International Workshop on Applied Materials for Science and Technology

Abstract Book

ISSN: 2462-9618 (En línea)

1st Edition, April 8-9, 2015, Barranquilla-Colombia

Universidad del Atlántico

Topics

- Synthesis and processing
- Characterization of Materials
- Magnetic Materials
- New Materials
- Thin film and Nanomaterials
- Modeling and Simulation
- Renewable Energy

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- CNR-IOM SLACS Cagliari, ITALY
- Université de Versailles St Quentin en Yvelines, FRANCE
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Content

Acknowledgements

The *Grupo de Física de Materiales (GFM)* and *Coordinación de los Programas de Ciencias Físicas* gratefully acknowledge to the *Rectoría Universidad del Atlántico* and the *Vicerrectoria de Investigación, Proyección social y Extención* for the financial support of this international event. In addition, we acknowledge especially to the international and national speakers for your participation.

Furthermore, the organizing committee acknowledge to the *Vicerrectoría de Bienestar Universitario*, the *Facultad de Bellas Artes*, the *Centro de Bienes y Suministros*, *Departamento de Servicios Generales* and the *Centro de Deportes* for your important collaboration.

General program

Wednesday 4/8/2015	
7:30–8:15	**Welcome Reception and Registration**
	Session I. (Centro de Convenciones Room)
8:30–10.30	Talks (International and national invited speakers)
10:30–11:00	**Coffee-break**
11:00–11:40	Welcome Speech
12:00–14:00	**Lunch**
	Session II. (Centro de Convenciones Room)
14:00–16:30	Talks
16.40–17:00	**Coffee-break / Artistic show**
Thursday 4/9/2015	
	Session III. (Centro de Convenciones Room)
8:30–1:30	Talks (International and national invited speakers)
10:30–11:00	**Coffee-break**
11:00–11:40	Talks
12:00–14:00	**Lunch**
	Session IV. (Centro de Convenciones Room)
14:00–15:30	Talks
15:30–16:00	Summary and Conclusions
16:00–17:00	**Poster Session**
17:30	**Cocktail / Artistic show**

Talks program

Session I. (Centro de Convenciones Room) Session Chair: Dra. Nathalie Montenegro	
Talk 1. 8:30-9:10	*MOCVD growth, dopin, and characterization of ZnO nanowires* Dr. Vincent Sallet – GEMAC CNRS – Université de Versailles, France
Talk 2. 9:10–9:50	*Magnetic and electrical properties on hybrid multiferroic bilayers deposited by sputtering technique at high oxygen pressures* Dra. Maria Elena Gomez de Pietro – G. Películas Delgadas – Universidad del Valle, Colombia
Talk 3. 9:50–10:30	*Ventajas del álgebra geométrica para aprender la Física* Dr. Philippe Eenens– Universidad de Guanajuato, Mexico

Session II. (Centro de Convenciones Room) Session Chair: Dr. Julio Trochez	
Talk 4. 14:00-14:30	*Synthesis and characterization of photoactive materials for medical and environmental applications* Dr. Carlos Diaz – GIFOQ – Universidad del Atlántico, Colombia
Talk 5. 14:30-15:00	*Raman spectroscopy for materials characterization* Dra. Margarita Correa – GFM – Universidad del Atlántico, Colombia
Talk 6. 15:00-15:30	*On the $CsHSeO_4$ high-ionic conductivity nature above 128 °C: a new interpretation* Dr. Ever Ortiz – GFM – Universidad del Atlántico, Colombia
Talk 7. 15:30-16:30	*A.C magnetic susceptibility and magnetization of amorphous alloy Composition of $Fe_{37}Co_{35}Nb_6B_{11}Si_{10}Cu_1$* Mr. Amilcar Orozco – CyCAM – Universidad del Atlántico, Colombia
Talk 8. 16:00-16:30	*Structural optimization of atomic systems with few degrees of freedom* Mrs. Beatriz Cogollo – Universidad de Cartagena, Colombia

Session III. (Centro de Convenciones Room) Session Chair: Dra. Margarita Correa

Talk 9.	*Modeling hybrid nanomaterials for photovoltaics*
8:30–9:10	Dr. Alessandro Mattoni – CNR-IOM SLACS Cagliari, Italy
Talk 10.	*Nanocristallization process of $Fe_{37}Co_{35}Nb_6B_{11}Si_{10}Cu_1$ alloy*
9:10-9:50	Dra. Zulia Caamaño – CyCAM – Universidad del Atlántico-Colombia
Talk 11.	*Modeling of materials under extreme conditions*
9:50-10:30	Dr. Javier Montoya - Universidad de Cartagena-Colombia
Talk 12. 11:00-11:40	*Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics* Dr. Carlos Pinilla – Universidad del Norte-Colombia
11:40-12:20	*Thermal and Electric Behavior of $Cs_3(HSO_4)_2(H_2PO_4)$ at temperatures above 300 K* MSc. Ismael Piñeres – GFM – Universidad del Atlántico-Colombia

Session IV. (Centro de Convenciones Room)

Sesión Chair: Dr. Ever Ortiz

Talk 13.	*Heusler Alloys: tunable multifunctional materials*
14:00–15:30	Dr. Julio Trochez -Universidad del Atlántico-Colombia
Talk 14. 14:30-15:00	*Secondary Ion Mass Spectrometry (SIMS) study of Metal Organic Chemical Vapour Deposition (MOCVD) semiconductors III-V hyperstructures* Dra. Diana Padilla – GEOEL – Universidad del Atlántico-Colombia
Talk 15.	*Buffer layers based on In and Zn to Thin Films Solar Cells*
15:00-15:30	Dr. William Vallejo – GIFOQ – Universidad del Atlántico-Colombia
Talk 16. 15:30- 16:30	*Growth and characterization of nanostructured multiferroic heterostructures by pulsed laser deposition technique* MSc. E. Linares – GFM – Universidad del Atlántico-Colombia

Poster Session. (Centro de Convenciones Room)

16:00-17:00

Síntesis y caracterización morfológica y estructural de $Fe_{65}Co_{35}$

Karla Echeverría – CyCAM – Universidad del Atlántico-Colombia

Estudio del comportamiento magnético y estructural del polvo nanoestructurado $Fe_{50}Co_{50}$ preparado por aleado mecánico

Jairo Orozco – CyCAM – Universidad del Atlántico-Colombia

Modelado del tamaño de partícula de nanopolvos de FeCo sintetizados por el método de aleado mecánico

Kevin García – CyCAM – Universidad del Atlántico-Colombia

Estudio de la devolatización termica y evaluación cinetica de la pirolisis del ceroxylon quindivense por medio de balanza termogravimetrica acoplada a un espectrometro de masas TG/MS

Cindy Ariza Barraza – GFM – Universidad del Atlántico-Colombia

Talks Session

Talk 1. MOCVD growth, doping, and characterization of ZnO nanowires

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Abstract. Semiconductor nanowires (SC-NWs) open new fields of investigation in fundamental physics, and offer unique opportunities for the future generation of electronics, photonics, sensors, actuators, energy, and medical applications. During the last decade, improvements in crystal growth and characterization at the nanometer scale made it possible to confront experimental observations and theoretical models. Today, an ensemble of advanced nano-characterization tools allows us to address the issues related to SC-NWs doping. A main ambition is to yield a clear understanding of the complex relations between doping, size reduction, surface effects and transport properties, in the light of structural, optical and electrical investigations at the nanoscale. Since p-type doping is still a debated issue for zinc oxide (ZnO), nanowire of this material has been taken as a "case study", in order to address some of the main issues that concern SC-NWs transport properties. In particular, we wanted to open the question whether size reduction (turning from a thin film to a nanowire) could make it easier to dope ZnO p-type.

In the presented work, ZnO nanowires have been grown by metalorganic chemical vapour deposition (MOCVD), and the incorporation of doping impurities has been investigated following in situ processes. Then we have taken benefit of the most advanced nano-characterization tools. Atom probe tomography has been developed and has yielded the spatial distribution of dopants. The incorporation and a first insight of the dopant properties have been also assessed through their optical signatures (photoluminescence, Raman). Scanning capacitance microscopy has been used to locally measure the type and the concentration of carriers. Finally, transport experiments in a single doped nanowire were carried out, including I(V) and cathodoluminescence coupled with e-beam induced current (EBIC).

Talk 2. Magnetic and electrical properties on hybrid multiferroic bilayers deposited by sputtering technique at high oxygen pressures

María Elena Gómez

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Abstract. Multiferroic materials exhibiting simultaneous ferroelectricity and ferromagnetism have potential applications in information storage and in the emerging field of spintronics, however, this properties in in most compounds is present below room temperature, limiting the practical applications. Extrinsic multiferroic hybrid structures, in which FM and FE compounds are artificially assembled, are promising candidates in exploration of robust cross-coupling effects at room temperature by exploiting the elastic coupling between the two constituents, leading to extrinsic magnetoelectric effects.

We addressed to deposit the ferromagnetic phase of the $La_{1-x}Sr_xMnO_3$ (LSMO) and the ferroelectric $BaTiO_3$ (BTO) or the multiferroic $BiFeO_3$ (BFO) for possible hybrid multiferroic heterostructures. We have optimized the growth parameters for depositing $BaTiO_3$ (BTO) / $La_{2/3}Ca_{1/3}MnO_3$(LCMO) / $La_{2/3}Ca_{1/3}MnO_3$(LCMO) and $BiFeO_3$ (BFO) / $La_{2/3}Ca_{1/3}MnO_3$(LCMO) / (001) $SrTiO_3$ by sputtering RF and DC, respectively, in pure oxygen atmosphere and a substrate temperature of 830°C. Keeping fixed the magnetic layer thickness (t_{LSMO}) and varying the thickness of the ferroelectric (t_{BTO}) or multiferroic (t_{BFO}) layer, we want to point out the influence of the thicknesses ratio (t_{BTO}/t_{LSMO} or (t_{BFO}/t_{LSMO}) on electrical and magnetic properties. From x-ray diffraction (XRD) analysis, we found the bragg peaks for LSMO maintain its position but BTO or BFO peak shift to lower

Bragg angle indicating a strained BTO or BFO film. Magnetization and polarization measurements indicate a possible multiferroic behavior in the bilayers. Hysteresis loop measurements of bilayers show ferromagnetic behavior due to the presence of the LSMO thin film. For the polarization measurements we used the LSMO layer as bottom electrode, and we evaporated circular (1.25 $x10^{-3}$ cm^2 of area) top electrodes of gold on the BTO layer, resulting in capacitor structures with saturation polarization of 20$\mu C/cm^2$. The performance of individual properties on FE and FM layers indicate a possible structure multiferroic at temperature near to 300 K.

Talk 3. Ventajas del álgebra geométrica para aprender la Física

Phillipe Eenens

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Abstract. En años recientes el álgebra geométrica ha generado un interés creciente como herramienta matemática con gran potencial teórico para la física y práctico para aplicaciones de cómputo e ingeniería. Pero en general sus partidarios ya eran especialistas en la física que el álgebra geométrica pretende explicar y en las matemáticas tradicionales que podría sustituir. Entonces ¿qué tan conveniente sería enseñarla a principiantes? En esta charla, basada en un experimento pedagógico realizado en Guanajuato, se presenta el álgebra geométrica tal como la descubre un alumno al inicio del pregrado y se discute su eficiencia pedagógica.

Talk 4. Synthesis and characterization of photoactive materials for medical and environmental applications

Carlos E. Diaz-Uribe

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Abstract. Technological application of materials with photochemical activity has expanded rapidly in recent years and has been several developments especially in field of energy, environment and health. Such materials play an important role in the photo-generation of reactive oxygen species, such as hydroxyl radical, superoxide anion radical, singlet oxygen and other, they have great useful to use in photodynamic therapy and the wastewater treatment to recalcitrant contaminants. Since three years ago,

Photochemistry and Photobiology Research Group at Universidad del Atlántico has worked in synthesis and characterization of organometallic of both free and supported sensitizers on different solid matrices in order to study their potential applications in photodynamic antimicrobial therapy and physicochemical study of the degradation of phenols, ionic dyes, polycyclic aromatic hydrocarbons among others. The characterization of these materials has been carried out by the techniques of FT-IR, UV-Vis, EPR, DLS, diffuse reflectance. Among the most active sensitizers are the tetracarboxyl-phenyl porphyrins and phthalocyanines. Studies show type of metal of coordination and type of organic and inorganic supports determine the possible application.

Talk 5. Raman spectroscopy for materials characterization

Margarita Correa

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Abstract. Modern science and technology of electronic materials requires design and development of new materials and heterostructures with excellent structural, optical, thermal, electric, magnetic and mechanical properties, along with a continuous decrease of its size and dimensions for device-purposes. This tendency imposes a challenge not only because of the synthesis and growth of materials but the way to characterize them in a nondestructive way. In this sense, Raman spectroscopy is a unique nondestructive tool for probing the structure and properties of a wide range of materials both organic and inorganic like polymers, biological, dielectrics, ferroelectrics, magnetic, multiferroics, carbon nanotubes, graphene, among others. Raman spectroscopy is based on the inelastic scattering of a monochromatic light that provides information about atomic vibration, structural transformation and dynamics in molecules. In this presentation, we will present a brief introduction to the technique, a few examples of its application to organic and inorganic nanostructured materials taken from literature, and some experimental results of our work on ferroelectric and multiferroic materials characterized by this technique.

Talk 6. On the $CsHSeO_4$ high-ionic conductivity *nature* above 128 °C: a new interpretation

E. Ortiz, I. Piñeres, M. Correa, DN. Montenegro, JC. Tróchez

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Abstract. By using simultaneous thermo-gravimetric and differential scanning calorimetric analysis, DSC-TGA, and modulated differential scanning calorimetric analysis, MDSC, x-ray diffraction (XRD) and electrical conductivity measurements, we have cheeked if the previously found phase transitions in $CsHSeO_4$ (at around 81, and 128 °C) behaves as those reported for $CsHSO_4$, or instead, they are truly physical transformations. The DSC-TGA results show that simultaneously with the DSC endothermic anomalies (at around 81, and 128 °C) two weight loss events appear, respectively. Moreover, the MDSC measurements show that full amount of heat flow belongs to the kinetic-component. Therefore, we conclude that the observed DSC endodermic anomalies are exclusively consequence of surface chemical decomposition, and thus the reported phase II and superprotonic-conducting phase for CHSe does not take place.

Talk 7. A.C magnetic susceptibility and magnetization of amorphous alloy Composition of $Fe_{37}Co_{35}Nb_6B_{11}Si_{10}Cu_1$

A. Orozco[1], Z. Caamaño[1], A. Rosales[2]

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Abstract. Amorphous FeCo-based alloys have been studied very much because of the excellent soft magnetic properties these alloys present, even above room temperature. The interesting magnetic properties allow these alloys can be used in technological applications at high temperatures and high frequencies, unlike conventional Fe-based magnetic alloys.

In this work, a study of the a.c susceptibility as a function of frequency and length in the magnetic amorphous alloy composition of $Fe_{37}Co_{35}Nb_6B_{11}Si_{10}Cu_1$ is presented. Frequency range was changed between 10 Hz and 5 kHz, and length of the sample between 10 mm and 4 mm, varying the magnetic field between -74 and 74 Oe. Also, the saturation magnetization values of $Fe_{72-x}Co_xNb_6B_{11}Si_{10}Cu_1$ (x = 30, 35 and 40 at. % of Co) amorphous alloys were obtained from their magnetic hysteresis curves recorded on a VSM. The samples were obtained by the melt-spinning technique. A. C. magnetic Susceptibility as the magnetization measurements were performed at room temperature.

Talk 8. Structural optimization of atomic systems with few degrees of freedom

B. Cogollo[1], J.A. Montoya[1,2]

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Abstract. Finding the most stable structure of a system, given only its chemical composition is a challenging problem. Predicting structure is important because by knowing the arrangement of the atoms in a material, we are able to understand its physical properties even if that material is under conditions which cannot be accessed experimentally or if that material has not yet been synthesized.

A methodology of crystal structure prediction using Random Sampling was applied in two cases from different areas of physics which are: a molecular oxygen system submitted to variations of pressure and a copper cluster with zero pressure in vacuum, with variations in the number of atoms of the system. We predict the ground state structure for each system, and when possible, calculated other properties and compared with other results.

Talk 9. Modeling hybrid nanomaterials for photovoltaics

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Abstract. Materials for third generation solar cells are synthesized by low-cost methods and are typically characterized by complex microstructures with a high degree of structural and chemical disorder.
For example, in nanocrystalline films the crystalline and the amorphous phases coexist in a hybrid order-disorder matrix. On the other hand, polymer-solar cells or dye-sensitized solar cells have a complex structure and chemical composition involving hybrid organic-inorganic interactions. The hybrid nature of such materials makes difficult the control of their properties and it represents a challenge for the development of a reliable predictive modeling.

In this talk, I will give an overview of the multi-scale modeling activity on hybrid nanomaterials for photovoltaics at the CNR-IOM, Cagliari (Italy). Model potential molecular dynamics and ab-initio methods are combined in a hierarchic multi-scale approach to generate realistic atomistic models. I will,provide examples related to the cases of: (i) amorphous-crystalline silicon films in order to study their microstructure evolution and the correlation between structure and electronic properties; (ii) polymermetaloxide interfaces with self-assembled molecular interlayers to engineer the photovoltaic properties; and (iii) hybrid perovskites by discussing the role of the organic and inorganic components in the recombination and photovoltaic properties.

Talk 10. Nanocristallization process of $Fe_{37}Co_{35}Nb_6B_{11}Si_{10}Cu_1$ alloy

Zulia Caamaño

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Abstract. Nanocrystalline FeCo base alloys are promising materials for use in power generation and power conversion applications. They must have good thermal stability and high-temperature soft magnetic properties. The formation of a nanocrystalline structure, through an appropriate heat treatment of the amorphous precursor, results in the improvement of soft magnetic properties.

In this work, the nanocrystallisation process of $Fe_{37}Co_{35}Nb_6B_{11}Si_{10}Cu_1$ alloy has been investigated using Differential Scanning Calorimetry (DSC), Thermogravimetry analysis under magnetic field measurements (TGM), X-ray diffraction (XRD), Mössbauer Spectroscopy (MS) and Vibrating Sample Magnetometry (VSM) techniques. DSC analysis showed the exothermic peaks attributed to the crystallization process of the sample. The values of Curie Temperatures of the amorphous and crystalline phases was estimated by means of TGM analysis. Heat treatments of the amorphous ribbons at different temperatures, in which crystallization occurs, caused the formation of α-FeCo nanograins surrounded by an amorphous matrix. The mean crystallite size, the crystalline volume fraction and the length between grains was calculated from fitting XRD patterns. The mean crystallite size was evaluated nearby 10 nm at the heat treatment temperature of 600 °C. Mössbauer spectra revealed the evolution of the nanocrystallization process of the sample with the increase of the heat treatment temperature. From the fitting of spectra, the hyperfine field contributions and spectral area of amorphous and crystalline components were calculated. The nature of the crystallization products as well as the phase structure within the partial crystallization of the sample was determined using MS combined with XRD results. The hysteresis curves

showed the magnetic softness of the samples and a saturation magnetization value about 116 emu/g, at higher heat treatment temperature, in comparison with the value obtained for the amorphous sample, which was around 106 emu/g.

Talk 11. Modeling of materials under extreme conditions

J.A. Montoya[1,2]

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Abstract. Carbon dioxide is commonly known, chemically, as a very stable molecule. In fact, CO_2 is a common byproduct of processes that involve a high release of energy, such as combustion and explosions. This study deals with the extreme conditions in pressure and temperature that are required in order to break the double carbon-oxygen bond (C=O) in pure CO_2. Studies in this area have resulted in the whole panoply of new extended phases currently known, both two-dimensional and three-dimensional, some of which bear no resemblance with any of the counterparts that are observed in isoelectronic systems such as SiO_2 or GeO_2. The molecular-bond destabilization upon applying extreme pressure and/or temperature is not unique to CO_2, in this regard; we also mention recent findings in O_2.

Talk 12. Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics

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Abstract. The equilibrium fractionation factor between two phases is of importance for the understanding of many planetary and environmental processes. Although thermodynamic equilibrium can be achieved between minerals at high temperature, many natural processes involve reactions

between liquids or aqueous solutions and solids. For crystals, the fractionation factor a can be theoretically determined using a statistical thermodynamic approach based on the vibrational properties of the phases. These calculations are mostly performed in the harmonic approximation, using empirical or ab-initio force fields. In the case of aperiodic and dynamic systems such as liquids or solutions, similar calculations can be done using finite-size molecular clusters or snapshots obtained from molecular dynamics (MD) runs. It is however difficult to assess the effect of these approximate models on the isotopic fractionation properties. In this work we present a systematic study of the calculation of the D/H and 18 O/ 16 O equilibrium fractionation factors in water for the liquid/vapour and ice/vapour phases using several levels of theory within the simulations.

Namely, we use a thermodynamic integration approach based on Path Integral MD calculations (PIMD) and an empirical potential model of water. Compared with standard MD, PIMD takes into account quantum effects in the thermodynamic modeling of systems and the exact fractionation factor for a given potential can be obtained. We compare these exact results with those of modeling strategies usually used, which involve the mapping of the quantum system on its harmonic counterpart. The results show the importance of including configurational disorder for the estimation of isotope fractionation in liquid phases. In addition, the convergence of the fractionation factor as a function of parameters such as the size of the simulated system and multiple isotope substitution is analyzed, showing that isotope fractionation is essentially a local effect in the investigated system.

Talk 13. Thermal and Electric Behavior of $Cs_3(HSO_4)2(H_2PO_4)$ at temperatures above 300 K

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Abstract. In the last decades, scientific efforts on research on ionic and superionic conductor materials have notably increased due to their potential application as electrolyte separators in fuel cells. Some compounds, such as CsH_2PO_4 and $CsHSO_4$, have been proposed for been used in fuel cells because there are literature reports of a low temperature transition from protonic conduction to superprotonic conduction at temperatures as low as 230 °C and 141 °C, respectively. These transitions have been attributed to structural phase changes at those temperatures. Recently, a new family of acid salts, called mixed salts, has been proposed

as electrolyte separators in fuel cells. One of the most representative compound of this family is $Cs_3(HSO_4)_2(H_2PO_4)$ which have a phase transition of superprotonic conduction above 119 °C, with conductivity values in the order of 10^{-3} S cm^{-1}. The sudden increment in conductivity has been explained in terms of a structural phase transition from monoclinic to cubic cell structure.Another possible explanation of the transition of protonic to superprotonic conduction showed by several acid salts, and that have been proposed by several authors, is that the high conductivity is the result of a partial decomposition that starts in the nucleations sites that are on the surface of the sample.

In the context of the scientific argument about the nature of the transformations at high temperatures in acid salts, in this work, systematic measurements using several techniques, such as DSC, TGA, TG-MS and impedance spectroscopy, have been employed to study the behavior of $Cs_3(HSO_4)_2(H_2PO_4)$ to contribute to enlighten the true nature (either chemical or physics) of the transition that this compound undergoes.

Talk 14. Heusler Alloys: tunable multifunctional materials

J. C. Tróchez, E. Ortiz, E. Solano

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Abstract. In the last two decades intensive studies has been done in materials with composition M_2TX (with M and T transition metal and X is a group III to V element of periodic table). The rich variety of physical and chemical properties in these compounds is a motivation for research in such materials. The compounds Ni_2MnGa and no stoichiometric $Ni_{2+(x+y)}Mn_{1+x}Ga_{1+y}$ are attracting to attention in condensed matter physics due to that Shape Memory Phenomena and ferromagnetism are present in all of them. Phase transition temperatures in these compounds can be tuned by small changes in the composition where stoichiometric dependence both electronic and structural properties is the most remarkable feature in these materials. In order to begin study in these compounds, we prepared polycrystalline samples by standard arc melting method. The composition of samples was $Ni_{2+x}Mn_{1-x}Ga$ with x= 0, 0.05, 0.10, 0.13, 0.19 and 0.22; after sintering we cut all samples in small pieces for carryout measurements of their thermal, structural and electric properties. We found that for samples with x= 0 and x=0.5 Curie temperature is below to that martensite-austenite. This fact will be useful for technological applications like actuators, because enhances their shape memory effect by using magnetic field. When x increases Curie and martensite-austenite temperatures are very close, where this is important

to increasing magnetocaloric effect. For x=0.22 martensite-austenite temperature rise and Curie decreases. All compounds show at room temperature tetragonal structure belonging to spatial group P4/mmm.

Talk 15. Secondary Ion Mass Spectrometry (SIMS) study of Metal Organic Chemical Vapour Deposition (MOCVD) semiconductors III-V hyperstructures

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Abstract. One of the most promising technologies in high efficiency solar cells is based on quaternary structures grown by epitaxial techniques as Metal Organic Chemical Vapour deposition (MOCVD). The semiconductors III-V structures are elaborated under tailored parameters, allowing the use of a broader area of the solar spectrum. Analytical techniques capable of providing accurate and precise information in cross sections about the composition and thickness of the layers are demanded. Secondary Ion Mass Spectrometry (SIMS) has been used for characterization of these structures due to its high depth resolution and sensitivity, stability and reproducibility. It was detected the diffusion process of Al and In across the cell interfaces and the layer diffusion over GaAs substrates. The Al diffusion was associated at incorrect incorporation of elements during growth process and the layer diffusion was associated at changes of manufacturing parameters. Such studies show the SIMS ability to diagnose of faults during the growth process, detection of impurities and incorrect diffusion of dopants that may affect the layer properties and the structure functionality.

Talk 16. Buffer layers based on In and Zn to Thin Films Solar Cells

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Abstract. Thin film solar cells are favorable option as renewable resource energy in mid term; these kinds of devices use a thin film about (40-100 nm of thickness) as buffer layer between absorbent layer and the transparent conductor oxide of the solar cells. Best results have reported conversion efficiency about 20% and, usually, this devices use CdS thin films as buffer layer, however this compound is highly toxic and, it has high adsorption coefficient at visible range. Different semiconductors could be used as buffer layers to replace conventional CdS buffer layers, and besides, different experimental method also could be used to obtain it. In this lecture we will explore different compounds and synthesis methods to fabricate alternatives buffer layers to be used in thin film solar cells.

Talk 17. Growth and characterization of nanostructured multiferroic heterostructures by pulsed laser deposition technique

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Abstract. Multiferroics materials (MF) are those having two or more ferroic orders such as ferroelectricity, ferromagnetism, and ferroelasticity. An important feature of these materials is that they may exhibit coupling of the different ferroic orders, being of particular interest the magnetoelectric (ME) coupling for their potential application in spintronics and nanoelectronics. The first investigated materials exhibiting magnetoelectric coupling were single phase. However, in these materials, the phenomenon was weak and observed at low temperatures, preventing or limiting its use in the development of new technologies. Currently, the looking for a room temperature magnetoelectric multiferroic is a very active research field worldwide. To overcome the problems presented with single phase materials, it has been proposed the synthesis and characterization of composites materials, following different geometries. In this approach, materials having electric and/or magnetic order are properly combined it to induce or enhance magnetoelectric coupling. In this research work, it is intended to design nanostructured multiferroic heterostructures to become a good candidate for room temperature magnetoelectric multiferroic. The investigated compounds, of the complex perovskites type, will be growth by pulsed laser deposition technique (PLD) on crystalline substrates such as MgO or SrO. Different techniques like XRD, Raman spectroscopy, SEM, impedance spectroscopy, ferroelectric testing, VSM, and SQUID will be used to characterize the structural, microstructural, magnetic and ferroelectric properties.

Poster Session

Poster 1. Síntesis y caracterización morfológica y estructural de $Fe_{65}Co_{35}$

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Abstract. Las aleaciones nanoestructuradas a base de Fe han sido de gran interés en la investigación básica del magnetismo y en aplicaciones tecnológicas. El interés radica en el tamaño nanométrico del cristalito, lo cual repercute en sus propiedades magnéticas. Las nanopartículas a base de aleaciones nanoestructuradas magnéticas se han potencializado como principal herramienta biotecnológica y en sistemas de grabación magnética.

La necesidad de obtener nanopartículas con propiedades magnéticas superiores que las de los materiales magnéticos precursores, impone la escogencia de aleaciones nanoestructuradas de FeCo, ya que estas aleaciones tienen las mejores propiedades magnéticas blandas, útiles en aplicaciones tecnológicas. El aleado mecánico ha sido uno de los métodos más utilizados en la síntesis de aleaciones nanoestructuradas de FeCo debido a su eficiencia y versatilidad. En este trabajo se sintetizaron aleaciones nanoestructuradas magnéticas de composición $Fe_{65}Co_{35}$ por el método de Aleado Mecánico de elevada energía; así mismo, se estudió la morfología y estructura de los nanopolvos obtenidos por SEM y DRX.

Poster 2. Estudio del comportamiento magnético y estructural del polvo nanoestructurado $Fe_{50}Co_{50}$ preparado por aleado mecánico

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Abstract. Actualmente ha habido un creciente interés en el estudio de materiales magnéticos nanoestructurados debido a su gran aplicación en aparatos de información. El interés del estudio se centra en las excelentes propiedades magnéticas que presentan estos materiales debido fundamentalmente a que el tamaño del cristalito obtenido es de orden nanométrico.
En este trabajo se realizó un estudio de la aleación magnética nanoestructurada de composición $Fe_{50}Co_{50}$, obtenida en forma de polvo por aleado mecánico, por medio de las técnicas de Difracción de Rayos X (DRX), Microscopia electrónica de barrido (SEM) y Magnetometría de muestra vibrante (VSM). Se estudió el comportamiento magnético y estructural de esta composición, en función de las condiciones de preparación. Así mismo, se comprobó la relación entre la estructura y las propiedades magnéticas blandas de la muestra objeto de estudio, importante no sólo desde el punto de vista de la Física del magnetismo sino también en sus aplicaciones tecnológicas.

Poster 3. Modelado del tamaño de partícula de nanopolvos de FeCo sintetizados por el método de aleado mecánico

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Abstract. En este trabajo se utilizó el modelo de Programación de Expresión Genética (PEG) para predecir el tamaño de partícula de nanopolvos de aleaciones bimetálicas y compuestos sintetizados por el método de aleado mecánico (AM). Por medio de este método, se han sintetizado un gran número de aleaciones nanocristalinas y compuestos

intermetálicos de manera exitosa, ya que se puede obtener el refinamiento de granos de material en forma de polvo.

El método de PEG es un modelo computacional basado en algoritmos genéticos, inspirado en la evolución biológica, el cual determina la capacidad de un programa para llevar a cabo una tarea de cálculo dada, en nuestro caso, el cálculo del tamaño de partícula de nanopolvos sintetizados por AM, por medio de los métodos de Rietveld, Willianson-Hall y Scherrer. La PEG ha sido utilizada para evaluar las propiedades mecánicas del cemento y del concreto; sin embargo, ésta aún no ha sido utilizada para nanopolvos de FeCo sintetizados por AM. A partir de los datos recolectados en la literatura para 86 muestras sintetizadas por AM, se comprobará la viabilidad de uno de los modelos de PEG de la literatura y posteriormente poderlo implementar utilizando *MatLab* para aleaciones nanocristalinas basadas en FeCo.