with a thickness of several micrometers comprises an alternating layer architecture of graphene oxide sheets and SnO_2 nanostructures, which imparts high mechanical stability along with extreme macroscopic flexibility. The influence of graphene oxide content on the mechanical properties of the paper (hardness and Young’s modulus) has been investigated by nanoindentation. It turned out that for a GO content larger than 50 wt%, the Young’s modulus of the paper is reduced while the hardness is preserved. In order to chemically reduce the GO sheets and thus enhance the electrical conductivity of the composites, the samples were subjected to thermal annealing. In this manner, the electrical resistivity of the paper could be substantially decreased by up to several orders of magnitude. In summary, our experiments demonstrate that a useful paper-like electrode material for Li-Ion batteries is accessible by taking benefit of the combined properties of SnO_2 nanoparticles and graphene oxide sheets.

P-53

TIO_2 NANOTUBE ARRAY SUPPORTED RuO_X ELECTROCATALYST FOR THE HYDROGEN EVOLUTION REACTION IN ACID SOLUTION

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Nanocomposite cathodes for the hydrogen evolution reaction (HER) were prepared by deposition of RuO_x catalyst particles on self-organized titania nanotube (TiNT) arrays of highly developed surface area following a procedure that involved the initial cathodic intercalation of H^+ into the TiNT walls and the subsequent two-step ion-exchange process. Anodically grown TiNT array substrates consisted of tubes of 184 ± 22 nm outer diameter, 133 ± 21 nm inner diameter and 25 ± 6 nm wall thickness, whereas the tube lengths were 7.2 and 16.4 µm depending on the applied anodization time. Transmission electron microscopy and energy dispersive X-ray spectroscopy analyses of obtained Ru-TiNT samples revealed that the concentration of RuO_x particles in the size range of a few nanometers was the highest at the surface of the TiNT layer and steadily decreased to a minimum value at about 4.5 µm inside the tubes. The capacitive behavior and electrocatalytic activity for the HER of Ru-TiNT nanocomposites, hydrogenated TiNT samples (H-TiNT) and compact TiO_2 were investigated in 1.0 M $HClO_4$ solution at room temperature by means of cyclic voltammetry, electrochemical impedance spectroscopy, Mott-Schottky analysis and steady-state polarization measurements. It was shown that cathodic hydrogenation treatment induced a four orders of magnitude higher concentration of electron donors in TiNT structures providing their quasimetallic behavior in the range of potentials corresponding to the HER, but exerted only a negligible effect on the conductivity and capacitive properties of compact TiO_2. A small quantity of highly dispersed RuO_x remarkably improved the electrocatalytic activity for the HER. Ru-TiNT cathodes exhibited a more than 250 mV lower overpotential for the HER with respect to bare H-TiNT substrates at the current density of -50 mA cm^{-2}. A decrease of the Tafel slope from about -120 mV/dec for H-TiNT samples to as low as -70 mV/dec for the Ru-TiNT sample with longer tubes was explained by the formal kinetics approach.

P-54

MULTIANALYTICAL EXAMINATION OF THE ARCHAEOLOGICAL CERAMIC FINDINGS FROM THE SITE OF KALE, SOUTHEASTERN SERBIA

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The site of Kale in Krševica near Bujanovac (southeastern Serbia) is a unique archaeological site recognized by archaeologists as a ‘meeting ground’ or a ‘crossroads’ of Greek and Celtic cultures. This fortified settlement, located in the South Morava River valley represents interesting social, cultural and historical phenomenon for archaeologists to investigate, offering a large quantity of archaeological material. According to the archaeologists some of the ceramic findings could be labelled as ‘Greek’, ‘Celtic’, or belonging to some other Iron Age cultures and were of special interest in the investigation. The most abundant group of the ceramic material, however, consists of local vessels produced after Greek models, similar to those from ancient Paeonia and Thrace.

Following this complex archaeological context, three groups containing about 30 ceramic fragments were formed according to the archaeologist’s knowledge, and were analyzed using pEDXRF spectrometry and FTIR analytical techniques. The aim of this study was to characterize elemental and mineralogical composition of the ceramic body material. The possibilities for distinguishing local ceramic products from the imported ones, were examined using analytical results and pattern recognition techniques.

P-55

RAW MATERIAL SELECTION STUDY OF THE POTTERY FROM THE MULTILAYER ARCHAEOLOGICAL SITE GRADIŠTE-IĐOŠ IN SERBIAN BANAT

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The archaeological site of Iđoš, located in south-central Great Hungarian Plain in Serbian Banat region was occupied periodically for over 5000 years, from Europe's first Neolithic farmers to the builders of an elaborate Late Bronze Age fortification. Its scale and character led to it being declared a site of great heritage importance. Lying between major cultural complexes in each phase, the luminal role of Iđoš underwrites the importance of the site for the research. The on-going revisionary archaeological research (BORDERLAND: ARISE project) explores three key phases and associated themes consequently bringing to the light a plenty of ceramic materials with the variety of information from the past.

By cross referencing three transformative periods using one site, it is possible to explore the human-environment interaction, with particular focus on defining domestic practices and the receptivity of influences from the major cultural complexes surrounding the site. By revealing the major information through a plethora of the analysis (macroscopic examination, thin section petrography, EDXRF, SEM and other) it is possible to reveal and cross-reference pottery function, style and production technology, procurement of rough material in order to help answering the questions of the interaction between landscape, environment and people through time, social boundaries between communities during the late Neolithic period, technological knowledge of the Iđoš inhabitants during different periods of prehistory.

Three different assemblages of the pottery excavated in Iđoš were analyzed by EDXRF spectrometry and obtained results have been presented together with the provenance study based on them and using pattern recognition techniques.

P-56

TILES MADE OF NATURAL HETEROGENEOUS MATERIALS FOR AN URBAN PLANNING APPROACH OF SPACE CLIMATIZATION: CERAMIC CLAY, ZEOLITE AND BENTONITE CLAY

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The aim of this study was preparation of various series of tiles in order to investigate the influence of their composition on the process of adsorption, i.e. moisture desorption. The combination of bentonite clay, zeolite and unfired ceramic clay can be used as adsorbent-moisture desorbent, which can be further successfully used in the construction of a buildings. The influence of adsorption and moisture desorption increases by increase of the zeolite content in the analyzed tiles. The significance of the bentonite clay is reflected in the fact that it increase moisture adsorption, but slows down its desorption. Sand in combination with wood chips increase porous nature of the tiles, which further decreases their ability to bind moisture. The optimization of the content of ceramic clay, bentonite clay, zeolite, wood chips, sand and plasticizers was done using an appropriate mathematical model of the studied process. An advantage of this approach is that tiles made of heterogeneous natural materials can be built into urban objects of different architecture and energy profiles. Their right position in a room would provide natural ventilation based on the changes in the air composition that would reduce the exchange of air with the environment, same as heating costs during the winter, cooling during the summer while using relatively similar air composition. The research showed that sand and ceramic clay provide quicker drying of the samples compared to the bentonite clay, polyphosphate and plasticizer.

Keywords: climatization, ceramic clay, zeolite, bentonite clay

P-57

RECYCLING OF COAL ASH FROM THERMAL POWDER PLANTS AND GLASS WASTES FOR FOAM GLASS

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The energy industry generates yearly great amounts of coal ash accompanied by a lot of work for transport and storage by landfill which cause negative environmental impacts such as leaching of potentially toxic substances into soils and groundwater. The best way to solve the disposal problem of ash is to decrease the quantity for disposal with utilization of such waste.

To deal with these problems, our paper assesses the recycling of coal ash generated in thermal power plants in conjunction with the re-use of waste glass. Due to its unique properties combination: i.e. thermal insulating, chemically corrosion resistance, lightweight, rigid, waterproof and low cost, these foam ceramic materials could be an alternative for application in building industry and other fields.

Oxide composition analysis (X-ray fluorescence, atomic absorption) indicates that it consists mainly of Al and Si oxides. The ash type is silico-aluminous with a composition close to clay lands, characterized by 45.6% SiO_2, 18.8% Al_2O_3. Some other constituents are CaO (10.45%), MgO (2.40%), Fe_2O_3 (8.72%) and in smaller quantities Na_2O (0.21%) and K_2O (1.44%). Most of the CaO and MgO are bound in sulphates and mixed oxides with SiO_2 and Al_2O_3. Preliminary measurements of radioactivity show the existence of ^{226}Ra and ^{232}Th, the irradiation on radiation protection being at a level, close but lower than of the health admitted norms. Such comprehensive characterization helps to find out the appropriate ways of ash recycling, giving also the useful information about the power plant combustion efficiency.

In this research the foam glass was obtained by high temperature foaming process. As main starting materials were used glass wastes and fly ash and bottom ash and as well as silicon carbide and carbon as foaming agents. Bulk density, expansion index and compressive strength in conjunction with structural and morphological analysis are presented in detail.

P-58

MODERN COMPUTATIONAL METHODS USED IN THE MODELING OF ADVANCED MATERIALS: BRIDGING THEORY AND EXPERIMENT

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In the first part, crystal structure prediction using simulated annealing in the lead sulfide [1] and zinc oxide [2] compound, calculated both using empirical potentials and on the *ab initio* level has been presented. The results were in good agreement with previous theoretical and experimental observations, and we have found some additional structure candidates as function of pressure. Furthermore, we have calculated their properties, focusing on structural, electrical and vibrational properties, and we also had good agreement with experimental results [1-3]. Next, we show calculations performed in the ZnO system using the novel prescribed path algorithm, where we have investigated the connectivity among experimental ZnO crystal structures on the energy landscape, and in particular transition states [4]. With the results of this study we were able to understand more about the influence of temperature in ZnO, to connect our results to the actual synthesis routes and get additional crystal and nanostructured candidates.

In the second part, the results for an *ab initio* minimization data mining approach, which combines two computational methods, have been presented. In this study we have investigated binary materials with elements from groups V, IV - VI, and III – VII, with the goal to identify chemical systems where recently proposed "5-5" crystal structure type might be experimentally accessible and, among others, TlF, SnO, SnS, SnSe, GeS, GeSe, PbO, PbS, ZnO and ZnS, were chosen for the study [5]. Finally, we present our current research on ternary ABX_3 compounds, where we show the results of $CaMnO_3$ system. In this theoretical study, we have further combined structure prediction and *ab initio* minimization data mining approach [6].

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P-59

DOPING EFFECT ON COORDINATION NUMBER IN CaMnO$_3$ PEROVSKITES

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The influence of yttrium amount on Mn–O bond angles and distances, tilting of MnO$_6$ octahedra and deformation due to the presence of Jahn-Teller distortion arround Mn^{3+} cation in Ca$_{1-x}$Y$_x$MnO$_3$ ($0 \leq x \leq 1$) was investigated. In general, tilting of *B*O$_6$ octahedra induces a distortion of *A*O$_{12}$ polyhedra which can result in a decrease of the *A* site coordination number. In order to estimate effective coordination of the *A* and *B* sites, bond valence calculations (BVC) were performed for *A* and *B* site cations. The reduced coordination is due to the movements of some of the anions too far away from the cation and can not be considered as a part of the coordination sphere. Different coordination numbers [CN = 12, 10, 9 and 8] can occur in perovskites as a result of different tilt schemes.

The coordination of cations occupying *A* site of the most *AB*O$_3$ orthorhombic perovskites is regarded as 8-fold rather than 12-fold, e.g. a four-fold antiprism with eight short *A*–O bonds in the first coordination sphere of the *A* cation. Four longer *A*–O bonds give rise to the second coordination sphere. Bond length analysis of the Ca$_{1-x}$Y$_x$MnO$_3$ ($0 \leq x \leq 1$) compounds shows that the *B* site cation enters the second coordination sphere of the *A* cation, as the *A*–O distances exceed the minimum *A*–*B* distance. If we apply criteria that *A*–*B* distance separates first and second coordination sphere, *A* cation in perovskite phase of the CaMnO$_3$ sample has 12-fold coordination. In the perovskites from Ca$_{0.95}$Y$_{0.05}$MnO$_3$, Ca$_{0.85}$Y$_{0.15}$MnO$_3$ and Ca$_{0.75}$Y$_{0.25}$MnO$_3$ samples *A* site cations are coordinated with 10 oxygen atoms. With further increase of *x*, the *B* cation moves closer to the *A* site coordination sphere, as demonstrated by the increase in the separation between the longest *A*–O bond and the *A*–*B* interatomic distance. Therefore, this results in 8-fold coordination number for *A* site cation in samples Ca$_{0.5}$Y$_{0.5}$MnO$_3$ and Ca$_{0.25}$Y$_{0.75}$MnO$_3$.

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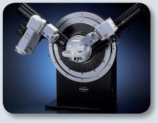

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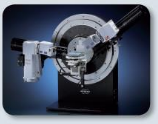

TWIN/TWIN setup for grazing incidence diffraction: Depth dependent information about phase composition, lattice parameters, microstructure, and residual stress

TWIN/TWIN setup for reflectometry, LYNXEYE detector switched to 90° position: Layer thickness, roughness, porosity chemical composition, and lateral structure

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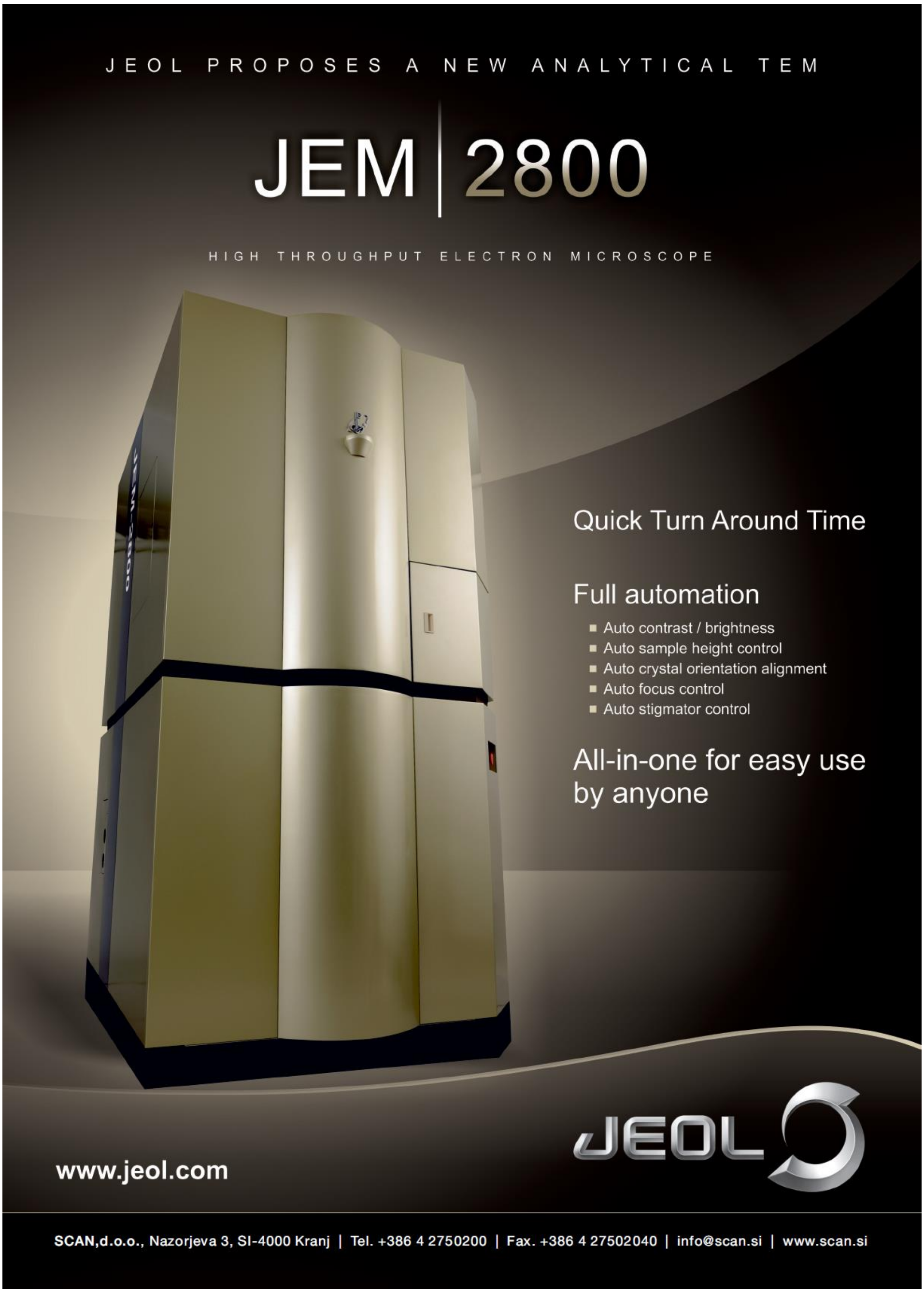

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