Oxides and related topics

1 - 1 – Hf influence on the magnetic behavior of hematite nanoparticles

Bercoff, P.G.,[1,2] Carpenco, J.,[3] Herme, C.,[3] and Jacobo, S.E.[3]

[1]*Facultad de Matemática, Astronomía y Física. Universidad Nacional de Córdoba. Ciudad Universitaria, Córdoba, Argentina.*
[2]*IFFAMAF, Conicet. Argentina.*
[3]*LAFMACEL, Facultad de Ingeniería, UBA. Paseo Colón 850, C1063EHA, Buenos Aires, Argentina.*

In order to study the influence of defects on the memory effect of hematite, Hf-doped hematite was synthesized by the self-combustion method. The obtained nanoparticles of 60 nm were characterized by x ray diffraction and magnetometry. Room temperature hysteresis loops show a paramagnetic contribution that slightly increases with Hf content and a very hard ferromagnetic contribution with coercivities which reach 6100 Oe for the sample with higher Hf content. Magnetization vs temperature data indicate that memory is enhanced while the Morin temperature is lowered with the doping, even when the concentration of Hf is as low as 1%. The results are interpreted in terms of the changes in the anisotropy introduced by the defects in the lattice.

1 - 2 – Electronic and Magnetic Properties of Double Perovskites A_2FeReO_6 (A = Ba, Ca)

Melo, J.I.[1] and Weht, R.[2]

[1]*Departamento de Fisica, FCEyN, UBA*
[2]*Gerencia de Investigación y Aplicaciones Comisión Nacional de Energía Atómica Avda General Paz y Consituyentes, San Martín, Argentina*

Double Perovskites with general formula $A_2BB'O_6$ have been subject of a very recent interest because the strong interplay among their electronic, magnetic and structural degrees of freedom. That richness comes as a result of the different possible elections for the A, B and B' sites. In this work we will concentrate our attention on systems with A = Ba and Ca, and BB'= FeRe. It has been shown that when going through A = Ba to Ca the system undergoes a metal-insulator transition (MIT) coincidentally to a structural transition, even though conduction band filling is not significantly changed. $Ba_2BB'O_6$ has been proposed to be a half metal with high magnetic transition temperatures and spin dependent transport properties, while $Ca_2BB'O_6$ seems to have a semiconducting transport behavior. We will present here several studies on the magnetic and electronic properties of these dobule perovskites, analyzing the possible mechanisms responsible for that metal insulator transition. To this end, we will use ab initio methods based on density functional theory that include electronic correlation effects via hybrid functionals and the LDA+U scheme.

1 - 3 – Cathodoluminescence and first principle study of defects in ZnO.

Mass, J.,[1] López, W.R.,[1] Ródriguez, J.A.,[2] and Jiménez, J.[3]

[1]*Departamento de Física, Universidad del Norte-Colombia.*
[2]*Departamento de Física, Universidad Nacional de Colombia.*
[3]*Departamento de Física de la Materia Condensada, Universidad de Valladolid-España.*

We have developed a theoretical-experimental study of optical and electronic properties of pure ZnO, with a Zn(O) vacancy and with a Li substitution. In order to study the electronic properties of the systems, we carry out first principles calculations in the Density Functional Theory (DFT) framework. To model the pure compound we consider a 32-atoms 2x2x2-supercell (16 O and 16 Zn). To represent a Zn(O) vacancy in the material, a Zn(O) atom is subtracted from the super-cell of pure ZnO. Subsequently, we substitute the vacant site with a Li atom simulating a Li concentration of 6.25%. With relation to optical properties, we performed measurements by cathodeluminescence on ZnO hydrotermics crystals, being observed a yellow-orange lumines-cence that can be associated to the presence of Li impurities or Zn vacancies. The analysis of the theoretical results and experimental measurements validates the fact that Li impurity and Zn vacancy are little deep acceptors that give rise to the luminescence band in the mentioned visible range.

1 - 4 – Influence of the B site ordering on the magnetic properties in the new $La_3Co_2MO_9$ double perovskites with M = Nb or Ta

Fuertes, V.C.,[1] Blanco, M.C.,[1] Franco, D.G.,[1] De Paoli, J.M.,[1] Pannunzio-Miner, E.V.,[1] Sánchez, R.D.,[2] Fernández-Díaz, M.T.,[3] and Carbonio, R.E.[1]

[1]*INFIQC, Dep. de Fisicoqca., Fac. de Cs. Qcas., UNC. Argentina.*
[2]*Laboratorio de Resonancias Magnéticas. Centro Atómico Bariloche. Argentina.*
[3]*Institut Max Von Laue Paul Langevin, Grenoble, France.*

Perovskite compounds are very interesting materials because of their potential technological applications. The ideal cubic perovskite structure can be seen like a three-dimensional corner-sharing network of BO6 octahedra, with a large A-cation occupying the cuboctahedral cavities. Double perovskites are formed with the general formula A2B'B"O6 were ions B' and B", in the ideal case, occupy different crystallographic sites. Usually, however, there is a certain degree of "anti-site" disorder, where a fraction of B'occupies the B" sites and vice versa. Usually, A is an alkali-earth ion, like Ca^{2+}, Sr^{2+}, Ba^{2+}. However, there are few reports of double perovskite materials in which the A site ion has been totally replaced by a small lanthanide Ln^{3+}. Magnetism in these compounds can be achieved when de B site ion is a transition metal cation with unmatched electrons. Magnetic properties, like ferromagnetism, or ferrimagnetism, in double perovskites are strongly dependent on their B cations order-disorder relationship. In the present work we describe the synthesis, structures and magnetic characterization of a new perovskite type family: $La_3Co_2MO_9$ with M = Nb, Ta. These phases were synthesized as polycrystalline powders by both standard ceramic and sol gel method, this last one by a tartrate-precursor decomposition. Their crystallographic formula can be written as $La_3(Co)_{2d}(CoM)_{2c}O_9$ for samples synthesized by solid state and as $La_3(Co_{2-x}M_x)_{2d}(Co_xM_{1-x})_{2c}O_9$ for those synthesized by the sol-gel method. Structural analysis was made through Rietveld refinement from XRPD and NPD data. All are insulator monoclinic double perovskites and can be well characterized in P 21/n SG. Anti-site disorder is noticeable larger in the sol-gel compounds case. Magnetic measurements were made in a commercial SQUID in the 10-300 K temperature range, with the objective to understand the effect that causes this disorder on the magnetic properties of these materials. M vs T measurements indicated that samples synthesized by solid state are ferromagnetic with TC c.a. 60 K, while those synthesized by the sol-gel method are antiferromagnetic materials with TN c.a. 20 K. The solid state method synthesized compounds have shown to be more B site ordered than sol-gel synthesized compounds. We assign different magnetic behaviours displayed by both compounds to these differences in antisite disorder. The refined magnetic cells are in agreement with magnetic measurements in both, ferromagnetic and antiferromagnetic cases.

1 - 5 – Magnetic microspheres for technological applications: Preparation and characterization

Podzus, P.E,[1,2] Daraio, M.E.,[1] and Jacobo, S.E.[2]

[1]*Grupo de Aplicaciones de Materiales Biocompatibles*
[2]*LAFMACEL*

One of the major applications of chitosan and its many derivatives are based on its ability to bind strongly heavy and toxic metal ions. In this study chitosan magnetic microspheres have been synthesized. Acetic acid (5% w /v) solution was used as solvent for the chitosan polymer solution (2% w /v) where magnetite nanoparticles were suspended in order to obtain a stable ferrofluid. The magnetic characteristic of these materials allows an easy removal after use if is necessary. Glutaraldehyde was used as crosslinker. The morphological characterization of the microspheres was carried by optical methods. The results show that the microspheres can be produced in the size range 500-700μm. Release kinetics of a model drug (KNO_3, as a possible fertilizer) and heavy metal complexation (Cu (II)) were analyzed. The drug release behavior can be modulated by crosslinking. The adsorption capacity for Cu(II) on chitosan microspheres was found to be in the order of 10% w /w.

1 - 6 – Microwave-absorbing characteristics of epoxy resin composites containing nanoparticles of NiZn and NiCuZn ferrites

Aphesteguy, J.C.,[1] Damiani, A.,[2] DiGiovanni, D.,[2] and Jacobo, S.E.[1]

[1]*LAFMACEL, Fac.Ingeniería, UBA*
[2]*División Antenas, CITEFA*

NiZn and NiCuZn ferrite nanoparticles (50-70nm) with the chemical formula $Ni_{0.5}Zn_{0.5}Fe_2O_4$ (NiZn) and $Ni_{0.35}Zn_{0.5}Cu_{0.15}Fe_2O_4$ (NiCuZn) were synthesized by a combustion synthesis method. The nanocrystallite of these materials were characterized by structural and magnetic methods. Saturation magnetization increases from 83 emu/g (NiZn) to 91 emu/g (NiCuZn). Magnetic permeability and dielectric permitivity were measured on sintered samples (pellets and toroids) in the frequency range of 1 MHz-1.8 GHz. Cu substitution in NiZn ferrite enhances permeability and magnetic losses. Tan δ (dielectric losses) at 1.3 GHz is close to 0.01 in NiCuZn while is much lower (0.006) in NiZn. These results are related to absorption properties in that microwave

range. In order to explore microwave-absorbing properties in X-band, magnetic nanoparticles were mixed with an epoxy resin to be converted into a microwave-absorbing composite and microwave behaviors of both materials were studied using a microwave vector network analyzer from 7.5 to 13.5 GHz. Cu substitution increases absorption intensity at 9 GHz while at another absorption frequencies (7.75 and 11.5 GHz) minor intensity is observed. Preliminary results on samples prepared under a moderate magnetic field are presented.

1 - 7 − Fluctuation conductivity of $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ (RE=Y, Sm, Gd, Dy, Ho, Yb) superconductors

Parra Vargas, C.A.,[1,2] Barrera B, E.W.,[1] Pimentel Jr, J.L.,[3] Pureur, P.,[3] Landínez Téllez, D.A.,[1] and Roa-Rojas, J.[4]

[1] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC*
[2] *Grupo de Física de Materiales, Escuela de Física, UPTC, Tunja*
[3] *Instituto de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, RS, Brasil*
[4] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC*

We report production and conductivity characterization of $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ (RE=Y, Sm, Gd, Dy, Ho, Yb) high temperature superconducting system. Samples were synthesized by the standard solid state reaction recipe. Rietveld-type refinements of x-ray diffraction patterns permit us to determine that the material crystallizes in a tetragonal structure. DC resistivity measurements show a bulk critical temperature Tc $\approx$ 75 K for the analyzed samples. In order to examine the effect of substitution of rare earth into the lanthanum structural sites on the pairing mechanism close to Tc, conductivity fluctuation analysis was performed by the method of logarithmic temperature derivative of the conductivity excess. We found the occurrence of Gaussian and genuinely critical fluctuations. Our results are in agreement with reports on non doped $LaBaCaCu_3O_{7-\delta}$ superconductor, but minor values of the coherence length of the fluctuation regimes were observed for the doped case. The correlations of the critical exponents with the dimensionality of the fluctuation system for each Gaussian regime were performed by using the Aslamazov-Larkin theory. From the reduced temperature of the three-dimensional Gaussian regime and the mean field critical temperature, the Ginzburg number for this superconducting material is predicted and the critical magnetic fields, critical current density and the jump in the specific heat at the critical temperature is theoretically determined. The genuine critical exponent is interpreted by the 3D-XY model as corresponding with the dynamical universality predicted by the E-model.

This work was partially supported by DIB, Colciencias on the project No. 1101-333-18707 and Centro de Excelencia en Nuevos Materiales, contract No. 043-2005.

1 - 8 − Magnetization fluctuation analysis and superconducting parameters of $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ (RE=Y, Sm, Gd, Dy, Ho, Yb) superconductors

Parra Vargas, C.A.,[1,2] Pimentel Jr, J.L.,[3] Pureur, P.,[3] Landínez Téllez, D.A.,[1] and Roa-Rojas, J.[1]

[1] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC*
[2] *Grupo de Física de Materiales, Escuela de Física, UPTC, Tunja*
[3] *Instituto de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, RS, Brasil*

In this work we report analysis of experimental data of the magnetization of $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ (RE=Y, Sm, Gd, Dy, Ho, Yb) superconducting systems. The data are analyzed in terms of thermal fluctuations on the magnetization excess $\Delta M(T)$ for different values of temperature in each sample. We describe a procedure for extracting the penetration depth λ_{ab}(T) ($\approx 2350\mathring{A}$) and the coherence length ξ_{ab} ($\approx 20.2\mathring{A}$) parameters from the magnetization, as a function of the applied magnetic field. This procedure was performed for polycrystalline samples of $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ by using the Bulaevskii, Ledvij and Kogan theory which analyzes the vortex fluctuation in superconducting materials within the Lawrence-Doniach framework. These data allowed to determine the characteristic temperature value T* (73, 58, 48, 57, 56, 71 K, for RE=Y, Sm, Gd, Dy, Ho, Yb respectively) in the magnetization curves for several magnetic fields. We calculated the data of magnetization excess from curves of Magnetization as a function of logarithm of applied field. We notice that the values for these superconducting parameters are in agreement with reports for high temperature superconductors. The obtained value of superconducting volumetric fraction is compared with the value obtained through the measurements of the Meissner effect.

1 - 9 – Ab initio study of vacancies in cubic zirconia

Taylor, M.A.,[1] Alonso, R.E.,[1] and Errico, L.A.[2]

[1]*Departamento de Física & Instituto de Física La Plata (IFLP, CCT-La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Casilla de Coreo 67, 1900 La Plata, Argentina*
[2]*Departamento de Física & Instituto de Física La Plata (IFLP, CCT-La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Casilla de Coreo 67, 1900 La Plata, Argentina and Universidad Nacional del Nordeste Bonaerense (UNNOBA), Monteagudo 2772, Pergamino, CP 2700, Buenos Aires, Argentina.*

Zirconia-based materials are in the focus of interest for many years because of their outstanding electrical and mechanical properties. They also show a rich variety of crystal structures depending on pressure, temperature, impurity/dopant content, growth conditions, etc. The addition of small amounts of impurities could stabilize the high temperature phases. These phases have applications ranging from solid oxide fuel cell electrolytes to catalyst substrates, and protective coatings. ZrO_2 has three polymorphs at atmospheric pressure: the low-temperature phase is monoclinic, and is transformed, on heating, to a tetragonal phase, and finally to a cubic phase. It is known that, cation-doped zirconia ZrO_2 with aliovalent cations such as Y, Ca, Sc, both stabilized the high temperature cubic phase and increase the number of oxygen vacancies enhancing anion conductivity. In the present work, we have performed an *ab initio* density functional theory study of oxygen vacancies in cubic ZrO_2. The equilibrium configuration and electronic structure of neutral and charged vacancies were calculated for two vacancy concentrations (2% and 0.5%). In all cases we determined the electric field gradient tensor (EFG) at the Zr-nucleus. From these results, we can evaluate the EFG distribution for each vacancy concentration and charge states. This distribution can be compared with experimental results obtained using Perturbed Angular Correlation technique.

1 - 10 – Experimental and *ab initio* study of the EFG at donor impurities in the Cr_2O_3:Ta semiconductor.

Darriba, G.N.,[1] Errico, L.A.,[1] Muñoz, E.L.,[1] Richard, D.,[1] Eversheim, P.D.,[2] and Rentería, M.[1]

[1]*Departamento de Física e IFLP (CCT La Plata - CONICET), Fac. de Cs. Exactas, UNLP, CC 67, 1900 La Plata, Argentina.*
[2]*Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany.*

In this work we report Perturbed-Angular-Correlation (PAC) experiments on $^{181}Hf/^{181}Ta$-implanted corundum Cr_2O_3 policrystals determining the magnitude and symmetry of the Electric-Field Gradient tensor (EFG). The measurements were carried out at 333 K after each step of a series of thermal annealings in air in the range 673–1273 K performed in order to obtain the maximum substitution of the Hf impurities at defect free Cr sites in the semiconductor crystal structure.

These results are analyzed in terms of self-consistent electronic structure FP-LAPW calculations in the dilute (1:4) Cr_2O_3:Ta system using the WIEN2k code. The calculations were carried out for diverse charge states of the impurities and are compared whit PCM calculations and with the EFG results coming from the PAC experiments using both $^{111}In/^{111}Cd$ and $^{181}Hf/^{181}Ta$ traces in the isomorphous α-Al_2O_3, α-Fe_2O_3 and Cr_2O_3 semiconductors.

This combined study enables the determination of lattice relaxations induced by the presence of impurities in the host and the charge state of the impurity donor level (Ta *5d*) introduced in the band gap of the semiconductor.

1 - 11 – Conductivity fluctuations in the two-dimensional anysotropic $CaLaBaCu_{3-x}Ga_xO_{7-\delta}$ Ssuperconducting material

Rojas Sarmiento, M.P.,[1] Landínez Téllez, D.A.,[1] and Roa-Rojas, J.[1]

[1]*Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC, Colombia*

Systematic conductivity fluctuation analyses on the $CaLaBaCu_{3-x}Ga_xO_{7-\delta}$; (x=0.06, 0.12, 0.18, 0.24, 0.30 and 0.36) system are reported. Samples were prepared by the standard solid state reaction recipe. Crystallographic tetragonal phase and lattice parameters were determined by x-ray diffraction experiments. Resistivity measurements were performed by using an AC low-frequency technique. Fluctuation analyses near the critical temperature Tc were made through the application of the Kouvel-Fisher method, e.g., the logarithmic temperature derivative of the conductivity excess. Close to Tc, results reveal the occurrence of three- and two-dimensional Gaussian fluctuation regimes, which are analyzed by the Aslamazov-Larkin theory. By the utilization of the Ginzburg-Landau theory, we experimentally determined the Ginzburg number. From the respective results, we calculated critical magnetic fields, critical current density and a jump in the specific heat for all Ga concentrations. Closer to Tc, a genuinely critical regime was identified. Scaling of our results permits to establish that the dynamics of the fluctuation system has the universality class described by the 3D-XY model. We performed conductivity fluctuation analysis in the $CaLaBaCu_{3-x}Ga_xO_{7-\delta}$; superconducting material. Close and above Tc, the conductivity fluctuation analysis reveal the occurrence of two fluc-

tuation regimes characterized by the critical exponents λ_{3D}=0.54 and λ_{2D}=0.95, respectively. These regions were interpreted as corresponding to 3D and 2D Gaussian regimes, respectively. Another intermediated regime was identified, which is related with fluctuations developed in spaces with fractal topology between three and two dimensionalities. Critical magnetic fields and critical current density were indirectly calculated from the Ginzburg number.

This work was partially supported by Colciencias, project No. 1101-333-18707, DIB and Centro de Excelencia en Nuevos Materiales, contract No. 043-2005.

1 - 12 – Electrical and magnetic properties of PMMA/Manganite composites

Artale, C.,[1] Fermepin, S.,[1] Forti, M.,[2] Latino, M.,[2] Quintero, M.,[1] Granja, L.,[1] Sacanell, J.,[1] and Polla, G.[1]

[1] *Division Materia Condensada, Unidad de Actividad Física, Centro Atómico Constituyentes, CNEA. Argentina.*
[2] *Instituto de Técnología "Jorge Sabato", UNSAM-CNEA. Argentina.*

Several manganite/insulator composites have been extensively studied in order to exploit their magnetic and electrical properties. In this context we explore the use of a polymer as the insulator, which gives the additional advantage of having a flexible sample. In this work, we present the synthesis and characterization of composites of $La_{2/3}Sr_{1/3}Mn_3$ (LSMO) and PMMA. We have obtained samples with different LSMO/PMMA ratio and a pure LSMO to use as a reference. We have performed a study of their structural and morfological characteristics, and their electrical and magnetic properties as a function of temperature and magnetic field. The magnetization results were dominated by the intrinsic LSMO magnetic properties without any appreciable influence related to the PMMA. Resistivity measurements showed an insulating behavior in the whole range of measured temperatures, indicating that the percolation threshold of LSMO grains has not been reached. A significant instability associated to the electric transport through the polymer have been observed. Although the magnetoresistance results of the flexible PMMA samples are large enough to be measured, their MR value is reduced compared to the reference LSMO. In the future we expect to improve the perfomance of this composite working closer to the percolation threshold of the system.

1 - 13 – Structural, magnetic and hyperfine interactions at the Fe sites of Fe-doped SnO.

Errico, L.A.[1] and Weissmann, M.[2]

[1] *Departamento de Física and Instituto de Física La Plata (IFLP, CCT-La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Casilla de Coreo 67, 1900 La Plata, Argentina Universidad Nacional del Nordeste Bonaerense (UNNOBA), Monteagudo 2772, Pergamino, CP 2700, Buenos Aires, Argentina.*
[2] *Departamento de Física, Comisión Nacional de Energía Atómica, Av. del Libertador 8250, 1429 Buenos Aires, Argentina*

Tin oxides SnO and SnO_2 have been a topic of interest in the last few years due to their technological importance and industrial applications. In fact, tin dioxide is used in many devices where transparent semiconductors are needed, such as thin heat reflecting foils, transparent electrodes, gas sensors, and solar panels, among others. In most cases, impurities are included in order to improve the response of the material. As an example, the interest in SnO_2 was recently renewed due to the discovery of high-temperature ferromagnetism in $Sn_{1-x}Co_xO_2$ films [Ogale et al., Phys. Rev. Lett. **91**, 77205 (2003)] with potential applications in spintronics. Also, in 2005, Punnoose et al [Phys. Rev. B **72**, 054402 (2005)] reported the development of room-temperature ferromagnetism in chemically synthesized powder samples of $Sn_{1-x}Co_xO_2$ samples and paramagnetic behaviour in $Sn1-xCo_xO$ samples. Results for the hyperfine interactions at ^{57}Fe (measured by Mössbauer spectroscopy) were also reported.

We present here our first results of a Density Functional Theory-based *ab initio* study of Fe-doped SnO. Calculations were performed assuming that Fe ions replace Sn indigenous atoms of the structure and including vacancies, in order to discuss their role in the hyperfine interactions and in the magnetic solutions. In all cases, the equilibrium atomic positions and electronic structure of the systems were determined and the hyperfine parameters at the Fe sites were obtained and compared with available experimental data

1 - 14 – Structural, magnetic and electronic behavior of Sr_2GdRuO_6 complex perovskite

Corredor, L.T.,[1] Velasco Zárate, J.H.,[1] Landínez Téllez, D.A.,[1] Fajardo, F.,[2] Rodríguez, J.A.,[2] and Roa-Rojas, J.[1]

[1] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, AA 14490, Bogotá D.C., Colombia*
[2] *Grupo de Estudios de Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá D.C., Colombia*

Magnetic long-range order and superconductivity do not usually coexist within a single thermodynamical phase. Discovery of the coexistence of the superconducting character and antiferromagnetic (AFM) ordering in Ru-1212-type $RuSr_2GdCu_2O_8$ compound has provided an opportunity for studying these antagonic phenomena in the same material. $RuSr_2GdCu_2O_8$ ruthenocuprate (Ru-1212) is characterized by a triple perovskitic cell similar to that of $YBa_2Cu_3O_{7-\delta}$, where Y and Ba are substituted by Gd and Sr, respectively, and the CuO_2 planes are separated from one another not by the Cu chains, but by RuO_6 octahedra. It is known that this material exhibits a superconducting transition $T_{SC} \approx$ 40 K and an AFM ordering with Néel temperature $T_N \approx 130$ K. In the fabrication process, double perovskite Sr_2GdRuO_6 is usually synthesized as precursor of ruthenocuprate material. This precursor contains the magnetic character of the ruthenocuprate superconductor. In this work, we present experimental and theoretical results of crystallographic lattice, magnetic feature and electronic structure of Sr_2RuGdO_6 complex perovskite. 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)Å, c=8.2223(7)Å, α=γ=90º and β=90.258º. Magnetization measurements reveal an AFM ordering for a Néel temperature of ≈ 33 K, which are attributed to Ru-O-O-Ru superexchange interaction and a ferromagnetic transition for a Curie temperature of ≈ 17 K, which are related with the Ru-O-Gd interactions. Calculations of electronic structure were performed by the Density Functional Theory. The exchange and correlation potentials were included through the LDA+U approximation. Density of states (DOS) study was carried out considering the two spin polarizations and several types of antiferromagnetism. Results show that Ru and Gd are responsible for the magnetic character in this material, which evidences a magnetic-semiconductor character.

This work was partially supported by DIB, Colciencias on the project No. 1101-333-18707 and Centro de Excelencia en Nuevos Materiales, contract No. 043-2005.

1 - 15 – First order reversal curves analysis of the temperature effect on magnetic interactions in La-Co substituted barium ferrites

Oliva, M.I.,[1] Bercoff, P.G.,[1] and Bertorello, H.R.[1]

[1] *IIFAMAF, UNC - CONICET*

First order reversal curves (FORC) distributions are a powerful tool for investigating hysteresis and interactions in magnetic systems and have been widely applied. La-Co substitution in barium hexaferrites has also been extensively studied . The most effective substitution to improve the magnetic properties (coercive field and energy product) is given by $x = 0.2$ in the formula Ba_{1-x} La_x $Fe_{12-x}Co_x$ O_{19}, so this stoichiometry is used in this work to prepare a sample and study its magnetic behavior as a function of temperature. The sample was structurally characterized by x-ray diffraction (XRD) and magnetically studied in a SQUID magnetometer. The temperature effect on the magnetic properties of a $Ba_{0.8}$ $La_{0.2}$ $Fe_{11.8}$ $Co_{0.2}O_{19}$ was analyzed by conventional ZFC-FC and magnetization (M) *vs.* applied field (H) curves. FORC distributions were used to study the dependence of the magnetic interactions with the temperature. FORC diagrams performed on the sample at different temperatures exhibit similar characteristics, such as the spread in the $h_c - h_u$ plane and a spread out of the h_c axes. These features are interpreted in terms of exchange-interacting particles and dipolar interactions, respectively. As the temperature decreases, stronger interactions are noticed.

1 - 16 – Bottleneck effect in the ESR of Ag doped with magnetic Gd and non-magnetic Sb ions

Vargas, J.M.,[1] Rettori, C.,[1] and Oseroff, S.B[2]

[1] *Instituto de Física "Gleb Wataghin", UNICAMP, Campinas-SP, 13083-970, Brazil.*
[2] *San Diego State University, San Diego, California 92182, U.S.A.*

The metallic Ag doped with Gd and Sb ions is an interesting model system for study the bottleneck effect associated to the localized spin-lattice relaxation mechanism. The Electron Spin Resonance (ESR) data of Gd^{3+} in both Ag:Gd and Ag:Gd,Sb systems reveal the existence of the bottleneck effect. As the Gd concentration increases the localized spin-lattice relaxation via an exchange interaction between the localized spin and the conduction electrons, **J**S.s, slow down gradually and the bottleneck effect is evidenced. The addition of non-magnetic Sb impurities to the Ag:Gd system enhance the localized spin-lattice relaxation rate via a conduction electron spin-orbit interaction, thus, breaking gradually the bottleneck effect. The bottleneck effect is quantified by the Korringa

rate (thermal broadening of the ESR linewidth) and the g-shift of the Gd^{3+} resonance.

1 - 17 − Magnetic and structural behavior of Sr_2ZrMnO_6 double perovskite

Llamosa P., D.,[1] Landínez Téllez, D.A.,[1] and Roa-Rojas, J.[1]

[1] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, A.A. 14490, Bogotá DC, Colombia*

We report synthesis and characterization of new Sr_2ZrMnO_6 manganite-like material. Samples were produced by the solid state reaction method with sinterization temperatures up to 1400^{o}C. X-ray diffraction experiments reveal the presence of (111) and (311) peaks, which are characteristic of the superstructure of a cubic complex perovskite system, space group Pm3m (#221). Lattice parameter a=7.86 Åwas obtained by means of Rietveld-type refinement, through the GSAS software. Magnetic properties were studied by using a MPMS Quantum Design SQUID. From measurements of magnetization as a function of temperature, we determine the occurrence of a paramagnetic-antiferromagnetic transition with a Néel temperature of 50 K. Curie-Weiss fitting allowed us to obtain the magnetic characteristic parameters. At temperature regimes below the Néel temperature, strong evidences of frustration and an irreversibility temperature between zero field cooling (ZFC) and field cooling (FC) measurements are observed. Curves of magnetization as a function of applied field were performed at T=4 K. Results show a hysteretic feature for Sr_2ZrMnO_6 magnetic material. This response is attributed to a possible antiferromagnetic canted ordering of magnetic spins, which give rise to an effective magnetization with the consequent hysteresis curve. From saturation magnetization and Curie-Weiss fitting we determine a magnetic moment of 3.8 μ_B.

This work was partially supported by DIB, Colciencias on the project No. 1101-333-18707 and Centro de Excelencia en Nuevos Materiales, contract No. 043-2005.

1 - 18 − Structural Characterization and multiferroic behavior of $La_{0.7}Sr_{0.3}MnO_3/BaTiO_3$ composites

Reyes Ortiz, M.C.,[1] Landínez Téllez, D.A.,[1] and Roa-Rojas, J.[1]

[1] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, A.A. 14490, Bogotá DC, Colombia*

We report synthesis and characterization of $La_{0.7}Sr_{0.3}MnO_3$ / $BaTiO_3$ composites for 40%, 50% and 60% of $BaTiO_3$ in a $La_{0.7}Sr_{0.3}MnO_3$ matrix. Materials were produced by the standard solid state reaction method. Structural parameters of both compounds were obtained by means of Rietveld-type refinement, through the GSAS software. $La_{0.7}Sr_{0.3}MnO_3$ crystallizes in a rombohedral structure (space group $R\bar{3}c$) with lattice parameters a=b=5.5142(1) Å, c=13.3674(2) Å; and $BaTiO_3$ in a tetragonal structure (space group P4mm) with a=b=3.9981(6) Å and c=4.0260(1) Å. Results of refinement and SEM images reveal that composites are constituted by separate non reactive crystallographic phases of $La_{0.7}Sr_{0.3}MnO_3$ and $BaTiO_3$ compounds. EDX spectra and semiquantitative analysis confirm that there are not impurities and only the expected compounds are present in samples. Electric polarization measurements reveal the ferroelectric character of the material and magnetic response show the hysteretic behavior of magnetization as a function of applied field, which characterizes ferromagnetic materials. From saturation magnetization and Curie-Weiss fitting we determine a magnetic moment of $3.7\mu_B$. These results confirm the multiferroic behavior of $La_{0.7}Sr_{0.3}MnO_3$/ $BaTiO_3$ composites, however, this response is more evident for 60% $BaTiO_3$ material.

This work was partially supported by Colciencias on the project No. 1101−333−18777, DIB and Centro de Excelencia en Nuevos Materiales, contract No. 043 − 2005.

1 - 19 − Weak field magnetic susceptibility fluctuations above the superconducting transition of $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ (RE=Y, Sm, Gd, Dy, Ho, Yb) superconductor

Parra Vargas, C.A.,[1,2] Pimentel Jr, J.L.,[3] Pureur, P.,[3] Landínez Téllez, D.A.,[1] and Roa-Rojas, J.[1]

[1] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC.*
[2] *Grupo de Física de Materiales, Escuela de Física, UPTC, Tunja*
[3] *Instituto de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, RS, Brasil.*

We report detailed experimental results of magnetic susceptibility for the $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ superconducting system, above and close to the superconducting transition. The data were obtained from 5 K up to 300 K, and applied field of 0.1 T, correspond to the so-called weak magnetic field limit. In this limit, the excess of magnetization is associated with the fluctuations of the vortex lines positions. These effects of thermal fluctuations on Mab can be quantified through the known "excess of diamagnetism" ξ_{ab}. but $T > T_C$. In this work we present a study of magnetic susceptibility fluctuations in the limit of weak magnetic fields, above the $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$; (RE=Y, Sm, Gd, Dy, Ho, Yb) high superconducting material. Samples were synthesized by the standard solid state reaction. For

the fluctuation analysis, we use the concept of excess of magnetization, based on the Lawrence-Doniach model (LD), which allowed to calculate the diamagnetism induced by thermal fluctuations in the normal state, in the vicinities of critical temperature T_{c0} (70, 54, 42, 52, 54, 70 K, for RE=Y, Sm, Gd, Dy, Ho, Yb respectively). It was demonstrated, by means of the analysis of the thermal fluctuations, that the $La_{0.5}RE_{0.5}BaCaCu_3O_{7-\delta}$ system shows an excellent 2D scaling behavior, also determining the value of the parameter B_{LD} ($\approx 7.66x10^{-3} \pm 2.28x10^{-3}$).

This work was partially supported by DIB, Colciencias on the project No. 1101-333-18707 and Centro de Excelencia en Nuevos Materiales, contract No. 043-2005.

1 - 20 − Synthesis, structural, and magnetic characterization of the oxide family Gd_3MO_7 (M = Nb, Ta, Sb).

Franco, D.G.,[1,2] Carbonio, R.E.,[2] and Nieva, G.L.[1]

[1] *CNEA - Centro Atomico Bariloche, Av. Bustillo 9500, 8400, S. C. de Bariloche, Rio Negro, Argentina*
[2] *INFIQC - Dpto de Fisicoquimica, Facultad de Ciencias Quimicas, Universidad Nacional de Cordoba, 5000, Ciudad Universitaria, Cordoba, Argentina*

Compounds of general composition A_3MO_7 where A^{3+} = La, Pr, Nd and M^{5+} = Nb, Ta, Sb, Ru, Mo, crystallize in an orthorhombic fluorite-related superstructure: the weberite structure. There are three different crystallographic sites for the cation, distorted cubic A^{3+} site, distorted pentagonal bipyramidal A^{3+} and the octahedral M^{5+} site. The M^{5+} cation is octahedrally coordinated to six oxygen ions and the MO_6 octahedra shares corners, forming a zigzag chain. In this structure slabs are formed in the bc plane, in which one dimensional MO_6 chains run parallel to the c-axis alternating with rows of edge shared AO_8 pseudo cubes consisting of one third of A^{3+} ions. These slabs are separated by the remaining two thirds of A ions which are seven-coordinated by oxygen ions. These compounds display a wide variety of physical properties depending on the electronic configuration of the metals ions and the interaction between the different metal sites. Fox example, when M is a d^0 or d^{10} cation the oxides are electronically inert. But when M^{5+} has a d^n configuration, the materials are electronically and magnetically active. In the case that A is also a magnetic ion, its magnetic moment can interact with the magnetic moments of the M^{5+} species, leading to a more complicated magnetic behavior. In this work we present the synthesis, structure and magnetic characterization of Gd_3MO_7 with M = Nb, Ta and Sb. These phases were synthesized as polycrystalline powders by standard ceramic method. All are orthorhombic, space group $C222_1$, determined through Rielveld refinement from X-ray powder diffraction data. Magnetic measurements were made in a commercial SQUID in a 5 – 400 K Temperature range. M vs T measurements indicated paramagnetic behaviour at room temperature for all the samples. The temperature dependence of the magnetic susceptibility obeys the Curie-Weiss law with a magnetic moment close to the expected value of 7.94 calculated assuming the free ion moment for 4f7 Gd^{3+}. In the case of Gd_3SbO_7 it is observed at round 125 K a deviation in the susceptibility, not observed en the case of Nb and Ta.

1 - 21 − Characterization of a mechanochemically activated titanium-hematite mixture: Mössbauer spectroscopy study

Cristóbal, A.A.,[1] Ramos, C.P.,[2] Botta, P.M.,[1] Aglietti, E.F.,[3] Saragovi, C.,[2] and Porto López, J.M.[1]

[1] *INTEMA*
[2] *GIyA - CAC - CNEA*
[3] *CETMIC*

Mechanochemical processes involving reactions between metals and crystalline oxides are of interest because their potential technological applications in structural, magnetic or electric materials. In addition they can contribute to the understanding of the natural occurring processes that lead to the formation of minerals and soils. The controlled studies of how the distribution of cations in the titanomagnetites takes place can help toward building a model for the nature of their magnetism and, since they are the primary carriers of rock and soil magnetism, are therefore intensively investigated in many experimental and theoretical studies. In behalf of a better comprehension of the thermal, physical-chemical, magnetic and hyperfine behavior, we have considered a titanium and hematite mixtures, with molar ratio Ti:Fe_2O_3 of 1:2, mechanochemically activated during different activation times. We have studied the development of new phases by X-ray diffraction (XRD), scanning electron microscopy, differential thermal analysis and Mössbauer spectroscopy. The evolution from the starting materials affected by different milling times and subsequent annealing show that the Ti reduces the Fe ions in the Fe_2O_3 lattice, partly to Fe^{2+} and partly to metallic Fe. All these techniques reveal mainly the formation of a solid solution (formed by ulvospinel and magnetite) and also the appearance of metallic iron.

1 - 22 – ESR characterization of $Zn_{1-x}Mn_xAl_2O_4$ spinel thin films

Saleta, M.E.,[1] Sánchez, R.D.,[1,2] Shapoval, O.,[3] Moshnyaga, V.,[2] and Samwer, K.[2]

[1] *Centro Atómico Bariloche (CNEA) and Instituto Balseiro (UNCu), S.C. de Bariloche (RN), Argentina.*
[2] *I Physikalisches Institut, Universiät Göttingen, Göttingen, Germany.*
[3] *Institute of Applied Physics, Academiei Strasse, Kishinev, Moldova.*

The spins in the geometrically frustrated magnets are located in a lattice, but the geometric constrains produce an impossible simple arrangement of magnetic moments. In the cubic spinel oxide with general formula AB_2O_4, the transition metal ions (sites A and B) are coordinated with different number of oxygen ions. The A ions coordinate with four oxygens (tetrahedral site) while the B ions have six neighbor oxygens (octahedral site). The $ZnAl_2O_4$ is an insulator and non-magnetic compound; it crystallized in a cubic ($Fd\bar{3}m$) space group. On the other hand, the $MnAl_2O_4$ spinel is a geometrically frustrated magnet. The Mn ions form a geometrically frustrated corner-sharing tetrahedral network (3D). The dominating interaction between the Mn^{2+} (S=5/2) is antiferromagnetic with a Neel temperature of T_N=40K [1]. In this work we present results on $Zn_{1-x}Mn_xAl_2O_4$ thin films (0<x<1). The films have been grown epitaxially on MgO(100) substrates by Metalorganic Aerosol Deposition technique (MAD) [2]. The morphology and structure of the films were studied by Scanning Electron Microscopy (SEM) and X-ray Diffraction (XRD), respectively. The magnetic properties were studied by dc-magnetization (SQUID) and Electron Spin Resonance (ESR). The ESR experiments were performed varying the angle (H, out of plane) and temperature from liquid He to room temperature. The ESR spectra of the substrate presents six principal lines which came from the Mn^{2+} impurities of the MgO. Between the 3^{rd} and the 4^{th} substrate lines there was observed an extra line, originated from the film, which we study in details. This additional line is asymmetric; the ratio a/b between the height from the base lines to the maximum (a) and from the base line to the minimum b is practically constant ($a/b \approx$ 0.90) at high temperature while at low temperature this value decrease significantly. On the other hand, $\Delta H_{pp} \approx 5$ Oe practically does not depend on the composition. Comparing the distance between peak to peak of the resonance h_{pp} with the same parameter of the 3^{rd} substrate line, we observed that the ratio between both distances increases with decreasing temperature down to 50-70K and after that it decreases monotonously. This behavior can be associated with the ESR susceptibility showing that magnetic correlations appear below 40-70 K, depending on the sample composition.

[1] N. Tristan, et al., Phys.Rev. B **72** 174404 (2005).

[2] V. Moshnyaga et al., Appl. Phys. Lett. **74**, 2842 (1999).

1 - 23 – Underscreened Anderson Lattice: Schrieffer-Wolff transformation and mean field treatment

Thomas, C.,[1] Simões, A.S.R.,[1] Lacroix, C.,[2] Iglesias, J.R.,[1] and Coqblin, B.[3]

[1] *Instituto de Física, UFRGS, 91501-970 Porto Alegre, Brazil*
[2] *Institut Néel, CNRS-UJF 38042 Grenoble Cedex 9, France*
[3] *L. P. S., UMR CNRS 8502, Université Paris-Sud, 91405 - Orsay, France*

We present a derivation of the Schrieffer-Wolff transformation for the Anderson Lattice Hamiltonian with a two-fold degenerate f-level in each site. The degeneracy of the f-electrons has been taken into account in order to describe uranium and other actinide magnetic compounds with a spin larger than 1/2, for example a total $S = 1$ spin for the f-electrons. The transformed Hamiltonian has several terms as in the $s = 1/2$ classical case, but we have obtained here both an exchange (Kondo) interaction between the $S = 1$ f-spins and the spins of the conduction electrons, and also an effective f-band term. This f-band term describes better the Underscreened Kondo Lattice model which has been recently developed to explain the Kondo-ferromagnetism coexistence observed in uranium compounds such as UTe [1].

[1] Perkins, N.B. *et al.*, Phys. Rev. B **76** (2007) 125101.

1 - 24 – Electric pulse-induced resistive switching in ceramic $YBa_2Cu_3O_{7-\delta}$ / Au interfaces

Acha, C.[1]

[1] *Departamento de Física, FCEyN, Universidad de Buenos Aires, Ciudad Universitaria, (C1428EHA) Buenos Aires, Argentina*

We shown the existence of a reversible, complementary and polarity dependant electric-pulse-induced resistance (EPIR) switching effects in Au / $YBa_2Cu_3O_{7-\delta}$ ceramic superconductor interfaces. Non-volatile high and low resistance states and transition regions between them are obtained as a function of the amplitude and polarity of the pulsing voltage. Relaxation processes of the resistivity after applying the pulses, not associated with heating effects, are also observed. We also report on the temperature sensitivity of these resistance hysteresis switching loops, where both the difference between high and low resistance states and the voltage needed to produce the switching decrease with increasing temperature. Our results are consistent with a mechanism for the EPIR effect based on oxygen electromigration.

1 - 25 – Sr_2YSbO_6 as a buffer layer for $YBa_2Cu_3O_{7-\delta}$ superconductor films

Ortiz-Diaz, O.,[1,2] Saldarriaga, W.,[3] Reyes, D.,[4] Cortes, A.,[4] Caicedo, J.M.,[4] Lopera, W.,[4] Landínez Téllez, D.A.,[2] and Roa-Rojas, J.[2]

[1] *Grupo de Física de Materiales, Universidad Pedagógica y Tecnológica Colombia, Tunja, Colombia*
[2] *Grupo de Física de Nuevos Materiales, CENM, Universidad Nacional de Colombia, Bogotá, Colombia*
[3] *Universidad Nacional de Colombia, sede Medellín, Colombia*
[4] *Thin Films Group, CENM, Universidad del Valle, Cali, Colombia*

We report growth and structural characterization of Sr_2YSbO_6 films over MgO singlecrystal by magnetron sputtering. This layer has been developed for growth of superconducting $YBa_2Cu_3O_{7-\delta}$ (YBCO) films with good superconducting properties such as critical current density value (J_c) in self–field at 75 K comparable with the J_c of the films growth over comercial $SrTiO_3$ substrates. These results and good lattice matching and chemical stability between Sr_2YSbO_6 and YBCO (reported in O. Ortiz–Diaz, *et. al.*, *Mod. Phys. Lett. B*, **18** 1035–1042 (2004)) make Sr_2YSbO_6 an ideal choice as the buffer layer for high performance superconductor coatings. For instance, Sr_2YSbO_6 material could be used in coated conductor tapes of YBCO with IBAD–MgO template.
This work was partially support by Universidad Nacional de Colombia on the 2nd call for financial support to postgraduate studies DIB 20301007460, code 8003080; by Universidad Tecnológica y Pedagógica de Colombia (UPTC); and by Centro de Excelencia en Nuevos Materiales (COLCIENCIAS) on the contract number 043–2005.

1 - 26 – Dynamical behavior of the phase transition of epitaxial $BaTiO_3$ from atomistic simulations

Sepliarsky, M.[1] and Tinte, S.[2]

[1] *IFIR, CONICET - Univ. Nac. de Rosario, 27 de Febrero 210 Bis, 2000 Rosario, Argentina*
[2] *INTEC, CONICET, Güemes 3450, 3000 Santa Fe, Argentina*

Using an atomistic shell model we study the temperature dependence of the ferroelectric properties of $BaTiO_3$ under biaxial compressive strain. Molecular dynamics simulations show that the first-order paraelectric to ferroelectric phase transition presents in bulk changes to a second-order one as a consequence of the in-plane constraint imposed by the mechanical boundary conditions. From the low temperature structure, the phase transition takes place in a finite range of temperature where the lattice parameter normal to the plane keeps approximately constant until T_c is reached. Histograms of local polarization reveal three different regimes of the dynamical behavior as a function of the temperature. At low temperatures in the ferroelectric phase, the distribution is unimodal centered at a finite value of P_z (out-of-plane polarization). In the transition region, the distribution turns bimodal with two unequal peaks at $+P_z$ and $-P_z$. Finally both peaks equal above T_c in the paraelectric phase.

1 - 27 – Structural properties, electric response and electronic feature of $BaSnO_3$ perovskite

Cuervo Farfán, J.,[1] Arbey Rodríguez, J. A.,[2] Fajardo, F.,[2] Vera López, E.,[3] Landínez Téllez, D.A.,[1] and Roa-Rojas, J.[1]

[1] *Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC, Colombia*
[2] *Grupo de estudio de Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC, Colombia*
[3] *Grupo de Superficies, Electroquímica y Corrosión, Escuela de Física, Universidad Pedagógica y Tecnológica de Colombia, Tunja, Colombia*

It has been observed that the semiconducting compound SnO_2 presents very good results as sensor. One important develop has been performed to study perovskite oxides for this relevant application. One perovskite material, which constitutes an excellent candidate for this technological application is $BaSnO_3$. Polycrystalline samples with single phase of $BaSnO_3$ were synthesized by using the solid state reaction method. Samples were characterized structurally by means the DRX technique. Rietveld refinement, by using the GSAS code, reveals that this material synthesizes in a cubic perovskite, space group P_{m3m} (121), with lattice parameter 4.117(6) Å. Electric response was examined through the Impedance Spectroscopy technique. Results of Nyquist and Bode diagrams, from an equivalent circuit, evidence the insulator character of material. We carried out a theoretical study by means of the calculation of the diagram of bands and the density of states of the $BaSnO_3$. Calculation was performed employed the Functional Density Theory (DFT), with the Approach of Generalized Gradient (GGA). DFT theory permitted to establish that $BaSnO_3$ material has an indirect semiconducting behavior. The gap of the material is at least 1.2 eV. There are differences between experimental and theoretical results because Wien2k program underestimates the gap value. Bulk modulus for this material was also determined to be 132 GPa.

This work was partially supported by Colciencias on the project No. 1101-06-17622 and Centro de Excelencia en Nuevos Materiales, contract No. 043-2005.

1 - 28 − Laser fluence effect on the morphology and magnetic properties of the barium hexaferrite thin films

Zandalazini, C.I.,[1,2] Oliva, M.I.,[3] Ferrero, J.C.,[1] Bertorello, H.R.,[3] and Rinaldi, C.A.[4]

[1] *Centro Laser de Ciencias Moleculares -INFIQC*
[2] *ANPCyT, FONCyT*
[3] *IIFaMAF - UN de Córdoba y CONICET*
[4] *CNEA- Laboratorio MEMS - Instituto de Nanociencia y Nantotecnología*

Pulsed laser ablation was used to deposit barium haxaferrite thin films on oriented silicon substrate. The depositions were made with a Nd YAG laser (1064 nm), varying the laser fluence, in vacuum at room temperature. The films were treated thermally to 1000 °C during 1 hour. The morphology and structural properties were analyzed by X-rays diffraction (XRD) and scanning electronic microscopy (SEM). The magnetic properties were studied with a vibrant sample (VSM) at room temperature and in a SQUID magnetometer for different temperatures and ZFC-FC curves. Ferrite deposited films have high crystalline anisotropy and sown a dependent coercive fields with the employed fuence, reaching similar values to the reported ones to ferrite bulk samples.

1 - 29 − *Ab initio* study of Cd-doped Sc_2O_3 semiconductor and comparison with ^{111}Cd PAC experiments

Muñoz, E.L.,[1] Richard, D.,[1] Errico, L.A.,[1,2] and Rentería, M.[1]

[1] *Departamento de Física e IFLP (CCT La Plata – CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, (1900) La Plata, Argentina.*
[2] *Universidad Nacional del Noroeste Bonaerense (UNNOBA), Monteagudo 2772, 2700 Pergamino, Argentina*

The combination of hyperfine techniques and theoretical simulations based on *ab initio* calculations has been shown to be a powerful tool to unravel structural characterizations in the atomic scale of impurities in solids. A recent example has been the study of SnO:Cd, where *ab initio* calculations [1] and Perturbed Angular Correlations (PAC) measurements were combined to describe the dynamic hyperfine interactions observed at ^{111}Cd impurities in the SnO semiconductor [2], originated in the electron-capture (EC) decay after-effects (AE) of the parent isotope ^{111}In. In this work, we present an ab initio study on the Cd-doped Sc_2O_3 semiconductor that enables a description of the dynamic interactions observed in PAC experiments using ^{111}In-implanted Sc_2O_3 samples. The theoretical study was performed at Cd impurities located at both cationic sites C and D of the Sc_2O_3 Bixbyite structure, using the Augmented Plane Waves + Local Orbital (APW+LO) method in the framework of the Density Functional Theory (DFT), with an impurity dilution of 1:48. We studied the EFGs for different charge states of the Cd impurity (neutral supercell and 1-electron added supercell). These theoretical results are compared with PAC results reported by Bartos et al. [3], in which an strong damping of the spin-rotation spectra was observed at low temperatures (lower than 600K). This damping is produced by dynamic hyperfine interactions that were correlated with the EC decay AE of ^{111}In probes. Our *ab initio* results are in excellent agreement with the experimental EFGs and can explain the origin of the dynamic interactions observed.

[1] L.A. Errico et al., Phys. Rev. B **75**, 155209 (2007).
[2] E.L. Muñoz et al. Hyp. Int. **138**, 37 (2008).
[3]A. Bartos et al. Phys. Lett. A **157**, 513 (1991).

1 - 30 − Experimental and *ab initio* study of ^{181}Ta-doped Sc_2O_3 semiconductor

Muñoz, E.L.,[1] Richard, D.,[1] Bibiloni, A.G.,[2] Errico, L.A.,[1,3] Eversheim, P.D.,[4] and Rentería, M.[1]

[1] *Departamento de Física e IFLP (CCT La Plata – CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, (1900) La Plata, Argentina.*
[2] *Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, (1900) La Plata, Argentina.*
[3] *Universidad Nacional del Noroeste Bonaerense (UNNOBA), Monteagudo 2772, 2700 Pergamino, Argentina*
[4] *Helmholtz-Institut für Strahlen- und Kernphysik (ISKP), Universität Bonn, Nussallee 14–16, 53115 Bonn, Germany*

Recently, experimental and *ab initio* studies of hyperfine interactions in solids has enabled to reinterpret erroneous assignments in previously reported PAC experiments in diluted semiconductor oxides. In particular, *ab initio* calculations in Ta-doped In_2O_3 semiconductor were used to reinterpret the hyperfine parameters dependence with the bixbyite lattice constant in these sesquioxides and a correct determination of the experimental electric-field gradients (EFGs) at defect free cation sites. The systems that need a revision of the hyperfine parameters are In_2O_3 and Sc_2O_3 among others, due to their smaller lattice parameters. In this work, we present ab initio calculations and results of new Perturbed Angular Correlations experiments on the ^{181}Ta-doped Sc_2O_3 semiconductor. The theoretical calulations were performed at Ta impurities located at both cationic sites C and D of the Sc_2O_3 structure, using the Augmented Plane Waves + Local Orbital (APW+LO) method in the framework of the Density Functional Theory (DFT), with an impurity dilution of 1:48. We studied

the EFGs for different charge states of the impurities (neutral cell, and removing 1 and 2 electrons). The PAC experiments were performed at La Plata with the PACAr spectrometer [1] in Sc_2O_3 polycrystalline pellets implanted with ^{181}Hf ($\rightarrow$ ^{181}Ta) ions at the ISKP ion accelerator. The samples were thermally annealed in air to eliminate the radiation dammage (at 673 K, 1173 K, 1273 K, and 1373 K, during 1h). The temperature dependence of the EFGs was determined at defect free cation sites C and D in the range 373 K-1173 K. The APW+LO results were found to be in excellent agreement with the new experimental values. Finally, the dependence of the hyperfine parameters with the lattice parameter of the bixbyite oxides was revisited.

[1] M. Rentería et al., Hyperfine Interactions (2008), in press (DOI 10.1007/s10751-008-9706-9).

1 - 31 − Perturbed Angular Correlation study of $Bi_2O_3 - Fe_2O_3$ system

Chain, C.Y.,[1,2] Quille, R.A.,[1,2] Fernández van Raap, M.B.,[1,2] and Pasquevich, A.F.[1,2]

[1]*Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Argentina – cc67 – 1900 La Plata, Argentina.*
[2]*Instituto de Física La Plata (CONICET), Argentina.*

The binary oxide $BiFeO_3$ exhibits ferroelectricity ($T_C = 830°C$) and antiferromagnetism ($T_N = 370°C$). This multiferroic material has received considerable attention in the last few years due to the potential applications in data storage, sensors, and devices for spintronics. $BiFeO_3$ has been reported as an incongruently melting compound that melts peritectically at $934°C$. In this paper results of a study of the solid state reactions of equimolar mixtures of Bi_2O_3 and Fe_2O_3 are presented. The phase transformations were monitored through the hyperfine interactions of radioactive ^{181}Ta impurities. The last isotope is an adequate probe for Perturbed Angular Correlations (PAC) studies. These isotopes appear in the oxides after the beta decay of ^{181}Hf , which were introduced in the oxide mixture as few atomic percent of HfO_2. We performed PAC studies of blends prepared mixing the oxides by ball milling. The samples were finally annealed under air at increasing temperatures in order to facilitate the solid state reactions. We used complementary techniques, such as X-ray Diffraction, Mössbauer Spectroscopy and Differential Scanning Calorimetry. After annealing at $850°C$, PAC measurements were carried out at several temperatures searching for the magnetic and ferroelectric phase transitions of $BiFeO_3$.

1 - 32 − Resistance switching in silver - TiO contacts

Gomez-Marlasca, F.,[1] Granja, L.,[1] and Levy, P.[2]

[1]*Materia Condensada, GIA, GAIANN, CAC -CNEA and Instituto de Nanociencia y Nanotecnología, CNEA, Gral Paz 1499 (1650) San Martín, Pcia. Buenos Aires, Argentina*
[2]*Materia Condensada, GIA, GAIANN, CAC -CNEA and Instituto de Nanociencia y Nanotecnología, CNEA, Gral Paz 1499 (1650) San Martín, Pcia. Buenos Aires, Argentina E-mail: levy@cnea.gov.ar*

Abstract. We study the electric pulse induced resistance switching on TiO - Ag contacts at room temperature by means of a multiterminal configuration. The "complementary effect" -in which the contact resistance of each pulsed electrode displays variations of opposite sign- is strongly influenced by the history of the pulsing procedure both during and after the pulse. Loops performed by varying the magnitude and sign of the stimulus at each pulsed electrode allow to disentangle their sole contribution at different stages of the process. The underlying mechanism for resistance switching of this nonvolatile, reversible and multilevel memory device is discussed in terms of electromigration of oxygen ions and vacancies.

1 - 33 − Differential thermal analysis to study metamagnetic transitions.

Quintero, M.,[1] Sacanell, J.,[2] Ghivelder, L.,[3] Leyva, A.G.,[1] and Parisi, F.[1]

[1]*Departamento de Física, Comisión Nacional de Energía Atómica AND Escuela de Ciencia y Tecnología, UNSAM, Buenos Aires, Argentina*
[2]*Departamento de Física, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina*
[3]*Instituto de Fisica, Universidade Federal do Rio de Janeiro,Rio de Janeiro, Brazil*

In this work we propose a method to perform differential calorimetric measurements using a commercial equipment. The method allows to identify metamagnetic transitions comparing the temperature between the sample and a reference, both in thermal contact with independent temperature sensors. By an adequate calibration is possible to determine the absolute temperature change and the heat related with the transition. The technique has been successfully tested using a sample with previously known magnetic properties and the obtained results were compared with those extracted from magnetic measurements.

1 - 34 – Peak Effect in type II superconductors: Stable and metastable vortex lattice configurations

Pérez Daroca, D.,[1] Pasquini, G.,[1] Chiliote, C.,[1] Lozano, G.,[1] and Bekeris, V.[1]

[1] *Departamento de Física, FCEyN, Universidad de Buenos Aires, Argentina*

Vortex lattice (VL) in type II superconductors may be considered as a model complex system where competing interactions give rise to a complex phase diagram. In this context the VL undergoes an order-disorder transition and the fingerprint is the anomaly known as the Peak Effect (PE). The static description (the nature of the O-D transition and the stability of ordered and disordered domains) as well as the related dynamics (the role of ac and dc external forces) in this region remain under discussion. We show results obtained in $NbSe_2$ and $YBa_2Cu_3O_{7-y}$ (YBCO) single crystals. In previous work we have shown evidence indicating that different physics governs the PE phenomena in both cases [1]. In this work, we explore the VL configuration landscape at each temperature (field) after applying different thermal and shaking protocols. In $NbSe_2$, shaking procedures allow us to access to the stationary configurations. Between the ordered and disordered phases we identify a region of stable phase coexistence [2]. On the contrary, as was shown in previous work, in YBCO different shaking waveforms lead the system in different robust metastable configurations [3]. The shaking frequency dependence and the relaxation mechanisms are analyzed.

[1] G. Pasquini and V. Bekeris, Supercond. Sci. Technol. **19**, 671 (2006); G. Pasquini et.al. Physica B **398**, 420 (2007).

[2] G. Pasquini, D. Pérez Darocca, C. Chilliote, G. Lozano and V. Bekeris, Phys. Rev. Lett. **100**, 247003 (2007).

[3] S.O. Valenzuela and V. Bekeris, Phys. Rev. Lett. **86**, 504 (2001); G. pasquini, D. Luna and G. Nieva, Phys. Rev. B 76, 212302 (2007)

1 - 35 – Atomistic modelization of the H-bonded ferroelectric KH_2PO_4

Lasave, J.,[1] Migoni, R.L.,[1] Kohanoff, J.,[2] Del Pópolo, M.G.,[3] and Koval, S.[1]

[1] *Instituto de Física Rosario, Universidad Nacional de Rosario and CONICET, 27 de Febrero 210 Bis, 2000 Rosario, Argentina.*
[2] *chool of Mathematics and Physics, Queen's University of Belfast, Belfast BT7 1NN, United Kingdom.*
[3] *School of Mathematics and Physics, Queen's University of Belfast, Belfast BT7 1NN, United Kingdom.*

KH_2PO_4 (KDP), the prototype compound of the family of H-bonded ferroelectric materials, is simulated by a shell model with adjusted interactions in order to reproduce recent ab initio results. Phonons, energy barriers, structure and the relative stability between the ferroelectric (FE) phase and the non-observed antiferroelectric one, are analyzed and compared to the available first-principles and experimental data. Finite temperature Molecular Dynamics simulations show satisfactory behaviour of the model within the FE phase.

1 - 36 – Coexistence of ferroelectric and antiferroelectric domain defects in the paraelectric phase of $NH_4H_2PO_4$ (ADP)

Lasave, J.,[1] Koval, S.,[1] and Migoni, R.L.[1]

[1] *Instituto de Física Rosario, Universidad Nacional de Rosario and CONICET, 27 de Febrero 210 Bis, 2000 Rosario, Argentina.*

Ammonium dihydrogen phosphate $NH_4H_2PO_4$ (ADP) is an antiferroelectric (AFE) compound belonging to the KDP-type family of hydrogen-bonded ferroelectrics. Recent ab initio results have shown that the optimization of the N-H-O bridges in ADP leads to the stabilization of the AFE state over a FE one. However, electron spin probe measurements have shown that domain regions of both phases may coexist above the critical antiferroelectric-paraelectric transition temperature. We have performed a first principles study of the relative stability and energetics of different AFE and FE defects embedded in a paraelectric (PE) matrix of ADP. Our analysis suggests that FE and AFE domains may coexist and are energetically more favorable than the pure PE phase (without defects) in accordance with the experiments.

1 - 37 − Synthesis and characterization of $Ln\mathrm{BaCo_2O_{5-d}}$ for cathodes of Solid-Oxide Fuel Cells

Hernández Sánchez, J.,[1,2] Sacanell, J.,[1] Leyva, A.G.,[1] and Lamas, D.G.[3]

[1] *Gerencia de Investigaciones y Aplicaciones, Centro Atómico Constituyentes, CNEA, Argentina.*
[2] *Departamento de Física, FCEN, UBA, Argentina.*
[3] *CINSO, CITEFA-CONICET, Argentina.*

Rare earth cobalt oxides with perovskite structure have been shown to be among the best candidates for cathodes of Solid-Oxide Fuel Cells (SOFCs). Their general formulae is $Ln_{1-x}Re_x\mathrm{CoO_3}$, where Ln is a lanthanide and Re an alkaline-earth.

Recently, it has been suggested that oxygen ion transport can be enhanced by inducing cation ordering of the lanthanide and the alkali-earth ion in these compounds, consistent of a layered structure alternating Ln and Re species in the A site of the perovskite.

In this work, we studied $Ln\mathrm{BaCo_2O_{5+d}}$ (LnBCO) (with Ln=La, Sm, Gd) materials and evaluated their electrochemical behaviour as cathode of SOFCs. The compounds were synthesized by the Liquid Mix method and the resulting powders were characterized by X-ray diffraction and scanning electron microscopy. Electrochemical impedance spectroscopy measurements were performed on symmetrical LnBCO/$\mathrm{CeO_2}$-$\mathrm{Sm_2O_3}$/LnBCO cells.

1 - 38 − Electron spin resonance and specific heat studies in the magnetoelectric effect $\mathrm{LiMPO_4}$ (M = Mn, Co, Ni, Fe) single crystals

Bufaiçal, L.,[1] Pagliuso, P.G.,[1] Li, J.,[2] Vaknin, D,[2] and Barberis, G.E.[1]

[1] *Instituto de Física, Unicamp, 13083-970, Campinas, (SP), Brazil*
[2] *Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames Iowa, USA*

We report X-band ($\upsilon \approx 9.5$ GHz) electron spin resonance (ESR) and specific heat measurements studies of $\mathrm{LiMPO_4}$ (M = Mn, Co, Ni, Fe) single crystals. This family of iso-structural orthophosphates has attracted much attention by virtue of their interesting magnetoelectric effect properties and their Li ionic conductivity that renders them potentiality electrode materials for lithium batteries. Surprisingly, only for $\mathrm{LiMnPO_4}$ compound an ESR signal is observed at high temperatures with a nearly isotropic g-value ˜2.0. The ESR linewidth with external field applied along the three principal crystallographic axes shows strong broadening as the temperature decreases toward the antiferromagnetic ordering ($\mathrm{T}_N = 33.8$ K) indicating the presence of short range magnetic correlations, as the increase of the linewidth accompany the magnetic susceptibility from room temperature to the magnetic transition. The specific heat capacity measurements of $\mathrm{LiNiPO_4}$ confirm the first order character of the magnetic commensurate-incommensurate transition recently reported by neutron scattering studies. By substituting Fe for Ni in $\mathrm{Li(Ni_{0.8}Fe_{0.2})PO_4}$ the transition becomes second order.

1 - 39 − Jahn-Teller effects in strongly correlated manganites

Fuhr, J.D.,[1] Avignon, M.,[2] and Alascio, B.[1]

[1] *Instituto Balseiro and Centro Atómico Bariloche, CNEA, 8400 San Carlos de Bariloche, Argentina*
[2] *Institut Néel, CNRS and Université Joseph Fourier, BP 166, 38042 Grenoble Cedex 9, France*

In manganites like $\mathrm{La}_x\mathrm{Sr}_x\mathrm{MnO_3}$, the interplay of several degrees of freedom, charge, spin, orbit and lattice displacements, determine the physical properties of the system. The interactions between these different degrees of freedom cannot be reduced to perturbation theory as in other materials. We have studied the effect on the strongly correlated Mn e_g electrons of the Jahn-Teller deformation of the O octahedra around each Mn ion. To obtain the energy of the system, we resort to a slave boson description for the electronic part and add an elastic term associated to the Jahn-Teller distortion. We present results on three particular phenomena: (i) the pressure-induced insulator to metal transition in $\mathrm{LaMnO_3}$ [1,2]; (ii) the Jahn-Teller transition with temperature [3]; and (iii) the appearance of JT distortion in the paramagnetic insulating phase of doped manganites [4].

[1] I. Loa et al., Phys. Rev. Lett. **87**, 125501 (2001).
[2] J.D. Fuhr, M. Avignon, and B. Alascio, Phys. Rev. Lett. **100**, 216402 (2008).
[3] Chatterji et al., Phys. Rev. B **68**, 052406 (2003).
[4] Mannella et al., Phys. Rev. B **77**, 125134 (2008).