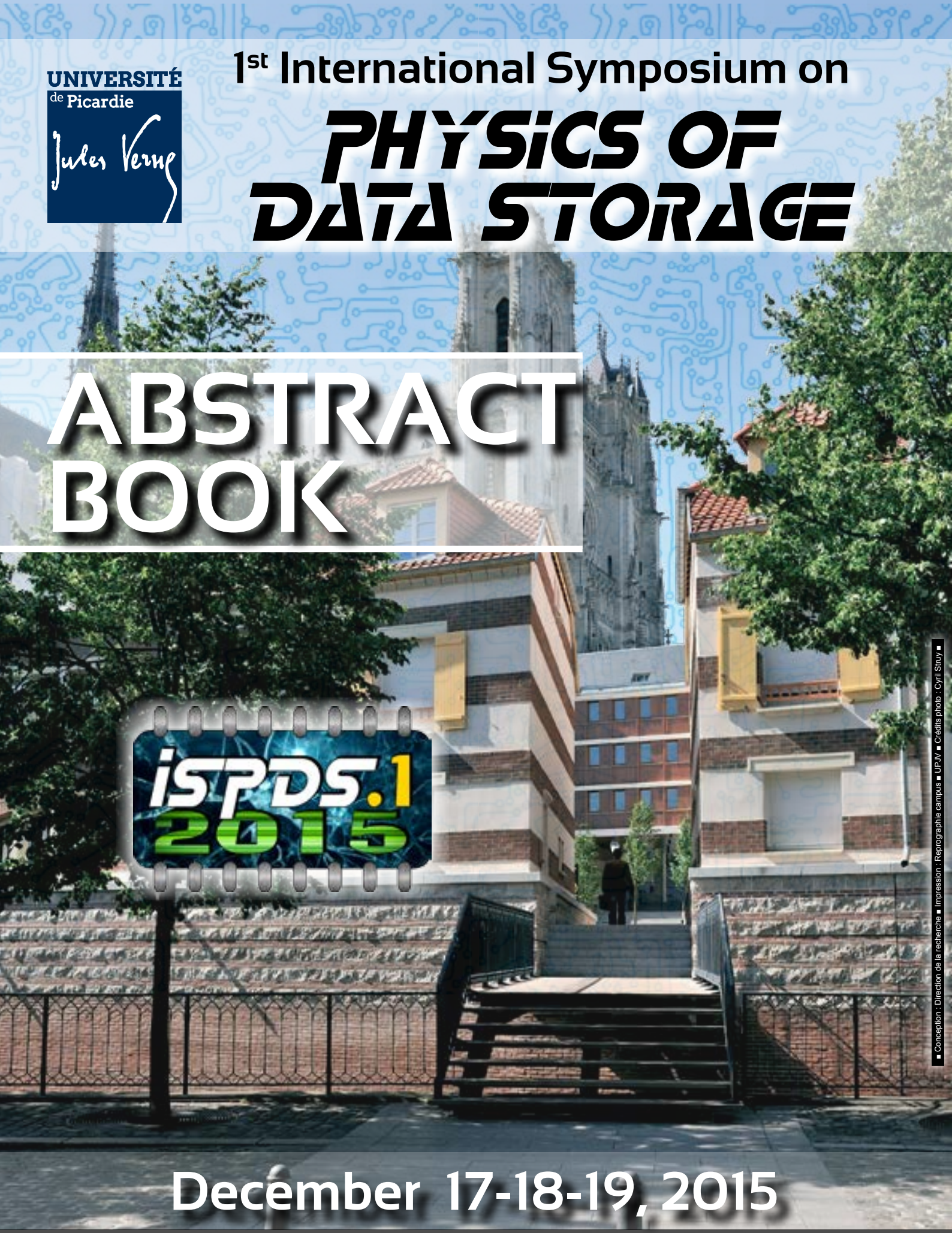
UNIVERSITÉ de Picardie Jules Verne

1st International Symposium on

PHYSICS OF DATA STORAGE

ABSTRACT BOOK



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Université de Picardie Jules Verne
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Welcome message

Dear Colleagues,

It is for us a real pleasure to welcome you at the **« 1st International Symposium on Physics of Data Storage (ISPDS-1) »** - website: https://www.u-picardie.fr/ispds1/index.html - *that is the beginning of a series of conferences, we hope to rotate between Universities voluntary researchers in the world. This conference is international and is interested in the field of physics of materials showing a memory effect: the retention and release of energy.*

As you know, various memory technologies have emerged throughout history. Today, the discovery of new technologies and new materials over the past two decades has helped to manufacture memory devices, less bulky, less expensive, consuming less energy, but always with a larger capacity and higher speed data transfer.

This first edition of the symposium ISPDS over two days, will permit:

- to round up specialists in this research field (theoretical and experimental),

- to discover the scientific community and research in the University of Picardy Jules Verne,

- to review the history of the evolution of storage memories and their implementation in physics and electronic devices, in computer memory to the younger generation today, through various scientific presentations.

In this symposium we will describe the state of art in fundamental scientific research on memories of the future, to reinforce collaborations that will allow us to meet industrial actors and to create links with the professional world partners; in order to generate employment, directly related to Scientific Research. ISPDS-1 will gather researchers at international scale, working in Physics of materials:

- ✓ ***Multiferroics***
- ✓ ***Memory storage devices***
- ✓ ***Switching phenomena.***
- ✓ ***Heterojunctions and semiconductors***
- ✓ ***Energy and environment***

We want to thank the members of the Scientific Committee, that becomes now the International committee for their availability: Profs. James SCOTT - Gustau Catalan - Gil Rosenman - Nadir Aliouane - Pierre Saint-Grégoire – Michael Karkut.

These professors strengthen cultural and scientific exchanges for successful research in the field of physical memory.

We recall that the financial support of the symposium was provided largely by:

- The University of Picardie Jules Verne in the quota of Bonus Quality Research

- The Picardy Region and the city of Amiens

- The Laboratory of Physics of Condensed Matter (LPMC)

We also thank the Journal, "Materials and Devices" which will publish the proceedings of the symposium.

Dr. Yaovi Gagou ***and*** ***A.I. Anna Cantaluppi***

Preface

It is a pleasure to provide this preface to the Abstracts for ISPDS-1.

I had hoped to participate actively in this meeting in Picardy, but medical problems prevent me from traveling. I am sorry to miss which from the program seems to be a very high-level conference, and I had looked forward to showing my wife Amiens and its beautiful cathedral.

The conference itself on data storage will undoubtedly attract a broad range of materials scientists and engineers. My own area of interest --ferroelectric memories -- has finally matured commercially, with Samsung manufacturing ferroelectric random access memories (FRAMs) for subway fare cards (similar to the London "oyster card") under the trade name "Felica" at millions of chips/month, packaged in Japan. These are now in use both in Tokyo and Washington. Equally important are the embodiments as cash-cards ("e-money") under the brand name "Edy".

New materials for FRAM applications may include tetragonal tungsten bronzes (under study both in Amiens by Dr. Gagou et al.) and our group (F. M. Morrison et al.) at St. Andrews University. Multiferroics seem to be the next target on the horizon for such applications, combining very fast (ns) electrical WRITE operations, very low power consumption (voltage-driven rather than current-driven), with magnetic non-destructive READ operations. Cell size is now submicron and prototypes up to 4 Gb have been tested.

The next decade should be a very productive era in this field.

With warmest wishes for a fine meeting,

Jim Scott
St Andrews

James F. Scott was born in New Jersey, USA, and educated at Harvard (B. A., physics 1963) and Ohio State University (Ph.D., physics 1966). After six years in the Quantum Electronics Research Department at Bell Labs he was appointed professor of physics at Univ. Colorado (Boulder), where he also served as Assistant Vice Chancellor for Research. He was Dean of Science and Professor of Physics for eight years in Australia (UNSW, Sydney, and RMIT, Melbourne), Professor of Ferroics in the Physics Department at Cambridge University, and since 2015 Professor of Chemistry and Physics at Univ. St. Andrews. His paper "Ferroelectric Memories" in Science (1989) is probably the most cited paper in electronic ceramics with 4000+ citations, and his text of the same title has been translated into Japanese and Chinese. He was elected a Fellow of the APS in 1974, and in 1997 won a Humboldt Prize and appointment as the SONY Corp. Chair of Science (Yokohama). He was awarded a Monkasho Prize in 2001 and in 2008 was elected a Fellow of the Royal Society (FRS) and recipient of the MRS Medal (Materials Research Society). In 2011 he was elected to the Slovenian Academy of Sciences where earlier he had won the Jozef Stefan Gold Medal. In 2014 he won the Thomson-Reuters Citation Laureate prize, which describes itself as a predictor of Nobel Prizes in Physics.

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ORALS

POSTERS

Orals

OR001

Dielectric properties and phase transitions of [001], [110], and [111] oriented Pb(Zn1/3Nb2/3)O3-6%PbTiO3 single crystals

Mouhamed Amin Hentati,[1,2] Hichem Dammak,[1] Hamadi Khemakhem,[2] and Mai Pham Thi[3]

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Phase transformations of [001], [110], and [111] oriented Pb(Zn1/3Nb2/3)O3-6%PbTiO3 (PZN-6%PT) single crystals have been investigated by means of dielectric permittivity and loss, x-ray diffraction and depolarization current as function of temperature (from 250 to 500 K). The unpoled samples undergo R-T-C phase transition sequence during zero field heating (ZFH), where R, T, and C are rhombohedral, tetragonal, and cubic phases, respectively. Under electric field (0.5 kV/cm), an intermediate orthorhombic (O) phase is induced between the T and R phases in the field cooling (FC) process. This phase reappears during subsequent zero field heating of the poled sample (zero field heating after field cooling: ZFHaFC). The existence range of this O phase depends on both the crystal orientation and the measurement conditions (FC or ZFHaFC). Finally, for the [001] direction, it was found that the piezoelectric activity of the intermediate phase is the highest.

OR002

Polar nanoregions and their influence: a case study of neodymium doped $Ca_{0.28}Ba_{0.72}Nb_2O_6$

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Relaxor ferroelectrics (hereafter relaxors) possess enormous piezoelectric and electromechanical response, which make them attractive for next generation sensors and actuators. A modern definition of relaxors came from one of its peculiar properties, the existence of local polar clusters with randomly oriented polarisation known as polar nanoregions (PNRs), whose first initiation takes place few hundred degrees above the Curie temperature *T*C at the Burns temperature *T*D. For more than five decades lead-based relaxors have been extensively studied, however, due to the disadvantage of volatility and toxicity of PbO, more and more research is encouraged in lead-free relaxors. Promising candidates are members of the tetragonal tungsten bronze (TTB) structure type. It is well accepted that relaxor properties are associated with these PNRs; however, the mechanism behind their formation is still a matter of debate. Here, a detailed description of PNRs induced relaxor behavior on Czochralski grown Neodymium doped $Ca_{0.28}Ba_{0.72}Nb_2O_6$ (CBN:Nd) single crystals will be presented. For the first time, a correlation between *T*D and *T*C in lead-free CBN type relaxor (pure & doped) will be reported, which is completely opposite in nature as observed in lead-based relaxors. Further, this correlation clearly describes the size effect phenomenon in lead free relaxors.

OR003

New Multiferroics: $GaFeO_3$ and $BaFe_{12}O_{19}$

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I will discuss new work on multiferroic switching in $GaFeO_3$ up to T = 410K. This is a ferromagnet with 0.3 Bohr magnetons per unit cell net magnetization and large (>20 macrocell/cm^2) polarisation. It is rather low-loss at room temperature and can be made as epitaxial films and single crystals. I will also discuss Quantum Critical Point studies (QCPs) in the multiferroic hexaferrites $BaFe_{12}O_{19}$, $SrFe_{12}O_{19}$, and $PbFe_3Ga_9O_{19}$. These are the most profitable commercial magnetic devices (3 billion euros/year) and used for magnetic stripe credit cards. The all exhibit ferroelectric QCPs with d=5 dimensionality and electric susceptibility temperature exponent 3.0; and the mixed Fe/Al compound exhibits a magnetic QCP.

OR004

Electrocaloric effect and Luminescence Properties of Lanthanide doped $(Na_{1/2}Bi_{1/2})TiO_3$ Lead free Materials

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Polycrystalline lead–free Sodium Bismuth Titanate (NBT) ferroelectric ceramics doped with rare earth element (RE) are prepared using solid state reaction method. Optical, ferroelectric and electrocaloric properties were investigated. The introduction of RE^{3+} ions in the NBT host lattice shows different light emissions over the wavelength range from visible to near infrared region. The ferroelectric *P-E* hysteresis loops exhibit an antiferroelectric-like character near room temperature indicating possible existence of a morphotropic phase boundary. The enhanced electrocaloric response was observed in a broad temperature range due to nearly merged phase transitions. Coexistence of optical and electrocaloric properties is very promising for photonics or optoelectronic device applications.

OR005

Flexoelectric Memories

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Research on flexoelectricity (polarization induced by strain *gradients*) has been fuelled by the realization that strain gradients scale in inverse proportion to size, leading to large effects at the nanoscale[1,2,3]. At small device sizes, the interaction between flexoelectricity and piezoelectricity in ferroelectric thin films and leads to new physical phenomena, including switchable mechanical properties, switchable "strain valves", mechanical writing of ferroelectric polarization and mechanical gating of memristor conductivity. All these phenomena can be grouped under a new category of new device functionality that one may term "flexoelectric memory". Here I will discuss the basic physics of flexoelectricity and the state of the art in flexoelectric memory effects.

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OR006

Switching processes of thin ferroelectric films in weak pulsing fields

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The motion of domain walls performing repolarization in ferroelectrics essentially depends on the value of the applied field and the temperature. For very strong applied fields the influence of lattice barrier associated with the lattice discreteness and the influence of lattice defects on the domain-wall motion can be neglected, and its speed increases linearly with the applied field. In the case of finite temperatures the barrier created by fixing factors, due to temperature fluctuations, can be overcome even in the fields below the critical value. As a result, the domain-wall motion, which is characterized by an activation law with barrier depending on the value of the applied field, appears. This type of motion is called “crawling” or “creep motion regime”. The speed of the motion of domain walls in this case is described by an exponential dependence on the external field $V \sim \exp[-C/E^{\mu}]$, where C – constant, and μ – the so-called dynamic exponent.

Character of overcome of stoppers by boundary, the values of critical exponent, and so, the speed of the domain-wall motion itself essentially depend on the system dimensionality. Knowledge of the laws of domain-wall motion in low dimensional ferroelectrics gives an additional possibility for practically important control of the speed of the domain-wall motion in thin-film ferroelectrics. The study of specified laws is dedicated to this work.

In present work, the polarization switching processes in lead titanate $PbTiO_3$ and lead zirconate titanate $Pb(Zr_{0.5}Ti_{0.5})O_3$ thin films in weak fields with rectangular pulses using the Merz method have been investigated. Deviation from the strictly exponential dependence of the speed of domain-wall motion in real ferroelectric materials is established. It is shown that for the studied thin films the exponent μ depends on the film thickness, temperature and on the film composition. With decreasing the film thickness an increase in the value μ is observed. At the same time the received value μ of lead titanate is more than those of lead zirconate titanate with the same thickness. With increasing temperature approaching the Curie point the coefficient μ decreases. The causes involving with the appearance of specified dependences are analyzed. It is shown that the observed increase of the dynamic exponent μ with decreasing the film thickness can be related to experimentally observed growth of the level of orientation of crystallites in polycrystalline film.

OR007

Voltage-induced Domain Growth Kinetics in Ferroelectric BST 80/20 Thin Films by Piezoresponse Force Microscopy

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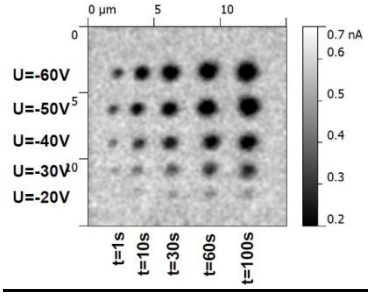
Previous and today's dynamic random access memories (DRAMs) have been advanced by mainly focusing on how to make memory cells small to realize high density DRAMs. The most critical challenges in gigabit density DRAMs are yield loss due to large die size and small feature size, standby current failure caused by large chip size and small data retention times owing to reduced charge packet in the memory cell. In the recent years thin film perovskite materials with high dielectric constant such as PZT, $SrTiO_3$ and $(Ba,Sr)TiO_3$ (BST) have been investigated as dielectric materials for future DRAMs [1].

In this work, we report a voltage-induced domain growth kinetics in ferroelectric BST 80/20 films (thickness 150 nm) fabricated by RF magnetron sputtering measured via piezoresponse force microscopy (PFM) [2,3]. The surface of the sample shows small grains which diameter ranges from 50 nm to 75 nm and roughness is less than 5 nm. Using the PFM mode to detect the out-of-plane polarization, the domain sizes were measured as a function of the applied writing voltage and the pulse time. As example Figure 1 show the result the local polarization effect via PFM. For the investigation of written domains on *as-grown* surface of the BST film the negative voltage pulses were applied to fixed locations within this area, thus we have an array of 23 *stable* domains created by applying voltage pulses of fixed height (V_{tip}=-20 V ÷ -60 V with step 10V) and various durations ranging from 1 to 100 s. The dynamics of domain growth is analyzed experimentally taking into account the strong inhomogeneity of the external electric field in the film.



OR008

Effect of in-plane biaxial strain on the phase transitions in ferroelectric/paraelectric superlattices

J. Belhadi [(1)], M. El Marssi [(1)], Y. Gagou [(1)], Yu. I. Yuzyuk [(2)], I. P. Raevski [(2)], H. Bouyanfif [(1)] and J. Wolfman [(3)]

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We present an x-ray diffraction (XRD) and a Raman-scattering investigation of the lead-free ferroelectric/paraelectric BaTiO3/BaZrO3 superlattices (SLs) deposited using pulsed laser deposition technique on MgO substrates buffered with $La_{0.5}Sr_{0.5}CoO_3$. We choose a modulation period of SLs approximately about 100Å, corresponding to a constrained $BT_{\Lambda/2}/BZ_{\Lambda/2}$ superlattice (SL) [1], and we have reconstructed $BT_{0.7\Lambda}/BZ_{0.3\Lambda}$ SL with 70 Å-thick BT and 30 Å-thick BZ layers [2-3]. We have demonstrated using X-ray diffraction and Raman spectroscopy that the polar axis in BaZrO3 layers is perpendicular to the plane of the substrate while BaTiO3 layers exhibit in-plane polar orientation. Using Raman spectroscopy we have studied the structural and dynamical behaviour of BT and BZ layers in the SL structure over a broad temperature range (25 ◦C ≤ T ≤ 480 °C). We found that the high strains in the SL produce a giant shift of the ferroelectric phase transition temperature in BT layers and stabilize the ferroelectric phase induced in BZ layers up to 450 °C. The observed stabilization of the ferroelectric state over a wide temperature range is very highly desirable for device applications.

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J. Appl. Phys. 116, 034108 (2014).
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OR009

$Bi_{0.5}Na_{0.5}TiO_3$ by Sol-Gel method: Synthesis and Characterization

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Key words: Piezoelectric, lead-free, Sol-Gel, thin films, BNT.

The lead zirconate titanate (Pb(Zr,Ti)O3 or PZT) are widely used in the microelectronics industry due to their ferroelectric and piezoelectric properties. However, due to the effects of lead toxicity, it has recently desired to develop lead-free piezoelectric materials for environmental protection.
The objective of this work is to synthesize a lead-free piezoelectric material by the Sol-Gel method: the bismuth sodium titanate (Bi0.5Na0.5TiO3 or BNT). Bismuth nitrate III penta-hydrate, sodium nitrate and titanium (IV) isopropoxide were used to prepare the solution of BNT. The solution is deposited by spin coating (at a speed of 3000 rpm for 20 s) on a Pt/Ti/SiO2/Si substrate. Then, the film was dried at 100°C for 5 min on a hot-plate in order to evaporate the solvent, and annealed in a rapid thermal processor (RTP).
The structural and morphological analyses studied by X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy (SEM) showed that the film annealed at 700°C with the rapid thermal processor (RTP) for 30 sec is dense and well crystallized in the rhombohedral perovskite phase.
The first results of electrical characterizations showed promising ferroelectric and dielectric performance. The relative permittivity and the dielectric loss were measured at 100 kHz, they are $\varepsilon r = 420$ and $\tan \delta = 0.07$, respectively, while the remnant polarization and coercive field are Pr = 12 µC/cm2 and Ec = 120 kV/cm, respectively, at 1 kHz.

OR010

Ferroelectric and photoelectrochemical properties of $Ba(Ti_{0.96}Mg_{0.013}Nb_{0.026})O_3$ ceramics

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Perovskite material (ABO_3) has been investigated intensively owing to their ferroelectric properties which are of great interest in several technological applications. On the other hand, the substitution in the A and (or) B site of ABO_3 lattice lead to perovskite compounds of complex formula such as $AA'BO_3$, $ABB'O_3$, $AA'BB'O_3$ …etc. In these perovskites, the statistical fluctuations of ions at the A and/or B site produce a local heterogeneity and thus yield ferroelectric compounds with a large variation in the Curie temperature [1].In addition, such compounds present large dielectric constants and wide space charge region interesting for solar applications, especially in photocatalytic hydrogen production [2].Nevertheless, the main ferroelectric materials are lead-based which cause serious environmental problem due the high toxicity and volatility of lead oxide during the preparation step. Then, to develop environment friendly materials, lead-free compositions were currently explored. In this way, numerous lead-free ceramics derived from $BaTiO_3$ were found to be interesting owing to their attractive ferroelectric and photocatalytic performances. Among this, we have evidenced previously photocatalytic behaviour in the ferroelectric $Ba_{0.785}Bi_{0.127}Y_{0.017}TiO_3$ and $Ba_{1-x}Eu_{2x/3}(Ti_{075}Zr_{0.25})O_3$ compositions [3-4]. In the present work, a new lead-free of $Ba(Ti_{0.96}Mg_{0.013}Nb_{0.026})O_3$ composition was explored. The materials were prepared by the conventional solid state reaction. The homogenized powder mixtures were dried at 100 °C for 3 h. The powder mixtures were calcined in a chamber furnace at 1200 °C for 2 h. The calcined powders were isostatically pressed at 300 MPa into disks of 8 mm in diameter and a thickness of ~2 mm. The powder compacts were sintered in an oxygen flow at 1300 °C for 2 h with heating and cooling rates of 5 °C/min in a platinum crucible. The XRD analysis reveal only the peaks related to the tetragonal perovskite phase. The complex dielectric permittivity measured on cooling from 470 to 150 K in the 10^2 -10^6 Hz frequency range, show classical ferroelectric behaviour with interesting parameters. This ferroelectric perovskite show photoelectrochemical properties with a gap of 2.90 eV, *n*-type conduction and a flat band potential of -0.57 V. As application, it is successfully tested for the eosin oxidation under solar light. At pH ~ 6.3, 90% of eosin (15 mg L^{-1}) disappears after 6 h of illumination for a catalyst dose of 2.5 g L

Keywords : *ferroelectric, relaxor, lead-free, perovskites.*

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OR011

Polarization rotation in ferroelectric tricolor PbTiO3/SrTiO3/ PbZr0.2Ti0.8O3 superlattices

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In ferroelectric thin films, the domain structure is directly controlled by the strain and the electrostatic environment. In tricolour ferroelectric/paraelectric superlattices, $PbTiO_3/PbZr_{0.2}Ti_{0.8}O_3/SrTiO_3$ (PT/STO/PZT 20-80), we have shown that tensile strain can be induced in the PT layers by the mismatch between the ferroelectric materials1. In this work we use laboratory and synchrotron x-ray diffraction to investigate the role of the SrTiO3 layers on the domain structure in these superlattices2. The out-of-plane and in-plane polar structure was studied by reciprocal space mapping using standard reflection geometry and grazing incidence diffraction, respectively. Satellite peaks were detected both around the *out-of-plane and the in- plane* superlattice Bragg peaks. We demonstrate the existence of 180° ferroelectric stripe nanodomains, induced by the depolarization field produced by the $SrTiO_3$ layers. Our x-ray investigations show that the polarization has both in-plane and out-of-plane components. This polarization rotation away from the film normal, is associated with the monoclinic Mc phase.
The role of the paraelectric layer is crucial in inducing the stripe nanodomain structure, whereas the polarization is rotated primarily by the effect of tensile strain which is induced by $PbZr_{0.2}Ti_{0.8}O_3$ in the $PbTiO_3$ layers. This work demonstrates that the tricolor paraelectric/ferroelectric superlattices constitute a tunable system to investigate the concomitant effects of strains and depolarizing fields. The ferroelectric/paraelectric tricolor superlattices offer an effective pathway to stabilize a rotation of the polarization, compatible with an enhancement of the piezoelectric properties.

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OR012

Sequence of structural transitions and electrocaloric effect in $(Ba_{1-x}Ca_x)(Zr_{0.1}Ti_{0.9})O_3$ ceramics

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Keywords: BZCT, structural phase transition, dielectric, ferroelectric, electrocaloric effect.

Abstract

The influence of the incorporation of calcium in lead-free ferroelectric Ba(Zr0.1Ti0.9)O3 perovskite on its structural phase transition, dielectric properties, ferroelectric behavior, and electrocaloric effect was investigated. X-ray diffraction study allowed the identification of a continuous solid solution in the composition range $0 \leq x \leq 20$ at %. Using dielectric and heat flow measurements two sequences of structural phase transitions were elucidated. The tetragonal-to-orthorhombic and orthorhombic-to-rhombohedral phase transitions temperatures were found to decrease with the increase of the Ca2+ content, while the cubic-to-tetragonal phase transition temperature remained constant in all the compositions. The adiabatic temperature change ΔT was calculated from the thermal variation of P–E hysteresis loops. The highest electrocaloric strength $\Delta T/\Delta E = 0.26$ K.mm/kV was found for the composition x=0.05.

OR013

Fabrication and dielectric properties of la/ca-co-doped barium titanate ceramics

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Key words: LBCT, sol-gel, DCS, SEM, generalized power law

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Abstract:
La/Ca-co-doped barium titanate ceramics powders La0.01(Ba1-xCax)0.99Ti0.9975O3 LBCT (x=0.01, 0.05 et 0.1) were prepared by sol-gel process through Destabilization of Colloidal Solution (DCS) **[1]**. The powders were heat treated at 900°C and pressed into discs and sintered in air at 1150°C, 1250°C and 1300°C for 4 hours. XRD analysis showed a good crystallization of the samples in the pure perovskite structure, and allowed determination of the crystallite size. Microstructure morphology was analyzed using Scanning Electron Microscopy (SEM), and the grain size of the samples was estimated. It was found that lanthanum doping has significant inhibiting effect on densification **[2,3],** but calcium appears to have a beneficial effect for the improvement of the densification of the material. Dielectric measurements were carried out with an impedance-analyzer in the temperature range from room temperature (RT) to 250°C, and for frequencies ranging from 100Hz to 1MHz. Data obtained from these measurements were fitted to the generalized power law.

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OR014

Synthesis and characterization of Aurivillius-type layered oxides

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Materials such Aurivillius structure constitutes a family of mixed oxides which is formed by the structure of perovskite layers separated by Bi_2O_2 groups. They play an important role in the chemistry of the solid state and materials science. The particular interest lies in industrial applications; they are used as best insulating ferroelectrics, as superconductors at high top performing critical temperature and also for energy storage, which involves placing an amount of energy in one place given to enable its subsequent use.

The aim of our work is part of a research program to be prepared by two different methods (dry, wet) and performs physico-chemical characterization of new phases with an applied focus.

In a first step, our choice fell on the family of phases derived from $Li_2Ge_4O_9$ because of the variety of opportunities it presents. Thus we are currently first define the optimal conditions for preparing compounds.

The powders of $SrBi_2Nb_2O_9$ (SBN) were prepared by a routine solid-state reaction technique, and by another way using an aqueous solution method. X-ray diffraction show that SBN Orthorhombic at room temperature as previously reported.

The comparison between the two synthetics has provid very effective for affording a means towards an environmentally friendly aqueous synthesis of the ferroelectric perovskite SBN at reduced temperature.

OR015

Electrocaloric effect in $Ba_{0.2}Ca_{0.8}Ti_{0.95}Ge_{0.05}O_3$ determined by a new pyroelectric method

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Keywords: pyroelectric current, electrocaloric effect, BCT, ferroelectric, ceramics.

The present letter explores the electrocaloric effect (ECE) in the lead free oxide $Ba_{0.8}Ca_{0.2}Ti_{0.95}Ge_{0.05}O_3$ (BCTG). The electrocaloric responsivity $\xi = (dT/dE)$ was determined by two different methods using the Maxwell relationship $\xi \propto (\partial P/\partial T)_E$. In a first well-known indirect method, P-E hysteresis loops were measured in a wide temperature range from which the pyroelectric coefficient $p_E = (\partial P/\partial T)_E$ and thus ξ were determined by derivation of *P*(*T*,*E*) data. In the second novel method the pyroelectric coefficient p_E and consequently the electrocaloric responsivity ξ was determined by direct measurements of the pyroelectric currents under different applied electric fields. Within the experimental error good agreement was obtained between two methods with ξ = 0.18 ± 0.05 10^{-6} K.m.V^{-1} was obtained at about 410 K.

OR016

On the crystal structures and phase diagrams in perovskites and TTB-type compounds

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Abstract

In the forthcoming decades, the humanity will face as a major risk, that of energy shortage since it may be expected that usual fuels as fossile or nuclear would quasi disappear in less than one century. Subsequent risks are the breakdown of information storage, and the breakdown of civilization was even evoked recently as a risk with high probability at a global level. In this context, research on materials for energy, and on those allowing reduction of energy consumption, in particular in relation with information storage, is of crucial importance.

In this respect, the perovskite and tetragonal-tungsten bronze type crystalline families occupy a big role in applications. They find applications for their piezoelectric properties as sensors and actuators, in nonlinear optics, and they may be used to recuperate energy from vibrations of structures, and for sourcing mobile electrical devices. In the context of energy, high temperature superconducting phases found in some of their representative, could find applications in the energy transportation with reduced loss over great distances. They are also used for their ferroelectric properties as thin films in FeRAM memories, that can be programmed at low voltage and with low energy, and recently some perovskite materials also found interest in new type photovoltaic cells.

In spite of a large number of papers dealing with these materials, the knowledge of such basic properties as the crystal structures of these materials still remain somewhat uncertain.

In this talk, we shall present different phases and situations found in composition - temperature phase diagrams and discuss the role of doping by various elements, that may destabilize some structures. As examples, the influence of lanthanum and tin introduction in lead zirconate and PZT ($PbZr_{(1-x)}Ti_xO_3$) considerably changes the sequence of phases found in temperature.

The possibility for a determining role of rigid unit modes (RUMs) on structural instabilities, on the observed dependence on composition and doping, and on pre-transitional effects is underlined by results obtained in these systems.

OR017

Interface Magnetoelectric Coupling in Co/Pb(Zr,Ti)O_3

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Research on spin electronics has been strongly influenced over the last decades by the discovery of alternative means to control the magnetization, i.e., other than by applying a magnetic field. An outstanding achievement of this research is the electric-field control of magnetic states[1], offering important advantages in terms of fast and dissipationless operations. Ferromagnetic and ferroelectric composite systems provide a particularly promising pathway towards the efficient electric-field control of the magnetization[2,3], owing to a strong magnetoelectric coupling (MEC).
In this talk, I will present our recent results on room temperature multiferroicity and interface MEC in Co/$PbZr_{0.2}Ti_{0.8}O_3$ (Co/PZT) bilayers. We explore the statics and the dynamics of the interface MEC in the sub-MHz regime by means of electric-field dependent optical measurements. A complex signal is obtained in Co(5-10nm)/PZT bilayers, revealing a multicomponent optical response. We propose a decomposition method to interpret these measurements and to extract the magneto-optical component related to MEC from the overall signal. The coupling mechanism in this system is found to be interface-mediated (*i.e.*, electronically driven), as further demonstrated by complementary methods based on X-ray magnetic circular dichroism measurements and first-principals calculations based on density functional theory. The frequency dependence of the magneto-electric hysteresis loops allows for an analysis of the dynamic properties of the interface coupling.

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OR018

Average particle sizes of magnetite nanoparticle coated with oleic acid

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Magnetite nanoparticles coated with oleic acid were prepared by co-precipitation method. The presence of magnetite it was evidenced by x-Ray Diffraction and Raman Spectroscopy Magnetite Particle size distributions are analyzed based on dc magnetic evaluation in Vibrating Sample Magnetometer (VSM). Using a log-normal distribution the experimental results were fitted. The average particle sizes, calculated by dc measurements, are in good agreement with the coherent domain length calculated by x-ray diffraction. This morphological evaluation was corroborated by AFM topography image. Magnetic evaluation versus temperature in argon atmosphere shows a transformation to maghemite then to hematite, but only on the nanoparticle surface. Moreover, from ac measurement in coated nanopowder, in the frequency range evaluated up to 100MHz, the superparamagnetic behavior can be affirmed. The Néel relaxation is observed about 22MHz. The proposed measurements combined with the analysis methods are useful for the characterization of ferrofluids, considered for biomedical applications.

OR019

Synthesis and photovoltaic application of Cu_2S thin films

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Polycrystalline copper sulfide (Cu_2S) thin films were deposited by spray pyrolysis using aqueous solutions of copper chloride and thiourea at substrate temperature of 200 °C. The deposited films were observed to be blackish brown in color, well adherent to the substrate, pin-hole free and uniform. The structural and optical properties of the films were carried out by means of X-ray diffraction and optical absorbance measurement techniques. XRD analysis showed that deposited films are chemically close to chalcocite, Cu_2S. The optical band gap was calculated to be in the order of 1.5 eV. These results allow us to use CuS_2 as an absorber material in the $CuS_2/\beta\text{-}In_{2-x}Al_xS_3$ p-n heterojunction solar cells.

Keywords *: copper sulfide, Thin films, Structural properties, Optical properties, Solar cells*

OR020

Voltammetric determination of paracetamol on carbon paste electrode modified by fluoroapatite:analytical application

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A carbon paste electrode modified with fluoroapatite was used for the voltammetric determination of paracetamol (PCT). The electrochemical sensing performances towards paracetamol were evaluated using electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV) and square wave voltammetry (SWV).In addition, the modified electrode (FAP-CPE) has also demonstrated excellent electrochemical activity toward PCT oxidation compared to that with unmodified carbon electrode. All the experimental conditions, which influence the electrochemical response of PCT, were studied and the optimum conditions were achieved. A sensitive and simple measurement with a good linear relationship in the range of 4.0×10^{-8}mol $L^{-1}$to 6.0×10^{-5}mol L^{-1}has been achieved for the determination of PCT. The detection limit obtained was 1.35×10^{-7}mol L^{-1}after 210 second of accumulation time. This methodology was proposed to determine PCT in river water, seawater, tablets and urine samples.

Keyswords : *fluoroapatite, square wave voltammetry, paracetamol.*

OR021

High efficiency of transmittance and electrical conductivity of V doped ZnO used in Solar cells Applications

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The full-potential linearized augmented plane wave method (FP-LAPW) based on the density functional theory (DFT) and Boltzmann's Transport theory, are employed to investigate theoretically the electronic structure, optical and electrical properties of vanadium -doped wurtzite ZnO with different concentrations (3.125%, 6.25%, 12.5%, 25%). The FP-LAPW based on the new potential approximation known as the Tran–Blaha modified Becke–Johnson exchange potential approximation (TB-mBJ). The calculated band structure and density of states (DOS) exhibit a band gap of pure ZnO (3.3 eV) closer to the experimental one. As well, our results indicate that the average transmittance in the 400 to 1000 nm wavelength region was 93%. We found that $Zn_{96.875}V_{3.125}O$ is the optimized composition of the V doped ZnO, which has the highest conductivity ($3.2\ 10^3\ (\Omega cm)^{-1}$) and transmittance. The high transmittance and electrical conductivity indicate that hexagonal V:ZnO system is a potential as material for solar energy applications.

Keywords **:** *FP-LAPW, TB-mBJ, transparent conductive oxide, electrical conductivity, Transmittance.*

OR022

Improved performance of the solar cells by the introduction of an ultra-thin layer of metal

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Abstract:

Efficiency of organic solar cells shows a strong improvement when the transparent conductive anode (indium tin oxide-ITO, aluminium-doped zinc oxide-AZO, fluorine-doped tin oxide-FTO), is covered with an ultra-thin metallic film. It is shown that the best results are achieved with a gold film (0.5 nm).
The efficiency of the solar cells using AZO or FTO is improved up to one order of magnitude, while in the case of ITO it is at least 50%. It is shown that if the matching between the work function of the anode and the highest occupied molecular orbital (HOMO) of the organic electron donor is the most important factor limiting the hole transfer efficiency, others factors such as transparent conductive oxide (TCO) surface roughness and adhesion of the organic layer are also key factors.

Key Word: Organic solar cells, transparent conductive anode, film, Efficiency

OR023

Modeling of magnetic properties (Cr/NiO/Ni) based multi-layers deposited by magnetron sputtering using Preisach model

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Abstract:

Ferromagnetism (F) behavior of a material is essentially due to an exchange interaction between aligned magnetic moments in the same direction allowing to a net magnetisation. However, the antiferromagnetism (AF) is originating from the exchange interaction but with antiparallel spins order. The contact between F- and AF- material leads to an exchange interaction at the interface of two materials, which induce an additional anisotropy in the whole system. Such characteristic is widely used in several electronic and magnetic areas such as digital storage, magnetic sensors technology, magnetic recording media, or domain stabilizers in recording heads based on anisotropic magnetoresistance.

In the present work, thin films of Cr/NiO/Ni are deposited on 5mmx5mmx1mm dimensions of glass substrates using the cathodic RF magnetron sputtering technique. The uniformity and homogeneity of the prepared films were controlled by varying both the power of the sputtering target, the target-substrate distance and the pressure of argon.

In order to test the Preisach Model, we carried out tests according to two directions: parallel and perpendicular to the substrate plan (VSM EV9) at room temperature. Good agreement has been found on comparing the hysteretic loops obtained in experiments and those obtained by theoretical model.

We conclude that Preisach is a powerful model to predict magnetic properties of magnetic multilayer systems.

OR024

Investigation of the photovoltaic effect in BiFeO3 thin films

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During the last years, multiferroic materials have gained great attention due to their fundamental physics and possible integration in advanced application. $BiFeO_3$ (BFO) appears actually as one of the most interesting, because it shows multiferroic properties at room temperature. Recently a peculiar photovoltaic effect has also been revealed in BFO with a large open circuit voltage Voc above the band gap. The photovoltaic effect (PV) was first interpreted as arising from the ferroelectric field separating the electrons from the holes. Such large Voc suggests several applications in optoelectronics and in non-volatile memories. In classical FERAM the information is encoded by the switchable spontaneous polarization defining the '0' and '1' states and a new PV FERAM concept has been proposed to avoid the destructive reading process used in classical FERAM. Indeed in photovoltaic FERAM the polarization state is simply inferred from the sign of the Voc under illumination. However the exact origin of the photovoltaic effect is obscured in standard capacitor geometry by the possible existence of a Schottky barrier, symmetry considerations, depolarizing field and the BFO complex rhombohedral ferroelectric domain structure. To better understand the observed PV effect and the possibility of using it in PV FERAM, we have grown by pulsed laser deposition BFO thin films with different thickness on buffered LaAlO3 substrates. A conducting 20nm thick SrRuO3 conducting buffer layer is used as a bottom electrode while Pt and ITO top electrodes were deposited. In order to understand the strain effects the thickness was tuned from 5.6nm to 350nm. Reciprocal space mappings and Raman spectroscopy were used to characterize the domain structure and symmetry. Ferroelectric properties were investigated using a Sawyer-Tower homemade system and piezo-force microscopy. Very large spontaneous polarization were measured and I(V) curves were collected at different temperatures to understand the transport properties (interface or bulk limited and the existence of a Schottky barrier). Photovoltaic responses were measured from the I(V) curves under illumination. PV effects under laser illumination of different wavelength (from 647nm to 488nm) and powers were investigated at different temperatures. Observed switchable Voc and Isc (short circuit current) will be presented showing a ferroelectric PV effect.

OR025

Characteristics of ZnO:Al thin films prepared by thermal evaporation technique

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Al-doped ZnO (ZnO:Al) transparent conductive thin films were deposited by thermal evaporation technique using ZnO powders on glass substrates at room temperature, after the deposition process, thin films were annealed at 300°C and 400°C for 2 h. The structural, electrical and optical properties of the ZnO:Al films with various dopants are studied. The X-ray diffraction spectra showed that ZnO:Al thin films are polycrystalline with the hexagonal structure. The optical transmittance spectra showed transmittance higher about ~ 92% within the visible wavelength region. Hence, the values of the gap were found to be between 3.12 to 3.28 eV. The electrical characterization obtained by four probes measurement in the order of 10 Ωcm.

Keywords: Thermal evaporation, thin films, ZnO:Al.

OR026

Structural and optical properties of ZnO:Co thin films prepared by ultrasonic spray pyrolysis method for DMS applications

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ZnO is an II–VI group semiconductor with a wide band gap of 3.37 eV and large exciton energy of 60 meV at 300 °K. Zinc oxide (ZnO) has been attracted a great deal of scientific attention because of their potential applications in the field of optoelectronics and data storage devices. In this fact, pure and Co-doped ZnO (ZnO:Co) nanostructured thin films with doping levels (0, 1, 3, 5, 7, 9, 11, 13 at%) and Ts = 350°C; were synthesized via a simple method: ultrasonic spray pyrolysis under atmospheric pressure. The structure of the as-prepared samples was characterized by X-ray diffraction (XRD) and Raman spectroscopy. Compared with the Raman spectra for ZnO pure films, the Co-doping effect on the spectra is revealed by the presence of three additional peaks around 235, 470 and 538 cm^{-1} due to Co incorporation. These results show that cobalt ions, in the oxidation state of Co^{2+}, replace Zn^{2+} ions into the ZnO lattice without changing its wûrtzite structure. The optical properties of the samples were studied by ultra-violet visible near infrared (UV-VIS-NIR) spectroscopy. These measurements shows absorption wells at approximately 570 (2.18 eV), 620 (2.02 eV) and 660 nm (1.88 eV) appearing in the spectra of the Co-doped samples in comparison with pure ZnO confirming XRD and Raman spectroscopy results.

PACS: 81.15.-z; 81.20.Ka; 78.30.Fs; 61.72.-y

Keywords: Nanostructured thin films; Chemical synthesis; Raman spectroscopy; microstructure.

OR027

Synthesis of nanomaterials of tio_2 and α-fe_2o_3 to remedy polluted waters with paracetamol

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The development of the industrial activity goes together to the increase of toxic substance. These emergent pollutants (drugs, pesticides, etc.) enter to surface waters mainly through the untreated residual waters, and through the residual waters coming from conventional waste water treatment stations, which are not designed to treat these recalcitrant substances. The Advanced Oxidation Processes (AOP) constitute a more and more studied and implemented alternative, because of its efficiency and relativity low cost. The aim of this work is to synthesize nanomaterials of TiO_2, α-Fe_2O_3 and TiO_2/α-Fe_2O_3 by different methods, to characterize them and to evaluate their ability to degrade paracetamol in aqueous solution. The obtained nanomaterials were characterized by different methods: X-rays diffraction (XRD), Fourier transform IR spectroscopy (FT-IR), energy dispersive X-rays fluorescence (ED-XRF), transmission electronic microscopy (TEM) and magnetization studies. The characterization with XRD evidenced the obtaining of each material, and their constituent phase. The particle size of each nanomaterial, determined by TEM, was smaller than 20 nm. The magnetization studies confirm the superparamagnetic character of the α-Fe_2O_3 compounds. The degradation tests were carried out with a concentration of 0.5 g/L of nanomaterial and 0.1 g/L of paracetamol, during 90 minutes of reaction and different reaction conditions, using heterogeneous photocatalysis and heterogeneous Fenton like system under UV and solar light. Approximately a 60% of pollutant was degraded with sun light, among 60% and 90% with UV light and around of 13% in dark.

Keywords: nanomaterials, heterogeneous photocatalysis, heterogeneous Fenton like system, paracetamol

OR028

Study of the influence of ultrasound on the determination of metals in samples of substrates from urban organic farms using different extraction methods

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Using ultrasonic bath and an ultrasonic probe they have been used to develop rapid BCR versions, providing great savings in the extraction time in relation to conventional agitation. The substrates used for the production of plants and vegetables vary in composition, so it is necessary to take into account possible organic and inorganic contaminants that may be present and alter the bioavailability in agricultural products bringing levels that do not comply with the provisions according to international laws.Among the pollutants are inorganic metals. To establish the impact of metals on substrates, it is not only necessary to consider the total content thereof, but also their mobility and bioavailability. In this paper a sample substrate was prepared about one kg, which led to a size less than 250 microns particle to ensure homogeneity and so the repeatability of the results for analysis. The digestion methods used for the extraction of metals in the samples were 1.Total digestion by EPA 3052 and 2. Sequential extraction of three stages of European Reference Bureau (BCR). It was determined the concentrations of bioavailable fraction of Cu, Fe, Mn and Zn in the sample substrate by atomic absorption spectrometry flame (EAA-Ll). The sequential extraction scheme allowed to know the phases to which are associated these elements contained in the sample analyzed and accordingly its bioavailability order. The results obtained were compared with the results of the total digestion.

Keywords : AAS flame. Sequential extraction. Metals. Substrates. Ultrasound probe. Ultrasonic bath

OR029

Resistive Switching in Graphene/ZnO Nanorod Heterostructures

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Graphene-based layer heterostructures have a great potential for use in high-performance electronics due to their fascinating electrical, thermal and mechanical properties. In particular, graphene/graphene oxide (G/GO) nanostructures could be used in the resistive switching devices because of their high speed, long retention time, low power consumption, high density, simple structure and multibit capabilities [1-2]. The resistive switching has been observed in vertical Graphene/ZnO nanorod nanostructures [3]. Graphene was grown by CVD on Ni films and transferred on SiO2/Si substrates [4]. ZnO nanorods were synthesized in aqueous solution at 110°C on graphene substrates [5]. The growth of ZnO nanorods has lead to the local oxidation of graphene layers. These Graphene/ZnO nanorod structures demonstrated resistive switching for low offset voltage due to the migration of the oxygen functional groups under the electric field. The ratio of the on/off currents was about 3 orders of magnitude. It was shown that resistive switching depends on a number of graphene layers in Graphene/ZnO nanorod nanostructures. Current-voltage (I-V) characteristics of the fabricated vertical structures with multi-layer graphene were studied by dc voltage sweep measurements. The results are illustrated in both Fig. 1a and b with the same I-V insets in a semilogarithmic scale. The shape of the I-V curve of the structure which have not been applied by electroforming voltage, shows the asymmetric rectification characteristic of the Schottky-type which was formed between multi-layer G and the n-type ZnO NRs, and the hysteresis loop became more pronounced when the ZnO NRs were biased positively (Fig. 1a). After the forming process (for 5 minutes with a forming voltage of -1 V applied to ZnO NRs), a pronounced increase in the resistance of the structure was observed. By increasing the positive bias voltage imposed on the top electrode, a pronounced sharp change in resistance from the high resistance state (HRS) to low resistance state (LRS) was observed at about 2.5?3 V. Subsequently, an opposite process could also be seen when sweeping the voltage reversely to negative values. The switching from the LRS to HRS occurs at about -0.7 V (Fig. 1b). Ratio of the currents “on” and “off” was about 103 (Fig. 1b insert). No resistive switching was observed in the vertical Graphene/ZnO nanorod structure with 1-2 layer graphene even after the forming process. The mechanism of resistive switching in the vertical Graphene/ZnO nanorod structures and a role of oxygen groups is discussed.

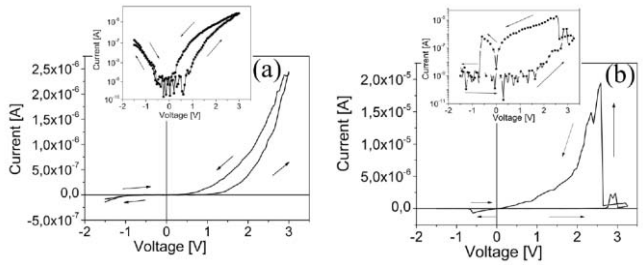

Fig. 1. I-V curve of the vertical G/ZnO structure with multi-layer G without (a) and after pre-forming at -1 volts (b), respectively. Insets of (a) and (b) are IV curves of vertical G/ZnO structure without and after pre-forming in a semilogarithmic scale, respectively.

The obtained results indicate that the proposed vertical memory structure based on ZnO nanorods and multi-layered graphene is promising for low consumption and high-density resistive memory.

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OR030

Ni/Fe and Mg/Fe layered double hydroxides and their calcined derivatives: preparation, characterization and application on dyes sorption.

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Abstract
In this study, Mg/Fe and Ni/Fe Layered double hydroxides (LDHs) intercalated with carbonate ions, (M^{2+}/Fe^{3+}) with molar ratio of 3, were synthesized by co-precipitation method. The as-synthesized materials and their calcined products (CLDHs) were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), thermo-gravimetric and differential thermal analysis (TGA–DTA), transmission electron microscopy coupled with energy dispersive X-ray spectroscopy (TEM-EDX) and inductively coupled plasma (ICP). The materials were used as adsorbents for the removal availability of dyes from aqueous, solution. Methylene blue (MB) and malachite green (MG), representative of cationic dyes, and methyl orange (MO) representative of anionic dyes were used. Adsorption experiments were carried out under different parameters such as contact time, temperature, initial dyes concentration and solution pH. Experimental results indicate a high degree of crystallinity for LDHs. The total weight losses after calcination were approximately 20.66 and 45.24%, respectively for Ni-LDH and Mg-LDH. Kinetic data fitted the pseudo-second order kinetic model. Adsorption process was spontaneous, endothermic for cationic dyes and exothermic for the anionic dye. Equilibrium sorption data fitted the Langmuir model in stead of Freundlich model. CLDHs had much higher adsorption capacities compared to LDHs.
Keywords: Layered double hydroxides; Dyes removal; Kinetics; Equilibrium; Thermodynamics.

OR031

A one-pot synthesis of nanostructured mesoporous TiO_2 films on graphite felt substrates for fast catalysis

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Key words: Waste effluents, NiO/TiO_2, Amido black.

Abstract

Many synthetic dyes are used in textile, paper, leather, ceramics, cosmetics, foods processing and ink industries. The majority of these dyes are azodyes, which are characterized by the presence of -N = N- group. Some of these dyes are toxic and may be hazardous to human health. At the time of production and application about 10 % of these dyes are lost as waste effluents. These effluent treatments involve physical, chemical and biological processes.

In this work, we propose a one-pot soft chemistry method for the homogeneous coating of graphite felt substrates with thin films of TiO_2. Variants of this method that are also reported here include the deposition of NiO/TiO_2 heterostructures on Graphite Felt. The photocatalytic activity of the different heterostructures is tested on amido black dye solution in a continuous flow set-up under a cold UV diode of 360 nm wave length. The choice of this dye has been made based on its widespread use for dying textile fibres, in biochemistry and because of its toxicity and pollution of waters.

The results show that the deposition NiO/TiO_2 on Graphite Felt can improve photocatalytic activity versus than TiO_2 alone and allows a total decolourization of dye.

OR032

Bioorganic Nanodots Memory Storage Devices

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Bioinspired nanoscale building blocks that are self-assembled from proteins and peptides, became an object of intensive research, due to integration feasibility of this new generation of bio-nanomaterials in diverse nanotechnological applications. These nanostructures exhibit exceptional physical properties [1] such as one of the strongest measured piezoelectric signal among biological structures [2], pronounced non-linear optical response [3]. They are used for efficient carbon electrode coating of supercapacitor electrodes [4], and demonstrate unique visible photoluminescent properties.[5]

Here we focus on a new class of nanodots of biological origin (Figure) self-assembled from chemically synthesized peptide biomolecules [6]. In this work peptide nanodots (PND) are composed from diphenylalanine (FF) biomolecules which are a core motif of Alzheimer beta amyloid polypeptide. We show that PND are stable organic dielectric nanocrystals of homogenous size, ~ 2nm size with energy gap ~4.0-5.0 eV possessing very low conductivity 10^{-13} $Sm{\cdot}cm^{-1}$. Transmission electron microscopy (TEM) of isolated PND shows that PND are molecular crystal particles that was also confirmed by the Fourier transform images displaying discrete diffraction spots, indicates the single crystalline structure. Mass- and secondary ion mass-spectrometry suggested that the PND is composed from a dimer of diphenylalanine molecules used in these work.

We employed these bioorganic nanounits for charge storage using PND arrays of high density and studied the ability of the PND monolayer to retain charge by using Kelvin Probe Force Microscopy (KPFM). We study their electron/hole trapping mechanisms at the nanoscale, and charge retention ability followed by fabrication of PND embedded into metal-oxide-semiconductor memory cell devices as charge storage nanoparticles for non-volatile memory [7].

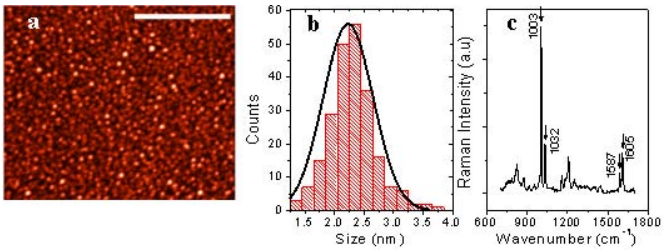

Figure : AFM morphology of the FF PND**.** (a) FF PND on Si surface. (b) Size-distribution histogram of (a). (c) Raman spectrum of (a) using a Raman NSOM apparatus.

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OR033

Vibrational spectroscopy study of $Ba_{0.15}Sr_{1.95}MgMoO_6$

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Double perovskite oxides of the type $A_2MM'O_6$, where A is an alkaline earth cation and M and M' are two heterovalent transition-metal elements show a large variety of physical and chemical properties. Because of the important applications of the double perovskites in diverse fields including ferroelectrics, superconductivity [1-3], colossal magnetoresistance effects, such as CMR discovery in Sr_2FeMoO_6 and ionic conductors [4-5].

Oxides with the perovskite structure in modern materials continue to grow. To contribute to a better investigation to follow structural phase's transition in this type of compounds, we have undertaken the synthesis by solid state method of large number of oxides $Ba_{0.15}Sr_{1.95}MgMoO_6$ using X-ray diffraction and Raman spectroscopy techniques.

We report in this work on the effect of Sr substitution at the A-site and on the high temperature induced phase transition in $Ba_{0.15}Sr_{1.95}MgMoO_6$**.** Their crystal structure was solved by Rietveld refinement of X-ray powder diffraction patterns.

The study with high-temperature Raman spectroscopy showed the phase transition from the cubic phase to tetragonal phase and thus confirming the X-ray diffraction results.

Keywords: *Double perovskite, Phase transition, Raman spectroscopy, X-ray diffraction,* $Ba_{0.15}Sr_{1.95}MgMoO_6$

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OR034

Spectroscopic studies of gamma irradiation and thermal effect of Copper doped silicate glass

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Abstract

Ion exchange process with irradiation and thermal treatment is an important method for obtaining cupper nanoclusters in glasses and provided an alternative way of forming metallic nanoclusters in glass to ion implantation. Samples of a commercial silicate glass have been subjected to ion exchange at 600°C in a molten mixture of $Cu(NO_3)_2$ and $NaNO_3$. The ion exchange process was followed by annealing at the temperature of 550°C for different time periods ranging from 10 to 582 min. Optical properties of the ion-exchanged glass are measured using UV–Vis absorption spectroscopy. The gamma irradiation induced holes and electrons in the glass structure leading to the creation of a brown colour, and copper ions trapped electrons to form copper atoms. The copper atoms diffused and then aggregated to form nanoclusters after heating at 550°C. The surface plasmon absorption of copper nanoclusters in the glass indicated that the nanoclusters radius grew between 1 and 10 nm with increasing of annealing time from 10 to 300 min and then saturated. Usually, the growth of metallic clusters in glass is considered as a diffusion-limited process. We found that our data can be fitted by a first order formation kinetic function, which confirmed the diffusion-control process. The average cluster radius R of the clusters is calculated. The Full width at half maximum (FWHM) is determined by assuming the absorption peak as a Lorentzian distribution.

OR035

C_{60} and C_{70} filling rate dependence on theoritical Raman spectra of carbon peapods

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Single walled carbon nanotubes (SCNT) can encapsulate small and large molecules, including C_{60} and C_{70} fullerenes [1]. Those systems consist of SCNTs in which fullerene molecules are inserted and called peapods. This hybrid system between fullerene molecules and SCNT has generated a lot of interest for future electronic applications. We focus on the calculation of the nonresonant Raman spectra of C_{60} and C_{70} peapods to determine the concentration of fullerenes in the single wall carbon nanotubes. The nonesonant Raman spectra are calculated in the framework of spectral moment method, together with a bond polarizability model. The present work extend the calculations to a larger range of peapod diameter (from 1.22 to 2.3 nm) where the C_{60} molecules form linear, zigzag, double helix and two molecule layers configurations. The changes of the Raman spectrum as a function of the orientation of the C_{70} molecules inside the nanotubes are also identified. The evolution of the average Raman intensity ratios between Raman mode of C_{60} and C_{70} molecules and nanotube as a function of the concentration of fullerenes has been analyzed and general good agreement is found between calculations and measurements. Our predictions validate the experimental method proposed in Ref. [2] to evaluate the concentration of C_{60} molecules inside the tube.

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OR036

Modeling of the influence of thermic treatment upon the mechanical properties of aluminum-copper & aluminum-copper-magnesium alloys

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Abstract

The aluminum possesses the qualities of lightness and resistance, it has also a large recycling capacity. The growing need of the respect for the environment and technological innovations, make aluminum a future metal. It has strong growth potential in the transport equipment, while remaining within a perspective of sustainable development. An important part of research and development focuses on the innovation of the new aluminum alloys. As it is the case with all pure metals, the properties of aluminum are weak. So it is suitable to strengthen them, specially the mechanical ones. Nevertheless, one can significantly improve these characteristics by means of cold hammering, thermic treatment or addition of alloy elements according to the case. Since the range of alloys is very extended, this allows finding that which is more convenient to the use envisaged constraints. Therefore the mechanical properties of aluminum can be modified with the addition of other metals, specially copper and magnesium.

In order to master and improve the quality and properties of the final products, the major industrial challenge lies in the possibility of controlling the morphology, size of microstructures that reside within the molded pieces, as well as their defects; this is the fundamental reason according to which we are more and more interested in mastering the growth and germination of such alloys, as well as the developing structures, at the time of solidification process. The modeling reveals as a valuable aid in the mastery of the formation of such heterogeneousness: segregation cells that are incompatible with industrial requirements.

On the one hand, the whole work focuses upon the modeling of the segregation phenomenon of the Al-Cu alloys, as well as the copper effect upon certain mechanical properties of aluminum, this consists basically of first studying the influence of homogenization, while systematically varying the three parameters: time, temperature and composition, then the influence of each of the copper diffusion according to the distance between the surface and the core of the ingot, on the other hand, The purpose of this work is to model the mechanical properties of Al-Cu-Mg alloys then the influence of magnesium addition upon the cooling process and the various mechanical properties of the aimed alloys. Usually, the microstructure and mechanical behavior of such alloys as Al-Cu, Al-Cu-Mg are directly influenced by some parameters such as composition, cooling velocity and homogenization process.

OR037

Broken-Symmetry Bent-Core Nematic Phases: Predictions and Reality

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Since the pioneering work of R. Meyer [1] on the flexoelectricity, the mesophases of bent-core molecules have attracted attention with their lower symmetry and outstanding polar properties. The discovery of strong polar order and broken chiral symmetry with two-fold degeneration in "banana" smectics [2,3] further enhanced the interest in the low-symmetry bent-core mesophases. Ten years ago, it has been suggested [4] that a similar symmetry breaking might be expected also in the nematic phases of achiral bent-core molecules. Due to the low, or even negative, bend elastic constant of the bent-core nematic, the ground state is no more uniform, as usual, but has a spatially modulated director orientation. Two possible modulated phases have been predicted, either with an oscillating splay-bend (SB) structure, or with twist-bend (TB) conical helix, with two-fold degenerated handedness. Independently, the TB state has been demonstrated [5] by Monte Carlo simulations of a model rigid, V-shaped molecule.
Recently, several experimental studies of achiral bent core mesogens [6-8] and achiral odd liquid crystal dimers [9, 10] reported low-symmetry nematic phases with spontaneous two-fold degenerated chirality. The observed behavior is similar to the one predicted for the spontaneously modulated TB and (in lesser extent) SB phases. However, the unambiguous identification of these phases remains difficult, the observed textures being much more complex than those predicted.
Here we extend the continuum model of ref. [4] to describe the behavior of the broken symmetry bent-core nematics under external "fields": applied a.c. or d.c. electric or magnetic field, surface anchoring in confined geometry, and moderate chiral doping. Analytically, and numerically when needed, we predict the "field"-induced variations of the modulated textures and the shift of the phase transitions between the two spontaneously distorted nematic phases and the uniform nematic. We estimate also the additional elastic energy related to the periodic distortion of the director in the modulated SB and TB phases. Based on our model, we propose simple experiments for the identification of the broken-symmetry bent-core nematic phases. Finally, we show that the strong decrease of the bend elastic constant in the uniform nematic phase before the transition to the TB one, $0<K33<<K22$, could be measured electro-optically in chirally doped bent-core nematic.

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OR038

Magnetoelectric domain control in multiferroic $TbMnO_3$

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The manipulation of domains by external fields in ferroic materials is of major interest for applications. In multiferroics with strongly coupled magnetic and electric order, however, the magnetoelectric coupling on the level of the domains is largely unexplored. We investigated the field-induced domain dynamics of $TbMnO_3$ in the multiferroic ground state and across a first-order spin-flop transition. In spite of the discontinuous nature of this transition, the reorientation of the order parameters is deterministic and preserves the multiferroic domain pattern. Landau-Lifshitz-Gilbert simulations reveal that this behavior is intrinsic. Such magnetoelectric correlations in spin-driven ferroelectrics may lead to domain wall–based nanoelectronics devices.

OR039

Voltage-induced Domain Growth Kinetics in Ferroelectric BST 80/20 Thin Films by Piezoresponse Force Microscopy

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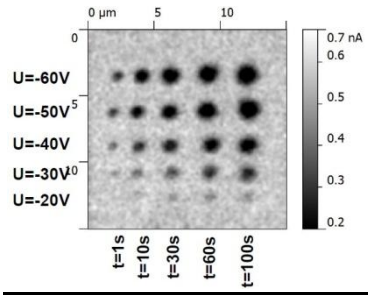
Previous and today's dynamic random access memories (DRAMs) have been advanced by mainly focusing on how to make memory cells small to realize high density DRAMs. The most critical challenges in gigabit density DRAMs are yield loss due to large die size and small feature size, standby current failure caused by large chip size and small data retention times owing to reduced charge packet in the memory cell. In the recent years thin film perovskite materials with high dielectric constant such as PZT, $SrTiO_3$ and $(Ba,Sr)TiO_3$ (BST) have been investigated as dielectric materials for future DRAMs [1].

In this work, we report a voltage-induced domain growth kinetics in ferroelectric BST 80/20 films (thickness 150 nm) fabricated by RF magnetron sputtering measured via piezoresponse force microscopy (PFM) [2,3]. The surface of the sample shows small grains which diameter ranges from 50 nm to 75 nm and roughness is less than 5 nm. Using the PFM mode to detect the out-of-plane polarization, the domain sizes were measured as a function of the applied writing voltage and the pulse time. As example Figure 1 show the result the local polarization effect via PFM. For the investigation of written domains on *as-grown* surface of the BST film the negative voltage pulses were applied to fixed locations within this area, thus we have an array of 23 *stable* domains created by applying voltage pulses of fixed height (V_{tip}=-20 V ÷ -60 V with step 10V) and various durations ranging from 1 to 100 s. The dynamics of domain growth is analyzed experimentally taking into account the strong inhomogeneity of the external electric field in the film.



$BiFeO_3$ codoping with Ba, La and Ti : Magnetic and structural studies

OR040

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Conventional solid state reaction method, from oxides and carbonates, was employed to prepare bismuth (Bi) based multiferroic systems. The pure $BiFeO_3$ (BFO) and codoped with Ba, La and Ti ($Bi_{1-x}Ba_xFe_{1-y}Ti_yO_3$, $Bi_{1-x-z}Ba_xLa_zFe_{1-y}Ti_yO_3$) with x,y,z = 0.1 were prepared stoichiometricaly. The structural and magnetic properties were investigated at room temperature. DRX measurements confirm the obtaining of the rombohedral perovskite structure of the BFO family system. For the undoped system, some reflections of undesired phases are present, while for the doped system only one phase is observed. The magnetic characterization at room temperature revealed remarkable differences between the ceramic samples. The results show that for undoped $BiFeO_3$ system, spontaneous magnetization is not observed at room temperature. Nevertheless, in doped one, a well-defined ferromagnetic behavior is observed at room temperature, possible, due to the suppression of the spatially modulated spin structure of BFO promoted by the reduction of the rhombohedral distortion and the weakening of the Bi-O bonds. The XPS results confirm the presence of oxygen vacancies and the coexistence of Fe^{3+} and Fe^{2+} in all the studied samples. Calorimetric measurements reveal that the dopant incorporation has not a direct effect in Néel temperature but possibly yes in ferroelectric-paraelectric transition.

OR041

History of Data Storage

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Various memory technologies have emerged throughout history. Today, the discovery of new technologies and new materials over the past two decades has helped to manufacture memories devices, less bulky, less expensive, less energy, but always with a larger capacity and higher speed data transfer.
Since the discovery of Vinyl records (1912, 1948 and 1970), data storage has evolved. It exploits progressively all physical properties of materials through Analog magnetic recording tape (1920) to Optical data recording (CD in 1979 by Phillips and Sony, DVD sold in 1983 and 1990), Magnetic hard drives, DD (1945), DRAM (1990) SDRAM (1995), New non-volatile storage, HDD, Flash, USB ... (2000) and Alternative technologies memories (2010), deposition of magnetic elements on strip chart ("magnetic tapes") or substrates (1920).
These technologies having 50 years old used before technologies on the audio market (Philips cassette) or 20 years (before the discovery of CDs) and 20 years in the market for video (VHS). Nowadays, with Magnetoelectric behavior, where variation in the magnetic field (induced current) orients the direction of magnetization and thus leads to write/read data. For magnetic hard drives the speed today reaches 3600 to 10,800 rpm.
New technologies using giant magneto resistance properties (GMR) reach 2TB of memory storage and Resistance switching effect in now also in progress.

Posters

P001

The investigation of pressure effect on the Optical properties, spontaneous polarization and effective mass: Ab initio study

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Optical properties and spontaneous polarization of cubic perovskite $BaHfO_3$ under pressure have been investigated using the Full Potential Linear Augmented Plane Wave (FP-LAPW) method as implemented in the Wien2k code, in connection with the Generalized Gradient Approximation (GGA).
The pressure is among the external factors that can affect physical properties of materials, we will show that the pressure affects the optical properties, more accurately it allows the reduction of band gap, and electronic polarization increases in a linear behavior.
These results confirm that $BaHfO_3$ is a piezoelectric material. Optical absorption and effective mass have been also studied.

Keywords **:** *Perovskite $BaHfO_3$; FP-LAPW; pressure; spontaneous polarization; Optical properties; effective mass*

P002

Lead potassium niobate $Pb_2KNb_5O_{15}$ thin film grown by Pulsed Laser Deposition

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Lead potassium niobate $Pb_2KNb_5O_{15}$ (PKN) was grown on different substrates using a Pt buffer layer. The dependence of the structural and transport properties of the PKN films on the deposition parameters are studied. PKN thin films were characterized by RHEED, X-Ray diffraction, electrical and optical measurements.
The out of plane orientation of PKN film depends on the oxygen pressure during the growth. PKN thin film is oriented [001] for low pressure and is oriented [530] for high pressure.
PKN thin film deposited on MgO substrate was found transparent and its refraction indices comparable to that of PKN single crystal.

Keywords ***:*** *Ferroelectric thin film**,** TTB-structure, PLD, RHEED, linear optical properties.*

P003

Structural, dielectric and impedance study of a new lead free ferroelectric $(Ba,M)(Ti,M')O_3$,M=Ca; Sr and M'=Sn; Zr ceramics

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Key words: Ferroelectric, Phase transition, Impedance, Piezoelectric.

The dielectric properties and microstructure of co-doped B-site and A-site $BaTiO_3$ solid solution of the type $(Ba,M)(Ti,M')O_3$ were investigated. The influence of extremely small amount of Sr, Sn, Zr and Ca dopants on the microstructure and the dielectric characteristics of $BaTiO_3$ were studied systematically. These compositions were designed using the conventional mixed oxide technique and the XRD analysis results indicated that no secondary phase was formed. The microstructure of sintered pellets was studied by SEM at room temperature. The dielectric measurements showed that the BSTZ ceramic present the highest permittivity at 25°C and 100kHz with the value of 2600, whereas the crystallite size was found to approach 32.3 nm. The $BaTiO_3$ ceramic with Sr at A-site has no phase transition above room temperature, while ceramics with Sn at B-site present ferroelectric – paraelectric transition with sharp transition. Finally, the ceramic with Zr at B-site exhibit normal ferroelectric-paraelectric transition with T_c=97°C. The effect of doping was been studied and analyzed using the AC complex impedance spectroscopy technique to obtain the electrical parameters of polycrystalline samples in a wide frequency range at different temperatures. The piezoelectric properties were also studied.

P004

Electric Field Deposition Behavior on Self-Polarization Effect in $LiNbO_3$ Thin Films

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Ferroelectric thin film integration with Si and other integrated device substrates has the potential to enable new modes of photonics integration as well as a new class of high work/volume piezoelectric devices for MEMS integration. Thin films of Lithium Niobate ($LiNbO_3$) posses a number of advantages over bulk material including the possibilities of producing step index profiles, selectively introducing dopants, and the fabrication of multilayer structures. The prospect of producing high quality (oriented and possessing low optical loss) thin films of $LiNbO_3$ on silicon substrates is particularly attractive because the silicon provides a rigid and flat substrate ideal for large area processing of devices by lithographic techniques and it allows for the integration of lithium niobate electro-optic and silicon integrated circuit technology. The studied LiNbO3films were deposited by applying the electric field during radio-frequencies magnetron sputtering of the single-crystalline target in Ar/O=1 atmosphere (0.6 Pa) on Si(110) substrate at 550 ºC. Atomic force microscopy measurements indicate that the surface roughness of the $LiNbO_3$ thin films was 4-10 nm, which meets the demands for practical waveguiding devices. The ferroelectric properties have been studied by visualization of the as-growth domain structure, recording induced ferroelectric states by piezoresponse force microscopy (PFM) using Scanning probe laboratory NTEGRA-Prima (NT-MDT, Russia). The asymmetry of the distribution of vertical PFM (VPFM) signal is a manifestation of the so-called self-polarization effect. The maximum of the VPFM histogram of this distribution is shifted toward negative (or positive) values of the piezoelectric response, which implies that the polarization vector in most grains is directed toward the upper (or lower) interface. In work discusses the possible mechanisms of the origin a self-polarization in $LiNbO_3$ thin films.

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P005

Dielectric measurements and Impedance spectroscopy studies of Ba_{2-x} Sr_x $CoWO_6$ (0 < x < 0.1)

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The double perovskite oxides with general formula Ba_{2-x} Sr_x $CoWO_6$ (0 < x < 0.1) show a large variety of physical and chemical properties, such as superconductivity, ferroelectricity, antiferroelectricity, piezoelectricity, various optical and magnetic properties or a combination of magnetic and electric interactions. Using X-ray diffraction and dielectric measurements, the results showed that Co containing compounds crystallize in a cubic system with the space group Fm-3 m. The dielectric permittivity and the loss tangent have been measured in a frequency range of 10Hz–1MH and in a temperatures range of 25–550◦C. The diffuse character of ferroelectric phase transition is well described by Santos-Eiras phenomenological model. Space-charge polarization, relaxation phenomena and free charges conductivity have been analyzed using dielectric and impedance spectroscopy. In paraelectric phase the Arrhenius activation energies were determined. Frequency dependence of ac conductivity at different temperatures obeys the Jonscher's universal law :
$\sigma_{ac} = \sigma_{dc} + A(\omega)^n$.

Keywords:
Double perovskites, Ferroelectrics, dielectric spectroscopy, Santos-Eiras model, impedance spectroscopy, Conductivity.

P006

Correlation between ferroelectrics and electrocaloric properties in $BaGe_xTi_{1-x}O_3$ ceramics, using direct and indirect methods

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Ferroelectric materials are of interest in various electronics applications, especially as cooler materials. The electrocaloric effect (ECE) was investigated in ferroelectric lead-free Ge doped $BaTiO_3$ ceramics. Direct measurements using high resolution calorimetry were compared to the two indirect measurements using the Maxwell relationship. In a first well-known indirect method, P-E hysteresis loops were measured in a wide temperature range and pyroelectric coefficient and thus the electrocaloric responsivity were determined by derivation of $P(T, E)$ data. In second method the electrocaloric responsivity was determined by direct measurements. Good agreement was obtained between different methods and large electrocaloric responsivity was found for some critical compositions around the dielectric maximum.

Keywords*:* Ferroelectrics, lead-free ceramics, electrocaloric, pyroelectric

P007

The hysteresis behavior of a ferroelectric or ferrielectric nanowire with core shell morphology

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By using the Quantum Monte Carlo simulation, the electric properties of a nanowire, consisting of a ferroelectric core of spin-1/2 surrounded by a ferroelectric shell of spin-1/2 with ferro- or anti-ferroelectric interfacial coupling, have been studied within the framework of the Transverse Ising Model (TIM). We have examined the effects of the shell coupling Js, the interfacial coupling JInt, the transverse field Ω, and the temperature T on the hysteresis behavior and on the electric properties of the system. The remanent polarization and the coercive field as a function of the transverse field and the temperature are examined. A number of characteristic behaviors have been found such as the appearance of triple hysteresis loops for appropriate values of the system parameters.

Keywords: Ferroelectrics; Transverse Ising model; Quantum Monte Carlo simulation; Hysteresis loop

P008

Dielectric and structural analysis of three-layered ferroelectric perovskites

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The Aurivillius systems with high Curie temperature or fatigue-free are possible candidates for applications in high temperature piezoelectric devices or non-volatile ferroelectric random access memories. The structure of these materials is represented by the equation $A_{m-1}Bi_2B_mO_{3m+3}$ where *m* is the number of perovskite blocks between $[Bi_2O_2]^{2+}$ layers. The $SrBaBi_2Nb_2TiO_{12}$ ferroelectric material belongs to the Aurivillius family with *m*=3. A previous structural study on this system, by using X-ray diffraction, has showed a tetragonal structure with space group *I4/mmm* at room temperature [1]. A cation sites mixing have been reported between *A* sites and bismuth sites into the $[Bi_2O_2]^{2+}$ layered structure [1]. The present work shows the dielectrics analysis for this material in a wide range of frequencies and temperature. Two anomalies (or peaks) are observed in the temperature dependence for the real dielectric permittivity, one near room temperature and the other one at high temperature. By using X-ray diffraction and Raman spectroscopy, in a wide temperature range, both anomalies are studied in order to evaluate phase transitions or another cause for the observed behavior, especially at room temperature.

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P009

Frequency response of interface states and series resistance in PolySi-oxide-cSi and PolySi-cSi structures

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The capacitance-voltage (C-V) and conductance-voltage (G/ω-V) characteristics of PolySi-oxide-Silicon (MOS) and PolySi-Silicon (MS) structures have been measured in the voltage range from -30 to +30 V and frequency range from 10 KHz to 1MHz. It is found that both the capacitance and conductance of the PolySi-oxide-Silicon (MOS) and PolySi-Silicon (MS) capacitors are very sensitive to frequency. The fairly large frequency dispersion C-V characteristic can be interpreted in terms particular distribution of interface states at Si/SiO_2 interface and the effect of series resistance. At relatively low frequencies, the interface states can follow an alternating current (AC) signal that contributes to excess capacitance.

P010

Study of aluminum oxide doped with terbium at different concentrations.

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Different emission intensities that occur in aluminum oxide powders correspond to different doping terbium concentrations, such sample powders were synthesized via evaporation technique. These were characterized using luminescence techniques, x-ray diffraction and Energy Dispersive Spectroscopy (EDS). The emission spectra for each of the distinct terbium doping percentages show terbium's typical transitions in 494, 543, 587 and 622nm, these correspond to $^5D_4 \rightarrow {}^7F_6$, $^5D_4 \rightarrow {}^7F_5$, $^5D_4 \rightarrow {}^7F_4$ and $^5D_4 \rightarrow {}^7F_3$, respectively. Such powders were excited at room temperature at λ = 380nm . X-ray diffraction results show the presence of both γ-400 phase and γ-440 phase at 45.90 degrees and 67.38 degrees for the two hour thermally treated compounds. EDS analyses indicate 60% of oxygen and 40% of aluminum with presence of terbium doping in the compound.

P011

Cartographiques et Minéralogiques d'une déformation polyphasée dans le massif de Znaga (Anti-Atlas Central)

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Le massif éburnéen de Zénaga dans l'Anti-Atlas central présente une déformation polyphasée. Cette étude a été faite à la suite des dernières données tectoniques et géochronologiques obtenues dans la boutonnière de Bou Azzer (D'Lemos et al. 2006, Admou et al. 2013, Soulaimani et al. 2013). Elle a pour but de faire une comparaison structurale entre la déformation dans ce massif et celle décrites dans la boutonnière.

Cette étude nous permis la réalisation d'une carte géologique et définir les ensembles géologiques de la partie nord du massif et de réaliser une étude structurale et microstructurale nous permettant de conclure aux points suivants :

1- Présence de deux ensembles : des granites orthogneisifiés et mylonitisés encaissés dans un complexe métamorphique formé de micaschistes et de migmatites renfermant des métabasites amphibolites et un réseau d'injection basques précoces et tardifs sur la foliation ;

2- Les granites sont de deux types : orthogneiss d'Azguemerzi (migmatitique) et des leucogranites de Tazenakht (alcalins) intrusifs dans les premiers. Ces deux types sont tous affectés par l'orthognessification et la mylonitisation (Ennih 2000, Saidi et al.2000) ;

3- L'étude structurale nous a permis de distinguer deux blocs structuralement différents :

- le bloc sud ou bloc d'Azguemerzi, caractérisé par une déformation ductile (orthogneissification et mylonitisation) orientée NE-SW (N60-N80) à composante dextre et dextre normale dominante. C'est la phase1 éburnéenne. Cette phase pourrait être associée au doming gneissique ;
- Le bloc de Taloust caractérisé par une déformation polyphasée bien visible : une phase 1 de déformation marquée par des structures orientées NE-SW et une autre phase 2 caractérisée par des structures orientées NW-SE (N120). Cette dernière a les mêmes orientations que la phase panafricaine B1. La limite entre ces deux blocs est dessinée par le cisaillement senestre ductile de Taloust.

Le déversement des structures dans la zone d'étude est globalement vers le NW, ce qui indique que lors de la collision des différents compartiments (croute éburnéenne et arcs panafricains), les déversement vers le SW connus dans la boutonnière de Bou Azzer se sont transformés en rétrochevauchements et en inversions structurales vers le nord ?.

En conclusion, la structuration du bloc de Azguemerzi est semblable à celle décrite dans la fenêtre de Tazigzaout, mais la nature des formations métamorphiques (présence de migmatites et de granites) et la datation à 2043 Ma obtenue par Thomas et al. (2002) rattachent ce bloc l'éburnéen !. Le bloc de Taloust pourrait être un bloc d'âge tonien à cryogénien inférieur fortement remobilisé et restructuré au panafricain au cours de la phase majeure panafricaine datée à 650 Ma ?!. Cette étude est préliminaire, elle devrait être appuyée par des datations géochronologiques.

Mots clés : Anti-Atlas central, Zenaga, Eburnéen, Panafricain, Mylonitisation, déformation polyphasée.

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P012

Effect of substrate on structural properties of aln thin films

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Keywords: AlN thin film, Magnetron sputtering, interface AlN/Si, XRD, HRTEM

This work investigates the growth mechanism and the crystallinity of AlN films elaborated by DC reactive magnetron sputtering at room temperature on different substrates (Al2O3, ZnO, AlGaN). Thanks to XRD, HRTEM and SAED studies a comparison has been made between each of these AlN films and AlN films deposited on Si(100) where we noticed at the AlN/Si interface a 3nm thick amorphous layer followed by a polycrystalline AlN layer, exhibiting crystallites mostly (100) oriented with few ones (002) oriented and a grain size of about 8nm.
The use of appropriate substrates such as Al2O3, ZnO or AlGaN showed that for the first two there was no significant improvement in the crystalline quality due to the amorphization of the layer due in particular to the presence of oxygen at the interface. In the other side, because of its lower sensitivity to oxygen and ion bombardment the substrate AlGaN proved to be favorable to epitaxial growth of aluminum nitride prepared by reactive magnetron sputtering at low temperatures. An AlN single crystal film of 800 nm was obtained on AlGaN substrate.

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P013

Impact of c-Si Substrate and front surface passivation on interdigitated back contact silicon heterojunction solar cell with 2D simulation study

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Abstract— This paper shows the interdigitated back contact heterojunction solar cell design that employed the advantage of amorphous/crystalline silicon technology. The front surface is passivated by a double layer of FSF doped (n++) crystalline silicon and silicon nitride, which also provides an anti-reflection coating. In the rear side the emitter and the back contact are formed by amorphous/crystalline silicon heterostructure and fabricate the rear junction of the cell. To achieve accurate IBC–SiHJ modeling, we use ATLAS 2-D device simulation software. We here focus on IBC–SiHJ structure on n-type c-Si simulations varying the values of the following parameters: bulk lifetime, surface recombination velocity at both front and back surfaces, bulk thickness for verified the influence of the substrate quality. The influence of these parameters has been tested by generating the current–voltage (I–V). We conclude that the solution to achieve high efficiency (21.47%) is a high crystalline substrate quality, low surface recombination velocity especially at the front surface.

Keywords: heterojunction; solar cell; amorphous silicon; crystalline silicon; interdigitated back contacts silicon heterojunction.

P014

The convergence of technologies, generates convergence in the regulations

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The convergence of nanotechnologies generates synergies among different technologies to say, nanotechnologies, neurotechnology, computers and biotechnology, these technologies must converge in their regulations, the application of medical devices in nanotechnologies should lead us to a link between the technical committee TC 210 and ISO technical committee 229 link that does not exist in our work in this moment. In this do an analysis of the management of risk from an optical NC-ISO 14971. Studying the global trend in this respect as imported for manufacturers medical Devices worldwide.

P015

Experimental study of one dimensional photonic crystal based on a mixture of (HMDSO / O2) deposed by PECVD

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Abstract

Over the last years, photonic band gap materials, also called photonic crystals, have been studied intensively and have received increasing demands from the scientific community due to their strong ability of manipulating and controlling photons. The photonic crystals are materials with a periodic distribution of the refractive index. The existence of a photonic band gap in these structures can prevent the propagation of light.

In this work we have elaborated a one-dimensional photonic crystal coated from a mixture of an organic composed the hexamethyldisiloxane (HMDSO) and oxygen (O_2), Our object is to obtain two layers B_1 and B_2 with two different refractive index from the same composed HMDSO, by varying the flow of HMDSO and the deposition time for each layer. In this study, PECVD technique has been used to produce an alternating layer of B_1 / B_2 which is our one-dimensional photonic crystal. After the optimization the thickness of each layer to obtain a good transmission, we studied the effect of the layers numbers of the photonic crystal on the spectra of transmissions and reflections. We have shown that a good band gap appears after 26 layers with a pseudo band gap 3.8ev. We have also introduced a defect in the structure by changing the thickness of one B_2 layer in the structure, we observed a frequency mode corresponding to this defect. We reproduced theoretically the spectra of transmissions and reflections that are in a good agreement with experimental results.

P016

Homogeneous switching mechanism in pure polyvinylidene fluoride ultrathin films

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Polarization switching kinetics is one of the key issues for future development of nanoelectronic devices based on ferroelectrics. Up to now, such kinetics still remains poorly studied despite its crucial impact on the device performances. Here, the switching mechanism in 11-nm-thick ferroelectric films of pure homopolymer of polyvinylidene fluoride is investigated. While the usual mechanism involves nucleation and growth of domains, a homogeneous ferroelectric switching is evidenced in such ultrathin films. Indeed, the dependence of the switching rate on applied voltage reveals a critical behavior with the existence of a true threshold field (of ∼0.26 GV/m) which is required to overcome the energy barrier to reverse the whole polarization homogeneously as suggested by Landau-Ginzburg mean-field theory. Such finding not only supports few previous works but also raises the question on the general aspect of such homogeneous mechanism that might exist in any other nanoscale ferroelectric materials.

P017

Phosphate sludge: analyze and physico-chemical characterization

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Morocco possesses around three-quarters of the world's phosphate reserves and is the third largest producer of phosphate (Benkhadra and El Abbaoui, 2008). During ore phosphate beneficiation, fluorapatite is separated from associated gangue minerals by a combination of various mineral processing units involving crushing and screening, washing, and/or flotation. These operations generate large volume of waste, which is stockpiled in tailings ponds (phosphate sludge ponds). For instance, in 2010, the amount of sludge was about 28.1 million metric tons. The growing dumped waste constitutes potential source of pollution, reduces arable lands and disfigures the landscape.

This sludge is removed by pumping to the spreading basin, near the laundry, which allows their storage.They are likely to bring undesirable elements, such as heavy metals(U, Cd, As, V, Cr, Zn, Cu, Ni ...),and organic pollutants and pathogens which must control the flow to ensure safety with respect to the environment.

Heavy metals can enter the food chain through the consumption of food and therefore are of concern regarding the potential impact on human health.Therefore a number of countries around the world have introduced standards for the maximum allowable concentration of heavy metals in sewage sludge for use in agriculture.

As currently there is no commercial means to eliminate these pollutants, their concentration in the sludge is critical regarding the possibilities for reuse.

In view of the huge amount of sludge generated by the OCP and to ensure the safety with respect to the environment,we proposed to develop this research with many industrial applications.

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P018

Possible onset of mesoscopic ferrielectricity in dechiralization lines dynamics of a pure Ferroelectric Liquid Crystal in confined geometry.

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Abstract

The influence of the electric bias field on SmC* phase of a new ferroelectric liquid crystal having large spontaneous polarization (120 nC/cm² at 110 Hz), short pitch and high purity, is studied in the frequency range 5 Hz - 1 MHz using a 7 microns thick cell in a planar alignment. Dielectric permittivity, polarization and optical measurements (dechiralization lines) have been investigated and shown a complex ferroelectric behavior. The density of the dechiralization lines are optically observed in accordance with dielectric response. Although these experiments exhibit Goldstone and Soft mode relaxations far from the SmC*- SmA phase transition, one can show dielectric and optic anomalies suggesting a possible onset of ferrielectric (f) ordering within the surface lattice of dechiralisation lines which we describe by phenomenological theory using a non-conventional Landau approach. This last has also the advantage to account for to the spectroscopic measurements.

P019

Magnetic characterization and superconducting properties of Nb_3Al by combustion synthesis

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In This paper, the synthesis of superconductive intermetallic compound, of crystallographic structure of type A15 (Nb_3Al) presenting a critical temperature of 18°K .we reported by using SHS (Self-propagating high-temperature synthesis) and electrothermal explosion (ETE) initiated by the heavy current (400 A), the obtained samples were characterized of the phase composition by the diffraction technique of the X-rays. Further studies have been carried out by scanning electron microscopy (SEM) and optical microscopy. Finally, the Magnetic properties were also investigated, for combution processers the magnetic behavior slightly softened becoming a semihard ferromagnetic.

Keywords: Thermal explosion, SHS, Nb_3Al intermetallic, superconductivity, magnetic.

P020

Fokker-Planck dynamic in a periodic Remoissenet-Peyrard potential

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In this work we present a study of diffusion mechanism of Brownian particle submerged in a symmetric periodic Remoissent-Peyrard potential which can represent the potential of a deformable substrate with deformability parameter S. Through this potential ions considered as Brownian particles can diffuse. This system is described by the Fokker-Planck Equation (FPE). We solve numerically (FPE) using the Method of Continuous Fraction Matrix (MCFM) to calculate the dynamic structure factor S(q,w). From S(q,w) some relevant correlations function are calculated. In particular, the half-line width $\lambda(q)$ of the peak of the quasi-elastic dynamic structure factor s(q,w) and the diffusion coefficient D(q). The results obtained in regime strong friction, and low temperature shows that the deformation of the substrate (S>0) involving potentials well-off (fig-1), leads to a diffusion mechanism described by a simple jump diffusion process with jump length close to lattice constant **a**. and the deformation of the substrate (S<0) involving potentials with wider wells (fig-2), leads to a dynamic of ions described by jump diffusion model with jump length close to constant **a** and also by liquid-like motion inside the unit cell.

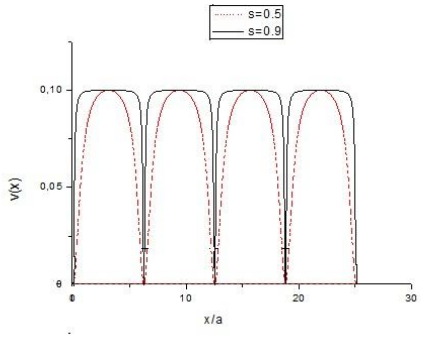

Figure 1: Representation of the potential of some positive values of the deformability parameter S.

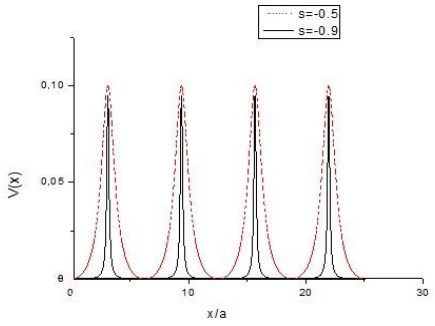

Figure 2: Representation of the potential of some negative values of the deformability parameter S.

P021

Magnetic and Electro Paramagnetic Resonance of Mn^{2+} and Gd^{3+} within the system $K_3Sr_2LnNb_{10}O_{30}$ (Ln = La, Gd).

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The present work reports on the effects of Mn^{2+} and Gd^{3+} substitution on the magnetic behaviour of polycrystalline tungsten bronze structure $K_3Sr_2LnNb_{10}O_{30}$ ceramics (Ln = La, Gd). Structures were found to crystallize with the tetragonal tungsten bronze structural type. Dielectric study carried out on the prepared ceramics has permitted to determine the temperature of phase transitions (Tc). Magnetic investigation and Electro Paramagnetic Resonance (EPR) studies have been conducted using manganese (II) and Gadolinium (III). Systematic EPR investigations were carried out versus temperature for the prepared samples. The recorded features are similar to those generally observed for disorder structures. The plot of total intensity versus temperature shows a sharp maximum at T_c, which is considered as a revelation of a phase transition.

P022

Theoretical study of the structural and optoelectronic properties of $NaXF_3$ (X =Ca, Sr)

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We present ab initio theoretical study of the structural, electronic and optical properties for fluoroperovskite $NaXF_3$ (X= Ca and Sr) compounds using full potential linearized augmented plane wave method (FP-LAPW) as implemented in Wien2k code. We employed the generalized gradient approximation (GGA) and the local density approximation (LDA) as exchange–correlation potential. We have calculated structural properties (the equilibrium lattice constant, the bulk modulus and its pressure derivative) and they are in good agreement with the available data. The calculations of the electronic band structures show that $NaCaF_3$ has an indirect bandgap, whereas $NaSrF_3$ has a direct bandgap. The contribution of the different bands was analyzed from total and partial density of states curves. We have presented the assignment of the different optical transitions existing in $NaCaF_3$ and $NaSrF_3$ compounds from the imaginary part of the dielectric function spectra with respect to their correspondence in the electronic band.

Key words: DFT, Ab-initio, Fluoroperovskite, Electronic structure, Optical properties.

P023

The magnetic properties of a nanoparticle with core/shell structure and disordered interface

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The phases diagrams and the magnetic properties of a spherical ferrimagnetic nanoparticle, consisting of a ferromagnetic core of spin-1/2 *A* atoms, a ferromagnetic shell of spin-1/2 *B* atoms, and a disordered interface in between which is characterized by a random arrangement of *A* and *B* atoms of A_pB_{1-p} type and a negative *A*-*B* coupling, are examined. The Monte Carlo simulation technique based on Metropolis algorithm has been used to study the effects of the concentration parameter p, the coupling between *B*-*B* atoms J_B, and the antiferromagnetic interface coupling J_{AB} on both critical and compensation temperatures. It is found that all the compensation temperature curves emerge from a critical concentration parameter p_c at T=0. On the other hand, the variation of the compensation temperature is very influenced by the variation of J_B and p. It is also found that three compensation points can appear for appropriate values of the system parameters. The compensation points of ferrimagnetic materials have potential use in magnetic recording materials.

P024

Ab-initio study of the mechanicaland thermal properties of the cubic $CsBeF_3$

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Abstract

We have investigated the structural, mechanical and thermal properties of a compound perovskite $CsBeF_3$ using the full-potential linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT) [1]. In this approach, both the local density approximation (LDA)[2] and the generalized gradient approximation (GGA)[3] were used for exchange-correlation potential calculation. The ground state properties such as lattice parameter, bulk modulus and its pressure derivative were calculated and the results are compared whit theoretical data. The elastic properties such as elastic constants, anisotropy factor, shear modulus, Young's modulus and Poisson's ratio are obtained for the first time.The thermal effect on the volume, bulk modulus, heat capacities C_V and Debye temperature was predicted using the quasi-harmonic Debye model, in which the lattice vibrations are taken into account.

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P025

Phase diagrams and magnetic properties of the transvers ising thin film

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Using the Monte Carlo simulation based on the Trotter-Suzuki formula, we examine the phase transitions of a transverse spin-1/2 Ising film. The critical transverse field of the film as a function of the exchange interactions, temperature, and film thickness are studied. We show that the critical transverse field is independent of the exchange interaction between the surface and the bulk (R1) when the surface coupling (Rs) is null. We also found that there are critical values of R1 and Rs, below which the critical transverse field remains constant and then increases. We also examine the hysteresis behavior and the coercive field.

Keywords: Transverse Ising film, Monte carlo Simulation, critical tranverse field, magnetic properties.
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P026

Vibrational properties of Single-Wall Boron nitride nanotubes inside Carbon nanotubes

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Carbon and boron nitride nanostructures are of considerable interest to researchers from many scientific areas due to their unique vibrational, electronic and mechanical properties. Recently, the synthesis of single-wall boron nitride nanotubes (SBNNTs) inside single-wall carbon nanotubes (SCNTs) have been reported [1].
The spectral moment's method [2] was shown to be a powerful tool for determining vibrational spectra (infrared absorption, Raman scattering and inelastic neutron-scattering spectra) of harmonic systems. This method can be applied to very large systems, whatever the type of atomic forces, the spatial dimension, and structure of the material. The calculations of vibrational properties of SBNNT inside SCNT (SBNNT@SCNT) are performed in the framework of the spectral moments method, using a classical force field. A Lennard–Jones potential is used to describe the van der Waals interactions between the inner and outer tubes.
We present the calculation results of the SBNNT@SCNT polarized infrared and Raman spectra as a function of the diameter and chirality of the inner and outer tubes. The diameter dependence of the wave number of the breathing-like modes, intermediate-like modes and tangential-like modes is derived. These predictions are useful to interpret the experimental data.

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P027

Lead-free ferroelectrics materials for electrical energy storage in capacitors

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Energy is the driving force of social development and all the human activities are based on energy, so energy consumption is the premise for social development. Life level is directly related to the energy consumption, and the increasing of comfortable life will need consume much energy. Energy is always insufficiency for people. How to make a good use of the limited energy has been subject discussed by people and attracted wide attention around the world recently. According to studies, the energy utilization rate is not high, as well as the capacity of energy storage materials is low. So it is necessary for human to find a way to improve energy utilization as far as possible. To develop high performance energy storage capacitor is one significant aspect of new energy resource exploiting. The function of capacitors is storing energy when the energy is sufficient and releasing the stored energy to use when energy is insufficient. At present, the batteries are the main equipment to store electric power, but due to the inherent deficiency of electrochemical cell, such as slow charging and discharging speed, high energy consummation, and potential safety problem and so on restrict the application of batteries in high power machinery such as electric vehicles. The capacitors with special physical storage mechanism has great advantage over the batteries for following advantages: not containing harmful metals (such as lead, etc.) will do not cause secondary pollution to the environment, much more charge and discharge cycle times, rapid charge and discharge speed, no change of form of energy during the charge and discharge process, being independent on the ambient temperature [1]. The BaTiO3 material has good dielectric properties, which make it the most used base material to elaborate high dielectric permittivity capacitors [2]. However, the variations of its dielectric permittivity with temperature are too important for a practical application. One can then carry out phases mixing to obtain a high dielectric permittivity, low losses and a Curie temperature within a range of use temperatures, typically from -25°C to 75°C. In particular, substitutions in the BaTiO3 perovskite cell can modify this material's dielectric characteristics in favour of the stability properties sought. The ceramic samples we have elaborated are based on classic ferroelectric materials such as BaTiO3, Ba1-xSrxTiO3, Ba1-xCaxTiO3 and Sr1-xCaxTiO3 and relaxors such as BaZrxTi1-xO3. Ceramics samples with 6 mm of diameter and 1 mm of thickness were prepared by the conventional solid-state reaction method [3]. The temperature and frequency dependence of the dielectric permittivity and loss-tangent of the samples were investigated from 100 K to 800 K and from 100 Hz to 1 MHz. Keywords: Lead-free materials, Capacitor, Ferroelectric, Relaxor.

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P028

Structural characterisation of ZnO/ Bi2O3 heterojunction prepared by solid state reaction at room temperature

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Two nanomaterials systems were developed. The first is composed of the bismuth oxide doped with cerium oxide, Bi2O3-CeO2 (SAN) and the second one is zinc oxide compound doped with bismuth oxide, ZnO-Bi2O3 (SWAN). Doping is used to increase the number of charge carriers and thereby optimizing the conductivity of these nanomaterials. The two material systems are developed with different experimental protocols: SAN is prepared by co-precipitation and SWAN, by solid state reaction.
We found through scanning electron microscopy, a very interesting architecturation to bismuth oxide coupled to ceria. Indeed, the compounds are grouped into rods which, in their rotation, are stacked to form pyramids. Architecturation in these systems is our new knowledge, which leads us to know more, control and see which parameters are predominant.
In addition, the SWAN system have a very promising architecturation for hetero-junction applications because, with a well-defined experimental protocol, its architecturation like leaflets with spikes and self-assembly can be used to create a junction with another semiconductor. This part of research has also helped us to confirm the nanometer grain size in both material systems. X-ray diffraction showed that the obtained powders are crystallized. The δ-Bi2O3 phase was obtained and stabilized at low temperature and the β-Bi2O3 phase was also stabilized instead of a metastable phase.

P029

Indirect and direct electrocaloric measurements in lead free BCZT ceramics

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Electrocaloric effect in lead-free $Ba_{0.95}Ca_{0.05}(Zr_{0.1}Ti_{0.9})O_3$ ceramic has been investigated by using two indirect methods. In the first classic approach, the electrocaloric temperature change (ΔT) was calculated from the Maxwell relation based on measured *P–E* hysteresis loops recorded at different temperatures. In the second approach, the ΔT was calculated from the Maxwell relation based on pyroelectric current measurements. The advantage of such approach is that it enables direct determination of the pyroelectric coefficient, which should be otherwise calculated from the hysteresis loops in the classic approach. Good agreement between methods was found near the cubic-to-tetragonal phase transition temperature with a significant electrocaloric responsivity of 0.30 K.mm/kV obtained by direct method.

Keywords: BCZT ceramics, electrocaloric effect, ferroelectric, pyroelectric.

P030

Study of Aluminum Oxide doped with at Different Concentrations

Sergio Humberto Ramirez Ramirez, Carlos Miguel Garcia Rosas and *Luis Mariscal Becerra*

Abstract

Different emission intensities that occur in aluminum oxide powders correspond to different doping concentrations of terbium, such sample powders were synthesized via evaporation technique. These were characterized using , x-ray diffraction and Energy dispersive spectroscopy (EDS). The emission spectra for each of the distinct terbium doping percentages show terbium's typical transitions in 494, 543, 587 and 622nm, these correspond to 5D4→7F6, 5D4→7F5, 5D4→7F4 y 5D4→7F3, .

When excited at room temperature at λ = 380nm. X-ray diffraction results show the presence of γ-400 phase and γ-440 phase at 45.90 degrees and 67.38 degrees for the two hour terminally treated compounds. indicate 60% of oxygen and 40% of aluminum with presence of terbium doping in the compound.

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