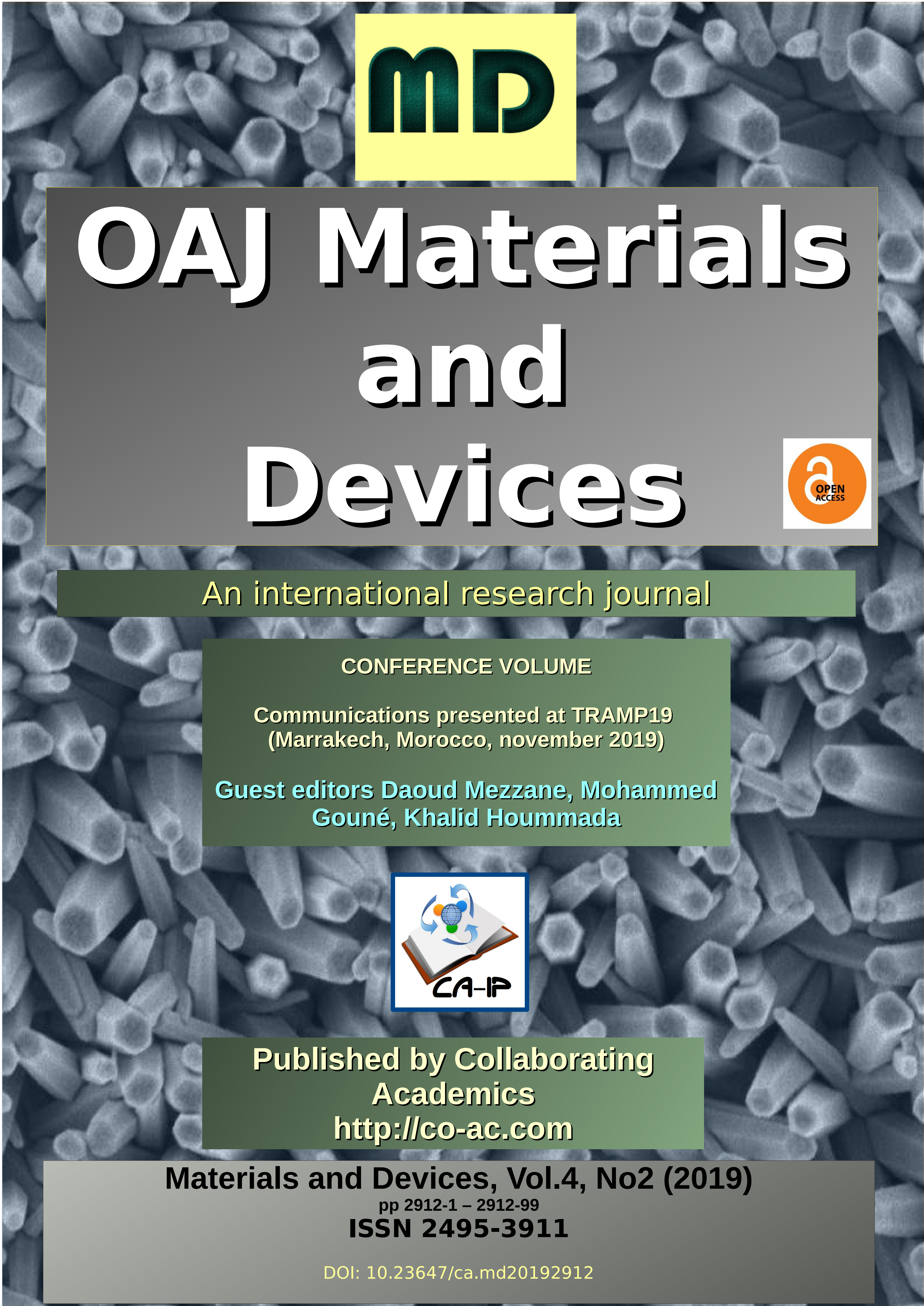

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(Updated on june, 21st, 2019)

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The topics covered by the journal are wide, it aims at publishing papers on :

- all aspects related to materials, namely according to their chemical formula (oxides, fluorides, carbon compounds, …, organic, inorganic), to their physical properties (conductors, super-conductors, semi-conductors, insulators, dielectrics,...), to their nature (crystalline or amorphous materials, liquid crystals, modulated systems, aperiodic materials, nanomaterials and nanostructured materials)… or environmental type (ecomaterials), or according to some specific applications. Papers on biomaterials, geomaterials, archeomaterials or on studies of ancient materials are also welcome. A particular attention is also paid on environmental studies related with materials. Authors are also encouraged to submit papers on theoretical studies applied to materials, including pure mathematical approaches, physical approaches, models, numerical simulations, etc.

- devices in a wide sense. Concerning Devices, the scope is restricted to those integrating given materials (for instance memories based on some specific magnetic materials) or those related to materials in their study or use (for instance specific instruments in materials science, devices of interest for the use of particular materials,...) . Papers on all types of such devices are welcome.

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People interested in this project are welcome ! Contact us to submit your proposals, ideas, suggestions, or to get involved in some actions !

Materials and Devices (ISSN 2495-3911) is a relatively new journal, and as such, is not yet indexed. However in future we shall consider as a priority task, to reach a significant impact factor for this journal.

ABSTRACTS BOOK

Cadi Ayyad University, Faculty of Sciences and Technologies Marrakech

7-9 November 2019
Marrakech, Morocco

The third International Symposium **TRAMP19** follows the previous successful events, **TRAMP14**, and **TRAMP17** and was held in the warm and hospital city Marrakech in Morocco, on 7-9 November 2019.

The Symposium was dedicated to the different aspects of the Materials Science and especially to advanced materials and their applications in energy, transport, medical and biological sectors. It has been a great opportunity for the junior and experienced scientists to share their knowledge on these hot subjects.

TRAMP 's objectives and topics of interest:

- Bring together a broad international community of scientists, engineers and PhD students.
- Provide opportunities to strengthen existing collaborations and exchange of ideas to bring new partnerships.
- Create a forum for researches and experts regarding to Nanomaterials, train students and young researchers.
- Synthesis, Characterizations and Properties of nanomaterials.
- Characterizations and Properties of Surfaces and Interfaces.
- Functional and Nanostructured materials.
- Nanostructured Thin Films.
- Metallurgy, Metal alloys and Corrosion.
- Synthesis and Applications of Nanocomposites.
- Nanomaterials for Energy and environment Applications.
- Nanomaterials Applications for Electronics, Medicine and Biotechnologies.
- Scanning Probe Techniques.

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- Laboratory of Condensed Matter and Nanostructures, University Cadi Ayyad, Morocco
- University Mohammed V, Rabat, Morocco (CNRST Priority Program PPR 15/2015)
- Institute of Condensed Matter Chemistry of Bordeaux (ICMCB), France
- Institute Microelectronic Materials and Nanosciences of Provence, Aix Marseille University, Marseille, France
- European Research and Innovation Network "Engineering of Nanostructures with Giant Magneto-Piezoelectric and Multicaloric Functionalities" HORIZON-RISE-ENGIMA.

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Plenary Speakers

PS001

MATERIALS SCIENCE OF NANOSTRUCTURES: UNDERSTANDING OF THE FUTURE

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ABSTRACT

The main feature of nanomaterials is the dependence of their properties on the size of the structural element. The main feature of nanotechnology is the ability to operate with nanomaterials that have a certain structure. Therefore, the diversity of structural forms increases every year by exponential low.

The escalation of complexity and variety of nanostructures is an intensive way of nanotechnology development today, alternatively to the combinatorics with chemical composition, which gives extensive growth. Examples are known: nanotubes, fullerenes – all first time have been predicted and obtained from carbon only and then were composed from other elements or chemicals. The same happened with 2D materials: from graphene to graphene-like sulfides, selenides, maxenes, and others.New structural forms and new materials with extraordinary properties are ahead.

The classical materials science is grounded on the study of relations between composition, structure and properties of materials, taking into account the processes of production and processing and production economics. In terms of physics and chemistry, we are accustomed to perceiving material through the prism of the energy of interatomic interaction. Classical materials science is first and foremost the science of bodies in which covalent chemical bonds with energy higher than 2 electron volts operate. In this coordinate system we consider the majority of material properties - strength and hardness, thermal conductivity and diffusion, ferroelectricity and luminescence. However, in nature, there are also low energy bonds, there are mechanisms providing self-assembly and self-organization of nanoparticles with the aid of weak bonds.

For the convergence of the two segments of materials science it is necessary to develop new processes with feedback, which allow to create new structures, new methods of analysis of these structures, new methods of control of process parameters. Development of multiscale modeling and design of new structures and materials is required. For example, methods of operating 2D materials are required to connect them to complex devices. It is possible to mix the maxenes evenly as a powder in the polymer and to obtain a screen from microwave radiation. It is possible to construct an ordered layered structure, an electronic device, by ordering the nanoparticles in an external field.

Keywords: strong chemical bonds, weak chemical bonds, complex nanostructures

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PS002

IS THE NANOPIEZOTRONICS BASED ON A PIEZOELECTRIC EFFECT?

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ABSTRACT

The nanopiezotronics refers to the research field on the coupling between semiconducting and piezoelectric properties of nano-objets. It was for instance observed that the mechanical deformation of flexible structures based on ZnO or III-nitride nanowires generates electrical spikes [1] or modifies their I/V characteristic. The piezoelectricity was claimed as the origin of these electro-mechanical couplings which could result on a broad range of new applications from nano-generators to nano-sensors [2].

In this talk, the spontaneous and piezoelectric polarizations of III-nitride materials will be described and the local study of the surface potential and piezocharges will be presented in order to investigate the nanopiezotronic signal obtained via conductive scanning probe microscopy in III-N nanowires. The results emphasize the negligible role of the piezoelectric effect [3], especially via the questioning of the giant piezoelectricity which was claimed to be present in such nanowires [4]. Several scanning force microscopy techniques dedicated to the local probing of electro-behaviors like the Kelvin probe force microscopy (KPFM) or the piezoresponse force microscopy (PFM) will be introduced during the presentation with a special care concerning their applications to semiconductors and related artifacts.

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PS003

THE RELATIONSHIP BETWEEN THE ENERGETIC PERFORMANCE OF RECHARGEABLE BATTERIES AND THE PROPERTIES OF THEIR ELECTRODE MATERIALS

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ABSTRACT

The depletion of fossil fuels and their drastic effects on the environment are becoming problematic. Hence, researchers were encouraged to use the clean renewable energies and to smoothly transit from thermal to electrical vehicles. Nevertheless, these two energetic applications require efficient energy storage technologies to fit with their impressive recent development. Owing to its high-energy density, long life cycling, lightweight and recyclability, lithium-ion batteries (LIBs) are widely used for portable electric devices along with electric vehicles (EVs). Sodium ion batteries (Na-ion) are also predicted to be promising low cost alternatives of the current lithium technology especially in large-scale applications. The concept of Li-ion and Na-ion consists of the reversible exchange of the alkali metal between the anode and the cathode materials, that constitute the main component of these two technologies. The energetic performances of the Li- and Na-ion (Capacity, Voltage, Energy, Cycling…) strongly depend on the structure and the physico-chemical performance of the electrode materials.

Through some recent investigations done in LCME Laboratory (UCA), this keynote will present a series of example elucidating the dependence of the storage performance of Li- and Na-ion batteries on the features of the electrodes.

Keywords: Energy Storage, Li-ion batteries, Na-ion batteries, Electrode Materials.

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PS004

ENTROPIC DESCRIPTION OF A Mg-BASED METALLIC GLASS FROM SERRATIONS STATISTICS

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ABSTRACT

Series of independent instrumented nano-indentation experiments were performed on a $Mg_{65}Cu_{12.5}Ni_{12.5}(Ce_{75}La_{25})10$ metallic glass at room temperature and at strain rates in the range of 1 to 0.3 s-1. The loading part of curves shows serrations which size and frequency of occurrence were measured using an automated procedure. It was conjectured, that (i) serration occurs through rearrangement of appropriate zone in the glass that should naturally scale with a multiple of an elementary domain size characterizing the deformation mechanism. (ii) As activated zones leading to serration are very few, the process should fit with rare event dynamics. Actually, serration sizes are well fitted by a Poisson distribution and the waiting times between successive serrations is consistent with the Poisson statistics. The model predicts an elementary domain which size scales with that of the activation volume of about 3 atoms, measured from nano-indentation near-creep tests at constant load in the same series of experiments (Thurieau et al, J. Appl. Phys. 2015). Dynamics of shear bands initiation, which is seemingly of avalanche type, is analyzed using the statistical approach proposed by Adam and Gibbs (J. Chem. Phys. 1965) to describe viscosity. An entropic description is proposed where elementary domains are associated to energy levels and able to cooperatively evolve to form avalanches (serrations).

PS005

FERROELECTRIC TOPOLOGICAL NANOMATERIALS FOR ULTRAFAST COMPUTING CIRCUITS WITH LOW ENERGY DISSIPATION

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ABSTRACT

Formation of unusual textures of polarization is imminent for nano-scale ferroelectric samples, films, rods, and granules, where the depolarization surface effects play a crucial role. The topologically protected stability of such textures and security of information storage is coming from polarization vorticity, provided by the condition of absence of the energetically-unfavorable depolarization charge. The endurance of ferroelectric formations with respect to high-energy irradiation makes them ideal for the aerospace industry, and the periodic domain walls structures can be used as a platform for terahertz radiation, generators and detection devices.

Polarization domains that alternate the surface charge distribution can be formed in ferroelectric thin films as an effective mechanism to confine the depolarization field to the near-surface layer and diminish the depolarization energy. However, their existence has long been considered as barely possible until the direct theoretical predictions [1,2] and experimental evidence [3,4] in thin oxide-based superlattices. Very recently we have demonstrated that the effective capacitance of ferroelectric layers with domains is negative [5,6]. This effect is explained by the opposite orientation of the depolarizing field with respect to the field-induced averaged polarization. This phenomenon is currently considered as the platform for the realization of the dissipation-free high-performance nano-circuits [7]. Moreover, in the sub-THz region, the resonance plasmonic effect can be induced by oscillating domain walls [8] and can be suitable for the design of the ultra-small low-energy THz chips.

Multi-vortex [9] and skyrmion [10] states can be formed inside ferroelectric cylindrical nano-dots and nanorods to reduce the depolarization energy. We study the topological stability of such states and target the multi-domain and topological excitations in FE nanodots as a platform for IT-secured multivalued logic units, breaking ground for neuromorphic computing [11,12].

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Keywords: ferroelectrics, THz radiation, nanoelectronics, multibit logic, negative capacitance

PS006

3D IMAGING OF MATERIALS CHEMISTRY AT THE ATOMIC-SCALE BY ATOM PROBE TOMOGRAPHY

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ABSTRACT

The technique of atom probe tomography (APT) enables atomic level microstructural characterization to be performed on a wide range of materials, from laboratory model to complex engineering alloys, to thin multilayer films, semiconducting structures and devices, and, since recently, to ceramic materials. The intrinsic performances of recent instruments will be presented, and well as their unique outcomes. Information on the size, morphology and compositions of coexisting phases, solute partitioning of the elements between the phases, and solute segregation to defects, like dislocation lines, interfaces and grain boundaries can be obtained down to the atomic scale. These informations lead to a more complete understanding of fundamental and service properties of complex engineering materials. The types of atomic level information that may be obtained with atom probe tomography are illustrated in a large variety of materials.

PS007

Toward material engineering and applications

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ABSTRACT

The inherent increasing demand in energy solutions and new technologies in various sectors such as transport and environment has prompted scientists to custom the materials design and properties for targeted application. Most of the newly developed materials are complex composites with more and more reduced size and dimensions. Special fabrication techniques have then emerged to make the processing possible and easily tunable. Among these techniques and the list is not exhaustive: Atomic Layer Deposition, Plasma Enhanced Chemical Vapor Deposition, Electron Beam & Thermal evaporators, Magnetron Sputtering, Electron beam and Photo lithography have attracted increasing interest due to their volatility and reproducibility. In parallel and to accommodate this progress made in nanomaterials, advanced characterization techniques such as High-Resolution Scanning Transmission Electron Microscopy (HRSTEM), Electron Energy Loss Spectroscopy (EELS), Scanning Near-field Optical Microscopy (SNOM), In situ experiments (TEM+AFM+SEM) and 3D imaging, appear as major tools to first evaluate the processing routes and parameters, then to correlate the fabricated materials to their targeted application. This duality, which consists of closing the loop between these two aspects fabrication and characterization in one hand and the material testing in the other hand, is a must to achieve cutting edge research and breakthrough.
Ultimately, this approach will allow better prediction of the material design for the desired application. In addition, as this approach lies in cross disciplines, it gives to scientists leverage to overcome the multidisciplinary aspect related to nanotechnology.

In this seminar, this approach will be applied to novel materials with special emphasis to the potential applications in energy harvesting & conversion, sensing, biology, and communications. These applications can find use in different domains such as space, transport and energy saving.

PS008

SOFT CALORIC LIQUID CRYSTAL-BASED MATERIALS

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ABSTRACT

Caloric effects are manifested in the heating or cooling a caloric material due to the application or removal, respectively, of the external field under nearly adiabatic conditions. Materials with large caloric effects, such as the electrocaloric (EC) and elastocaloric (eC) effects, have the promise of realizing new solid state refrigeration techniques [1, 2]. First proof of such conceptual cooling devices was produced from relaxor ferroelectric ceramic and polymer thin films [3, 4], but with rather low power density, due to the relatively large EC inactive regenerator mass [5]. The natural idea is to replace such regenerator with the EC active dielectric fluid, such as liquid crystals (LCs), which may improve the power density of EC cooling devices. Another soft material, called liquid crystal elastomers (LCEs), are good candidates with large elastocaloric effect with potentially better elastocaloric responsivity than shape memory alloys wires, in which the eC temperature change of 40 °C was observed at 0.8 GPa stress field [6].

In this contribution a review of recent direct measurements of the large EC effect in LCs and large eC effect in LCEs [7, 8] will be given. In smectic liquid crystalline materials and mixtures of LCs with functionalized nanoparticles the EC effect exceeding 8 K was found in the vicinity of the isotropic to smectic A phase transition. Direct EC measurements indicate that the EC response is significantly enhanced by the latent heat [9]. Further, the results of direct measurements of the eC in side-chain and main-chain (MC) LCEs will be presented. The eC change of temperature of about 1 K was observed in MCLCEs. However, both soft materials can play a significant role as active cooling elements and parts of thermal diodes or regeneration material in development of new cooling devices.

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Keywords: electrocaloric, elastocaloric, liquid crystal, liquid crystal elastomers

Invited Speakers

IS001

NANOCRYSTALLINE MULTIFUNCTIONAL Pr-Co COMPOUNDS: PERMANENT MAGNETS, MAGNETIC REFRIGERATION AND HYDROGEN STORAGE

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ABSTRACT

Rare-earth transition metal intermetallics RM_n, where a rare earth (R) is combined with a transition metal (M), are attractive compounds for their technological magnetic application. Of all them, only the R-3d intermetallics ever exhibit a significant magnetic moment on the M partner. This group is the subject of this work.

After presenting the relevant theoretical models for magnetism in R-3d intermetallics the crystallographic relations between the stoichiometry are discussed. Following a detailed treatment, the overall magnetic properties are summarized. The characteristics of the intermetallic compound RMn are depending on the nature of the metals involved and the stoichiometry of the compound.

We focus here in the Pr-Co binary system, it forms several intermetallic compound which have structural and magnetic properties enough different. These compounds can crystallize in hexagonal and rhombohedral structures depending on annealing temperature. The structures of PrCox compounds derived from the structure of the compound by replacing PrCo5 third of rare earth atoms by a pair of atoms of transition metal smaller. The crystal structure of Pr2Co7, as well as Pr5Co19 compounds, can be constructed by the substitution of Co atom by the rare earth atom in each mesh PrCo5, as well as the PrCo3 and PrCo2 compounds, by an ordered substitution of atoms. These compounds exhibit magnetic properties that can be exploited to produce soft, hard or semi-hard magnetic materials. The origin of these unique magnetic properties is mainly due to the coexistence of two complementary types of magnetism: magnetism characteristic of localized 4f electrons of the rare earths and itinerant magnetism of the 3d electrons of the transition metals.

Moreover, we report that the insertion of a light element such as carbon or hydrogen, allows to increase the Curie temperature of these systems. The related hydrides present a reversible cycle of absorption/desorption.

We also report on the study of the magnetocaloric effect (ME) of the intermetallic Pr-Co type. It shows that the ME effect is sensitive to the stack configuration. The temperature dependence of the magnetization (M vs. T) and the Arott plots around the second order magnetic transition for Pr5Co19 and Pr2Co7 compounds are reported. These results indicate that Pr-Co compounds could be good candidates for permanent magnets, but also for magnetic refrigeration at high temperature and for hydrogen storage.

Keywords: nanomaterials, permanent magnets, magnetic refrigeration, hydrogen storage, energy.

IS002

LEAD-FREE AND ANTIFERROELECTRIC MATERIALS AS ELECTROCALORIC COOLANTS

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ABSTRACT

The request for greener heat-management technologies has recently developed significant interest in new electrocaloric (EC) effect-based cooling devices that have the potential to replace the existing cooling technics [1,2].

In this contribution the direct measurements of the large EC effect in antiferroelectric, lead-based and lead-free ferroelectric materials [3,4] will be presented. Specifically, the negative EC effect in antiferroelectric PZSTN, n/95/5 PLZT and PBZ ceramics will be investigated by direct experiments. Here, it is demonstrated that both negative and positive EC response can be arbitrarily invoked in antiferroelectric materials by properly controlling the electric field and temperature. In addition, the large positive EC response observed by direct experiments in lead-free BCTZ-based ferroelectric materials will be reviewed.

A prototype of electrocaloric based cooling device using a regeneration technique will be presented, its properties reviewed and compared to existing caloric prototypes.

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Keywords: antiferroelectric, ferroelectric, electrocaloric, dielectric, lead-free

IS003

CHARACTERIZING THE POROSITY IN THIN BST FILMS BY LASER-ACOUSTIC WAVES.

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ABSTRACT

Porosity may be harmful for the properties of thin films. Depositing dense films is often the aim of the technological development, although there are also applications requiring adjusting a special amount of pores in the film. In thin films, the pore dimension is in the sub-micrometer range so that detecting the pores is difficult. The laser-acoustic technique is shown to be able to indicate an enhanced porosity in thin films. It is based on surface acoustic waves and yields Young's modulus of the film. The elastic modulus of the material is distinctly influenced by porosity. It reduces with increasing porosity and depends also on the shape of the pores. Test series of BST ($Ba_{0.65}Sr_{0.35}TiO_2$) thin films with porosity were deposited on $Pt/TiO_2/SiO_2/Si$ substrate. The laser-acoustic tests yielded elastic moduli for the films that were up to 24% lower compared to the value of the bulk material. The lowering of Young's modulus was found to correlate with increasing porosity. For the manufactured BST series a pore volume fraction up to approximately 7% was estimated. A theory for Young's modulus depending on porosity, also taking into account the pore shape, was employed to deduce information on the pore structure from the laser-acoustic results .

Key words: BST thin films, texture, porosity, laser acoustic waves.

IS004

STRUCTURAL, DIELECTRIC AND ENERGY STORAGE PROPERTIES OF NEODYMIUM NIOBATE WITH TETRAGONAL TUNGSTEN BRONZE STRUCTURE

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ABSTRACT

The present work reports on the effects of Nd3+ substitution on the structural, dielectric and energy storage behaviour of polycrystalline Ba2NaNb10O30 (BNN) ceramics. The ferroelectric lead-free Ba2Na1-xNdX/3Nb5O15 ceramics were prepared by conventional solid-state reaction technique. The room temperature X-ray study and Raman investigations have allowed to evidence the stabilization of a tetragonal tungsten bronze structure with P4bm as space group for all studied compound. Dielectric study carried out on the prepared ceramics has permitted to determine the temperature of phase transitions (Tc). It was found that the dielectric constant increased with increasing the amount of Nd in BNN matrix. Room temperature energy storage property was determined using P-E hysteresis loops. The optimum discharge density was found for x= 0.7 with Wrec = 18,1 mJ.cm-3) at 1KHz.

Keywords: Tetragonal Tungsten Bronze, Dielectric, Energy storage.

IS005

BENEFIT OF PRESSURE IN THE SINTERING PROCESS

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ABSTRACT

Pour atteindre certains objectifs, la conception de procédés originaux de synthèse dans la gamme de pression (1 bar – 60 kbar (6 GPa)) a mené à l'obtention de matériaux impossibles à élaborer par tout autre procédé. Le service de synthèse Hautes Pressions (HP) étudie l'effet de P pour l'obtention de matériaux et la maitrise des transitions de phase. Ces matériaux peuvent être sous forme de monocristaux, micro/nano-cristallites, polycristaux (par frittage pour l'obtention de céramiques) et de monolithes (par densification et/ou consolidation de matériaux pulvérulents). Le procédé HP est maitrisé sous forme gaz, liquide et solide; le milieu fluide en condition hydrothermale (état souscritique ou supercritique) permet par le biais du phénomène de dissolution-précipitation, la croissance de monocristaux et le frittage de poudres (céramiques, métalliques).

L'impact de la PRESSION au travers de ses principales caractéristiques (faible énergie mise en œuvre en comparaison avec la température (T), accroissement de la réactivité chimique, diminution du volume, force motrice) est étudié pour une grande variété de domaines d'applications : piézoélectricité, photonique, biomatériaux, outils d'usinage.

Des exemples de l'intérêt de la RESSION seront donnés pour les exemples suivants:

- Diminution de T de frittage / consolidation / densification, par son effet de Force motrice, afin de :
  - ⇒ Limiter la croissance granulaire,
  - ⇒ Favoriser la phase basse température : SiO_2 quartz (transition α-β à 573°C),
  - ⇒ Préserver la composition initiale du biomatériau (conservation d'éléments volatils: OH^-, H_2O, CO_2),
  - ⇒ Augmenter le domaine de stabilité thermique évitant la décomposition : BP [$T_{decomp.}$ = 1130°C]: $T_{fritt.}$ = 1600°C/5 GPa, MgB_2 [$T_{decomp.}$ = 830°C]: $T_{fritt.}$ = 1200°C/5 GPa,
- Orientation de la réaction chimique dans le sens de la synthèse conduisant à la phase la plus dense : diamant (c-C) au détriment du graphite (h-C),
- Initiation d'une nouvelle microstructure plus fine par la maitrise des changements de phase (matériaux polymorphes) soit à l'état solide (Al_2O_3: γ -> α) ou bien soit à l'état liquide par dissolution d'une phase et précipitation d'une autre phase (SiO_2: amorphe -> cristallisé),
- Frittage de matériaux réfractaires (borures, nitrures, carbures) pour atteindre une densité améliorée en comparaison avec les procédés à plus basse pression (c-SiC),
- Frittage de phase stable qu'à haute pression (c-C, c-BN),
- Densification de céramiques avec une porosité proche de 0% (céramiques transparentes) ou à forte porosité (biomimétisme structure osseuse)

Divers procédés HP seront présentés pour la synthèse de matériaux / multimatériaux / composites sous forme dense (*HP-HT, HP-SPS, HyS, HIP, ..*) et poreux (*HyS, FIP, HIP, CIP, UAP, ..*), mais également pour l'obtention de matériaux sous forme de monocristaux (*HyCG, HyS*) et micro/nano-cristallites (*HyCr*), la purification de matériaux naturels (*HyPu*) et la décontamination athermique (sanitisation à froid: Pascalization) de biocomposites dont l'un des constituants est thermo-instable (*HHP, HPP*)

IS006

THE ROLE OF MECHANICAL FIELDS AND STRESS RELAXATION ON AMORPHOUS/CRYSTALLINE TRANSITION OF NANOSCALE SILICON NITRIDE IN -Fe

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ABSTRACT

The need to reduce the fuel consumption of vehicles, improve passenger safety and the new global standards for the CO2 emission force the automotive industry to rapidly develop new materials with higher mechanical properties and lower density. The attractive properties of nanoscales Si3N4 in terms of both density and strengthening make them excellent candidate for nitriding applications in the transportation industry. Upon nitriding of Fe-Si binary alloys at 570°C, a very large amount of Si3N4 forms in the -Fe matrix as an amorphous phase of size-dependent cuboidal morphology whose density is very low (1.8 g. cm-3). Upon denitriding at the same temperature, a transition from amorphous Si3N4 to crystalline Si3N4 was observed. This change in structure is associated with a change from the cube-like morphology to a hexagonal prism shape and an increase of density from 1.8 g. cm-3 to 3.6 g. cm-3.

In this paper, the understanding of such an evolution was addressed through an approach based on numerical modelling that couples both stress field and the diffusion-controlled growth of nanoparticules of Si3N4. The role of the anisotropy of stress fields, the elastic strain energy stored in the material, the pressure jump at the interface between Si3N4/-Fe and the stress relaxation phenomenon on the stability of both amorphous and crystalline nanoparticles were discussed. The results obtained open new avenues for developing new lighter materials for transportation.

IS007

DESIGN, MICROSTRUCTURES AND PROPERTIES OF HIGH ENTROPY ALLOYS AND COMPLEX CONCENTRATED ALLOYS

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ABSTRACT

High entropy alloys (HEAs) and complex concentrated alloys (CCAs) based on 3d transition metals (3d TM CCAs) and refractory elements (RCCAs) are widely studied as candidates for structural and functional materials. 3d TM CCAs usually have FCC or duplex FCC+BCC microstructures, while RCCAs usually have BCC-based phases. In fact, many 3d TM CCAs and RCCAs have both disordered solid solution and long-range ordered phases, i.e. FCC+L12 and BCC+B2 respectively, giving the opportunity to produce precipitation-strengthened alloys. Besides, low stacking fault energy FCC HEAs/CCAs are susceptible to deformation twinning which imparts excellent strength-ductility combination by increasing strain hardenability. This talk steps back over the rapid development of HEAs/CCAs to discuss their principles and the new concepts they introduce, their microstructures and properties, their design strategies, and will develop ideas to guide future efforts. We will also explore different processing routes with the aim to evaluate the effects on the microstructure and tensile properties of 3d TM CCAs.

IS008

DISCOVERY OF A FeCoNiPdCu HIGH-ENTROPY ALLOY WITH EXCELLENT MAGNETIC SOFTNESS

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ABSTRACT

The author reports on the discovery of a magnetically soft high-entropy alloy of composition FeCoNiPdCu, which performs comparably to the best commercial soft magnets for static and low-frequency applications. Properly heat-treated FeCoNiPdCu develops nanostructure that can be viewed as a two-phase bulk nanocomposite of randomly intermixed FeCoNi magnetic domains and PdCu nonmagnetic “spacers”, both of 2–5 nm cross dimensions. Due to the nanometric size, the FeCoNi domains are magnetically single-domain particles, and since the particles are exchange-coupled across the boundaries, exchange averaging of magnetic anisotropy takes place, resulting in an almost vanishing coercive field and excellent magnetic softness. The formation of a two-phase nanostructure favorable for the exchange averaging of magnetic anisotropy is a consequence of specific values of the binary mixing enthalpies for the chosen elements. Though high-entropy alloys are generally considered to be random solid solutions of multiple elements on a topologically ordered crystal lattice, clustering of the atoms into preferential chemical environments on a nanoscale essentially determines their magnetic properties. Experimentally, the magnetic properties of the FeCoNiPdCu high-entropy alloy are compared to the commercial, magnetically soft non-oriented silicon electrical steel [1].

Keywords: high-entropy alloy, bulk nanocomposite, magnetism, magnetic softness

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IS009

MAGNETOELECTRIC EFFECT IN CHEMICALLY DISORDERED PEROVSKITE MULTIFERROICS

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ABSTRACT

Multiferroics are materials having two or more order parameters (for instance, magnetic, electric or elastic) coexisting in the same phase. They have emerged as an important topic in condensed matter physics due to both their intriguing physical behaviors and a broad variety of novel physical applications they enable. The unique physical properties of multiferroics originate from the complex interactions among the structural, polar and magnetic long-range order parameters. In magnetoelectric (ME) multiferroic materials, besides of the linear and biquadratic couplings of magnetic and electric order parameters, quadratic paramagnetoelectric (PME) effect should exist in the paramagnetic phase below the TC temperature of the paraelectric-to-ferroelectric phase transition, where the electric polarization is non-zero. In general, the quadratic ME coupling is much less studied in magnetoelectrics than the linear coupling while the former one can be even larger than its linear counterpart in antiferromagnetic (AFM) materials. Large ME coupling in AFM multiferroics, especially in ceramic samples, are attractive for applications in ME memory elements and spintronics as AFM domains are almost unsusceptible to external magnetic fields that preserves well the stored information. The coupling between ferroelectricity and antiferromagnetism offers an intriguing possibility of electric field control and switching of AFM domains.

It is aim of this report to present results of comprehensive study of the ME effect in chemically disordered perovskite multiferroics based on ferroelectric-antiferromagnets Pb(Fe1/2Nb1/2)O3 [PFN] and Pb(Fe1/2Ta1/2)O3 [PFT]. Usage of ceramic samples enables performing dielectric and ME response measurements up to 400-500 K without marked influence of conductivity. However, main attention is paid to low (T<150 K) temperatures, where the ME coupling coefficient is extremely large (as compared to the well-known multiferroic BiFeO3) and shows strong nonlinearity. We also present the results of ME measurements in PFN ceramics with 900 and 1800 switching of electric polarization in the AFM phase which demonstrate that the alignment of electric domains leads to corresponding alignment of magnetic domains. The behavior of the ME coupling between disordered (dynamically or statically) spin ensemble and polarization in case of spin-glass or superparamagnetic phases was studied as well. Extremely large ME response is demonstrated in magnetoelectrics with superparamagnetic phase. Phenomenological Landau theory of phase transitions is used to explain experimental data.

Keywords: multiferroic, magnetoelectric, multifunctional material, magnetoelectric

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IS010

PROBING STRUCTURAL AND MAGNETIC PROPERTIES OF THIN FILMS BY ^{57}Fe MÖSSBAUER SPECTROMETRY

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ABSTRACT

In this talk, recent advances of 57Fe conversion electron Mössbauer spectrometry (CEMS) for the analysis of thin films will be presented. Examples of applications will include various functional materials such as multiferroic thin films [1-2] and diluted magnetic semiconductors [3]. For multiferroic bismuth ferrite (BiFeO3) thin films, we will show that both strain and magnetic field destabilize the cycloidal spin structure (figure 1), resulting in a critical magnetic field sharply reduced from the bulk value [4].

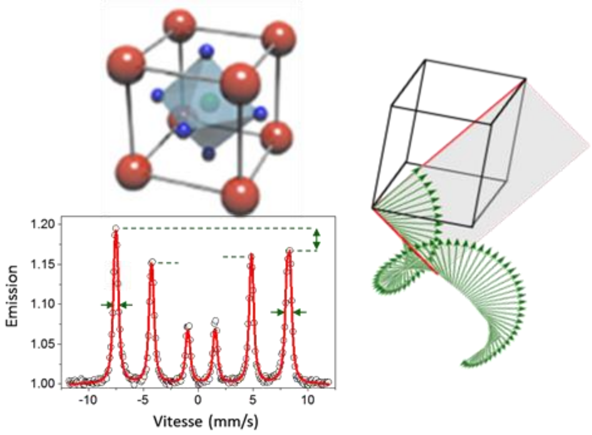

Figure 1: Mössbauer spectrum at 300 K of a 70-nm thick (001) BFO thin film grown onto GSO substrate and corresponding cycloidal spin structure derived from the fit.

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Keywords: thin film, multiferroic, Mössbauer spectrometry, magnetism.

IS011

ELECTROCALORIC EFFECT IN FERROELECTRIC COMPOSITES AND DOMAIN STRUCTURE

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ABSTRACT

Climate global warming is becoming a very serious problem all over the world, so that everyone must play their part in helping to save our planet.

It should be noted that industrial production alone generates nearly 51% of greenhouse gases. Among these greenhouse gases, there are coolants used in cooling devices. Freon and these analogs are also poisonous gases that are not environmentally friendly, so they must be disposed of in the future. The alternative will be to produce cooling based on the barocaloric (BCE), magnetocaloric (MCE), piezocaloric (PCE)or electrocaloric effect (ECE).

Physics based on these physical properties is gaining importance in order to replace the cooling gases with the solid material and the applications could take place massively in the near future, if the variation of the electrocaloric temperature approaches the 10 K for a material under a reasonable applied field.

In this presentation, we investigated the electrocaloric effect of phase transition region in ferroelectrics in general and those based on BaTiO3. At first, we were interested in the effect of doping to decrease Curie temperature towards room temperature and then on the amplification of the ECE. The first goal is reached. With regard to the amplification of the ECE our work continues on the study of the grain size effect and the control of domain structure and the combination of ferroelectric materials. The obtained results on the ferroelectric composites based on BCTL or BTSr and the perspectives were highlighted.

IS012

MECHANISMS DURING THIN FILM REACTION AND THEIR INFLUENCE ON THIN FILM PROPERTIES

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ABSTRACT

Thin films are essential bricks of many nanostructures used in nanotechnology devices. For example, the gate of complementary metal oxide semiconductor (CMOS) transistors is a stack of several nano-films of different electrical properties, typically: 20 nm-thick SiO_2/ 5 nm-thick monocrystalline doped-semiconductor/ 2 nm-thick SiO_2/ 10 nm-thick HfO_2/ 3 nm-thick TiN/ 20 nm-thick highly-doped polycrystalline Si/ 20 nm-thick silicide/ W 1^ST^ metallic contact. In order to get the desired properties, some layers composing the nanostructure need to be made of given phases containing several elements (given structure and composition). In this case, the desired phase needs to be grown after deposition, often using solid-state reaction. To this aim, several reaction processes can be used to form the phase of interest, such as thin-film reactive diffusion, which is a usual process in industry ("Salicide" process in microelectronics for silicide growth, for example). However, the reaction process type is expected to influence the structure and the atomic distribution of the obtained layer, and thus, could modify the film properties. Consequently, the growth process should be wisely chosen.

This study presents the influence of two types of solid-state reaction, reactive diffusion (RD) and non-diffusive reaction (NDR), on the chemical, structural, and magnetic properties of ferromagnetic Mn_5Ge_3 and MnCoGe thin films, potentially interesting for Ge-based spintronics. In our case, RD-mediated growth is characterized by a strong initial composition gradient and "long-range" atomic transport during the film growth, while NDR takes place without composition gradient and without long-range atomic transport. The comparison of these two opposite methods illustrates the influence of atomistic processes taking place during solid-state

crystal growth, such as atomic transport, on the properties of the obtained crystal. The results show also how the control of atomic transport could allow thin film properties to be modified.

IS013

DYNAMICAL PROPERTIES OF FERROELECTRIC THIN FILMS AND SUPERLATTICES

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ABSTRACT

Ferroelectric thin films and artificial superlattices composed of alternating ferroelectric layers usually exhibit better functional parameters than bulk materials of the same compositions or even can have new properties, not reachable in the bulk.

Epitaxial $Ba_{0.5}Sr_{0.5}TiO_3$ (BST0.5) thin film, bi-color artificial $BaTiO_3/Ba_{0.5}Sr_{0.5}TiO_3$ (BT/BST) and tri-color $BaTiO_3/Ba_{0.5}Sr_{0.5}TiO_3/SrTiO_3$ (BT/BST/ST) superlattices were grown on cubic single crystal (001)MgO substrates by pulsed laser deposition using alternating focusing of the laser beam on stoichiometric BT, BST, and ST targets. The bi- and tri-color superlattices were symmetric with the modulation periods of Λ = 135 Å and 143 Å, consequently. The total thickness of the grown BT/BST and BT/BST/ST superlattices was 1000 nm, while that of the BST-film was 600 nm. For comparison, the $Ba_{0.5}Sr_{0.5}TiO_3$ (BST05) ceramics sample was prepared by conventional solid-state reaction method from stoichiometric mixtures of $BaCO_3$, $SrCO_3$, and TiO_2 raw materials.

The structural parameters of the layers were determined by X-ray diffraction. Near- and sub-Terahertz dynamics of soft and Debye-type central modes was studied by the polarized Raman spectroscopy of the BT/BST*x* superlattices in the temperature range of 80-500 K. Based on the temperature dependence of the polar modes we revealed the phase transitions temperatures in the studied heterostructures. In the sub-THz frequency range of the *XZ* spectra, we observed the coexistence of the Debye-type central peak and soft mode in bi-color $BaTiO_3/Ba_{0.5}Sr_{0.5}TiO_3$ superlattice.

This work was supported by internal grant No. VnGr-07/2017-23 of Southern Federal University, Russia, and by H2020-RISE-ENGIMA action

Keywords: ferroelectrics, Raman spectroscopy, lattice dynamics, crystal structure, phase states

IS014

CONTRIBUTION TO THE IMPROVEMENT OF LIGHT EMITTING DIODES BASED ON NITRIDES

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ABSTRACT

Nowadays, the commercial success of light-emitting diodes (LEDs) has encouraged researchers to focus on the achievement of even higher efficiency optoelectronic devices. However, the improvement in the performance of LEDs is limited by some issues related to the active region and template properties, which have to be ameliorated. Commonly, sapphire substrates are used for the nitride material growth. Nevertheless, the large mismatch with nitride templates is considered as a source of significant number of defects, which reduce LED's luminescence. In order to overcome these drawbacks, we have proposed novel technology, so-called "SiN treatment". This technique has been proved to be very promising method for nitride material growth. It is a simple and cost effective technology, which introduces a randomly in-situ SiN nano-masking on sapphire substrate. We have elaborated Si-doped GaN template layer and nitride-based multiple quantum well (MQW) light-emitting diodes with GaN buffer layer using SiN treatment by metalorganic vapor phase epitaxy (MOVPE). It is shown that optical properties of InGaN/GaN MQWs depend on the defect density of elaborated templates. Thereafter, we report an enhancement of the emission of MQW LEDs using SiN treatment, compared to the MQW LED emissions deposited on a conventional GaN buffer layer.

keywords: GaN, MOVPE, SiN treatment, LEDs.

Orals

OR001

WEAR AND FRICTION BEHAVIOR OF THE POROUS TiNiCu ALLOY FOR BIOMEDICAL APPLICATION

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ABSTRACT

Porous TiNiCu alloys are used in wide and different engineering applications due to their excellent mechanical properties such as ductility, strength, toughness, etc. Also, these alloys have a good resistance to corrosion and the excellent biocompatibility properties, the demands increased to use it in different medical applications. The biomedical application of these alloys requires good structural and surface biocompatibility. It is characterized by the damage caused by the implant-tissue interaction. This damage is related to products released by friction. For this purpose, the objective of this work is the study of the tribological behavior of porous TiNiCu alloys, using two static partners: alumina ball and bone pion.In this research work, porous TiNiCu alloys were prepared from the pre-alloyed powders. The milling was realised using a planetary ball mill for 10 hours an under argon atmosphere. The The milled TiNiCu powders were then sintered at temperatures of 950°C for 7h.The results of the investigation confirm that wear degradation is manifested by the abrasive mechanism for both partners. The addition of copper improves the tribological properties of the alloys developed by decreasing the coefficient of friction.

Keywords: TiNiCu alloys, sintering, wear.

OR002

DESIGN OF A BIO-FLEXIBLE PIEZOELECTRIC NANOGENERATOR FOR BIOMECHANICAL ENERGY HARVESTING

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ABSTRACT

Over the last decade, the research and development of piezoelectric and sensing devices based on functional piezoelectric materials has made significant progress [1]. Piezoelectric nanogenerators (NGPs) are increasingly becoming a new energy conversion source with promising capabilities for mechanical energy harvesting using piezoelectric materials at the nanoscale [2]. So far, the market for piezoelectric devices is largely dominated by lead-based generators based on PZT ($PbZr_{1-x}Ti_xO_3$) systems because of their excellent piezoelectric properties. However, lead is toxic and harmful to the environment and our health [3]. Consequently, it is highly desirable to develop environmentally friendly piezoelectric materials whose piezoelectric properties would be comparable to those of lead-based components [4].

In this regard, lead-free ceramic $Ba_{0.85}Ca_{0.15}Zr_{0.10}Ti_{0.90}O_3$ (BCZT) with excellent dielectric, ferroelectric and piezoelectric properties were embedded in the biodegradable polylactic acid (PLA). BCZT fillers were elaborated by low-temperature hydrothermal route and functionalized via core-shell structuration using polydopamine layer (PDA). BCZT/PLA nanocomposite films were elaborated by solvent casting method. The core-shell structuration of BCZT particles leads to an enhancement of the dielectric, ferroelectric and energy storage performances. Finally, BCZT/PLA eco-friendly and bio-flexible nanogenerator was designed to have an insight on the output performances.

Keywords: Lead-free ceramic, biodegradable polymer, nanocomposite, piezoelectric nanogenerator, energy storage.

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OR003

PHOTOCATALYTIC AND PHOTOLUMINESCENT PROPERTIES OF A SYSTEM BASED ON $SmPO_4$ NANOSTRUCTURE PHASE

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ABSTRACT

In the present work, we investigate the structural, microstructural, vibrational, photocatalytic and luminescence properties of the system $SmPO_4$ thermally treated at 900 °C. Polycrystalline sample was elaborated using a coprecipitation technique. The sample was then characterized using X-ray diffraction, Scanning electron microscopy, Infrared spectroscopy, Raman spectroscopy and photoluminescence analyses under UV excitation. X-ray diffraction profile analyses showed that the monoclinic phase $P2_1/n$ was observed. The scanning electron microscopy experiments showed a homogeneous distribution of morphologies and indicated that $SmPO_4$ was in nano-sized particle. Attributions of Raman and FTIR vibrational modes were proposed. For the photocatalytic activity, UV-visible spectrophotometer has used to analyze the evolution of photodegradation of rhodamine B. Photoluminescence (PL) properties of $SmPO_4$ nanoparticle has been investigated and reported.

Keywords: Samarium phosphate $SmPO_4$, luminescence properties, co-precipitation technique, photocatalytic activity, diffraction techniques, spectroscopy methods.

Acknowledgments

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OR004

HIGHLY TEXTURED Ge(Sn) THIN FILMS GROWN BY MAGNETRON SPUTTERING ON Si(100)

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ABSTRACT

CMOS Si-Photonics is currently considered as a key technology for the development of the future generation of communication systems. In particular, Ge(Sn) semiconductor alloys have received increasing attention since it should allow the integration of laser in the CMOS technology [1], which is an essential brick still missing in Si-Photonics technology. Indeed, Ge(Sn) films are expected to be compatible to the CMOS technology, and to exhibit a direct bandgap for Sn concentrations higher than 10 at.%. Furthermore, Ge(Sn) should possess carrier mobility exceeding both the carrier mobility in Ge and Si. However, the low Sn solubility in Ge (≤ 1 at%) and the large lattice mismatch between α-Sn (6.489 Å) and Ge (5.646 Å) or Si (5.431 Å), complicate the epitaxial growth of Sn-rich Ge(Sn) layers on Si substrates. Growth techniques, such as chemical vapor deposition (CVD) and molecular beam epitaxy (MBE), were shown to be able to grow Sn-rich Ge(Sn) thin films in epitaxy on Si(001) substrate, exhibiting good crystalline properties [2]. Nevertheless, magnetron sputtering is one of the CMOS-compatible techniques the most cost-effective for mass manufacturing. This technique was shown to be able to produce Ge(Sn) thin films deposited on Si or Ge with reasonable electrical properties and high Sn concentration, allowing for the production of efficient Ge(Sn)-based devices [3].

The present work aimed to study Ge(Sn) thin film elaboration on Si(100) substrate, using magnetron sputtering. $Ge_{1-x}Sn_x$ thin films with $0.04 \leq x \leq 0.13$ were deposited at room temperature (RT) or at 360 °C on Si(100) substrates, with or without the pre-deposition of a Ge buffer. The film growth kinetics was studied by in-situ XRD, while the film microstructure was investigated using XRD and SEM, and their surface state was studied by AFM. In situ XRD measurements show a strong kinetic competition between Ge(Sn) crystallization and Sn incorporation, complicated by Sn melting and de-wetting, limiting the possibilities of Ge(Sn) layer production. Ge and Sn phase separation can lead to strongly inhomogeneous layers, with probably amorphous Ge inclusions. However, Sn selective etching using a 5% HF solution can be used to improve the surface state of the films. RT deposition leads to the growth of polycrystalline Ge(Sn) layers, while the subsequent deposition of a Ge buffer and the Ge(Sn) film at 360 °C allows the growth of a strongly textured Ge(Sn) layers, probably in epitaxy on the Si(001) substrate, with a good surface state and a high Sn incorporation (~ 13 at%).

Key words: Si photonics, CMOS, Ge(Sn), magnetron sputtering, epitaxy.

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OR005

DIELECTRIC AND ENERGY STORAGE STUDY FOR THE ITO/$BiFe_{0.95}Mn_{0.05}O_3$/$SrRuO_3$/$SrTiO_3$ HETEROSTRUCTURE

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ABSTRACT

During the last years, multiferroic materials have gained great attention due to their fundamental physics and possible integration in advanced applications, especially in energy storage. BiFeO3 (BFO) appears actually as one of the most interesting, because it shows multiferroic properties at room temperature. The lack of dielectric study in the BFO thin film present an obstacle to this integration. To remedy this, a BFO thin film was elaborated by pulsed laser deposition, and a dielectric dependency in frequency and temperature is investigated. The dielectric relaxation study, noticed two origins, the translational hopping process, and the dipole frictional losses. The energy storage is deduced from the measured polarization hysteresis loop.

Keywords: energy, dielectric, thin film, multiferroic.

OR006

$LaCoO_3$ THIN FILMS AS GAS SENSOR

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ABSTRACT

Gas sensors recently attracted attention of researchers for application in harsh environment for example in car industry [1]. Electrochemical sensors with perovskite $LaCoO_3$ sensing electrodes deposited on Yttrium Stabilized Zirconia (YSZ) is promising configuration. Cubic YSZ is a well-known ionic conductor widely used in gas sensor application. In literature there is few works concerning tetragonal YSZ as ionic conductor in gas sensor. Tetragonal phase is characterized by high chemical stability and high mechanical properties. Perovskites are popular sensing materials [2]. In this work thin films of $LaCoO_3$ were deposited on YSZ (9,5 % mol) and (3,5%) substrates by Pulsed Laser Deposition (PLD) method at 750 °C and 850 °C in presence of oxygen. The sensors are in the configuration $LaCoO_3$/YSZ/Pt and will be used for the detection of NOx gases. The influence of the deposition temperature and of nature of the substrate on the morphology of the sensing electrodes ($LaCoO_3$ thin films) was investigated by Transmission Electron Microscopy (TEM) X Ray Diffraction (XRD) Scanning Electron Microscopy (SEM). The resistance variation of $LaCoO_3$ layers under NO_2 was also tested. Sensors were exposed to various concentration of NO_2 in the temperature range 25 °C - 700 °C.

Keywords: gas sensors, thin films, $LaCoO_3$, PLD, NO_2

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OR007

HYBRID THIN FILMS FOR CATALYTIC DEGRADATION OF DYES

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ABSRACT

During the past twenty years, oxidation techniques have been emerged as new processes for treat of wastewater containing high concentration of non-biodegradable and / or toxic pollutants. Photocatalytic degradation is one of these techniques which is capable whether partially or completely mineralizing various organic molecules. Titanium dioxide TiO2 is the most widely used as photocatalyst, because of its photo-stability and low costs, however, the photocatalytic efficiency of this material is limited by the fact that its particles are harmful [1] for biological bodies. A new promising material is based on hybrid composite of bismuth oxide and carbon deposited on thin films using spin coating and PECVD techniques. In this work, we present a brief description of the microstructure of the deposited thin films and the results of photodegradation tests carried out on indigo carmine and methyl orange dye solutions diluted in distilled water. The results showed a total discoloration of the solutions, thus a loss of associated chromophores. The apparent kinetics of the discoloration reactions were calculated basing on the Langmuir - Hinshelwood model and studied according to the different deposition parameters of our BiOC films.

Keywords: catalytic degradation, dye, thin film, titanium dioxide, apparent kinetics.

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OR008

EFFECT OF THE WO_3/Nb_2O_5 RATIO ON THE STRUCTURAL, ELECTRICAL AND ENERGY STORAGE PROPERTIES OF $BaO–Na_2O–Nb_2O_5–WO_3-P_2O_5$ GLASS–CERAMICS

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ABSTRACT

Ferroelectric glass-ceramics are promising composite materials with dual properties, of high dielectric permittivity and high dielectric breakdown strength. In this context, new phosphate glass-ceramics $2BaO-0.5Na_2O–2.5[(1-x)Nb_2O_5–xWO_3]-1P_2O_5$ (x=0, 0.1, 0.2, 0.3 and 0.4) designated B0, B1, B2, B3, B4 respectively, were prepared by the controlled crystallization technology and then crystallized at high temperature of 760 °C for 10 hours. Subsequently, the obtained glass-ceramics were studied by Differential Scanning Calorimetry (DSC), X-ray powder diffraction (XRD), Raman and impedance spectroscopy. All of these techniques allowed the identification of $Ba_2Na_4W_2Nb_8O_{30}$ phase with tungsten bronze structure embedded in the glassy matrix. The density of glass-ceramics was found to increase with increasing tungsten content to reach a maximum at x =0.3 and then decreases. Dielectric and conductivity parameters were found to be governed by the presence of oxygen vacancies. The dielectric constants of all the samples exhibited excellent stability from 25 °C to 150°C °C and low dielectric losses less than 0.03. Room temperature energy storage property which depends on the composition X, was performed using *P-E* hysteresis loops of the glass-ceramics. The optimum recoverable density of 25.6 $mJ/cm^3$was obtained for B3 with an energy efficiency of 73.77% under the electric field of 90kV/cm.

Keywords: Phosphate; Glass-ceramics; Structural and Dielectric properties; Energy storage; WO_3.

OR009

ELECTRICAL TRANSPORT PROPERTIES OF MULTI-CONTACT INTERFACES AND SPOTS NUMERICAL IMAGING FROM SURFACE PROFILOMETRY

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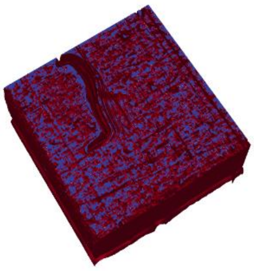
ABSTRACT

Though widely used in many industrial applications, discrete interfaces arising from contacting metal pieces are poorly understood. That field has attracted the attention of most engineers or researchers to respond to the acute need for a better understanding of both the physical and mechanical processes acting within such interfaces and open new ways to the control and optimization of these interfaces.

The major obstacle to a physical understanding of such interfaces originates from their structural and functional complexity. Due to their discreteness consisting of a sparse array of mechanical spots with typically micron size scales, their structural complexity is tightly connected to the random surface geometry of the contacting materials. On the opposite side, their functional complexity regards multiphysical aspects such as the strongly coupled thermal and electrical transport properties and their sensitivity to the mechanical conditions imposed to the interface. The mechanical spots contribute the electrical properties both individually through their shape and size and collectively through their elastic interactions. The interface structure is a basic knowledge which allows computing its transport properties whenever a model of electron transport is available.

Our approach to discrete interfaces relies on the prior determination of the interface structure from surface profilometry and numerical imaging of the spots. The surface profiles data processing with a specific numerical code provides the spots array, its evolution with the compression force, the statistical spots sizes and shapes distribution as well as the mechanical stresses. The electrical properties are extracted from the numerical simulation of an electron transport model restricted to constriction effects. In a second step, these predictions are compared to electrical and mechanical stresses data obtained on copper/copper interfaces allowing the validation of the numerical model and a further interpretation of the physical processes acting within the contact.



Simulation of the mechanical contact between a cooper plate and a flat rigid surface

OR010

MULTILAYER DEVICES FROM THIN FILMS OBTAINED BY TAPE CASTING

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ABSTRACT

Creation of thin $BaTiO_3$ tapes for use as a dielectric layers in ceramic multilayer capacitors is a challenging goal because it is the most efficient way to increase an MLCC capacity. The use of nanopowders as the basis for tapes is promising because it allows obtaining of films with low thickness and roughness close to the linear dimensions of one nanoparticle. It is a guarantee of improving the performance of multilayer devices without increasing their size, which is consistent with the tendency of miniaturization. Adaptation of high productive film formation method like tape casting to create layers with thickness of less than 1 µm from an affordable electrotechnical materials is a promising and challenging goal.

The $BaTiO_3$ nanopowder was used to create tapes of dielectric layers and a mix of Ni/NiO powders was used for conductive layers. Tapes with the thickness from 5 µm to less than 1 µm were created by the tape casting method. The rheological behavior of all casting suspension was studied and casted tapes were characterized. Surface roughness comparable with the diameter of 1 particle was achieved. From obtained tapes, a few types of multi-layer composites with different layers thickness were assembled using isostatic lamination. Obtained multi-layer composites were successfully annealed and sintered without cracking or delamination.

Keywords: tape casting, thin films, MLCC, nanopowders, sintering.

OR011

EFFECTS OF CONCENTRATION AND TEMPERATURE ON THE RHEOLOGICAL PROPERTIES OF NANOFLUIDE GRAPHENE / SLIDEWAY OIL

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ABSTRACT

Nanofluids are colloidal solutions composed of particles with nanometric size, suspended in a liquid. Their astonishing thermal properties have been the subject of intense investigation during the last decade. In this study, the effects of the volume fraction of graphene nanopowder and temperature were studied on the rheological properties of the slideway oil as a base fluid. For this purpose, nanofluids based on graphene were prepared using a two-step process. In addition, in order to evaluate the morphology and the stability of the nanoparticles, a scanning electron microscope analysis was performed on these samples. The results of the SEM analysis indicated a uniform dispersion of nanoparticles. In addition, the results of the experiments indicated that with increasing temperature, the viscosity of the nanofluid decreases. In addition, it has been found that the dynamic viscosity of the nanofluids, having a solid volume fraction of less than 1%, is lower than that of the base fluid. For fractions from 1%, the dynamic viscosity of the nanofluid increases with the solid volume fraction. Finally, the addition of these nanoparticles can also modify the Newtonian behavior of the base fluid, and then the behavior of the nanofluids strongly depends on the volume fraction in nanoparticles.

Keywords: Graphene, slideway oil, nanofluid, viscosity, rheological properties, volume fraction, temperature

OR012

INTERACTIONS BETWEEN TRANSFORMATIONS DURING INTERCRITICAL ANNEALING OF A HIGH-FORMABILITY STEEL

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ABSTRACT

High strength steels are widely used in the automotive industry to help reduce the average weight of vehicles without compromising passengers safety [1]. Manufacturing these steels involves a cold-rolling step before intercritical annealing, during which a certain volume fraction of austenite is formed. The austenite decomposes upon cooling into several products (usually martensite) and gives the steel its final microstructure.

The steel mechanical properties are dependent on the volume fraction of the phases composing the microstructure, but also on their chemistry, their morphology and their spatial distribution. This latter property is essential to ensure good formability. Consequently, it is of prime importance to not only understand *how* austenite forms during intercritical annealing, but also *where*. During intercritical annealing, several transformations occur simultaneously, such as recrystallization, cementite precipitation, microalloying elements precipitation and austenite formation. These transformations interact with each other [2–5]. For example, microalloying elements hinder recrystallization [5], whereas incomplete recrystallization tends to accelerate austenite formation kinetics and leads to banded microstructures [2,4].

In this study, we used a model for microstructural evolutions during intercritical annealing to show how these transformations interact with each other, and how cementite precipitation, often neglected in available literature, should be considered to properly model recrystallization and austenite formation kinetics.

Keywords: cementite, recrystallization, precipitation, austenite, intercritical annealing

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OR013

OBTAINING PURE STOICHIOMETRIC LEAD TITANATE WITH SIZE CONTROL

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ABSTRACT

Lead titanate ($PbTiO_3$) is a well-known material for its unique ferroelectric and piezoelectric properties. Despite on the toxicity of the Pb-content material it still attracts high attention due to the wide spectrum of the properties such as switchable polarization, piezoelectricity, high non-linear optical activity, pyroelectricity and high dielectric behavior. Due to the toxic nature of the PbO volatile material at high temperature and problems connected with large lattice distortion during cubic- tetragonal phase transition around 773 K, it's important to reduce the synthesis temperature. In this context synthesis method and condition, which has the crucial role on the temperature, should be well matched. There're various methods of $PbTiO_3$ nanopowders preparation such as conventional mixed-oxide, mechanochemical synthesis, Pechini-type processes, hydrothermal process, sol-gel processing. Among them, the most appropriate in context of phase purity, stoichiometry precise control, particle size, homogeneity and production effectivity, is Pechini method, thermal decomposition of the organic precursor. Crucial role in the obtaining product with desire characteristic in this method is determination of the precursor optimal precipitation condition and optimizing the heat treatment condition of its precursor. In present work $PbTiO_3$ with tetragonal structure was obtained with Pechini and hydrothermal methods. The effect of lead titanyl oxalate precipitation conditions (starting reagents, pH, C solution) and precursor thermal decomposition mode on the final decomposition temperature and morphology of lead titanate nanopowders were investigated. Thermogravimetric analysis of lead titanil oxalate was performed to investigate the optimal calcification regime. Hydtothermal method of $PbTiO_3$ obtaining was used to compare with Pechini method in view of morphology characteristic. The obtained powders of lead titanate were analyzed by scanning electron microscopy and X-ray analysis. The optimal mode of calcination of lead titanate oxalate has been determined, taking into account the variety and low melting point of lead oxides in order to obtain the pure phase of lead titanate. The final temperature for the $PbTiO_3$ crystallization is 823 K. The sizes of the $PbTiO_3$ nanoparticles obtained with Pechini and hydrothermal methods are 8-75 nm (with aggregate sizes of 166-500) and 83-333, respectively. Comparison of hydrothermal method and Pechini methods in terms of morphology control for $PbTiO_3$ obtaining was performed

Keywords: lead titanate, Pechini method, hydtothermal method, size control

OR014

ELABORATION OF THERMOELECTRIC Mg-Ag-Sb THIN FILMS

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ABSTRACT

The increase of functionality of mobile technologies leads also to an increase of energy consumption, limiting the autonomy of mobile devices. In this context, new technologies allowing for environmental energy harvesting (EH) are currently investigated. These EH devices should allow the autonomy of mobile devices to be extended by either partially recharging the battery of the device or allowing some operations to be performed without using the energy stored in the battery.

In the case of technologies such as micro-sensors, microelectronics integrated circuits (IC) etc. for which part of the energy is thermally lost, the integration of thermoelectric devices appear as a potential EH solution. In this case, the integrated thermoelectric device should be based on nanostructures, such as thin films, elaborated with industrial processes compatible with the complementary metal oxide semiconductor (CMOS) technology [1], and the material working-domain should be around room temperature. BiSbTe and Bi2Te3 are known as the best compounds operating at room temperature [2-3]. However, these materials are toxic and scarce, motivating the development of alternative materials.

The ternary compound α-MgAgSb was recently shown as a serious potential candidate for room-temperature thermoelectric applications. It is a less-toxic *p*-type thermoelectric material exhibiting a ZT ~ 1 close to room temperature, which can be increased by doping [4]. However, this material was only studied in its bulk state, using elaboration methods incompatible with CMOS technology.

In this work, the elaboration of MgAgSb thin films by CMOS-compatible magnetron sputtering is investigated for the first time. The film microstructure is characterized by as X-ray diffraction and scanning electron microscopy, and compared to the film Seebeck coefficient measured between –50 and +50 °C.

Keywords: Thermoelectric materials, Mg-Ag-Sb, thin film, Seebeck coeficient

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OR015

THE EFFECT OF Sn DOPING ON STRUCTURAL, FERROELECTRIC, DIELECTRIC AND ELECTROCALORIC PROPERTIES OF $Ba_{0.9}Sr_{0.1}TiO_3$

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ABSTRACT

The lead-free ferroelectric materials $Ba_{0.9}Sr_{0.1}Ti_{1-x}Sn_xO_3$ with x = 0, 0.02, 0.05, 0.07, 0.10 and 0.15 (abbreviated as BSTS) were prepared using the conventional solid-state method. The effect of Sn substitution on the crystal structure, ferroelectric behavior, dielectric and electrocaloric properties of BSTS ceramics have been systemically investigated. The X-ray diffraction (XRD) patterns show that the samples have well crystallized into perovskite structure suggesting the substitution of Ti^{4+} by Sn^{4+} in BST lattice. With increasing Sn-content, the enhancement of the dielectric permittivity was observed for ($0 \leq x \leq 0.10$) and the ferroelectric transition temperature (T_C) was found to shift towards the room temperature (T_C = 33°C for x = 0.10). A Typical P–E hysteresis loops were observed for the investigated compositions and they were confirmed the ferroelectric-paraelectric phase transition. Electrocaloric effect (ECE) of BSTS ceramics was studied by using the indirect method from P-E hysteresis loops using the Maxwell relation.

Keywords: BSTS ceramics, Electrocaloric effect (ECE), X-ray diffraction, ferroelectric.

OR016

PHASE FORMATION BETWEEN NI THIN FILMS AND InAs SUBSTRATE

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ABSTRACT

As conventional Si CMOS scaling approaches the end of the roadmap, III-V based MOSFETs are seriously being considered as an alternative technology to continue Moore's law.[1] To realize high-performance III-V MOSFETs, reliable contact metals for S/D with low contact resistance is essential, especially in highly scales devices [2]. An atomic level understanding of the metal-semiconductor solid-state reaction can shed light on material-electronic property interactions at nano-scale, especially when the intentional or unintentional defects are present. The best candidate as III-V material is the solid solution InGaAs, with the adequate proportion in order to be able to grow in epitaxy with Si. Despite the large interest for this material, fundamental studies on the metal reaction have principally focused on GaAs and very few on InAs. We have focused our research on this last ternary system (Ni/InAs). Ni has been deposited on InAs(100) substrate to form a 100 nm thick film. The first phase formed during the solid state reaction has been identified as Ni_3InAs with a NiAs hexagonal structure. It grows in epitaxy from an initial layer formed as deposit. The ternary phase is stable up to 250°C but from this temperature a new phase appear. The solid state reaction has been followed by in situ x-ray diffraction and the phase formed during the first stage has been characterized carefully using HRTEM. The relation of epitaxy between the phase and InAs substrate has been established and is different from the one found for the similar system Ni/GaAs.

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Keywords: III-V materials, thin films, solid state reaction, epitaxy, contact

OR017

IN SITU AND REAL TIME STUDY OF GRAVITY EFFECTS ON THE SOLIDIFICATION MICROSTRUCTURE FORMATION

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ABSTRACT

Mechanical properties of materials are deeply related to the solidification microstructure, which results from the solidification conditions such as the thermal history and gravity-related phenomena. The understanding of the relationship between the final grain structure and the processing conditions is thus crucial to improve industrial products. In this work, we will present a study of the gravity effects on the dynamic of the microstructure formation. It is well known that gravity-related phenomena such as thermo-solutal convection caused by density gradients in the melt, and buoyancy when the liquid phase is denser than the solid phase or vice-versa, are unavoidable and can affect drastically both the grain number and their morphology. The aim of our study is to investigate directional solidification experiments of refined Al-20wt.%Cu alloys, using in-situ and real time X-radiography. Experiments were carried out on sheet-like samples (thickness ≈ 250 µm) in the laboratory device SFINX (Solidification Furnace with IN situ X-radiography), for two different furnace orientations with respect to the gravity direction:

- Horizontal orientation where the main surface of the sample is perpendicular to the gravity direction. For this configuration the gravity related phenomena are limited in the thickness of the sample.
- Vertical orientation where the main surface is parallel to the gravity direction. For this position, the temperature gradient can be either parallel to gravity (upward solidification) or antiparallel to gravity (downward solidification). The gravity effects are significant in the liquid phase of the sample for this configuration.

The comparison of the grain formation mechanisms during the experiments performed with the same solidification parameters (growth velocity and temperature gradient), but with the two different configurations (horizontal and vertical) allows us to reveal the different effects related to the presence of gravity and that affect the grain structure. The main phenomena highlighted from this comparison and that affect drastically the grains structure formation are the grain floatation during the upward solidification due to the buoyancy force, and the Cu-enriched plume formation during the downward solidification.

Keywords: Solidification, X-radiography, convection, grain structure, gravity, buoyancy.

OR018

EFFECT OF Sr DOPING ON THE CONDUCTION PROCESS IN THE COPPER CALCIUM TITANATE CERAMICS SYNTHESIZED BY SEMI WET METHOD

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ABSTRACT

In this report, strontium (Sr) doped Calcium Copper Titanate $Ca_{1-x}Sr_xCu_3Ti_4O_{12}$ with two values x=0 and x=0.05 commonly known as CSCTO ceramics have been obtained by using the semi wet route synthesis method. Rietveld refinement shows that the powders crystallize in the cubic perovskite related structure with Im3 space group. Scanning Electron Micrograph (SEM) analysis shows that the average grain size of ceramics becomes larger when Sr doping is considered. Both DC and AC electrical conductivity are investigated throughly in the temperature and frequency ranges between [373-653K] and [20Hz-1MHz], respectively. The values of the average activation energies for CSCTO-0 (x=0) and CSCTO-5 (x=0.05) were found to be 612meV and 576meV, respectively. In Fact, Sr doping has an effect on the broadening of the impurity band that can lead to a dramatic decrease in the activation conduction energy of CSCTO ceramics. A systematic study of AC electrical conductivity reveals that the predominant conduction mechanism existing in these ceramics is generated by large polaron hopping process. This mechanism has also been identified by the modulus analysis and confirmed by comparing the hopping polaron size with the lattice parameter.

Keywords: Copper Calcium Titanate, semi wet route, low temperature, electrical properties, OLPT.

OR019

LAYERED $Na_{0.66}[Co_1\text{-}yTiy]O_2$ CATHODES FOR NEXT GENERATION SODIUM-ION BATTERIES

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ABSTRACT

Rechargeable Sodium-ion batteries are regarded to be promising for next generation storage devices i.e. grids thanks to the rich and natural abundance of sodium and as a consequence low price. In addition to that, sodium-ion batteries exhibit similar electrochemical mechanism as commercial lithium-ion batteries. Commercialized by Sony in 1991[1], $LiCoO_2$ has received tremendous success as positive electrode material for lithium ion batteries. This was the main reason that motivated researchers to investigate first Na_xCoO_2 as alternative for the sodium-ion technology. In comparison to its lithium counterpart, the Na_xCoO_2 structure show numerous potential steps during electrochemical sodium intercalation/deintercalation. This suggests more complicated phase transitions. The aim of this work is to elucidate the effect of increasing titanium contents on the structural properties and electrochemical performances of $Na_xCo_yTi_{1-y}O_2$ (y=0, 0.05;0.1; 0.2; 0.3; 0.33) system in Na half-cell. $Na_xCo_yTi_{1-y}O_2$ compositions were synthesized through the solid state method, the sodium electrochemical intercalation/deintercalation in the potential window 2-4.2V was investigated via diffraction using synchrotron radiations. The crystal structure of all compositions was stable over the cathodic potential window.

Inactive titanium has drastically reduced the number of potential steps and limited the biphasic domains observed in the case of $Na_{0.66}CoO_2$. The combined effect of cobalt and titanium has shed light on a powerful candidates in terms of structural stability at high voltages and stable capacity for next generation sodium ion batteries.

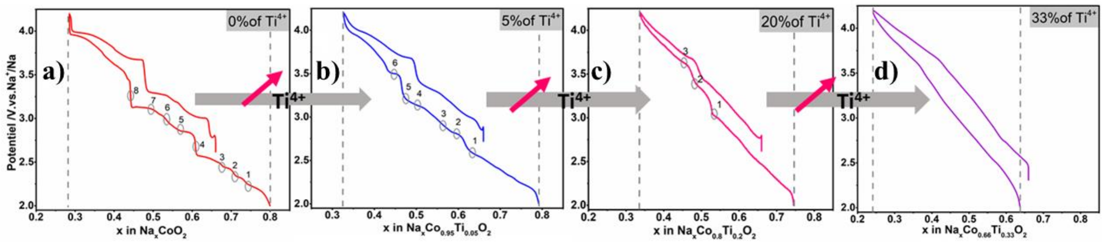

Figure 1: Galvanostatic Cycling test with Potential Limitations involving $Na_xCo_{1-y}Ti_yO_2$ with different titanium concentrations at sodium half-cell in the potential range 2 and 4.2V

Keywords: Sodium-ion Batteries, Layered Structures, $Na_{0.66}Co_{1-y}Ti_yO_2$,

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OR020

STRUCTURAL, THERMAL, ELECTRICAL AND ELECTROCALORIC PROPERTIES OF LEAD-FREE BCZT-BCT SOLID SOLUTION

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ABSTRACT

Lead-free $BaTiO_3$ (BTO) and its solid solutions (BST, BCT, BZT, BCT-BZT) have a wide range of applications in many fields including electronic industries, such as positive temperature coefficient devices, infrared detectors, multilayer ceramic capacitors (MLCC), lead-free piezoelectric transducers, microwave tunable dielectrics , because of their enhanced dielectric, ferroelectric, piezoelectric and electrocaloric properties [1–2]. $Ba_{1-x}Ca_xTiO_3$ (BCT) solid solution has been reported as a promising MLCC, dielectric filters and piezoelectric actuators[3]. In recent years, an increase interest in the development of lead-free piezoelectric and electrocaloric materials such as $(1-x)Ba(Zr_{0.2}Ti_{0.8})O_3–x(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT-BCT) system by dint of its excellent electromechanical properties[4]. In this study, $(Ba_{0.8}Ca_{0.2})(Zr_{0.02}Ti_{0.98})O_3$-$(Ba_{0.8}Ca_{0.2})TiO_3$ solid solution in weight ratio 1:1 abbreviated BCZT-BCT was synthesized by solid state reaction method. Structural, dielectric, thermal, ferroelectric, alongside to electrocaloric properties were thoroughly investigated. In-situ Raman spectroscopy results confirmed the existence of tetragonal phase at Room temperature. X-ray diffraction and the differential thermal analysis (DSC) measurements of BCZT-BCT ceramic were used to highlight the phase transition from tetragonal to cubic at 115 °C. High dielectric permittivity (ε'~ 9000), low dielectric loss (δ ~0.02) were found at Curie temperature T_c=115 °C. The coercive field of BCZT-BCT was found to be less than 2 kV/cm.

Keywords: Lead-free ceramic, solid solution, phase transition, dielectric, ferroelectric

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OR021

MICROSTRUCTURAL EVOLUTION OF DISSIMILAR METAL WELDS DURING AGEING: AN APT/EBSD INVESTIGATION

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ABSTRACT

The integrity of the welded joints made to assemble the various components of a nuclear reactor is very important for the proper functioning of the power plant. The joints are used to assemble at least two different materials, and the welding operation of these heterogeneous materials involves metallurgical and chemical phenomena, leading to atomic redistributions. Furthermore, atomic redistribution in the joint vicinity can be modified (grain boundary segregation, precipitation…) during ageing at the service temperature, modifying the mechanical properties of the polycrystalline materials.

A new narrow gap design of Dissimilar Metal Welds (DMW) for nuclear plants has been developed recently using inconel52 as filler metal, in order to join the main components of the nuclear island made of bainitic low alloy steel (LAS), with the main coolant line pipes made of austenitic stainless steel 304L type.

In this work, the [inconel52/LAS] side of the DMW is studied, since the rupture of fracture toughness specimens in the brittle to ductile domain takes place in this area. Due to the temperature gradient cause by the welding procedure, four different zones are generated in the joint vicinity, exhibiting different structural and chemical properties: i) a carbide band at the [inconel52/LAS] interface, a heat affected zone deeper in the LAS composed of two zones ii) a carbon depleted zone and iii) a carbon non-depleted zone, and finally iv) the base LAS metal. The aim of this work is to study the metallurgical changes in these four zones due to thermal ageing. X-ray diffraction, **EBSD, SEM**, and atom probe tomography are used to investigate both structural (dislocation density…) and chemical (grain boundary segregation, precipitation…) evolutions, in the case of five different ageing states, obtained by five different annealing conditions. This work is a first attempt to establish a link with the mechanical behavior of DMWs.

Keywords: DMWs, ageing, APT, Segregation, Mechanical behavior

OR022

ENHANCED OF MAGNETOELECTRIC COUPLING IN MFe_2O_4/PZT/ MFe_2O_4 (M=Ni,Co) : A MONTE CARLO SIMULATION

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ABSTRACT

Based on the Monte Carlo simulation, ferroelectric, magnetic and magnetoelectric properties of $NiFe_2O_4$/PZT (NFO/PZT), $CoFe_2O_4$/PZT (CFO/PZT), $NiFe_2O_4$/PZT/$CoFe_2O_4$ (NFO/PZT/CFO) and $NiFe_2O_4$/PZT/$NiFe_2O_4$ (NFO/PZT/NFO) heterostructures were carried out. The effect of the temperature on magnetization, electric polarization and their susceptibilities have been examined. The determination of the interfacial magnetoelectric coupling interaction $\mathbf{J_{me}}$ in NFO/PZT interface and CFO/PZT interface permitted to predicte the magnetoelectric voltage coefficient inNFO/PZT/CFO and NFO/PZT/NFO heterostructures. Interestingly, a high magnetoelectric voltage coefficient of 762.7 and 2080 mV/(cm.Oe) was predicted in NFO/PZT/CFO and NFO/PZT/NFO, respectively. Moreover, the effect of $\mathbf{J_{me}}$ on **M-H** and **P-H** hysteresis loops and magnetoelectric voltage coefficient was studied.

Keywords : Monte Carlo simulation ;magnetoelectric properties ; heterostructures; M-H and P-H hysteresis loops ; magnetoelectric voltage coefficient.

OR023

SYNTHESIS AND CHARACTERIZATION OF Bi_2O_3 BY SELF ASSEMBLY PHENOMENON FOR RHODAMINE B PHOTODEGRADATION

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ABSTRACT

In recent years, semiconductor photo-catalysts attracted many researchers due to their promising

applications in the removal of environmental pollutants, such as the photo-degradation of organic dyes. Furthermore, self-assembled 3D architectures of these materials can increase their catalytic

performances. For this purpose, we investigate the relationship between the architecture via the selfassembly phenomenon of bismuth oxide (Bi2O3), a semiconductor which exhibit an interesting bandgap, and its photo-catalytic activity for the degradation of one of the most important organic dye. In our study, we report the fabrication of various morphological bismuth oxides (Bi2O3) by a self-assembly process of bismuth oxalate at room temperature. Under controlled pH, bismuth oxide was successfully synthetized from oxalate precursor, by an aqueous precipitation method using bismuth (III) nitrate hydrate, nitric acid and oxalic acid. The elaborated sample was dried and calcined for two hours. The powders were structurally, morphologically and thermally characterized using X-ray diffraction (XRD), Scanning electron microscopy (SEM) coupled with energy dispersive X-Ray analysis (EDS), Thermogravimetric analysis coupled with differential thermal analysis (TGA/TDA). The photodegradation performance of the as prepared photo-catalyst was evaluated on the degradation of Rhodamine B using UV visible spectrometer.

Keywords: Bismuth oxide Bi2O3, self-assembly phenomenon, photo-degradation, Rhodamine B

OR024

STRUCTURAL, ELECTRONIC, MAGNETIC, AND MAGNETOCALORIC PROPERTIES IN SEMICONDUCTORS TRI-CHALCOGENIDES (TMTC) WITH THE CHEMICAL FORMULA ABX_3

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ABSTRACT

As one of the rare ferromagnetic semiconductors tri-chalcogenides (TMTC) with the chemical formula ABX_3 (A = Mn, Cr; B = Si, Ge; X = S, Se, Te) has recently attracted a great deal of attention as a potential candidate for next-generation high-performance nano-spintronic devices. In this study, the density of states, band structure and optical properties have been studied by Ab-initio calculation. Respectively, the magnetic and magnetocaloric properties have been performed using Monte Carlo simulation by adopting various models, including the three-dimensional (3D) Ising model and the 3D Heisenberg model. The Curie temperatures were reported to increase as the number of layers is reduced. [1-2]

Keywords : magnetocaloric, Heisenberg, tri-chalcogenides, optical properties, nano-spintronic.

OR025

STRUCTURAL, DIELECTRIC AND ELECTROCALORIC PROPERTIES OF (Ba$_{0.85}$Ca$_{0.15}$)(Ti$_{0.9}$Zr$_{0.1-X}$Sn$_{X}$)O$_{3}$ CERAMICS ELABORATED BY SOL-GEL METHOD

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ABSTRACT

Ferroelectric ceramics (Ba$_{0.85}$Ca$_{0.15}$)(Ti$_{0.9}$Zr$_{0.1-x}$Sn$_{x}$)O$_{3}$ (x=0.00, 0.02, 0.04, 0.06) were prepared by a sol-gel method. Structural investigation revealed the co-existence of tetragonal (*P*4*mm*) and orthorhombic (*Pmm*2) symmetries at room temperature for the undoped ceramic, while only a tetragonal structure (*P*4*mm)* was observed for the doped ceramics. Dielectric measurements indicate a dielectric relaxation process at high temperatures which is essentially related to the hopping of oxygen vacancies $V^{\cdot\cdot}_{O}$. Furthermore, a down shifting of the Curie temperature (T$_{C}$) with increasing Sn^{4+} doping rate has been revealed. The temperature profiles of the Raman spectra unveiled the existence of polar nanoregions (PNRs) above the Curie temperature in all ceramics. The ferroelectric properties were found to be related to the microstructure. Electrocaloric effect was investigated in this system that revealed an electrocaloric responsivity of 0.225×10^{-6} K m/V for the composition with x = 0.04 Sn doping, where other remarkable physical properties were also observed.

Keywords: Sol-gel, polar nanoregions, phase transition, electro-caloric.

OR026

ARSENENE MONOLAYER AS AN OUTSTANDING ANODE MATERIAL FOR (Li/Na/Mg)-ION BATTERIES: DENSITY FUNCTIONAL THEORY

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ABSTRACT

Arsenene, a single layer arsenic nanosheet with a honeycomb structure, has attracted increasing attention recently due to its many exceptional properties. In this paper, the density functional theory (DFT) calculations are employed to investigate and compare the interaction of Li, Na or Mg ions with the arsenene monolayer. On purpose, to be used as anodes in lithium, sodium, and magnesium ion rechargeable batteries. The results indicate that the Li, Na and Mg adatom preferably adsorbed on the valley sites, with a negative adsorption energy of -2,55; -1,91 and -1,10 eV, respectively, introducing strong binding between alkali-metal and arsenene monolayer which is important fact for battery application. Also, it is found the arsenene exhibit a high theoretical specific capacity up to 1430,91 mAh/g for Li and Mg and 1073,18 mAh/g for Na, which are extremely higher than the commercially used graphite anode (372 mAh/g) in Li-ion batteries. Furthermore, the diffusion barrier energies of Li, Na and Mg ions are calculated using the nudged elastic band method. The activation energy barriers of these ions show isotropic behavior for the different pathway (X, Y, and diagonal directions) where the obtained values are 0,16; 0,05 and 0,016 eV, for Li, Na, and Mg ion, respectively. Our findings indicate that the high capacity, low open circuit voltage, and ultrahigh barrier diffusion make the arsenene a good candidate for application as an anode material for rechargeable batteries.

Keywords: First principal calculations, 2D materials, Li-batteries, Na- batteries, Mg-ion batteries

OR027

STRUCTURAL, DIELECTRIC AND MAGNETIC PROPERTIES OF MULTIFERROIC (1-x) $La_{0.5}Ca_{0.5}MnO_3$ - (x) $BaTi_{0.8}Sn_{0.2}O_3$ LAMINATED COMPOSITES

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ABSTRACT

High performance lead-free multiferroic composites are desired to replace the lead-based ceramics in multifunctional devices applications. Laminated compounds were prepared from ferroelectric and ferromagnetic materials are step toward this aim. In this work, we present laminated ceramics compound by considering the ferromagnetic $La_{0.5}Ca_{0.5}MnO_3$ (LCMO) and the ferroelectric $BaTi_{0.8}Sn_{0.2}O_3$ (BTSO) in two different proportions. Compounds (1-x)LCMO-(x)BTSO with x=1 and 0 (pure materials) were synthesized by the sol gel method and x=0.7 and 0.5 (laminated) compounds were elaborated by welding appropriate mass ratios of each pure material by using the silver paste technique. Structural, dielectric, ferroelectric, microstructure and magnetic characterizsation were conducted on these samples. X-ray scattering results showed pure perovskite phases confirming the successful formation of both LCMO and BTSO. SEM images evidenced the laminated structure and good quality of the interfaces. The laminated composite materials have demonstrated a multiferroic behaviour characterized by the ferroelectric and the ferromagnetic hysteresis loops. The enhancement of the dielectric constant in the laminated composite samples is mainly attributed to the Maxwell-Wagner polarization.

Keywords: ferroelectric, ferromagnetic, laminated composites, multiferroics.

OR028

EFFECT OF MINERALIZER ON MICROSTRUCTURE AND ELECTRICAL PROPERTIES OF FORSTERITE

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ABSTRACT

Olivine materials were recently subjected to extensive studies, due to their high performance as cathode for Mg rechargeable battery. Previous works were focused on the study the effect of microstructure and element doping on electrical properties and electrochemistry performance of Mg_2SiO_4.

In this work, the effect of cation alkaline salts MCl ($M=Na^+$, K^+) used as mineralizer on structural, microstructural and electrical properties of Mg_2SiO_4 was investigated. Pure forsterite single phase Mg_2SiO_4 was synthesized by sol-gel method and the final powder was characterized by X-ray Diffraction and confirms the synthesis of pure materials. TGA shows that the synthesized samples with NaCl have a lower temperature of the initial formation of forsterite than those prepared with KCl. SEM was carried out to evaluate the morphology of sintered ceramics and their bulk densities were measured by Archimedes method and Electrical measurements were carried by Electrical impedance spectroscopy.

Keywords: Forsterite; Mg-Battery; Sol-gel route; Electrical impedance spectroscopy

OR029

CO-SUBSTITUTION EFFECT ON TUNING THE PHYSICAL PROPERTIES IN THE NEW PEROVSKITE SERIES $Ba_{1-X}La_XTi_{1-X}Fe_XO_3$ ($0 \leq x \leq 1$): STRUCTURAL, MAGNETIC AND OPTICAL INVESTIGATIONS TOWARD HIGH PERFORMANCE MATERIALS

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ABSTRACT

The search of new cheap, efficient and stable materials in different fields such as energy storage, solid oxides fuel cells, catalysis or electrocatalysis [1] has brought perovskites materials to be the foremost studied materials. Perovskite materials crystallize in different structures under the general formula (ABO_3), where A is a rare or alkaline earth element and B is a transition metal cation. Their extremely thermodynamically stable atomic arrangement and their structural flexibility and ability to accommodate a wide range of the periodic table elements make it possible for researcher to enhance, tune or induce their macroscopic properties [2]. The present work report the physical properties dependence to the structural and composition variation of a novel perovskite series ABO_3-type material. A solid solution of perovskite series $Ba_{1-x}La_xTi1_{-x}Fe_xO_3$ with $0 \leq x \leq 1$ has been prepared using the conventional solid state reaction technique. The structural investigation using the Rietveld refinement method allowed the identification of two phase transitions. The optical response of the studied perovskites showed large board absorption in the UV-Vis domain with a shift toward the visible domain as the amount of La^{3+} and Fe^{3+} ions increases. Magnetic measurements were carried out and strong response of ferromagnetic behavior where the temperature dependent magnetization at 500 Oe under field-cooled (FC) and zero field cooled (ZFC) modes shows characteristic of magnetic frustration or spin glass-like behavior.

Keywords: Perovskites, phase transition, band gap, ferromagnetic, visible light absorption.

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OR030

ROLE OF Fe^{3+} AND Cr^{3+} CATIONS SUBSTITUTION ON THE MAGNETIC AND MAGNETOCALORIC PROPERTIES OF $(La_{0.6}Pr_{0.1})Sr_{0.3}MnO_3$

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ABSTRACT

In this work, we report the effect of (Fe/Cr) doping on structural, magnetic and magnetocaloric properties of $(La_{0.6}Pr_{0.1})Sr_{0.3}Mn_{0.95}(Fe/Cr)_{0.05}O_3$ polycrystalline manganite compounds. The samples were prepared using a standard solid state reaction, X-ray powder diffraction (XRD) shows that all the samples crystallize in a rhombohedral phase with R-3c space group. The morphological study showed that the grains are irregularly spherically-shaped and have a micrometric size, while the chemical composition spectra confirm the presence of all the predicted elements. Magnetic measurements indicate that the ferromagnetic double exchange interaction is weakened with Mn-site doping, resulting in a shift in T_C from 360 K (for undoped Mn-site) to 320 K (for Fe doped Mn-site) and to 350 K (for Cr doped Mn-site). The samples present a high saturation magnetization which exceeds 78 emu/g and a very low coercive field ranging from 60 Oe to 170 Oe at 5 K. The magnetic entropy change (ΔS_M) and the relative cooling power (RCP) values have been estimated from the magnetization measurements at temperature beside the Curie temperature. The maximum of magnetic entropy change, under an applied magnetic field of 5 T, reaches a value of 2.73 J/(kg.K) in the case of $La_{0.6}Pr_{0.1}Sr_{0.3}MnO_3$ compound. This value decreases in the case of the (Fe/Cr) doped products. The RCP values have been found in the range of 300-320 J/kg. These results confirm the effect of Mn-site doping on the studied properties, which were explained by the weakening of the double exchange interaction.

Keywords: Magnetocaloric properties, manganite, double exchange interaction, magnetic entropy change, relative cooling power.

OR031

PHOTOCATALYTIC ACTIVITY OF TiO_2/ZIRCONIUM PHOSPHATE NANOCOMPOSITES FOR THE REMOVAL OF ORANGE G FROM AQUEOUS SOLUTIONS

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ABSTACT

Zirconium phosphates (ZrP) organomodified by cetyltrimethylammonium bromide (CTAB) were functionalized by the titanium precursor. The TiO2 photocatalyst attached to zirconium phosphates were then characterized using various techniques such as X-ray diffraction (XRD), Infrared spectroscopy (IR).The calcination at different temperatures of the raw precursor samples thus obtained has allowed the development of inorgano-inorganic TiO2-ZrP nanocomposite materials in which TiO2 crystallizes under the most photoactive variety: anatase and which remains remarkably stable until at 900 °C as shown by temperature-programmed XRD. Further, the photocatalytic activity of the resulting nanocomposites samples were evaluated for the removal of Orange G (OG) from aqueous solution as a model dye pollutant. The photocatalytic activity performances were found to be better for TiO2-ZrP nanocomposite treated at 900 °C, compared to the supported photocatalyst treated at 500 and 600 °C.

Keywords: Zirconium phosphates**,** cetyltrimethylammonium bromide, organomidification, photocatalyst.

OR032

NEGATIVE CAPACITANCE INVESTIGATIONS IN $Pb(Zr_{0.2}Ti_{0.8})O_3$ /$SrTiO_3$ SUPERLATTICES

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ABSTRACT

The negative capacitance phenomenon, evidenced in ferroelectric/paraelectric heterostructures, has aroused a great interest since it could provide a way to reduce the power consumption of field-effect transistors (1). This negative capacitance effect was shown to be strongly related to 180° stripe domain structure, produced to minimize the electrostatic energy, arising from the depolarization field. Ferroelectric/paraelectric superlattices geometry provides a means to investigate the negative capacitance phenomenon as shown by Zubko et al (2). By alternating individual ferroelectric layers with dielectric layers, it is possible (1) to produce ferroelectric domains, which are isolated from surface or film-substrate interfaces, and (2) to modify the electrostatic boundaries and mechanical strains, which strongly influence the negative capacitance effect.

Here we present experimental results on a series of Pb(Zr0.2Ti0.8)O3 /SrTiO3 superlattices in which we evidence 180° stripe polar nanodomains. The structural characteristics of these superlattices and the influence of the multidomain state on the ferroelectric phase transitions, as well as the temperature dependent dielectric susceptibility will be presented. The electrostatic effect in the superlattice is confirmed by a noticeable reduction of the Curie temperature. The temperature dependent dielectric susceptibility measurements, between 300K and 680K, give the indication that a negative capacitance was stabilized within the ferroelectric layers. We will show that these experimental results validate the Ginzburg-Landau model that predicted a stable negative regime in the ferroelectric layers within the Pb(Zr0.2Ti0.8)O3 /SrTiO3 superlattices.

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Keywords: Ferroelectric, superlattice, negative capacitance, dielectric measurements, XRD.

OR033

MONTE CARLO SIMULATION OF THE MAGNETIC PROPERTIES OF BULK $CoFe_2O_4$ VS $CoFe_2O_4$ NANOPARTICLES

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ABSTRACT

Nano-structured materials, counter to bulk the ones, have proven their various applicabilities with the increased demand for size reduction materials. Cobalt ferrite is considered as one of the most important material in the spinel family because of its interesting properties such as good chemical stability, low synthesis cost, high coercivity and significant saturation magnetization. These properties influence the magnetic properties of the material, in particular, the maximum energy product (BH) max, which is the main characteristic of a permanent magnet. In this study, we report the magnetic properties of bulk $CoFe_2O_4$ ferrite and the size effect on the magnetic properties of single nanoparticles of $CoFe_2O_4$ using Monte Carlo simulation with the Ising model. Periodic and free boundaries conditions were used to simulate bulk and nanoparticles, respectively. Saturation magnetization increases with the increase of the particle size towards bulk value. Small squareness ration (Mr/Ms) is observed for bulk particles, while a large values was shown in single nanoparticles. The performance of the cubic shaped $CoFe_2O_4$ ferrite was evaluated in term of the maximum energy product. It is found that bulk cobalt spinel ferrite exhibits a maximum energy product of 0.19 MG.Oe at room temperature. However, a large value of 2.83 MG.Oe was found for cubic shaped nanoparticles of 21nm. The obtained results pave the way for the development of $CoFe_2O_4$ spinel ferrites for permanent magnet applications.

Keywords: $CoFe_2O_4$ ferrite, Monte Carlo, Energy product**,** permanent magnet.

OR034

NOVEL BIOHYBRID AEROGELS BASED ON CELLULOSIC AND COBALT METALLIC NANOPARTICLES: EFFICIENT CATALYSTS FOR GREEN REDUCTION REACTIONS

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ABSTRACT

Heterogeneous catalysis has played an important role in chemical reactions and environmental remediation, there is a growing need for environmentally benign, economic and highly active catalysts. Metal and metal oxide nanoparticles (NPs) have attracted a lot of attention due to their excellent catalytic activities in different organic transformation reactions. But, their applications is limited because of their self-agglomeration in solution which reduces their catalytic performance. In this study, a cellulose nanomaterial (Cellulose nanofiber, CNF) was employed as solid support and stabilizer agent for the highly active cobalt nanoparticles via in situ green and facile synthesis as an environmentally benign material.

The structure of synthesized organic-inorganic hybrids Co/CNF is characterized by field emission scanning electron microscopy, energy dispersive spectroscopy, Fourier transform infrared spectroscopy and X-ray diffraction. The hybrid aerogel nanocomposites Co/Cell-CNF demonstrated excellent catalytic activity for the reduction of 4-nitroaniline (4-NA) to 4-aminoaniline (4-AA) in water with NaBH4. Even with a very low amount of catalyst was also found to be good enough to achieve 100% reduction of 4-NA with a higher reaction rate (8 min).

The heterogeneous nanocomposite catalyst was easily isolated from the reaction mixture by simple filtration and reused 5 times without significant loss of its catalytic activity.

Keywords: cobalt nanoparticles; composite; green chemistry; nanocellulose; recyclability.

OR035

EFFECTS OF (CaO, NiO AND ZnO) ADDITIVES ON THE CRYSTALLIZATION BEHAVIOR AND MECHANICAL PROPERTIES OF CORDIERITE SYNTHETIZED FROM A MOROCCAN CLAY

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ABSTRACT

The cordierite (2MgO, $2Al_2O_3$, $5SiO_2$) is a magnesium aluminosilicate that presents a very significant technological interest, and constitutes a promising candidate in many applications thanks to its physicochemical properties. Cordierite precursors were prepared by solid-state reaction from a Moroccan clay named “Ghassoul”. This later contain a large amount of silica SiO_2 and has the ability to consolidate by heat treatment at 1000 ° C, hence its use as a raw material for the synthesis of cordierite.

The purpose of this study is to investigate the effects of additives on the crystallization behavior of cordierite. In this regard, three additives were used (ZnO, NiO and CaO) with a percentage of 5%. The mineralogical analysis show that the use of additives affect the nature of the secondary phases present. The use of zinc oxide and nickel oxide leads to the formation of an appreciable amount of spinel and protoenstatite. Unfortunately, the presence of nickel oxide and zinc oxide

could not improve the crystallization temperature of cordierite; while, the presence of the calcium oxide blocks completely the formation of cordierite.

The addition of the additives has a strong influence on the mechanical behavior of the sample; it leads to the deterioration of the mechanical properties following the increase of the porosity. Nevertheless, the sample without adding additive remains to have the best mechanical properties.

Keywords: Cordierite, Ghassoul, additives, mechanical properties.

OR036

EFFECT OF BaO-Bi_2O_3-P_2O_5 GLASS ADDITIVE ON STRUCTURAL AND DIELECTRIC PROPERTIES OF $BaTiO_3$ CERAMICS

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ABSTRACT

A phosphate Bi_2O_3-BaO-P_2O_5 (BBP) glass is added to $BaTiO_3$ ceramics (BT) to investigate its influence on densification, rearrangement of structural units, and dielectric properties of the elaborated composites. The BT ceramic is elaborated by the solid-state method while the glasses BaO-Bi_2O_3-P_2O_5 (BBP) are synthetized by melting-quench process. The synthesized composites are labeled BT-xBBP (x = 2.5, 5, and 7.5 wt %) where x stands for the glass content in weight percent. It is found that the glass addition induces a decrease of their densification and helps their sintering at lower temperatures. A composite (x=5) exhibits the lowest sintering temperature at 900°C. The composition dependence of the dielectric properties shows that a material (x= 5) has the highest dielectric constant at room temperature. The P-E plots are carried out and the energy storage parameters (density and efficiency) of the composites are determined. These parameters are affected by the porosity and the remnant polarization of the composites.

Keywords: Phosphate, glasses, composite, dielectric properties, energy storage.

OR037

MAGNETO(DI)ELECTRIC EFFECTS IN BARIUM-LEAD M-TYPE HEXAFERRITES

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ABSTRACT

Hexagonal ferrites (Ba,Pb)$Fe_{12}O_{19}$ are completely new family of magnetic quantum paraelectrics and significance of the FeO_5 bipyramid structural units of M-type hexaferrites goes beyond quantum paraelectrics only. In principle, a variety of dielectric materials could be expected on the basis of the non-d^0 electric dipole while electric polarization in conventional ferroelectric oxides usually involves nonmagnetic transition-metal ions with an empty d-shell. The deviation from «rule of empty shell» will lead to the appearance of new magnetoelectric multiferroic.

We investigated interaction of dynamically disordered magnetic ion in a bipyramidal unit with a stereo-active lone pair of lead ion in the crystal structure of solid solutions $Ba_{1-x}Pb_xFe_{12}O_{19}$ (x =0, 0.3, 0.5, 0.7, 0.9, 1) by single-crystal X-ray diffraction (Beamline P24 Chemical Crystallography, PETRA III at DESY) and THz-spectroscopy in temperature range of 10-300 K. Spectroscopic studies shown the presence of a number of low-frequency lines (below 50 cm^{-1}) below 100 K for solid solutions with x = 0.9. This indicate the activation of lattice vibrations involving large structural blocks or/and appearing of electromagnon excitation. Reciprocal space maps inspection clearly shown significant thermal diffuse scattering for $Ba_{0.1}Pb_{0.9}Fe_{12}O_{19}$ single crystal in contrast to other investigated samples. Thereby, active disorder in the magnetic subsystem can be controlled by substituting a divalent metal with a stereoactive lone pair in M-type hexaferrites $Ba_{1-x}Pb_xFe_{12}O_{19}$. Previously, a similar result for M-type hexaferrites was achieved only by substitution of iron ions in the multisublattice magnetic system. We shown a simpler and more technologically advanced way of influencing the magnetoelectric effect in these compositions. The proper balance between the long-range Coulomb interaction and short-range Pauli repulsion in a FeO_5 bipyramid would favor an off-center displacement of the magnetic Fe^{3+} ions, which induces a local electric dipole in M-type hexaferrites $Ba_{1-x}Pb_xFe_{12}O_{19}$ solid solutions.

The reported study was funded by RFBR, project number 17-02-01247.

Keywords: quantum paraelectrics, multiferroics, XRD, THz-spectroscopy, hexaferrites

OR038

ELECTROSTATIC ENERGY STORAGE DENSITY IN $\mathbf{Na_{0.5}Bi_{0.5}TiO_3}$ BASED MATERIALS FOR POTENTIAL HIGH-TEMPERATURE CAPACITOR APPLICATION

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ABSTRACT

Energy storage is one of the vital technologies for a judicious utilization of energy, aiming to meet the challenge of fossil fuel depletion. Furthermore, due to the concern about climate change and atmospheric pollution, great interest has been devoted to energy storage devices based on lead-free materials that present high storage capacity. One of the new areas of interest is a high energy density at high operating temperatures (>300°C) for use in applications in which materials are subjected to harsh operating conditions, such as in power electronics, deep-well oil and gas exploration, and hybrid vehicles applications. Sodium bismuth titanate (Abbreviated as NBT) is considered as one of the promising candidates for energy storage applications due to its interesting properties. However, pure NBTsuffers fromhigh conductivity andlarge coercive field. Doping with rare earth elements was found as an appropriate way toenhance the physical properties of NBT. In the present work, we examine the influence addition of Dysprosium element on the structural, electrical, and energy storage properties of$\mathrm{Na_{0.5}(Bi_{1-x}Dy_x)_{0.5}TiO_3}$ $\mathrm{(xDyNBT)}$ system. Interestingly, the inclusion of Dy^{3+} allows not only asubstantial decrease of the coercive fieldand increasethe resistivity of pure NBT but also to ahigh stability of the dielectric permittivity (ε) over a wide temperature range $(\sim 90 - 510°\mathrm{C})$ with $\Delta\varepsilon \leq \pm 15\%$ variation. Further, the studied system was found to exhibit improved energy storage density of (1.2 J/cm^3) at high temperatures (200°C). The obtained results are very promisingand open a great potential for high temperature power electronics applications.

Keywords: NBT, Dielectric properties, High temperature stability, Energy storage, Capacitor

Posters

P001

THE THEORETICAL AND EXPERIMENTAL CHARACTERISTICS OF NOVEL MATERIAL BASED ON STRANDBERG-TYPE HYBRID COMPLEX $(C_6H_{10}N_2)_2[Co(H_2O)_4P_2Mo5O_{23}].6H_2O$

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ABSTRACT

The hybrid strandberg complex materials have attracted intensive interest due to their multifunctional properties. In this work, we report the structural, electronic and optical properties of the novel synthetized compound $(C_6H_{10}N_2)_2[Co(H_2O)_4P_2Mo_5O_{23}].6H_2O$, investigated successfully by the First principle calculations, based on the density functional theory (DFT). The nanocrystals of $(C_6H_{10}N_2)_2[Co(H_2O)_4P_2Mo_5O_{23}].6H_2O$ with triclinic structure were characterized by X-ray powder diffraction (XRD). The profiles of the density of states and the optical spectra including the real and imaginary part of dielectric function were presented and analyzed in detail, the *results* are in *good agreement* with experimental measurement. It is found that the compound presents a high absorption coefficient in the visible range. A systematic analysis of the experimental and theoretical results shows a good band gap and a high optical property, which reveals promising original material for advanced in optoelectronic and photovoltaic applications.

Keywords: $(C_6H_{10}N_2)_2[Co(H_2O)_4P_2Mo_5O_{23}].6H_2O$, Optical properties, absorbance, electronic structure, DFT.

P002

FEATURES OF SINTERING OF MULTILAYER OBJECTS

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ABSTRACT

The development of nanotechnology stimulates the improvement of methods for obtaining and researching thin films. Today, thin films have a very wide range of applications, from functional coatings to the manufacture of multilayer systems such as capacitors or fuel cells.

One of the most productive methods for obtaining thin films is tape casting. With this method, our team managed to get film about 1 µm in thickness. But this thickness has been reached in the green body sample, that ıs why more interesting fact is thickness after heat treatment. After all, the removal of the organic component can lead to significant shrinkage during sintering.

Thus, the main aim of this study is optimization of sintering process of thin films and the study of competing processes of mass transfer at different heating rates. Thin films were prepared from paste based on nanosized BaTiO3 powder with a particle size of 20-25 nm. The study of the kinetics of sintering process will be carried out in a dilatometric installation. And ınvestigation of grain growth and porous structure will be conducted at various stages of sintering, at temperatures range from 700 to 1200 °C. The resulting samples wıll be examined by using a number of techniques: optical profilometry method, XRD, microscopy, and others.

Keywords: thin films**,** tape casting**,** kinetics of sintering**,** dilatometry, profilometry method.

P003

STRUCTURAL AND DIELECTRIC PROPERTIES OF SODIUM NIOBATE CERAMIC $NaNbO_3$ WITH GLASS ADDITIONS

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ABSTRACT

$NaNbO_3$ is a ferroelectric material which has claimed the attention of researchers and designers of equipment owing to its unique physical properties and as a basis for a class of ecologically benign active materials. Hence, $NaNbO_3$ has been studied by several workers. However, less work has been reported on $NaNbO_3$ glass-ceramics. In the present work, $NaNbO_3$ has been synthesized by solid state sintering technique while the glasses has been synthesized by the conventional melt-quenching technique. The $NaNbO_3$ ceramics were synthesized by adding different contents of glass into $NaNbO_3$. Two composites with different glass weight percentage have been elaborated and sintering at different temperatures. Density measurements, Raman spectroscopy, and Scanning Electron Microscopy are used to characterize their structural study. Electrical properties of the composite samples are carried out by impedance spectroscopy in the frequency range of 10 Hz to 1 MHz under various temperatures from 300 to 473 K.

Keywords: phosphate glasses, Sodium niobate, composite, Raman spectroscopy, SEM, dielectric properties.

P004

LARGE ELASTOCALORIC EFFECT IN LIQUID CRYSTAL ELASTOMERS

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ABSTRACT

Caloric effects are manifested in the heating or cooling a caloric material due to the application or removal, respectively, of the external field under nearly adiabatic conditions. Materials with large caloric effects, such as the elastocaloric (eC) effect, have the promise of realizing new solid-state refrigeration techniques [1]. Soft materials, called liquid crystal elastomers (LCEs), are good candidates exhibiting a large elastocaloric effect with potentially better elastocaloric responsivity than shape memory alloy wires, in which the eC temperature change of 40 K was observed at 0.8 GPa stress field [2, 3]. In this contribution a review of recent direct measurements of the eC effect in LCEs will be given. The eC temperature change of about 1 K was observed in MCLCEs at relatively small stress field of 0.6 MPa [4]. Soft materials can play a significant role as active cooling elements and parts of thermal diodes or regeneration material in the development of new cooling devices.

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Keywords: elastocaloric, liquid crystal, liquid crystal elastomers

P005

MAGNETOCALORIC PROPERTIES OF THE $LaFe_{13-X}Si_X$ ALLOYS: AB INITIO CALCULATIONS AND MONTE CARLO SIMULATION

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ABSTRACT

Magnetic refrigeration techniques based on the magnetocaloric effect (MCE) have recently been demonstrated as a promising alternative to conventional vapor-cycle refrigeration. In the present work, the $LaFe_{13-x}Si_x$ alloys ($1.0 \leq x \leq 1.6$) has been studied by using Density Functional Theory implemented in Quantum Espresso package. Giant magnetocaloric properties are determined in the framework of Monte Carlo simulation and the Means field Theory. These properties are summarized into thermodynamic quantities. The results indicate that the $LaFe_{13-x}Si_x$ alloys exhibit a large magnetic entropy change over a wide temperature range.

Keywords: $LaFe_{13-x}Si_x$ alloys, magnetocaloric materials, DFT, Monte Carlo, Means field Theory.

P006

COBALT DOPED COPPER OXIDE THIN FILMS FOR SOLAR SELECTIVE ABSORBERS APPLICATION

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Abstract:

In this study, undoped and cobalt doped copper oxide thin films were deposited by RF sputtering. In addition, the covered surface was varied to investigate the effect of doping percentage on the structural, electrical, morphological and optical properties of the obtained thin films. All the obtained thin film samples have good solar selectivity (>12) with low thermal emittance (<7%) and high solar absorptance (>92%). The Co:CuO thin films possess high solar-selectivity value of 12 and thus could be suitable and used as a novel candidate material for selective absorber films in solar collectors for thermal energy conversion.

Keywords: Cobalt doped CuO; thin films; optical properties; structural and electrical properties; RF sputtering; selective absorber and emissivity.

P007

ZINC CHLORIDE AS PRECURSORS TO ELABORATE ZINC OXIDE WITH SPIN COATING TECHNIQUE

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ABSTRACT

The zinc chloride is one of the precursors used to deposited the zinc oxide (ZnO) thin films by sol-gel spin coating technique from aqueous solution onto glasses substrates at optimum conditions. The effect of the concentration of precursor on the structural, optical and electrical properties of ZnO thin films has been investigated. The X-ray diffraction analysis showed typical patterns of the hexagonal ZnO structure for all films. The films were polycrystalline with the (002) preferred orientation. The grain size and optical band gap were evaluated for different concentrations. The optical transmittance measurements of ZnO thin films showed that all films are transparent in the visible regions and decrease with increase the $ZnCl_2$ concentration. The film with 0.4 M $ZnCl_2$ has a high crystallographic quality with an energy band gap of 3,36 eV.

The produced ZnO thin films at optimum conditions may be useful for specific applications as transparent n-type windows in solar cells for sensor devices where large surface areas are needed.

Keywords: Zinc oxide; Thin films; Nanoparticles; Zinc chloride; Spin coating.

P008

Al:ZnO PROPERTIES IMPROVEMENT BY Mg CODOPING AS OPTICAL WINDOW

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ABSTRACT

In the present work, we first studied the influence of aluminum doping on the structural and optical properties of zinc oxide thin films. Thus, thin layers of zinc oxide have been successfully deposited by the sol-gel technique on glass substrates under optimized experimental conditions. The pH of the solution and the annealing temperature were maintained at 10 and 500 ° C respectively. Thin layers of ZnO were doped at different Al concentrations (1%, 3%, 5% and 7%). The results of XRD showed that all the films lost the preferential orientation according to the (002) plane, while the UV results showed a decrease of the transmittance as soon as the Al concentration exceeded 1%. This deterioration in optical properties led us to co-dope thin layers of ZnO by (Mg, Al) in order to improve the optical and structural properties. Therefore, in a second step, we opted for co-doping by simultaneously introducing aluminum and magnesium in varying proportions. The whole molar amount of impurity was maintained constant and equal to 5%. The results show that with the increase in the Mg percentage, the preferential orientation of the films according to (002) improves and the transmittance reaches 80%. The optimized results were obtained for a co-doping concentration (Al-Mg) with a ratio of 2/1.

P009

THERMO-RAMAN STUDIES AND ELECTRICAL PROPERTIES OF THE $Sr_{1.15}Na_{1.7}Nb_4W_{1-X}Mo_XO_{15}$ CERAMICS

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ABSTRACT

The $Sr_{1.15}Na_{1.7}Nb_4W_{1-x}Mo_xO_{15}$ ($0\leq x\leq 1$) ceramics, labeled SNNbWM-x, were elaborated by the solid state route. Their structures were studied by X-ray diffraction and Raman spectroscopy and their electrical properties were investigated by impedance spectroscopy. X-Ray patterns of the ceramics reveal that the substitution of tungsten by molybdenum induces a full solid solution and the compounds crystallized in single-phase tetragonal tungsten bronze (TTB) with space group P4bm. Raman spectra of the SNNbWM-x compounds highlighted the vibration modes of the different cations involved in the TTB structure and showed a small peak's displacement according to the Mo/W ratio. The Raman peak position temperature dependence studies had allowed to identify the presence of a phase transition around the temperature Te = 270°C in each compound. The investigation of the electrical properties of the SNNbWM-x samples in the frequency range 20 Hz–10^6Hz at various temperatures from room temperature to 550°C showed that theses ceramics exhibited a phase transition around 270°C in agreement with the thermo-Raman studies.

P010

AB-INITIO CALCULATION AND MONTE CARLO SIMULATION OF THE MULTIFERROIC RMnO$_3$

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ABSTRACT

Muliferroic are multifunctionnal materials which exhibit more than one type of ordernig including magnetic, electric and elastic order. While there are numerous technological application for magnetic and ferroelectric. In this work will be focused on the electronic and magnetic properties of the pervoskite RMnO3 where R is rare earth (R=Tb) using ab-initio calculation and Monte Carlo simulation (MCS), Firstly, we calculate the electronic and magnetic properties using the full-potential augmented wave (FP-LAPW) implemented in the wien2ka code, we also present the results of densities of states of two up and down spin polarisations, then we will establish a physical model to describe our system, we calculate the exchange coupling and the crystal filed. Finally, we study Monte Carlo simulation and we will compare these results with the experimental results to prove that this multifarroic exhibit also magneto-caloric coupling and can be used for Magnetic refrigeration.

Keywords: muliferoiic, FP-LAPW, Monte Carlo,magntocaloric,Magnetic refrigeration,Wien2ka

P011

SYNTHESIS OF KESTERITE THIN FILMS: INFLUENCE OF ANNEALING IN VACUUM

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ABSTRACT

In this work, we studied the structural, optical, and electrical properties of the quaternary and ternary compounds of the kesterite structure as a function of the annealing temperature. The chemical solution was an aqueous solution based on copper, zinc, tin and sulfur precursors. The thin layers were deposited on soda lime glass plates by the pneumatic spray method. The product was sprayed onto the glass plates initially put down on a heating plate raised to 380 ° C. The obtained layers were then annealed at 400 ° C and 500 ° C for 20 min in vaccum. We have confirmed the existence of a kesterite phase by XRD. This structure has also been checked by Raman spectroscopy which shows the two peaks characteristic of kesterite. The chemical composition of the samples follows the initial stoichiometry giving ratios between the elements of the compound in agreement with the expected composition. The optical transmission of the layers was in average around 60% for quaternary compounds, and lower for the ternary compounds. The optical gaps were determined to lie between 2.02 eV and 2.21 eV in agreement with results reported by a majority of authors. The found optical and electrical properties are encouraging in the perspective of integration of such layers in photovoltaic devices.

Keywords: CZTS, CZS, XRD, thin films, optical transmission, band gap, photovoltaic

P012

PLASMA ELECTROLYTIC OF ZINC: THE FORMATION OF MICRO-ARCS OR SPARKS ON THE ZINC AT HIGH VOLTAGE

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ABSTRACT

For several years, one of the main objectives of many processes is to fulfill the requirements of environmental standards, and to avoid the use of toxic reagents as hexavalent chromium or nickel salts. In this framework, the processes based on electrochemical conversion as anodizing can be interesting alternatives. At low voltage, below the dielectric breakdown of the interface, several processes of zinc anodizing in alkaline media were already studied for anticorrosion properties or photo-catalytic applications. Moreover, many works have been devoted to the knowledge of the zinc oxidation mechanism, especially the dissolution–passivation phenomenon at low potential because of the technical importance of aqueous alkaline batteries made from this metal. At low potential, the anodic layers are mainly constituted by zincite, ZnO, and zinc hydroxide if the alkaline media is at low carbonate concentration. At high voltage, during the dielectric breakdown and the formation of micro-arcs or sparks, the development of ceramic-type coatings seems to be possible because of the high temperature reached in the electric discharges occurring at the "metal/oxide/electrolyte" interface.The aim of this work is to describe the electrochemical behavior of zinc in a large anodic voltage range (until 300 V namely beyond the dielectric breakdown) by using a DC regime. This study focuses on the influence of the KOH concentration and the presence of additives, such as silicates and aluminates. Different in-situ electrochemical measurements in a two-electrode cell allowed a better understanding of the anodizing process with respect to the composition of the "metal/oxide/ electrolyte" interface. The anodized coatings or oxide layers were characterized by different metallographic analyses: scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy, and X-ray diffraction.

Keywords: Zinc, micro-arc oxidation (MAO), plasma electrolytic oxidation (PEO).

P013

STRUCTURAL, DIELECTRIC AND IMPEDANCE SPECTROSCOPY ANALYSIS OF LEAD FREE($Ba_{0,85}Ca_{0,15}Zr_{0,1}Ti_{0,9}O_3$) CERAMICS SYNTHESIZED BY SOL-GEL METHOD

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ABSTRACT

In recent decades, there is an increasing attention paid to ferroelectric and ecological materials,
both in scientific research and technology developments. In the present work, a lead free ceramics Ba 0,85Ca0,15Zr0,1Ti0,9O3(BCZT) was prepared by sol-gel method. Morphological and structural properties of BCZT were investigated by SEM and XRD technique confirmed by Raman spectroscopy at room temperature, respectively. Dielectric characteristics were analyzed
by Impedance spectroscopy. Rietveld refinement indicates the formation of a single phase compound with a tetragonal structure of space group P4mm. The ceramics sintered at 1350°C
exhibits a dense microstructure. The dielectric measurements of BCZT were studied as a function of temperature in the frequency range of 100Hz-500 kHz. The variation of dielectric constant (ε’) shows a maximum value of ~4700 at the ferroelectric-paraelectric phase transition
(Tc= 64°C). The Diffuse nature of the transition is well described by Santos–Eiras phenomenological model. Impedance spectroscopy analysis over the frequency range of 100Hz to 500 kHz presents mainly grain and grain-boundary contribution above 266°C.

Keywords: dielectric materials, sol-gel method, phase transition, diffuse nature,

P014

UNOCCUPIED ELECTRONIC STRUCTURE OF GRAPHENE DERIVED TWO-DIMENSIONAL SUBSTRATES

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ABSTRACT

The possibility of opening a gap in the electronic structure of the two-dimentional (2D) material known as graphene continues to be investigated for the development of nanoelectronics. Another approach consists to further elaborate new 2D materials with original electronic properties. Such 2D materials can be derived from a graphene layer or a functionalized graphene layer. By decomposition of silicon carbide SiC at 1200 °C under ultra-high-vacuum it is possible to obtain several 2D substrates. Depending on the annealing time it is possible to elaborate the so called buffer layer (BLG) also named zero-layer graphene, a monolayer graphene above the BLG, a bilayer graphene above a BLG and so on until full graphitization resulting in a multi-layer graphene substrate. Hydrogenation of a BLG substrate under different temperature conditions allows to obtain two additional substrates called H-BLG and QFSG for quasi free standing graphene, this QFSG being a decoupled monolayer graphene floating above an underlying hydrogenated substrate.All these 2D substrates have distinct electronic behaviour which may be interesting for the development of nano-electronic devices including zero gap seconductor, correlated insulator... Using photoemission an inverse photoemission experiments we have studied the electronic properties of these substrates. We show for example that it is possible to modify these properties by performing nitrogen implantation in mono or bilayer graphene. From the respective properties of the H-BLG and QFSG a route is suggested for the large scale production of graphene based devices [1].

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Keywords : graphene, electronic properties, 2D materials, nanoelectronics.

P015

HYDROGEN STORAGE IN SOLID FORM

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ABSTRACT

The hopes of using hydrogen as an energy carrier are severely dampened by the fact that there is still no safe, high-density method available for storing hydrogen. We investigate the possibility of storing hydrogen on one of carbon's family ''Graphene" , Recently, several studies on graphene, the one-atom-thick membrane of carbon atoms packed in a honeycomb lattice, have highlighted the potentialities of this material for hydrogen storage and raise new hopes for the development of an efficient solid-state hydrogen storage device. Here we review on-going efforts and studies on functionalized and nanostructured graphene for hydrogen storage and suggest possible developments for efficient storage/release of hydrogen under ambient conditions. We have tried to calculate the storage properties of hydrogen on a graphene sheet by using the pseudo potential quantum espresso and calculate the density of state and band structure by using the GGA aproximation and then we calculated the band energy of the complete system.

Keywords: Quantum espresso, Hydrogen storage, Band structure, Density of states, Graphene

P016

EFFECT OF IONIC LIQUIDS AND HUMIDITY ON IONIC CONDUCTIVITY FOR CARBOXYMETHYL CHITIN BASED SOLID POLYMER ELECTROLYTE

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ABSTRACT

Carboxymethyl chitin (CMChit) has the potential to be used as a solid polymer electrolyte (SPE), it gives an ionic conductivity of the order of 10^{-6} Scm^{-1} in plain films. 1-Butyl-3-methylimidazolium chloride and 1-Butyl-3-methylimidazolium acetate (BMIM[Ac]), two types of ionic liquids (ILs) were added to the CMChit-SPE to improve the ionic conductivity. The films were prepared by solution casting method then conditioned in different atmospheres of different relative humidity. The Films prepared were characterized using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Field-emission scanning electron microscopy (FESEM-EDX), Differential scanning calorimetry (DSC), Electrochemical Impedance Spectroscopy (EIS) and linear scanning voltammetry (LSV). In controlled humidity, BMIM[Cl] showed an optimum of ionic conductivity in the order of 10^{-4} S cm^{-1} and electrochemical stability of 1.93 V, by the addition of only 30wt. %. On the other hand, for BMIM[Ac], the optimum was reached with the addition of 40 wt.% for the same order of ionic conductivity and electrochemical stability of 2.93 V.

Keywords: carboxymethyl chitin, solid polymer electrolyte, ionic liquids, humidity.

P017

PULSE-POWER INTEGRATED-DECAY TECHNIQUE FOR THE MEASUREMENT OF THERMAL CONDUCTIVITY OF NANOFLUID GRAPHENE IN GLYCEROL/WATER

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ABSTRACT

We present experimental results of the thermal conductivity of nanofluid prepared by dispersing nanoparticles of graphene in glycerol/water at various concentrations in mass fraction. The measurements have been performed by the pulse-power integrated-decay technique for the measurement of thermal conductivity of nanofluid. A self-heated thermistor probe is used to deliver heat and also to measure the temperature response.

Our experimental technique allows a very accurate determination of the enhancement in the thermal conductivity of the fluids due to the presence of dispersed nanoparticles. Measured enhancements compare well with some of the values published so far in the literature.

Keywords: nanofluid, graphene, glycerol, thermal conductivity.

P018

MODELING THE ADSORPTION OF HYDROGEN IN THE METAL ORGANIC FRAMEWORK (MOF5, CONNECTOR): $Z(C_8H_4O_4)_3$

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ABSTRACT

Metal-organic frameworks (MOFs) are thought to be a set of promising hydrogen storage materials; The electronic structure of porous metal-organic framework-5 MOF-5 of composition Zn4O 1,4- benzenedicarboxylate was investigated with an *ab initio* method. The purpose of this work allowed us to study the structural stability, the electrical properties of the MOF-5 type organometallic materials [Zn4O(C8H4O4)3] and their Connector (metal oxide centers) to Zinc base were studied using the first calculations based on the functional density theory (DFT) and using the Quantum Espresso code and the PBE-GGA approximation. With determination of adsorption energy to contribute to a better understanding of the fundamental interactions of H2 with MOF-5. The adsorption energy of the hydrogen molecule in MOF-5 was studied taking into account the favorable adsorption sites (Metallic, Carboxylic and Cyclic) and orientations (vertical, horizontal, inclined) with the energy of Coupling based on the calculation of the first and second adsorption sites. In addition, the interaction between the hydrogen molecule and MOF-5 is very stable and more adsorption in the organic part (Cyclic site).

Keywords: DFT; Hydrogen storage; Metal organic framework; Adsorption energy

P019

STRUCTURAL AND MICROSTRUCTURAL ANALYSIS OF ECOLOGICAL AND NANOSTRUCTURED BCZT THIN FILMS

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ABSTRACT

Today, energy storage and environmental protection are the major challenges; therefore, researches have been carrying out studies in order to develop environmentally-friendly nanomaterials with high energy density. In this study, we have developed thin films of $Ba_{0,85}Ca_{0,15}Ti_{0,9}Zr_{0,1}O_3$ (BCZT) by sol-gel via spin-coating on $Pt/Ti/SiO_2/Si$ substrates; and heat-treated at 750°C/30min. The SEM micrographs showed that the six-layers BCZT films are dense and homogeneous and the XRD reveled the presence of single perovskite phase at room temperature. Likewise, in order to prepare BCZT nanorods thin films, firstly, uniform and homogeneous TiO_2 nonorods have grown on FTO substrates via the hydrothermal process. Then, Ca ions were added to the rutile phase of TiO_2 nonorods to form $CaTiO_3$ (CT) perovskite phase confirmed by X-ray diffraction analysis. In a last step, this CT perovskite nonorods will be doped by Ba and Zr ions to obtain BCZT nanostrctured thin film that is a potential candidate for energy storage application.

Keywords: BCZT, energy storage, hydrothermal, nanorods, sol-gel, spin-coating.

P020

CURED CUTTLEBONE/CHITOSAN-HEATED CLAY COMPOSITES: MICROSTRUCTURAL CHARACTERIZATION AND PRACTICAL PERFORMANCES

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ABSTRACT

Clay-based materials composed of geopolymers and natural fibbers, among others, could be suitable composites for building construction. So, in this study, composites of a heated kaolinitic-illitic clay and cuttlebone or chitosan (up to 10 mass%) were etched with a NaOH solution (6 M), shaped as briquettes and cured at 83 °C for up to 30 days. The microstructure of the cured composites was investigated, and some of their practical performances were evaluated. The results showed that metakaolinite and illite - to some extent-, and a portion of Na+ ions were involved in the formation of zeolite (chabazite) and Na-carbonate respectively. Moreover, layers of cuttlebone or chitosan were built up around the clay particles, and the thick layers developed in the cuttlebone and in the chitosan-rich composites affected differently the zeolization process. Chitosan versus cuttlebone favoured zeolization by facilitating the ions mobility, and the illite reactivity. By referring to the mechanical/physical properties of the cured NaOH-etched heated clay, the bending and the compressive strengths of the cured composites as well as their water absorption increased by two-to three times. The strengthening of the composites was related mainly to the reduction of porosity (up to 40% for the cuttlebone-rich composite).

Keywords: Heated Clay-Cuttlebone-Chitosan-Alkali-activation-Microstructure

P021

COMPOSITES WITH FERROELECTRIC PROPERTIES IN As_2S_3-Sb_2S_3-SbI_3 SYSTEM

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ABSTRACT

Studies of nanoscale ferroelectric materials are important in the view of both fundamental and practical aspects. The experience of obtaining crystallites in amorphous matrices, especially well known for II-VI chalcogenides, also inspires the fabrication and investigation of glass-embedded nanoscale ferroelectric chalcogenidebased materials which are interesting with respect to size-related effects and possible applications. In our recent studies we present the technology of synthesis and results of investigations of glasses in new As_2S_3-Sb_2S_3-SbI_3 system.The glasses of As_2S_3-Sb_2S_3-SbI_3 system with content As_2S_3 45, 40, 35 and 30 mol.%, Sb_2S_3 – 27.5, 30, 32.5, 35 mol.% and SbI_3 – 27.5, 30, 32.5, 35 mol.% were prepared by vacuum melting method (~0.01 Pa) of the relevant mixture of As_2S_3, Sb_2S_3 and SbI_3 components, preliminary synthesized from high-purity elemental substances. Glassy As_2S_3 was obtained by cooling a homogenized for 48 h melt from 780 K in air. Polycrystalline Sb_2S_3 and SbI_3 were obtained by slow cooling the homogenized for 72 and 12 h melts from 900 and 445 K, respectively, to room temperature. During the synthesis, we applied the stepwise increase in temperature. The melts were periodically mixed. The melts of As_2S_3-Sb_2S_3-SbI_3 system were homogenized at 820-850 K for 24-36 h. Cooling of the melts was carried out into cold water. Nanoheterogenous structure of glasses in As_2S_3-Sb_2S_3-SbI system established on the basis of Raman spectra investigations. Their structural network is formed by only binary structural groups with heteropolar bonds (AsS_3, SbS_3, SbI_3, AsI_3) and contains small amount fragments with S-S bonds. Raman spectra of $(As_2S_3)_{30}(Sb_2S_3)_{35}(SbI_3)_{35}$ glasses annealed at 348 K for 48h and at 328 K for 2h clearly exhibit distinct peaks at 55, 72, 113, 139 and 320 cm^{-1}. All these peaks are characteristic for crystalline SbSI Raman spectra measured at 300 K into different scattering configurations. This fact is a good agreement with the earlier data reporting on the annealing induced crystallization of SbSI phase from $(As_2S_3)_{100\ x}(SbSI)_x$ and $(Sb_2S_3)_{100-x}(AsSI)_x$ glasses.

Keywords: nanomaterials, chalcogenides, spectroscopy, glasses, ferroelectrics**.**

P022

EFFECTS OF VOLUME CONCENTRATION AND TEMPERATURE ON THE THERMAL AND RHEOLOGICAL PROPERTIES OF ALUMINUM OXIDE /WATER NANOFLUID

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ABSTRACT

Nanofluids are colloidal solutions composed of Nano-sized particles suspended in a liquid that surprising thermal properties have been the subject of intense research over the past decade. This work aims to study the influence of the temperature and volume concentration of nanoparticles dispersed in a base fluid on the thermal conductivity and dynamic viscosity of the nanofluid in homogeneous suspension Aluminum oxide / water, without surface pre-treatment.

Keywords: Nanofluid, Nanoparticles, Thermal conductivity, Dynamic viscosity.

P023

ELECTRIC AND THERMAL INSULATOR GLASS-CERAMIC BASED ON CORDIERITE FROM COAL FLY ASH

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ABSTRACT

Cordierite-based glass-ceramics have been successfully produced from coal fly ash (80.74 wt.%), magnesium hydroxide, and aluminum hydroxide. The phase crystallization was followed by thermogravimetric and differential thermal analysis, X-ray diffraction, Fourier transform infrared, and scanning electron microscope. The properties of sintered materials in the range 900-1200 °C such as apparent porosity, bulk density, and mechanical parameters were measured. The results show that the increase in firing temperature from 900 °C to 1200°C induces the transformation of coal fly ash component and magnesium oxide to α-cordierite with high purity. The formation of cordierite at 1200 °C involves the densification of ceramic body and the decrease in apparent porosity to 22 %. The obtained cordierite-based ceramic exhibit a thermal conductivity (1.12 W/m.°K) and compressive strength (128 MPa), which promote its application as a thermal insulator. Also, the dielectric constant (ε = 9.5 at 1MHz) measurement shows that the obtained ceramic can be useful as insulator for electric and electronic applications.

Keywords: Cordierite; Coal fly Ash; Thermal insulator; Dielectric

P024

STUDY OF THE EFFECT OF COMPOSITION AND TEMPERATURE ON THE STRUCTURE STABILITY AND OPTICAL PROPERTIES OF NEW TELLURIUM BASED DOUBLE PEROVSKITES

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ABSTRACT

The continual development of technology has caused a depletion of all kind of energy resources and climate change with non-predictable consequences. Extensive efforts to change to renewable energies and implementing new and alternatives energy concept are required. Perovskite materials have shown potential in the energy field being one of the most promising materials, such as hybrid perovskites for solar cells, solid oxide fuel cells and refrigeration technologies[1,2]. Double perovskite structure typically has the chemical formula A2BB'O6. Depending on the elements residing at A and B sites, different crystalline structures are possible, resulting in specific electronic and magnetic properties. Fundamental understanding of the structure stability and phase transitions of these materials, under different synthesis conditions, is very important for optimizing the next generation applications-tailored energy conversion devices.

In the present study, the mechanisms of self-doping together with continuous composition modulation in the Ba3-xSrxTeO6 ($0 \leq x \leq 3$) system are investigated. For $x \leq 1$, the exceeded Sr substitutes Ba on the B-site as Ba2(Ba1-xSrx)TeO6; while for $x>1$, Sr substitutes partial Ba at A-site as (Ba2-ySry)SrTeO6 (here, $y=x-1$). The structure stability and phase transition of compounds are studied using X-ray diffraction, and Raman spectroscopy at ambient and elevated temperatures. At ambient temperature, a systematic structure transition (I41/a → $\mathrm{R}\overline{3}\mathrm{m}$ → $\mathrm{R}\overline{3}$ → $\mathrm{R}\overline{3}\mathrm{m}$ → C1) was determined, with x increasing from 0 to 3. At elevated temperatures (up to 570 °C) all structures tend to merge to the single cubic phase $\mathrm{Fm}\overline{3}\mathrm{m}$, indicating an expanded bonding length and a greater atomic thermal motion. The optical properties of the Ba3-xSrxTeO6 ($0 \leq x \leq 3$) system were part of the paper objective in investigating the substitution effect on the optical response. The optical properties of the compounds were significantly dependent to the symmetry change in the system and a shrink in the band gap energy values was observed as the amount of the strontium increase, at some specific amount of the substitution, some unusual behaviour were observed.

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P025

A COMPARATIVE STUDY OF STRUCTURAL AND DIELECTRIC PROPERTIES IN LEAD-FREE $BaTi_{0,89}Sn_{0,11}O_3$ CERAMICS SYNTHESIZED BY SOLID STATE AND SOL-GEL

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ABSTRACT

Ferroelectric barium stannate titanate (BTSn) possesses a high dielectric constant coupled with the possibility of shifting the Curie temperature toward room temperature by changing the Sn content. Therefore, it is an interesting material for applications such as capacitor, bolometer, actuator and microwave phase shifter. $BaTi_{0,89}Sn_{0,11}O_3$ ceramics were synthesized by solid state method and sol-gel in order to realize a comparative study of two compounds and to establish a correlation between their structures and their dielectric properties. The crystalline structure, the unit cell parameters and the phase composition were ascertained by the Rietveld refinement. The average grain size estimated from the microstructure was found to be about 1.5 µm for the solid-state derived ceramic and 4-14 µm for the sample prepared by sol-gel method, respectively. Complex impedance spectroscopy results revealed a classical ferroelectric behavior and diffuse nature of the ferroelectric-paraelectric phase transition in each of the two samples, and highlighted the effect of grain size and density on the dielectric properties: permittivity, dielectric losses and conductivity.

Keywords: BTSn, solid state, sol-gel, structural properties, dielectric properties, impedance spectroscopy, ferroelectricity, phase transition temperature.

P026

TiO_2 PHOTOCATALYSIS: HYDROGEN PRODUCTION

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ABSTRACT

TiO_2 is extensively used in a variety of applications for photocatalysis and-hydrogen evolution. The development of new materials, is strongly required to provide enhanced performances with respect to the photocatalytic properties and to find new uses for TiO_2 photocatalysis.To produce the hydrogen by using solar energy, we have been studied the band gap, and optical properties of TiO_2 compound, which is considerate one of the most promising photocatalyst used of water splitting.For this purpose, the doping of TiO_2 has been studied with non-metallic elements and the use of one, two and three dimensional TiO_2 as a photocatalyst. The aims of this research are studying the crystal structure, the optical properties and the photocatalytic activity of TiO_2.

Keywords: Photocatalysis, Hydrogen, Visible-light, TiO_2, Photocatalyst

P027

STUDY OF THE ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF MATERIAL $DyMn_2O_5$ USING AB-INTIO AND MONTE-CARLO SIMULATION

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ABSTRACT

We use Ab-inition methods with the density functional theory (DFT) to study the electronic and magnetic proprieties of multiferioc DyMn2O5.Our goals are to determine the band gap the magnetic anisotropy and exchanges couplings between the magnetic ions. The density of states show an semiconductor behavior in the ferrimagnetic state of DyMn2O5 at Fermi level and there is a small band gap, confirming the experimental fact that DyMn2O5 as a typical semiconductor. The exchange couplings between the magnetic ions were calculated using the Heisenberg model by including only the nearest neighbor interactions, all by selecting stable magnetic configurations. The magnetic properties of the ferrimagnetic DyMn2O5 compound were studied using Monte Carlo simulations.

P028

COMPARATIVE STUDY OF THE SOLID STATE REACTION OF Ni/GaAs AND Ni/InAs

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ABSTRACT

Recently, research has turned to III-V semiconductors for the development of future electronic and optoelectronic devices at the nanoscale [1]. The semiconductor III-V InGaAs with well-defined proportions is the most studied to substitute Si on MOSFET technology [2]. With the same lattice parameter, it can be deposited on Si substrate. Good electric contact between metal and III-V still remains a challenging issue for several applications. In one possible integration flow, the fabrication of these contacts is based on the reactive diffusion process in the same way as with Si substrates allowing to improve the ohmic resistance contact between III-V semiconductors and metal [3-4]. However, as a first step to simplify the understanding of the different phenomena that can occur the study of different manufacturing processes has been focused on GaAs and InAs rather than on InGaAs.

For this, we have studied the nature and the sequence of the phases formed for the two systems Ni / GaAs and Ni / InAs, where Ni is deposited by sputtering. We have used in this study X- Ray Diffraction in-situ and ex-situ with different diffractometers (two circles and four circles), Scanning and Transmission Electronic Microscopies. The solid-state reaction between a Ni film and GaAs and InAs substrates during annealing (below 400 °C) gives a ternary intermetallic as the first phase formed for two systems, they are in epitaxy with the substrate and have the same hexagonal structure. This phases are Ni3GaAs [5] and Ni3InAs phases. Moreover, the texture of the Ni3GaAs phase is different from the Ni3InAs phase. At high temperatures (above 400 ° C), we observe for both systems the presence of new phases. These are hexagonal and cubic structures for the Ni / InAs system and just one phase hexagonal for the Ni/ GaAs.

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Keywords*:* Ni/GaAs, Ni/InAs, epitaxy, Ni_3GaAs, Ni_3InAs, reactive-diffusion, formation kinetics, in-situ structural characterization.

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