

Oxides and related topics

1 - 1 – Behavior of thermal expansion coefficient of $\alpha - MoO_3$ in function of the concentration of Nd^{3+}

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The molybdenum trioxide (MoO_3) and neodymium (Nd) has excellent physical and chemical properties that have made them useful in different applications. For example, the MoO_3 has been used as thermal sensor (thermochromic), in information display screen (photochromic), as cathode material in solid-state micro batteries and as gas sensor. On the other hand, the Nd^{3+} due to their photo emissive properties has been used mainly as active element in laser systems; it is important remember that the photoluminescence related with the neodymium is produced only by interaction with the crystal field of a suitable host material. In order to establish the physical mechanisms that determine the inclusion of neodymium in MoO_3 structure several samples were prepared, using the technique of liquid phase reaction, mixtures with different molar concentrations of Nd (0.1% to 20%). The mixtures were subjected to heat treatment, starting from room temperature to reach 823K, and analyzed in situ by X-ray diffraction (XRD). From the XRD analyses were calculated x_i (with $x=a, b, c$ lattice parameters) of molybdenum trioxide as a function of molar concentration Nd^{3+} ion, and allow us calculate thermal expansion coefficients ($\alpha_a = 7.7402 \times 10^{-4} \text{ } \dot{A}/^{\circ}C$, $\alpha_b = 5.7012 \times 10^{-5} \text{ } \dot{A}/^{\circ}C$, and $\alpha_c = -3.1031 \times 10^{-6} \text{ } \dot{A}/^{\circ}C$); the composition of these materials were determinate by X-ray dispersive spectroscopy (EDS). From the EDS analyses were found that the mixtures have concentrations of the 4.00to8.00%atomic the Nd.

1 - 2 – Behavior of the irreversibility line in the new superconductor $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$

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The irreversibility properties of high-Tc superconductors are of major importance for technological applications. For example, a high irreversibility magnetic field is a more desirable quality for a superconductor [1]. The irreversibility line in the H-T

plane is constitutes by experimental points which divides the irreversible and reversible behavior of the magnetization. The irreversibility lines for series of $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$ polycrystalline samples with different doping were investigated. The samples were synthesized using the usual solid state reaction method. Rietveld-type refinement of x-ray diffraction patterns permitted to determine the crystallization of material in a tetragonal structure. Curves of magnetization ZFC-FC for the system $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$, were measured in magnetic fields of the 10 Oe to 20000 Oe, allowed to obtain the values for the irreversibility and critical temperatures. The data of irreversibility temperature allowed demarcating the irreversibility line, $T_{irr}(H)$. Two main lines are used for the interpretation of the irreversibility line: one of those which supposes that the vortexes are activated thermally and the other proposes that associated to T_{irr} , it happens a phase transition. The irreversibility line is described by a power law. The obtained results allow concluding that in the system $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$ a characteristic bend of the Almeida-Thouless (AT) tendency is dominant for low fields and a bend Gabay-Toulouse (GT) behavior for high magnetic fields. This feature of the irreversibility line has been reported as a characteristic of granular superconductors and it corroborates the topological effects of vortexes mentioned by several authors [1,2].

[1] Dawood Ahmad, Tae Kwon Song, Insuk Park, G. C. Kim, Y. C. Kim. Current Applied Physics 10 (2010) 1345-1348. [2] P. Rodrigues Jr, J. Schaf, P. Pureur, Phys. Ver. B 49, 15292 (1994).

1 - 3 – Synthesis, structure and magnetic properties of the double perovskite Sr_2SbMnO_6

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We report the structural and magnetic properties of the perovskite Sr_2SbMnO_6 , which has been synthesized by the standard solid state reaction recipe. Crystalline structure was studied by means of Rietveld refinement of X-ray diffraction data. This study indicates that the structure is tetragonal, space group 128.

The magnetic behavior was studied for several temperatures between 5 and 300 K, through measurements of magnetization in function of field, AC and DC susceptibility in function of temperature and ZFC–FC magnetization curves. The ZFC and FC curves show a magnetic transition/glassy freezing at ~ 13 K and was observed that the behavior is not pure Curie Weiss; also, at 300 K $\text{Sr}_2\text{SbMnO}_6$ show a pure paramagnetic behavior. Was studied field dependence of magnetization data at 8 K, which show that there are ferromagnetically coupled clusters in the ordered/glassy state. However, there are significant details that distinguish the observed behavior from a standard spin glass. The measurements of AC susceptibility at 125 Hz and 1000 Hz show two peaks, one of these indicating the magnetic transition glassy at 13 K, and the second about 40 K show up the beginning of glassy dynamics. These results are in agreement with reports of other authors.

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1 - 4 – Evolution of the structural ordering of the $\text{Sr}_2\text{SbMnO}_6$ perovskite in function of temperature

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Polycrystalline samples of $\text{Sr}_2\text{SbMnO}_6$ material has been synthesized by means of the conventional solid state reaction method, using powder oxides SrO , MnO_2 and Sb_2O_3 . Our route of synthesis differs of others reported in the literature by the use of SrO instead of SrCO_3 as the precursor of the Sr. X-ray diffraction (XRD) pattern obtained was studied by means of the Rietveld refinement method. This study reveals that the $\text{Sr}_2\text{SbMnO}_6$ material has tetragonal structure, space group 128. Furthermore, XRD patterns were registered for temperatures between 25°C and 1400°C . The Rietveld refinements of these patterns show that the structure correspond to the space group 128 until 200°C , change to space group 87 for temperatures between 300 and 1000°C and, finally is cubic, space group 225 for temperatures above 1000°C . Additionally, is discussed the evolution of the lattice parameters in function of the temperature. The study of this material is important because it has been attracted the attention due to its ferroelectric and magnetic properties.

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1 - 5 – Critical temperature above 92 K in a new superconducting material $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$

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We report the synthesis, structural ordering and superconducting measurements of a new material $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$, which was made by means of the conventional solid state reaction method, based on commercial oxide powder precursors. To determine the crystal structure of the $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$, the X-ray diffraction pattern was refined by Rietveld method. This study reveals that the material has a single phase with complex orthorhombic perovskite structure, space group 25.

Results of magnetization measurements in function of temperature show that the $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$ material undergoes a superconducting transition at $T_c \sim 98$ K. This results are in agreement with the observation of a high transition temperature in $\text{Y}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ system, reported by Aliabadi et. al[1].

This work was partially supported by the Dirección de Investigaciones (DIN) of the Universidad Pedagógica y Tecnológica de Colombia (UPTC).

[1] A. Aliabadi, Y. Akhavan Farshchi and M. Akhavan, *Physica C*, **469** 2012–2014, (2009).

1 - 6 – Production and characterization of the type Superconducting Perovskites $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$, (RE= Y, Sm, Dy, Ho)

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In this work we report the synthesis and characterization of the system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Y, Sm, Dy, Ho), in order to reproduce the results reported by A. Aliabadi et. al.[1] about the $T_c \sim 100$ K for the superconducting system $\text{Y}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ and, to evaluate the superconductor behavior of $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ samples (RE=Sm, Dy, Ho). The system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Y, Sm, Dy, Ho), was produced by the method of solid state reaction following a thermal process similar to that used for the superconductor RE:123 and different to that used by Aliabadi. The experimental results obtained by the technique of X-Ray Diffraction and Rietveld analysis show that these samples have the expected

crystal structure. On the other hand, the resistivity measurements of samples produced ensure the superconductor transition in the system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Y, Sm, Dy, Ho), with critical temperatures near $T_c = 96\text{K}$ for the system $\text{Y}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ and a T_c above 92K for the system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Sm, Dy, Ho). This work opens a new avenue of research in the area of superconductivity for systems RE:358.

This work was partially supported by the Dirección de Investigaciones (DIN) of the Universidad Pedagógica y Tecnológica de Colombia (UPTC).

[1] A. Aliabadi, Y. Akhavan Farshchi and M. Akhavan, *Physica C*, **469** 2012–2014, (2009).

1 - 7 – Shot noise in HTc superconductor quantum point contact system.

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We study the electrical transport properties of a quantum point contact between a lead and a High Tc superconductor. For this, We use the Hamiltonian approach and non-equilibrium Green functions of the system. The electrical current and the shot noise are calculated with this formalism. We consider $d_{x^2-y^2}$, d_{xy} , $d_{x^2-y^2} + is$ and $d_{xy} + is$ symmetries for the pair potential. We find that for d_{xy} symmetry there is no a zero bias conductance peak; for $d + is$ symmetries there is a displacement of the transport properties. From shot noise and the current, the Fano factor is calculated and we find that it takes values of effective charge between e and $2e$ depending on the pair potential symmetry, it is explained by the diffraction of the quasiparticles in the contact. These results are compared with the obtained for a plain junction.

1 - 8 – Magnetic properties and structural characterization of $\text{Sr}_2\text{RuHoO}_6$ complex perovskite

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We report an experimental study of the crystallographic lattice, morphologic characteristics and magnetic feature of $\text{Sr}_2\text{RuHoO}_6$ complex perovskite, which is used as a precursor in the fabrication process of the superconducting ruthenocuprate $\text{RuSr}_2\text{HoCu}_2\text{O}_8$. The samples were produced through the standard solid state reaction. A careful Rietveld

refinement of the experimental X-ray diffraction patterns shows that the material crystallizes in a monoclinic structure, which belongs to the $P21/n(\#14)$ space group, with lattice parameters $a = 5.7719(6)\text{Å}$, $b = 5.8784(5)\text{Å}$, $c = 8.1651(9)\text{Å}$, and tilt angle $\beta = 90.200^\circ$. The calculated tolerance factor of material was 0.9170, which is in agreement with a monoclinic crystallographic cell. The inter-atomic distance and occupancy calculated through the Rietveld refinement of experimental data is reported too. Micrograph of Scanning Electron Microscopy for $\text{Sr}_2\text{RuHoO}_6$ double perovskite, obtained from ETD detector, show the granular characteristic of material with mean size between 2.0 and $7.5\mu\text{m}$. Through semiquantitative Energy Dispersive X-ray analysis, we determined that the composition of the material is 98% in agreement with theoretical values calculated from stoichiometry of $\text{Sr}_2\text{RuHoO}_6$ material. From the structural, morphologic and compositional characteristics we deduced that no other crystallographic phases or impurities are present in the sample. Magnetic susceptibility measurements reveal the occurrence of an antiferromagnetic behavior for a Néel temperature $T_N = 10.1\text{K}$. From the Curie-Weiss fitting of the paramagnetic regime we obtain an effective magnetic moment of $11.31\mu_B$. The antiferromagnetic ordering is attributed to Ru-O-O-Ru superexchange interaction and a ferromagnetic transition for a Curie temperature of 17K , which are related with the Ru-O-Gd interactions.

1 - 9 – Formation of a magnetic composite by reduction of Co-Nd doped strontium hexaferrite in a hydrogen gas flow

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Co-Nd strontium hexaferrite nanoparticles synthesized by the self-combustion method were treated in a hydrogen flow at different temperatures and times. The samples were characterized structurally by scanning electron microscopy and x ray diffraction and magnetically with a vibrating sample magnetometer. Phase identification showed decomposition of the hexaferrite structure into Fe_3O_4 , Fe_2O_3 and different strontium mixed oxides. The sample treated at 500° for 30 minutes shows good magnetic properties due to the formation of a magnetite/hexaferrite composite. In this case saturation magnetization is very close to the original sample while the coercivity slightly diminishes. The hexagonal phase is almost completely transformed into non-magnetic oxides at a reducing temperature of 500° for 120 minutes. The obtained results are analyzed in terms of the phase composition and of the magnetic susceptibility of the studied samples.

1 - 10 – Impedance spectroscopy and structural properties of the perovskite-like $\text{Sn}(\text{Ba},\text{Sr})\text{O}_3$ stagnate

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In the last decades, the study of perovskite materials has attracted great interest of researchers in the ceramics area due their physical and chemical properties at several temperatures, which are required for technological applications. In this work we perform an exhaustive study of structural, electrical and transport properties in bulk samples of the perovskite stagnate $\text{Sn}(\text{Ba},\text{Sr})\text{O}_3$. The synthesis of the $\text{SnBa}_{1-x}\text{Sr}_x\text{O}_3$ compounds was performed by the solid state reaction recipe. Seven tablets were obtained with different concentrations of $\text{SnBa}_{1-x}\text{Sr}_x\text{O}_3$ with $0 \leq x \leq 1$. The crystallographic structure was studied by the X-ray diffraction technique and the analysis of the experimental data was performed from the Rietveld refinement by using the GSAS code. Results reveal that the material synthesized in a Pnma structure (space group #62). The approximate grain size was found from experiments from Scanning Electron Microscopy images to be $2\mu\text{m}$. The semi-quantitative composition was established from Energy Dispersive X-ray experiments, which permitted to establish that the chemical compositions of our samples are 97% in agreement with the expected stoichiometry. The response of the impedance as a function of frequency at room and low temperatures were obtained by the Impedance Spectroscopy technique from 10.0mHz up to 0,1MHz, also obtaining the respective equivalent circuit, using the fitting the Cole-Cole diagrams. Electric polarization measurements for SnSrO_3 and SnBaO_3 were determined through polarization experiments, using a polarization equipment produced by Radiant Technologies. Curves of polarization as a function of applied electric fields reveal the hysteretic behavior which is characteristic of the ferroelectric materials. From the saturation polarization it was determined that SnSrO_3 and SnBaO_3 have dielectric constants of 64.7 and 95.2 respectively. The ferroelectric parameters for these materials are presented and discussed.

1 - 11 – Size Dependent Ferroelectric Polarization in BaTiO_3 Nanocrystals Probed by Electron Holography

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In bulk ferroelectric crystals and thin films, the paraelectric to ferroelectric phase transition is accompanied by the formation of polarization domains to minimize the system energy with respect to the depolarization field and mechanical strain. While experimental data is available for thin perovskite films only few studies address the electric polarization properties of ferroelectric nanocrystals. Hence, it is yet to be established what is the minimal nanocrystal (NC) size and geometry that could support the ferroelectric crystal phase in the absence of external support such as a substrate, metal electrodes or adjacent high dielectric constant material. It is not established experimentally whether a small isolated NC exists as a single ferroelectric domain, or that its high depolarizing field causes other forms of ferroelectric order. Here, we present images of ferroelectric polarization in isolated BaTiO_3 (BTO) NCs obtained with nanometer resolution using off-axis electron holography, above and below the Curie temperature (T_C). It is found that the polarization magnitude within 20-55 nm NCs is size dependent, forming complex configurations in the larger nanocrystals with polarization values surpassing the bulk values quoted in the literature. In addition, the polarization appears to decay or re-orient near free NC surfaces to minimize the depolarization energy.

1 - 12 – Magnetotransport Properties in Manganite $\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3$ (FM) and $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ (AF): A Monte Carlo Approach

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Manganese perovskites have recently been the focus of renewed interest, due to the "colossal" magnetoresistance (CMR) effect and the coupled metal-insulator and magnetic transitions displayed at the

spin-ordering temperature TC by some of these compounds. In this work, a magnetotransport properties simulation of ferromagnetic (FM) $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ and antiferromagnetic (AF) $\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3$ is presented and discussed. Our study is addressed by using the Monte Carlo method. Moreover, magnetic Kronig-Penney model based on the thermodynamics of a Heisenberg can be used for describing the colossal magnetoresistance (CMR) phenomenon for the FM phase and insulating behavior for the AF phase. The model consists on tunnelinglike transmission process of hopping electrons in a magnetically dynamic lattice containing magnetic clusters. In this model, electrical transport features are mainly governed by the magnetic states, neglecting the lattice strain effects. By means of the theoretical fundamentals described here, intrinsic temperature and field dependences of the resistivity and magnetoresistance, typically observed in these manganites were obtained and analyzed.

1 - 13 – Effect of the heat treatment conditions on the synthesis of Sr-hexaferrite

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The effect of the heat treatment conditions under oxygen atmosphere on the $\text{SrFe}_{12}\text{O}_{19}$ (Sr-M ferrite) synthesis is analyzed. We study the effect of the partial evacuation of the gases of decomposition of the organometallic precursor on the phase composition of different samples. An accurate structural analysis of samples obtained between 250 °C (with Sr-M crystallite size, \varnothing , around 20 nm) and 500 °C (\varnothing 40 nm) is reported. From the structural analysis two secondary phases, hematite and maghemite, are identified. The amount of secondary phases (between 10% and 30%) can be manipulated through the control of the heat treatment conditions, and therefore, this constitutes a methodology to manipulate the phase composition of the nanopowders. The influence of secondary phases on the magnetic properties of the samples is also studied. The quantitative determination of phases is performed by structural refinement of X-ray powder patterns, by using Rietveld analysis. Magnetic study is done by Magnetization vs Temperature and Magnetization vs Applied Magnetic Field.

1 - 14 – Copper adsorption on magnetite chitosan composites: a kinetic and equilibrium study

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The accumulation of heavy metals in water is an important environmental problem, caused by industrial effluents. One possibility for removing these contaminants is the use of adsorption on biopolymers, such as chitosan. It is of interest to prepare an adsorbent material with magnetic properties, allowing the separation of the material with a magnet.

A composite of magnetite and the biopolymer chitosan was prepared as microspheres and used to adsorb copper ions which were chosen as model of contaminant metal in water. Fe_3O_4 particles of nanometric size were obtained by the oxidative hydrolysis of a FeSO_4 solution. The ferrofluid made of magnetite nanoparticles and chitosan was transferred dropwise on the surface of an alkali solution to form microspheres, which were then crosslinked with glutaraldehyde. The resulting material contained 35% w/w of chitosan, determined gravimetrically.

The adsorption of copper on the surface of the magnetic microspheres was studied in a batch process, with different aqueous solution of Cu (II) concentrations ranging from 40 to 1100 ppm. The residual metal concentration in solution was determined by a spectrophotometric method.

Kinetic and equilibrium aspects of the adsorption process were studied. The time-dependent Cu (II) adsorption data were well described by a pseudo-second-order kinetic model. Moreover, it was found that the equilibrium data fitted well to the Langmuir isotherm, with a maximum adsorption capacity of 500 mg Cu per g chitosan.

The microspheres were removed after use with a magnet and following a chemical treatment with a complexing agent the material could be reused as an adsorbent.

In conclusion, the prepared microspheres have proved useful in the removal of copper ions through an adsorption process whose kinetic and equilibrium characteristics have been analyzed.

1 - 15 – High Temperature-induced phase transitions in $\text{Sr}_2\text{GdRuO}_6$ complex perovskite

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We report experimental and theoretical study of crystallographic lattice and electronic structure of $\text{Sr}_2\text{GdRuO}_6$ complex perovskite, which is used as precursor in the fabrication process of superconducting ruthenocuprate $\text{RuSr}_2\text{GdCu}_2\text{O}_8$. Samples were produced by the standard solid state reaction. Rietveld refinement of experimental X-ray diffraction patterns shows that material crystallizes in a monoclinic structure, which belongs to the $P2(1)/n$ (14) space group, with lattice parameters $a=5.8019(6)$ Å, $b=5.8296(5)$

\AA , $c=8.2223(7)$ \AA , and tilt angle $\beta=90.2580^\circ$. Measurements of X-ray diffraction in the range between 298 K and 1273 K show that lattice parameters a , b and c of complex perovskite Sr_2GdRuO_6 suffers volume expansion in the three coordinate axes. The results show that as temperature increases the value of cell parameter c increases approximately linearly, while the values of cell parameters a and b tend to be equal and the tilt angle β decreases to 90° . The value of cell parameter a increases approximately linearly and takes the value of cell parameter b at temperature of 753 K. From this temperature the values of two parameters are similar, and arguably presents a phase transition in complex perovskite Sr_2GdRuO_6 , when the tilt angle β tends to $90.073(3)^\circ$. In Agreement with these results have a tetragonal structure, in which $a=b$, c is arbitrary and $\alpha=\beta=\gamma=90^\circ$. Then the complex perovskite Sr_2GdRuO_6 adopts an tetragonal perovskite structure with space group $Ibmm$, which is characterized by rotation of GdO_6 octahedra about the pseudocubic two-fold axis.

1 - 16 – Resistive switching in ceramic multiferroic $\text{Bi}_{0.9}\text{Ca}_{0.1}\text{FeO}_3$ oxide

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Resistive switching (or RS) [1] is defined as the reversible change of the resistance of a material under the application of electrical pulses. RS in transition metal oxides has been observed in many binary and complex compounds, being the basis for the development of novel non-volatile resistance random access memories (RRAM). While in the case of binary oxides the RS effect is believed to arise from the creation/destruction of conducting filaments, in complex oxides the effect is interface-related, that is, it takes place at the interface between a metal electrode and the oxide, playing a key role the presence of oxygen vacancies that modulate the interface resistance. Here we study the RS effect in ceramic samples of the multiferroic oxide $\text{Bi}_{0.9}\text{Ca}_{0.1}\text{FeO}_3$ with different metallic electrodes. Samples were prepared by means of standard solid state reactions. We show by means of Mössbauer spectroscopy that the Fe valence remains unchanged (3+) upon Ca doping, suggesting a charge compensation mechanism via formation of oxygen vacancies. We studied the dependence of the RS effect with the type of electrode and with the intensity and number of pulses. RS values of up to 100 per cent were obtained, a figure that is lower than that found in thin films samples [2]. We argue that this is due to the low electrical fields achievable in ceramic samples with metallic electrodes separated by distances of the order of millimetres. In addition, the RS effect is found to relax with time, with typical relaxation times that depend on the number and intensity of the

previously applied electrical pulses. We rationalize our results by considering the Nernst-Planck equation and the migration of oxygen vacancies to and from the metal-oxide interface.

[1] A. Sawa, *Materials Today* 11, 28 (2008)

[2] C.-H. Yang et al., *Nature Materials* 8, 485 (2009)

1 - 17 – Magnetic behavior of Mg - Al - Zn - Fe mixed oxides from precursors layered double hydroxide

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Mixed oxides of Mg-Al-Zn-Fe were obtained by calcination of layered double hydroxides (LDH) prepared by coprecipitation reaction with hydrothermal treatment. The structural characterization of precursors and the mixed oxides was carried out by X rays diffraction, showing a increases of ZnO phase with the increase of the zinc content. Magnetic behavior was studied by vibrating sample magnetometer (VSM) and by a superconducting quantum interference device (SQUID) showing both ferromagnetic and superparamagnetic behavior depending on both particles size and composition.

1 - 18 – Structural, Magnetic and Electric behavior of new $\text{Ba}_2\text{TiMoO}_6$ material

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The $\text{A}_2\text{BB}'\text{O}_6$ double perovskites tend to order in a NaCl-type superlattice structure. Compounds where A is an alkaline earth cation and B= Cr, Fe, Mg; B'= Mo, Re, are ferromagnetic [1]. Interest in this type of compounds was revived because they exhibit

properties like intrinsic tunneling-type magnetoresistance (TMR) at room temperature [2], show evidence of electronic conductivity attractive for applications as anodes or cathodes in solid-oxide fuel cells [3] and half-metallicity [4]. These characteristics suggest the possible technological applications of perovskites in magnetoelectronic devices and make them promising candidates for future spin electronics. We report synthesis and characterization of the new $\text{Ba}_2\text{TiMoO}_6$ material. X-ray diffraction experiments reveal characteristic reflections for complex perovskite systems. A Rietveld refinement of the diffraction pattern shows that $\text{Ba}_2\text{TiMoO}_6$ crystallizes in a tetragonal structure, which corresponds to the space group $P_{4/mmm}$ (#123), with lattice parameters $a = b = 3.906 \text{ \AA}$; and $c = 11.732 \text{ \AA}$. Images of scanning electron microscopy (SEM) reveal small, sphere-shaped grains from $3.0 \mu\text{m}$ up to $5.0 \mu\text{m}$ size.

Measurements of the magnetization as a function of temperature after Zero field cooling and field cooling were carried out by using a MPMS Quantum Design SQUID magnetometer. We find paramagnetic behavior down to 5 K. Electric polarization curves were measured by means of a radiant ferroelectric tester, which include a 10 kV source for experiments in bulk samples. Hysteresis curves of the polarization as a function of the applied voltage exhibit a ferroelectric response for $\text{Ba}_2\text{TiMoO}_6$.

[1] A.K. Azad, S.-G. Eriksson, S.A. Ivanov, R. Mathieu, P. Svedlindh, J. Eriksen, H. Rundlöf, J. All. Comp. 364 (2004) 77-82.

[2] T.S. Chan, R.S. Liu, G.Y. Guo, S.F. Hu, J.G. Lin, J.-F. Lee, L.-Y. Jang, C.-R. Chang, C.Y. Huang, Solid State Commun. 131 (2004) 531-535.

[3] P. Karen, A.R. Moodenbaugh, J. Goldberger, P.N. Santhosh, P.M. Woodward, J. Solid State Chem. 179 (2006) 2120-2125.

[4] C.M. Bonilla, D.A. Landínez Téllez, J. Arbey Rodríguez, E. Vera López, J. Roa-Rojas, Physica B 398 (2007) 208-211.

1 - 19 – Growth of Ba-titanate and Ba-hexaferrite bilayers: effect of BTO layer in magnetic properties of BaM phase

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Bilayers of barium titanate, BaTiO_3 (BTO) and barium ferrite, $\text{BaFe}_{12}\text{O}_{19}$ (BaM) were grown by Pulsed Laser Deposition, using (100) LaAlO_3 substrate in the BaM/BTO configuration and (0001) Al_3O_4 substrate in BTO/BaM configuration, maintaining identical conditions of growth in both

samples. Stoichiometric control of the plasma emission during the deposition of BTO and BaM films was made by optic emission spectroscopy (OES). The structural characterization was achieved by X-ray diffraction and preferential growth it was found for the BTO phase in the BaM/BTO bilayer, and for BaM phase in the BTO/BaM bilayer. The magnetic properties of BaM phase was studied by SQUID magnetometer over a temperature range of the 5-300K and for different magnetic field applied. The dependence with temperature of the coercive field and squareness ($Sq = M_R/M_S$) present strong influence with structural characteristic of BaM, besides, significant differences were found between $Sq(T)$ of BaM single phase and the squareness of BTO/BaM bilayer, both deposited on Al_3O_4 , indicating the influence of BTO layer.

1 - 20 – Displacive Disorder, Anti-site Disorder and Magnetic Properties of Cubic Pyrochlores $\text{Bi}_2\text{MM}'\text{O}_7$ with $\text{M} = \text{Sc, Cr, Mn}$ and Fe and $\text{M}' = \text{Nb, Ta}$ and Sb

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Pyrochlore oxides are being the subject of renewed interest because of their many interesting applications. Specifically those with formula $\text{A}_2\text{MM}'\text{O}_7$ were recently informed to be alternative cathodes for IT-SOFCs [1]. Proton conductivity has also been observed in doped $\text{Sm}_2\text{Sn}_2\text{O}_7$ [2] and dielectric properties were informed for doped $\text{Bi}_{1.5}\text{Zn}_{0.92}\text{Nb}_{1.5}\text{O}_{6.92}$ [3]. Many other important applications make the synthesis of new pyrochlore oxides and their fundamental studies a very interesting area of research. The typical pyrochlore compound has the general formula $\text{A}_2\text{B}_2\text{O}_7$, with a cubic crystal structure Fd-3m (SG 227), and it is well described as $\text{A}_2\text{B}_2\text{O}_6\text{O}'$ comprising two interpenetrating sublattices with the formulae $\text{A}_2\text{O}'$ and BO_6 . Non spherical ions (like Bi^{3+}) inside the classic cubic structure can be accommodated through displacive disorder. This disorder results in the appearance of hkl reflections where $h = 4n$, $k = 4n$, and $l = 2n$. Its appearance is rationalized by a static displacement of the A ions toward the surrounding ring of O atoms. The synthesis of new $\text{Bi}_2\text{MM}'\text{O}_7$ pyrochlores with a combination of both, a magnetic ion and a spectator ion on the M sites (where $\text{M} = \text{Sc, Cr, Mn}$ and Fe and $\text{M}' = \text{Nb, Ta}$ and Sb) have been selected as an interesting family to study their fundamental properties. They were successfully synthesized

by solid state method, from stoichiometric quantities of the corresponding binary oxides and appropriated thermal treatments. XRD patterns, combined with Mössbauer spectroscopy for Fe containing compounds, allowed establish the displacive disorder and site disorder presence for all compounds. Their structures were refined by Rietveld analysis of PXRD patterns, and the comparison between the ideal cubic and displaced cubic pyrochlores was carried too. Resulting cell parameters are consistent with the M^{3+} cation in high spin configuration in octahedral coordination. Magnetic measurements were made in a commercial SQUID in the 10-300 K temperature range, and they allowed observe a wide range of magnetic characteristics, starting by expected diamagnetism for Sc pyrochlores, and indications of magnetic frustration for Fe pyrochlores.

[1] R. Martínez-Coronado, A. Aguadero, C. de la Calle, M.T. Fernández and J.A. Alonso, *J. Power Sources* (2010) (In press). [2] K.E.J. Eurenus, E. Ahlberg, C.S. Knee, K.E.J. Eurenus, E. Ahlberg and C.S. Knee, *Solid State Ionics* (2010) (In press). [3] A. Mergen, H. Zorlu, M. Özdemir and M.Yumak, *Ceramics International* (2010) (In press).

1 - 21 – Zero-valent iron nanoparticles and magnetite as solid catalysts for benzene degradation

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Fenton's reagent, a solution of hydrogen peroxide and ferrous iron catalyst, is used for an in-situ chemicals oxidation of organic contaminants. Recent studies of Fenton's reaction are concentrated on improving the remediation technique by minimizing the addition of extrinsic materials into subsurface systems and by using environmentally benign chemicals. Natural iron catalyst as a means of minimizing the extrinsic chemical addition was examined by many researchers. Although still in the emerging phase, zero-valent iron nanoparticles represent a highly promising agent of environmental remediation technologies. Nanoparticles containing magnetic materials such as Fe_3O_4 , Fe_2O_3 are particularly useful for imaging and separation techniques. They are considered to be biologically and chemically inert. The high ratio area/volume increase the catalysts properties. In this work we report the preparation and characterization of a magnetite ferrofluid and zero-valent iron nanoparticles by the method of ferric iron reduction by sodium borohydride. A comparative kinetic analysis between magnetite and zero-valent iron nanoparticles for the degradation of an aqueous solution of benzene is presented. The results are related to previous experiences developed in our laboratory with ferrous sulphate with the traditional Fenton's method. The experiences were performed at 20°, at a fixed molarity of benzene, hydrogen peroxide and catalyst. Prelimi-

nary results indicate that zero-valent iron nanoparticles show promising results compare to magnetite at one hour.

1 - 22 – Characterization of magnetite nanoparticles used for adsorption of As

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Magnetite may be used for remediation purposes, because of its physical properties that allow a magnetic separation of the oxide from polluted natural and industrial sources. In this work we characterize several samples of pure and doped nanomagnetites used for the adsorption of As(V), a ion that originates in some natural processes of mineral dissolution, mining operations and through the use of fertilizers and pesticides [1-3]. We have obtained nanosized pure magnetite (MP), doped Mn-magnetite (MMn) and doped Co-magnetite (MCo) by a chemical co-precipitation method using $FeCl_2 \cdot 4H_2O$ and $FeCl_3 \cdot 6H_2O$ in the molar ratio $\frac{1}{2}$. The ionic force was increased to assure the formation of nanoparticles [4]. The doped samples were obtained by replacing 10% of the Fe(II) ions by Co(II) and Mn(II) using $CoCl_2 \cdot 6H_2O$ and $MnCl_2 \cdot 4H_2O$. To analyze the influence of the preparation media on the morphology and hyperfine properties of the obtained particles, similar series were prepared in urea 0.4 M (samples named MPUREA, MCoUREA, and MMnUREA).

The effect of the dopants and the preparation media on the magnetite nanoparticles was evaluated by 77K Mössbauer spectrometry, FTIR, SEM and EDS measurements. The adsorption studies were performed at 25 °C, using 0.1 KNO₃, As(V) (40 ppm) and 80 mg of the iron oxide. The pH was kept at 4.00 using KOH 0.1N and HNO₃ 0.1N.

[1] Silva J., Mello J., Gasparon M., Abrahao W. and Jong T., *IMWA Symposium 2007: Water in Mining environments*, R. Cidu and Frau (Eds), 27th-31st 2007.

[2] Li Y., Wang J., Zhao Y., Lun Z., *Separation and Purification Technology*, (2010) 73, 264-270.

[3] Boddu V., Abburi K., Talbott J., Smith E., Haasch R., *Water Research*, (2008) 42, 633-642.

[4] Vayssières L., Chanéac C., Tronc E., Jolivet J.P., *Journal of Colloid and Interface Science*, (1998) 205, 205-212

1 - 23 – Structural stability and electronic properties study of the Sr_2MnSbO_6 perovskite

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The Sr_2MnSbO_6 perovskite has been reported as a ferroelectric and ferromagnetic compound in the tetragonal I4m phase and exhibits very interesting dielectric properties in the cubic Fm-3m phase, that make it a technological alternative for use in microelectronics devices. In addition, it is also very interesting the co-existence of both ferromagnetic and ferroelectric phenomenon, which is very important in spintronic applications such as the spin valves, reading devices in magnetic disks and recording devices.

In this work, first-principles calculations have been performed to study the structural and electronic properties of the Sr_2MnSbO_6 perovskite in cubic (Fm-3m), tetragonal (I4m) and P4/mnc phases. The calculations are performed in the framework of the spin density functional theory (DFT). We have employed the full potential linearized augmented plane waves (FP-LAPW) method as implemented in the WIEN2k code. The exchange and correlation effects were treated using the generalized gradient approximation (GGA), and the local density approximation (LDA). (GGA)+U approaches has been used in order to describe the strong on-site Coulomb repulsion among the localized d-Mn electrons; the results are compared with experimental results. Also we present a structural stability analysis based on fitting of the total energy values to the Murnaghan equation of state and a thermodynamic study of the phase transitions was carried out by means of the calculations of the Enthalpy. On the other hand, the study of the electronic properties was carried out by means of the representation of the bands structure and the densities of states for the two spin polarizations, which this show the half-metallic behavior in the cubic phase while that in the tetragonal phases is comported as semiconductor material.

1 - 24 – Electronic Structure of α - Al_2O_3 Slabs: a local environment study.

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In this work we performed an *ab initio*/DFT study of structural and electronic properties of the (001) α - Al_2O_3 surface. For this study we used two methods

with different basis set: the Augmented Plane Wave plus local orbital (APW+lo) and a linear combination of numerical localized atomic orbital basis sets, employing the Wien2K code and SIESTA code, respectively. In order to calculate the structural and electronic properties of the reconstructed surface, we calculated the final equilibrium atomic positions with the SIESTA code and then we calculated the Electric-Field Gradient (EFG) tensor with the APW+lo code at the optimized positions. Using this procedure we found equilibrium structures with less energy than those obtained by using only the APW+lo method. The EFG tensor and the local structure for Al were study as a function of the depth from the surface, for relaxed structures. We found that distances down to 6 Å from the surface are sufficient to converge the EFG and the Al-O distances to bulk values. The predicted bulk EFG is in good agreement with the experimental results. These results can be used for local probe purposes, for example in the case of doping, with important sensitivity for probes located close to the top of the surface, in particular for distances lower than 6 Å

1 - 25 – Study of the formation of $Co_3(BO_3)O_2$ by oxidation of Co_3B nanoparticles

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Until recently, the physical properties of the homometallic cobalt ludwigite, $Co_3(BO_3)O_2$, were unknown. The interest in this compound is due to the low-dimensionality of its structure, that is composed of low-dimensional subunits in the form of three-leg ladders, and the unexpected strong ferromagnetic ordering observed below 42 K that do not occurs in the compound $Fe_3(BO_3)O_2$ that have similar structure. The goal of our work is study the formation of the $Co_3(BO_3)O_2$ during the oxidation of Co_3B nanoparticles and the effect of antiferromagnetic spurious phases in its magnetic properties. The nanoparticles were prepared by reduction of Co^{2+} ions by sodium borohydride in 2-propanol and its specific surface area obtained by application of BET method in the N_2 adsorption isotherm is 52 m^2/g . Thermogravimetric analysis of oxidation process of these nanoparticles, combined with X ray diffratograms (XRD) of samples calcined in different temperatures, showed the formation process of the phases Co_3O_4 , $Co_3(BO_3)_2$ e $Co_3(BO_3)O_2$. The Rietveld analysis of XRD patterns revealed that the sample calcined at 800 °C is composed by 55.3% of $Co_3(BO_3)_2$ and 44.7% of Co_3O_4 , while the sample calcined at 900 °C is formed by 71.7% of $Co_3(BO_3)O_2$, 13.8% of $Co_3(BO_3)_2$ and 14.5% of Co_3O_4 . The magnetization curves of the sample calcined at 800 °C show features similar to the Co_3O_4 nanostructures, possibly due to the entanglement of the phases. An increase of coercivity of

the phase $\text{Co}_3(\text{BO}_3)_2\text{O}_2$ due to the presence of antiferromagnetic phases was observed. The results of this work contribute to understanding of the formation of $\text{Co}_3(\text{BO}_3)_2\text{O}_2$ that will allow in a future work the control of the preparation process and the study of the particle size effects in its magnetic properties.

1 - 26 – Dynamic hyperfine interactions in $^{111}\text{In}/^{111}\text{Cd}$ -doped ZnO semiconductor: PAC results supported by *ab initio* calculations

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During the last 25 years, dynamic hyperfine interactions have been observed in several Time-Differential γ - γ Perturbed-Angular-Correlation (PAC) experiments when the probe isotope ^{111}Cd , obtained after the electron-capture (EC) decay of its parent ^{111}In , was used in certain semiconducting and insulator oxides. These dynamic interactions are originated in the electronic relaxation of the probe atom, usually called "after-effects" (AE), which follows the EC decay of the ^{111}In isotope. This relaxation must occur during the life time of the intermediate-sensitive-nuclear state of the γ - γ cascade, time-window in which we measure the hyperfine interaction at the probe nucleus with external fields by means of the PAC technique. Up to now it was believed that the ECAE can only be detected if the probe atom was a non-isovalent impurity in the system under study.

Following these ideas, we present here results of PAC experiments performed in an oxide, ZnO, where the ^{111}Cd probe atom is an isovalent impurity. But this time the observed behavior will be analyzed enlighten by recent *ab initio* calculations of the electric-field gradients (EFG) as a function of the charge state of the Cd atom.

PAC experiments carried out on ^{111}In -diffused polycrystalline ZnO have been performed in order to measure the EFG at (^{111}In (EC) \rightarrow) ^{111}Cd nuclei located at the cation site of the ZnO crystal structure. The PAC experiments were performed in the temperature range 77 K-1075 K. The presence of dynamic hyperfine interactions with low intensity was observed, fitting the spectra with a perturbation factor based in the Båverstam and Othaz model [U. Båverstam et al., Nucl. Phys. A 186, 500 (1972)]. The experimental results were compared with *ab initio* calculations performed with the Full-Potential Augmented Plane Wave plus local orbital (FP-APW+lo) method, in the framework of the Density Functional Theory

(DFT), using the Wien2K code. The dependence of the EFG at the Cd sites as a function of the charge state of the supercell was determined. From this *ab initio*-experimental comparison we can correlate the strength dynamic hyperfine interaction with the dependence of the EFG on the charge state of the impurity Cd atom.

1 - 27 – Synthesis and characterization of thin films of Zn-Mn - Al - O system obtained by PLD

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Among semiconductor II-IV compounds, oxide zinc (ZnO) is one of the most promising for technological applications for its optical, electrical, piezoelectric and magnetic properties. In particular ZnO films exhibit unique properties that are appropriate for devices and magnet-optics applications. Incorporating aluminum and manganese allows obtaining a material known as diluted magnetic semiconductor (DMS) that continues showing a high bandwidth prohibited, retains its transparency in the visible range and is able to generate a magnetic order at room temperature. Starting from precursors ZnO, MnO_2 and Al_2O_3 , by conventional ceramic method were obtained powders, ZnO + 3% wt. of Al, + 2% ZnO at. Mn, + 2% ZnO at. Mn + 3% wt. of Al, and ZnO + 5% at. Mn + 3% wt of Al. These materials cold pressed to make the targets employees in pulsed laser deposition (LDP). (Deposits were made using a Nd-YAG (532 nm) laser in atmosphere oxygen on a substrate (SI 100) / SiO_2 /nitride) at 450 °C. The structural properties-obtained by DRX - and magnetic properties of powders and films were compared. Also the films were characterized surface and morphologically; determining presence of oxide of zinc and other oxides of Mn in powders samples. Also Zn oxide is detected in all films. Contrary to expectations, ferromagnetic ordering has not been detected, in films at room temperature.

1 - 28 – Structural and magnetic properties of pyrochlore $Gd_{2-x}M_xRu_2O_7$ (M = Ho, Y)

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Compounds with the pyrochlore structure, face centered cubic $A_2B_2O_7$, have been intensively studied in recent years due to its variety of properties arising from the different elements that can occupy the sites A and B. In this work, we present a systematic study of structural and magnetic properties the ruthenium pyrochlores $Gd_2Ru_2O_7$ as well as the effect of doping Gd site in the structure $Gd_{2-x}M_xRu_2O_7$ (M= Ho and Y). The X-ray diffraction patterns were analyzed by Rietveld refinement, allowing the identification of single-phased compounds and verification of the lattice parameter contraction with increasing doping concentration according to Vegard's law, independent of the dopant. The study of magnetic properties show that doping with Ho and Y, in site of Gd ions causes an increase and a dilution in magnetic moment of the compounds, respectively. The Curie constant and Weiss temperature calculated from experimental data show an indication of antiferromagnetic ordering below 35 K, in both compounds studied. It was verified that the addition of Ho increases the magnetic response of the material and decreases sharply the magnetic irreversibility present in the pristine sample, observed in the temperature range 9 - 16K. We conclude that by adding Ho one can tune the magnetic ordering of the sample by changing it from antiferromagnetic, in the absence of Ho, to ferromagnetic in the absence of Gd. It is observed that the Y doped samples preserves the magnetic order of the compound. It presents an antiferromagnetic order for all the dopant concentration studied. Nevertheless, it was also found that by increasing Y one can get a spin glass behavior. Work financed by CAPES, CNPq and FACEPE.

1 - 29 – Magneto-optic study of the behavior of magnetic domains walls in ferrimagnetic garnet films placed over samples with in-plane magnetization.

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Magneto-optic (MO)imaging is based on Faraday rotation of a linearly polarized incident light beam illuminating a sensitive MO layer placed in close contact to the sample. For in-plane magnetized layers of $Lu_{3-x}Bi_xFe_{5-y}Ga_yO_{12}$ ferrimagnetic garnet films, zig-zag domain formation occurs whenever the sample stray parallel field component changes sign. In this work we study the behavior of zig-zag domain walls that appear when the garnet is placed over samples with in-plane magnetization like audio tapes recorded with different signals. We describe the zig-zag walls considering the anisotropy, exchange and magneto-static energies in the Neel tails and the contribution of an applied magnetic field. Using different recorded signals we have been able to control the gradient of stray parallel field component on the garnet, changing the distance between domains and the size of zig-zag walls. We could even avoid the appearance of these zig-zag domain walls and obtain closed domains structures. We also study the behavior of the domain walls when an external magnetic field is applied parallel to the sample.

1 - 30 – Magnetic properties of Co doped $CeO_{2-\delta}$ nanopowders.

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The development of spintronics has promoted the study of materials with strong coupling between their electric and magnetic properties. For that kind of applications, the materials should have a high spin polarization and also present structural compatibility with existing semiconductors. Among materials that meet these requirements are the diluted magnetic oxides such as Co doped CeO_2 . The pure compound is a diamagnetic insulator, but on doping with magnetic ions like Co, Mn or Fe, the system can become paramagnetic or ferromagnetic. The great capability to accommodate oxygen vacancies in its structure seems to be the responsible for this particular behavior. In this work we study the magnetic properties of Co doped CeO_2 nanopowders, as a function of doping and the relative concentration of oxygen vacancies, by performing thermal treatments of the samples in a vacuum chamber. Our results indicate that magnetism is enhanced in samples with higher concentration of oxygen vacancies.

1 - 31 – *Ab initio* study of F-centers in alkali halides

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The structural and electronic properties of an electron trapped at vacant anion sites in alkali halides (F-center) have been investigated using *ab initio* band-structure calculations with the super-cell method. Despite of the underestimated transition energies we could obtain a qualitative agreement with the known experimental UV/Vis absorption energies.

We used the Full-Potential Linearized Augmented Plane Waves plus local orbital (FP-APW+lo) method in the framework of the Density Functional Theory (DFT), with a vacancy dilution of 1:64 in order to determine the spatial electronic charge density and the vertical transition energies.

1 - 32 – Electric-Field Gradients at ¹⁸¹Ta impurities in Sc₂O₃ semiconductor

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In this work we present a combined *ab initio* and experimental study of ¹⁸¹Ta-doped Sc₂O₃ semiconductor. An extrapolation to 0 K of the experimental electric-field gradient (EFG) results obtained by Perturbed Angular Correlations (PAC) as a function of temperature suggested a reinterpretation of the charge state of the impurity in this semiconductor.

The experimental temperature dependence of the EFGs at ¹⁸¹Ta probes located at defect-free cation sites C and D of the Sc₂O₃ structure was determined in the range 373 K - 1173 K.

The theoretical calculations were performed at diluted Ta impurities located at both cationic sites, using the Full-Potential Augmented Plane Wave plus Local Orbital (FP-APW+lo) method in the framework of the Density Functional Theory (DFT), with a impurity dilution of 1:32. The structural atomic relaxations and the EFGs were studied for different charge states of the cell in order to simulate different ionization states of the double donor Ta impurity (with a

neutral cell, and removing 1 or 2 electrons from the cell). These APW+lo results were found to be in excellent agreement with the experimental values.

1 - 33 – Dielectric and impedance spectroscopy studies on YBa₂Cu₃O_{7- δ} -Sr₂YSbO₆ composites

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We have studied the dielectric behaviour of YBa₂Cu₃O_{7- δ} -Sr₂YSbO₆ composites as a function of YBa₂Cu₃O_{7- δ} and Sr₂YSbO₆ volume fractions. Frequency dependence of complex impedance spectroscopy studies have been investigated in the frequency range from 1 Hz to 100 kHz. The experimental results showed that the composite undergoes a change in the electric behaviour, from resistive to dielectric for ~ 0.24 YBa₂Cu₃O_{7- δ} volume fraction. Fitting of permittivity in function of YBa₂Cu₃O_{7- δ} volume fraction shows a percolative behaviour, with a sudden change of permittivity value at percolation threshold of 0.24. The critical exponent for the permittivity is $u = 0.78$, which is in agreement of percolation theory. The complete study of the dielectric characteristics in function of volume fraction of components and of the frequency is discussed.

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1 - 34 – Structural and Magnetical properties of La(Fe, Cr, Mn)O₃ nanostructured systems

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The nomenclature *multiferroics* has been used to name materials in which two or more ferroic ordering simultaneously, i. e., ferroelectrics, ferromagnetics, and ferroelastics coexist in the same phase [1,2]. These materials have attracted innumerous researchers because of its perspectives of both fundamental physics and practical applications have to offer [3]. Although there exist many works in literatura devoted to the materials in bulk form, few works in these nanostructured materials have been reported in literature.

Besides, these materials are not easy to produce as single phase. In this sense, we have studied the synthesis process of $LaMTO_3$ (MT = Mn, Cr and Fe) in both bulk and nanostructured form using co-precipitation method. X-ray diffraction results added to the Rietveld refinement analysis confirm the formation of the crystalline phase of $LaFeO_3$, $LaCrO_3$ and $LaMnO_3$ identified as system orthorhombic, rhombohedral and orthorhombic, respectively with particles average size among 25 and 70 nm, calculated using Scherrer equation. DC-magnetization measurements carried out on a magnetometer SQUID point out an increasing in the magnetization with decreasing particles size. Beside, the magnetization measurements as a function of temperature show a change in T_N for samples obtained at different temperature, in which we have associate to the particle size. These results show to be promise with respect to the possibility of making small multiferroic nanostructures for future technological applications. (CNPq)

[1] T. Kimura *Phys. Rev. B*, **67**, 180401 (2003).

[2] G.A. Smolenskii and I.E. Chupis, *Sov. Phys. Usp* **25**, 475 (1982).

[3] Y. Wang, *Appl. Phys. Letters*, **88**, 142503 (2006).

1 - 35 – Non equilibrium Thermodynamics and entropy production spectra: a tool for ferrimagnetic materials characterization under electromagnetic field applied

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The entropy production and its evolution in the frequency domain upon application of electromagnetic fields to ferrite materials has been investigated. The spectral entropy of $NiZn$ ferrites doped with different amount of SiO_2 has been studied by numerical simulation. The system under the application of oscillating electromagnetic field is out of equilibrium, since there are entropy production due to dielectric and magnetic polarization. A system subjected to applied electromagnetic fields $E(\omega)$ and $H(\omega)$ at constant temperature T has been considered. For the numerical simulation of the behavior of the entropy production due to the magnetic relaxation a recent published causality model has been used. For the dielectric relaxation the well known Cole-Cole model has been used. The behavior of the entropy as a function of the frequency with the correlation of the amount of SiO_2 has been analyzed in terms of entropy production due to increasing the electric resistance between the boundary grains and the response of the magnetic

and dielectric properties. Entropy production related to magnetic response could be associated with domain wall resonance and spin rotation relaxation. Entropy production related to dielectric processes could be associated with the delay of the different components of the polarizability as a function of the frequency of the applied field and the correlation with the transport charge mechanism in the material. Then the entropy spectra will be transformed in a tool for ferrimagnetic material analysis

1 - 36 – Hyperfine interactions and site localization of Sc impurities in Sapphire

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Single electric-field gradient (EFG) obtained from γ - γ Perturbed Angular Correlation (PAC) experiments at $^{111}\text{In}/^{111}\text{Cd}$ impurity sites in $\alpha\text{-Al}_2\text{O}_3$ have been already reported in the literature [1,2]. In these works the hyperfine interaction observed were assigned to ^{111}Cd probes localized at substitutional cation sites in the corundum structure. Nevertheless, other authors [3,4] claimed that the ^{111}Cd isotope could be localized at interstitial sites after the electron-capture decay of ^{111}In .

In this work we present a theoretical study of Sc impurities in $\alpha\text{-Al}_2\text{O}_3$ performing electronic-structure *ab initio* calculations for different impurity charge states and site localizations (substitutional and interstitial) and compare the EFG predictions (in magnitude, orientation and symmetry) with preliminary experimental results obtained in singlecrystals doped with the $^{44}\text{Ti}/^{44}\text{Sc}$ probe. The structural relaxations and the electronic properties induced by the presence of the Sc impurity at both sites (substitutional and interstitial) in the $\alpha\text{-Al}_2\text{O}_3$ lattice are also discussed. The *ab initio* calculations were performed with the FP-APW+lo (Full-Potential Augmented Plane Wave plus Local Orbitals) in the framework of the Density Functional Theory, using the Wien2K code. From the comparison between theory and experiment both substitutional and interstitial scenarios are possible, in order to explain the two hyperfine interactions present in this impurity-host system.

[1] S. Habenicht, D. Lupascu, M. Neubauer, M. Uhrmacher, and K.P. Lieb, *Hyp. Int.* **120/121**, 445 (1999).

[2] J. Penner and R. Vianden, *Hyp. Int.* **158**, 389 (2005).

[3] J.G. Marques, A.A. Melo, J.C. Soares, E. Alves, M.F. da Silva, K. Freitag, *Nucl. Instr. and Meth. in Phys. Res. B* **106**, 602 (1995).

[4] G. C. Farlow, P. S. Sklad, C. W. White and C. J. McHargue, *J. Mater Res.* **5**, 1502 (1990).

1 - 37 – Magnetic properties of lamellar aluminosilicate structure rich in Fe

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Layers of Si-Al-O can be formed when the ratio $O/(Si + Al) = 2.5$ is obeyed, giving rise to lamellar structures aluminosilicates type, which have interesting physical properties, eg, transport and controlled release of drugs in anti-cancer therapies. In natural samples, there is a very high possibility of ionic exchange, allowing the formation of a lamellar structure consisting of transition metals, particularly iron. Natural samples from the coast of Sergipe, Brazil were collected, washed and separated from sand by a permanent magnet. Analysis by SEM,EDS, XRF and XRD showed a Biotite-like mineral as the major component of the sample. SEM show clearly a lamellar structure presented by typical true micas and in the association with the high level of Iron showed by EDS and XRF analysis and, with help XRD phase identification, this material has a ferriphlogopite-like structure. Another phase founded was a clinocllore-like mineral, namely chamosite and goethite. When in raw mode, the original sample showed the presence of quartz, rutile and possibly crossite. Magnetic measurements (saturation magnetization, remanence magnetization and coercive force) and the anisotropy constant $K(T)$ have been determined at room temperature and at low temperatures using magnetic fields up to 7 T. Influenced by the lamellar structure, the average value of K for an applied field parallel to the lamellae, was 2082 and 3.3 *emu.Oe/g* at 2 and 300 K, respectively. For an applied magnetic field perpendicular to the lamellae, was 1338 and 3.8 *emu.Oe/g* at 2 and 300 K, respectively. The H_c versus T curve showed a minimum of 34 Oe about 15 K due to the presence of pseudo-single-domains probably formed by the buildup of $\alpha FeOOH$, revealed by analysis of SEM.

1 - 38 – Synthesis and structural and electrical characterization of new materials $Bi_3R_2FeTiO_{15}$

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In this work we report the synthesis of polycrystalline samples of Bi_5FeTiO_{15} (BFT) and $Bi_3R_2FeTiO_{15}$ compounds with

$R = Nd, Sm, Gd, Dy, Ho, Yb$. The materials were synthesized by the standard solid state reaction recipe from high purity (99.99%) powders. The structural characteristics of materials were analyzed by x-ray diffraction experiments. Results reveal that materials crystallized in orthorhombic single-phase structures and space group to be $Fmm2$, Rietveld refinement by the GSAS code was performed, taking the input data from the ICSD 74037 database. Measurements of polarization as a function of applied electric field were carried out by using a Radiant Technology polarimeter. We obtain a hysteretic behavior, which is characteristic of ferroelectric materials that can be used as nonvolatile memories. Rapid growth is appreciated on the $2E_c$ and $2P_r$ with increasing external electric field applied to polarize the compound.

1 - 39 – Magnetic properties of the disordered barium titanium manganite $BaTi_{1/2}Mn_{1/2}O_3$.

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Oxides materials with perovskite structure are outstanding examples of materials used in technological applications as well as in fundamental studies in condensed matter physics because of the observed ground states which include multiferroicity, high-temperature superconductivity, colossal magnetoresistive effects, ionic conductivity, etc. The ideal formula unit is ABO_3 , where A is a large cation, e.g. K, Sr, Ba, La, and B is a smaller cation like Ti, Mn, Co, Ni. When a second (B') transition metal atom is added to the above structure, an ordered double perovskite type structure $A_2B'B''O_6$ (where $B', B'' = 3d, 4d, 5d$ metals) as well as a disordered $AB'_{1/2}B''_{1/2}O_3$ perovskite-type structure might be formed, which have attracted great attention due to their potentiality as magneto-electronic devices.

In this work we present the results of the low temperature specific heat and magnetization measurements as well as the high temperature magnetization data of the barium titanium manganite $BaTi_{1/2}Mn_{1/2}O_3$. This 12R-type hexagonal perovskite is a modest dielectric insulator at room temperature with high permittivity at both radio and microwave frequencies and its magnetic behavior as a function of temperature remains unclear. We have performed detailed specific heat and magnetization measurements as a function of the applied field and temperature in order to understand the detailed magnetic behavior of the Mn^{+IV} ions. Our results show

the presence of a ferromagnetic phase at high temperature ($T > 300$ K) coexisting with a previously reported low temperature antiferromagnetic phase. We evaluate and discuss the mechanisms that drive the coexistence of the magnetic interactions.

1 - 40 – Magnetic measurements in double perovskite $\text{Ca}_2\text{FeMoO}_6$ single crystal

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In the 1990's decade materials exhibiting colossal magnetoresistance (CMR) were widely studied due to technological interest. A range of compounds were found to exhibit intrinsic CMR, most of them are manganese perovskites based on LaMnO_3 . A few years later, some members of the family of double perovskites of composition A_2MTO_6 ($A =$ alkali earths, $M, T =$ transition metals) have been proposed as halfmetallic ferromagnets, as an alternative to perovskite manganites. We focused our attention on the Ca analogue of the A_2FeMoO_6 family. $\text{Ca}_2\text{FeMoO}_6$ perovskite has been prepared in single crystalline form by a floating zone technique as described elsewhere.[1] This high quality material has been studied by X-ray powder diffraction (DRX), thermal analysis, and magnetic measurements. The crystal structure is monoclinic, space group $\text{P}2_1/\text{n}$, with $a = 5.41(1)$ Å, $b = 5.52(1)$ Å, $c = 7.71(2)$ Å, and $\beta = 89.9(8)^\circ$ at room temperature (RT). The crystal contains alternating FeO_6 and MoO_6 octahedra, considerably tilted due to the relatively small size of the Ca^{2+} cations. Magnetization as a function of temperature indicates a Curie temperature of 380 K, in agreement with the obtained by others authors in polycrystalline sample.[2] The dependence of magnetization with magnetic field at 5 K, 100 K and 300 K are typical of a ferromagnet with a saturation magnetic moment of approximately $2.1 \mu_B$, $2.0 \mu_B$ and $1.4 \mu_B$ per formula unit, respectively. Magnetism indicate a large component of itinerancy for down-spin Fe t_{2g} electrons. M

[1] L.B. Barbosa, D. Reyes Ardila, J.P. Andreetta, *Journal of Crystal Growth* 254 (2003) 378-383

[2] J.A. Alonso, M.T. Casais, M.J. Martínez-Lope, J.L. Martínez, P. Velasco, A. Muñoz and M.T. Fernandez, *Chem. Mater.* 12, (2000) 161-168.

1 - 41 – Electromagnetic properties of lithium zinc ferrites doped with aluminium

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Ferrites form a very good class of electrical materials because of their high resistivity and low loss behaviour, and hence have vast technological applications over a wide range of frequencies. Ferrites assume special significance in the field of electronics and telecommunication industry because of their novel electrical properties which makes them useful in radiofrequency circuits, high quality filters as electromagnetic interference (EMI), rod antennas, transformer cores, read/write heads for high digital tapes and other devices. The dielectric properties of ferrites are dependent on several factors, such as method of preparation, heat treatment, sintering conditions, chemical composition, cation distribution and crystallite size. We present the results of the effect of Al substitution on the magnetic and electrical properties of $\text{Li}_{0.2}\text{Zn}_{0.6}\text{Fe}_{2.2-x}\text{Al}_x\text{O}_4$ ferrites (where $0 \leq x \leq 0.5$) prepared by the standard ceramic technique. The characterization has been performed using XRD, SEM, magnetic and dielectric response in frequency. XRD analysis confirms that the system exhibits polycrystalline single phase cubic spinel structure only to low dopant content. Dielectric loss tangent are lower by replacing in the whole frequency range analyzed. Doping decreases the conductivity of the ferrite in more than two orders of magnitude. Reflection losses has a maximum near 50MHz for $x=0$ and they decrease significantly to high levels of aluminium. these ferrites can be used as EMI devices.

1 - 42 – Determination of critical exponents of inhomogeneous Gd films

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An understanding of thermal phase transition behavior of inhomogeneous ferromagnets has been an outstanding problem in the science of magnetism. On the other hand, homogeneous magnetic films have been an important case study due to the fact that their universality class is relatively well understood and adequate fabrication methods have been devised. In this work, we explore the role of inhomogeneity on the critical behavior of Gd films. The films were prepared as $\text{Cr}(50\text{nm})/\text{Gd}(100\text{nm})/\text{Cr}(50\text{nm})$ multilayers grown onto $\text{Si}(110)$ single crystal substrates by

means of ultra high vacuum sputter deposition. The sample inhomogeneity was controlled by annealing at different temperatures, $T = 500, 400,$ and 200 C). VSM magnetometry was used for the magnetization M vs. T measurements at different external fields H . To extract the critical exponents and the distribution of intrinsic Curie temperatures T_c we applied a linear superposition theory [1] which views the $M(T)$ dependence as a distribution of power laws centered at specific T_c s. We found that this method allows us to extract reliable values of the critical exponents for all annealing temperatures, which enabled us to study the effects of disorder onto the universality class of Gd-films.

[1] A. Berger et al., J. Appl. Phys. 91, 8393 (2002)

1 - 43 – Synthesis and characterization of cobalt-doped manganese oxides

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In this work, cobalt doped and undoped manganese oxides materials were synthesized by soft chemical reactions, specifically by oxido-reduction method, which allows us to generate metal mixed oxide. The synthesized materials were characterized using chemical analysis which shows the presence of cobalt, XRD reveals a spinel type structure and SEM analysis shows morphology with fine aggregate of particles. Vibrating sample magnetometry was used to determinate the hysteresis loops at different temperatures. We observed different magnetic behavior, when the manganese oxide material is cobalt doped.

1 - 44 – Structural and electronic properties influenced by high pressure in $\text{La}_{0.325}\text{Pr}_{0.300}\text{Ca}_{0.375}\text{MnO}_3$

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Because of the strong coupling between their different degrees of freedom (i. e. magnetic, electronic and structural), manganites are nowadays one of the most studied in the family of strongly correlated electrons systems. The enormous capacity of tuning its properties by the application of moderated

external excitations (magnetic and electric field, hydrostatic pressure, etc.) converts manganites in one of the most investigated systems for potential technological applications. The effect of high pressure in the structure of manganites is one of the less studied topics, mainly due to the complexity of the experimental procedure. In this work we have studied the temperature-magnetic field-pressure phase diagram of $\text{La}_{0.325}\text{Pr}_{0.300}\text{Ca}_{0.375}\text{MnO}_3$ using magnetization (M), X ray diffraction (XRD) and resistivity (R) measurements. At room pressure, we observed a paramagnetic state above 220K, followed by a region of coexistence of ferromagnetism and charge ordered phase between 200K and 75K, and a purely ferromagnetic state below 75K. The existence of all these phases has been shown by different techniques like M , XRD and R . In this presentation we will show the effect of external applied pressure on the transport and the structure up to 300kbar. We will correlate the crystallographic and the electronic phases in order to clarify the phase diagram.

1 - 45 – Magnetic Hydrophobic Nanocomposites: Silica Aerogel/Maghemite

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In this work we present a new material: Magnetic hydrophobic aerogels (MHA). It consists of iron-oxide nanoparticles hosted in hydrophobic silica aerogels. In this work, we discuss about the fabrication and characterization of this nanocomposite. We also investigate the relation between the MHA's porosity and magnetic nanostructure.

Silica aerogel/iron oxide nanocomposites were fabricated by means of the sol-gel process followed by supercritical drying. The gel obtained in this process was synthesized from tetraethylorthosilicate (TEOS) and methyltrimethoxysilane (MTMS), with a molar ratio $\text{MTMS}/\text{TEOS} = 0.5$. MTMS was added to achieve the aerogels' hydrophobic property. As Fe oxide precursor, we incorporated iron nitrate. We fabricated samples with different $m_{\text{Fe}}/m_{\text{Si}}$ ratios: 0.083, 0.207, and 0.330. The molar ratios $\text{alcohol}/\text{TEOS} = 2.3$ and $\text{H}_2\text{O}/\text{TEOS} = 1.8$ were kept fixed in all of them.

The structural and magnetic properties of $\text{Fe}_2\text{O}_3 - \text{SiO}_2$ nanocomposite porous aerogels were systematically investigated by XRD, Mössbauer Spectroscopy, TEM, SQUID magnetometry and with SAXS and XAF by using synchrotron radiation at LNLs.

These materials exhibit an accessible internal porous structure, both in the meso and in the micro

scale. Porosity structure was studied by SAXS and displays the typical fractal power law behaviors with primary particle radius of 20 nm.

Field cooled and zero field cooled magnetization curves indicate that the composites behave as an assembly of non-interacting superparamagnetic nanoparticles for the three compositions studied. The samples become blocked at a temperature TB between 27 and 40K.

Direct magnetic particle size determination is not an easy task because these materials exhibit low crystallinity and low contrast for TEM. Here we attempt this determination using SAXS: hydrophobicity allows the aerogel to be loaded with an organic liquid to lower the silica/porous contrast and highlight the nanoparticle/silica contrast. Contrast studies and the feasibility of a direct determination of magnetic structure from the scattering data are discussed.

The results provide new insights into innovative materials and on the relation between the compositional and microstructural features, and the properties of magnetic nanocomposite.

1 - 46 – Specific Loss Power of ferrofluids under Radiofrequency fields

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Ferrofluids (FF) are liquid suspensions of magnetic nanoparticles. When FF are submitted to a radiofrequency (RF) magnetic field, the nanoparticles dissipate energy. In the case of single domain particles two relaxation mechanisms exist, known as Néel and Brown mechanisms. Néel relaxation depends on particle magnetic anisotropy, whereas Brown relaxation depends on fluid viscosity. Both types of relaxation depend on temperature and particle size, but through different functional expressions. Except for the infrequent situation in which the two relaxation times are equal, relaxation occurs almost entirely by one of the two mechanisms.

In this work we study aqueous FFs of $Zn_xFe_{3-x}O_4$ ($0 \leq x \leq 0.5$). We have determined the FF Specific Loss Power (SLP), defined as the power dissipated per mass unit of nanoparticles, as a function of RF field parameters (amplitude H_0 and frequency f) and FF concentrations. H_0 was varied up to 700Oe and discrete f values between 160 kHz and 260 kHz were used. The nanoparticles mass/water volume ratio, $R = m_{NP}/V_{FF}$, was varied from about 1 g/l to 10 g/l.

We observed that measured SLPs did not depend on R . On the other hand, SLP f and H_0 dependences deviate slightly but clearly from the behaviors found

in the literature. It was reported that SLP depends linearly and quadratically with f and H_0 , respectively [1]. The experimental results indicate that for field amplitude larger than about 500 Oe, SLP increases at a slower rate than predicted by the power H_0^2 law, suggesting saturation effects. Simulations based on the Stoner-Wholfahrt model modified for finite temperature conditions, give a consistent account of the observations. The simulations illustrate how the M-H minor loops shape determines the previously mentioned dependences.

[1] Kallumadil, M., Tada, M., Nakagawa, T., Abe, M., Southern, P., Pankhurst, Q.A., *Journal of Magnetism and Magnetic Materials* 321 (2009) 1509-1513.

1 - 47 – Electrical transport properties of manganite powders under pressure.

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We have measured the electrical resistance of micrometric to nanometric powders of the $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ (LPCMO with $y=0.3$) manganite for hydrostatic pressures up to 4 kbar. By applying different final thermal treatments to samples synthesized by a microwave assisted denitration process, we obtained two particular grain characteristic dimensions (40 nm and 1000 nm) which allowed us analyze the grain size sensitivity of the electrical conduction properties of both the metal electrode interface with manganite (Pt / LPCMO) as well as the intrinsic intergranular interfaces formed by the LPCMO powder, conglomerate under the only effect of external pressure. We also analyzed the effects of pressure on the phase diagram of these powders. Our results indicate that different magnetic phases coexist at low temperatures and that the electrical transport properties are related to the intrinsic interfaces, as we observe evidences of a granular behavior and an electronic transport dominated by the Space Charge limited Current mechanism.

1 - 48 – Resistive switching topology in metal-complex oxide interfaces

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In order to determine the key parameters that control the resistive switching mechanism in metal-complex oxides interfaces, we have studied the electrical properties of metal / YBa₂Cu₃O₇ (YBCO) interfaces using metals with different oxidation energy and work function (Au, Ag, Pt) deposited by sputtering on the surface of a YBCO ceramic sample. By analyzing the IV characteristics of the contact interfaces and the temperature dependence of their resistance, we inferred that ion migration may generate or cancel conducting filaments, which modify the resistance near the interface, in accordance with the predictions of a recent model.

1 - 49 – Electric transport through nanometric CoFe₂O₄ thin films investigated by conducting atomic force microscopy

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The ferrimagnetic insulating spinel CoFe₂O₄ (CFO) is considered a promising candidate material for spintronic devices, e.g as spin filtering tunnel barrier capable to work at room temperature. However, although spin filtering through CFO thin films has been successfully demonstrated, up to now reported efficiencies are clearly below expectations.

In the search of optimized CFO thin films, we have used conducting atomic force microscopy (CAFM) to perform a systematic study of electric transport through thin (1-8nm) CFO films deposited on SrRuO₃ thin film bottom electrodes. Samples were grown on (111) and (001) oriented SrTiO₃ substrates using either rf sputtering or pulsed laser deposition (PLD).

Experimental procedures to investigate tunnel transport through thin insulating films by CAFM are revised. The potential of differently prepared CFO films for the use as spin filtering barrier is assessed. Samples prepared by PLD on SrRuO₃/SrTiO₃ (001) are found to offer improved properties compared to rf sputtered CFO thin films.

1 - 50 – Light induced negative magnetoresistance in ZnO Films.

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Transient photoconductivity and magnetotransport measurements were used to investigate the spin interaction in pure ZnO thin films grown under N₂ pressure. Light induced temperature dependent negative magnetoresistance was measured at 300K in ZnO films growth on c-plane Al₂O₃. There is a correlation between the magnetoresistances and the existence of defect-induced magnetic order already reported in these films. The oxygen and/or nitrogen 2p orbitals are responsible of the magnetic exchanges interaction. The experimental results support theoretical predictions of photoinduced ferromagnetism interaction in diluted magnetic semiconductors.

1 - 51 – Effects of Dopant Cation Order in 3D and Layered Perovskite Manganites

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The 3-dimensional and layered La,Sr-doped manganites, (La_{1-x}Sr_xMnO₃)_n·SrO, exhibit a delicate interplay between charge, spin and orbital degrees of freedom which gives rise to a number of intriguing collective states. Depending on cation doping (x) and dimensionality (n), these materials can exhibit ferromagnetic, antiferromagnetic, charge and orbital ordering. Recently, our group has shown that ordering the A-site cations through the atomic-monolayer control of molecular beam epitaxy can uncover additional physics in the 3-dimensional (3D) systems, including a metal-insulator transition, higher anti-ferromagnetic ordering temperatures, and modulated in-plane ferromagnetic and antiferromagnetic ordering as a function of depth. Here, we investigate the effects of A-site cation order on the magnetism, transport and magnetotransport of two related systems: (1) the 3D, ferromagnetic and colossal magnetoresistant La_{1-x}Sr_xMnO₃ (x=1/3) and (2) its 2-dimensional analog, single layered La_{1-x}Sr_{1+x}MnO₄ (x=1/3), which in bulk only exhibits a spin-glass phase below 20K. We find that in both systems, while the in-plane magnetism appears largely unaffected

by the dopant cation order, the out-of-plane magnetism perpendicular to the cation-ordered sheets is enhanced. Additionally, in the single layer manganite, large differences in magnetic anisotropy and low temperature transport mechanisms between the cation ordered and disordered films suggest that ordering the dopant cations in this layered compound results in a new preferred orbital ground state.

1 - 52 – Electric Pulse Induced Resistive Switching Contacts for Non Volatile Memory Devices

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Non volatile memory concepts for electronic applications are presently based on resistance change rather than in charge storage. Electric pulse induced resistance switching (RS) was shown to produce useful retention time capability for massive applications. Several basic and applied research teams are presently devoted to the study of transition metal oxides contacted through metal electrodes driven by appealing fast switching and scalability.

We study manganite (LaPrCaMnO) and titanium dioxide (TiO) samples contacted with metallic electrodes, under different experimental conditions. Evidence for an oxygen diffusion mechanism by means of electric transport measurements was obtained using the Hysteresis Switching Loop procedure in which pulses of varying amplitude determine the state of the interface, and a small bias is used to test the remnant state, in a loop mode. Obtained results can be explained by oxygen vacancy detrapping at the oxide-metal interface. Besides, we study the characteristics of RS applying a closed-loop control protocol of the amplitude pulse to attain a certain resistance level.