Posters

Magnetic Oxides and related topics

1 - 1 – Characterization of rust layers formed on carbon steels submitted to total immersion tests in NaCl solutions

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Coupons of low carbon steels were submitted to total immersion tests in 0.2M of NaCl solutions, during 1.9, 7 and 14 days. A study of the composition of the adherent (AR) and nonadherent (NAR) rusts by means of Mössbauer spectroscopy (MS) and diffuse reflectance infrared Fourier transform (DRIFT), is presented. The morphology of the rusts was analyzed through scanning electronic microscopy (SEM). In addition, the corrosion rates, measured by the gravimetric method, are presented. The experimental results revealed the presence of magnetite, goethite, lepidocrocite and akaganeite in the AR samples. In the 1.9 and 7 days NAR samples, lepidocrocite and superparamagnetic goethite were found, while in the 14 days samples, non stoichiometric magnetite was additionally found. The parameter **missing**, which measures the amount of corroded iron that completely converts into AR, was calculated for all immersion times. Finally, the effects of the immersion times and the grain sizes of the corrosion products on the corrosion rates were also investigated.

1 - 2 – Exchange bias effect in nanogranulated composites of antiferromagnetic superconductros and ferromagnetic manganite

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We report the synthesis, crystallographic characterization and magnetic response of $RuSr_2GdCu_2O_8 - La_{0.67}Sr_{0.33}MnO_3$ composites. Separated compounds of $RuSr_2GdCu_2O_8$ and $La_{0.67}Sr_{0.33}MnO_3$ were solid-reacted from powder precursors. Transport measurements of $RuSr_2GdCu_2O_8$ were effectuated by electrical resistivity. It was observed that for a critical temperature of 39 K this material experiments a superconducting transition. Magnetization curves evidenced a paramagnetic to antiferromagnetic transition with Néel temperature of 132 K. This material was mixed with ferromagnetic $La_{0.67}Sr_{0.33}MnO_3$ to form a 50% volumetric composite. Structural characterization was performed by using the x ray diffraction technique. Results show that there is not chemical reaction between $RuSr_2GdCu_2O_8$ and $La_{0.67}Sr_{0.33}MnO_3$ compounds. Magnetic response of composites was performed by measurements of magnetization as a function of applied magnetic field. Hysteretic behavior for low magnetic fields below the Néel temperature of antiferromagnetic material, reveal an asymmetry of the hysteresis curves, which is characteristic of the exchange bias effect. For strong magnetic fields the ferromagnetic character is dominant and the asymmetry disappears.

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1 - 3 – Synthesis and structural ordering of a potential ferromagnetic material Bi_2CrCuO_6

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A new complex perovskite oxide Bi_2CrCuO_6 (BCCO) has been synthesized by solid state reaction method. X–ray diffraction measurements and Rietvekd analysis revealed that a new material has a structure characteristic of monoclinic $A_2BB'O_6$ perovskite family. Furthermore, compositional analysis of BCCO was performed by energy dispersive X–ray (EDX) measurements, which showed that there is no impurity traces. BCCO was predicted as a promising candidate to ferromagnetic material by *ab initio* density functional theory study (Y. Uratani *et. al.*, *Physica B* **383** 9–12 (2006)).

1 - 4 – Electrical and percolative behaviour of $Ba_2NdZrO_{5.5}$–$YBa_2Cu_3O_{7-\delta}$ composites

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We have synthesized an insulator material $Ba_2NdZrO_{5.5}$ (BNZO), which was found, by X–ray diffraction analysis, chemically non reacting with $YBa_2Cu_3O_{7-\delta}$ (YBCO) superconductor material. These materials form a system where the particles of superconductor and insulator materials are found coexisting in a composite with two separate phases. We have prepared several samples of BNZO–YBCO composites with differents volumetric fraction (Vol %) of YBCO. We have performed resistivity measuremts, at room temperature, in function of Vol % of YBCO in these composites. The results are studied and discussed in the frame of the percolation theory.

1 - 5 – Preparation of magnetic and conductive Ni-Gd ferrite-polyaniline composite

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In this work the addition of Gd in the structure of nickel ferrites obtained from mixed Gd, Fe and Ni citrates has been investigated in order to explore the possibility of Gd for Fe substitution in the solids. Particles of $NiFe_{1.95}Gd_{0.05}O_4$ were coated with polyaniline (PANI) during the in situ polymerization of aniline in aqueous solution. Different ratios aniline/ferrite were selected in order to study magnetic and conductivity properties with increasing fraction of PANI. Transmission electron microscope reveals a core-shell structure with particle size near 50 nm. The PANI-ferrite composites were characterized by XRD and IR spectroscopy. The changes of the magnetic and conductive properties after polyaniline coating were investigated. The introduction of Ni-Gd ferrite nanoparticles significantly affects the conductivity and magnetic properties of resultant ferrite-polyaniline nanocomposites. Upon polyaniline coating, both the conductivity and the blocking temperature decrease. The coercivity is almost unchanged, while the saturation magnetization drastically decreases. The prepared solids are suitable to be used in electronic devices.

1 - 6 – Morin Transition and memory effect of ball-milled and annealed hematite

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Fine particles of hematite (mean size 60 nm) were produced by ball-milling a mixture of hematite and pure Fe and annealing at 1000 °C. XRD and Mössbauer spectroscopy show that only $\alpha-Fe_2O_3$ is present in the final product, with lattice and Mössbauer parameters that correspond to crystalline hematite.

ZFC and FC magnetization measurements were performed from 5 to 300 K, at different applied fields. Two magnetic regimes were observed: one with a low temperature Morin transition at T_{M1}= 97 K and another one at $T_{M2} \sim$ 250 K. The high temperature transition shows a hysteretic behavior as the FC curve has a lower T_{M2} than the ZFC curve. This unusual behavior for hematite is attributed to a bimodal volume distribution of particles. The role of interacting volumes is also taken into account to describe the observed results.

The memory effect is clearly observed in magnetic measurements that start from different remanence states and explained as dependent on the magnetic ordering of the particles.

1 - 7 – Large magnetocaloric effect in $La_{1-x}Ag_yMnO_3$ manganites at room temperatures

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In recent years, magnetic materials exhibiting the so-called magnetocaloric effect (MCE) in the vicinity of room temperature have received much attention in view of their possible practical applications. The idea of creating a solid state cooler capable of operating in the vicinity of room temperature is highly attractive. For this reason, there is an extensive search for new materials suited for solid-state cooling machines working in this temperature range. Perovskite like manganites, in which the MCE is quite strong and occurs in the vicinity of room temperature, are also among the candidate materials.

In this paper we present the results of investigation of the thermal and magnetic properties (specific heat, thermal conductivity, thermal diffusivity, magnetocaloric effect) of silver-doped manganites of the $La_{1-x}Ag_yMnO_3$ system. A series of $La_{1-x}Ag_yMnO_3$ manganites were prepared (with x=0.1; 0.15; 0.2 and y=0.1; 0.15; 0.2) correspondingly to systematically study the effect of substitution on thermal and magnetic properties. The temperature dependences of the magnetocaloric effect are investigated by direct measurements. The specific heat and thermal diffusivity were measured by ac-calorimetry method, and thermal conductivity was estimated as their product. Anomalies observed on the temperature dependences of all measured parameters. Giant temperature changes with magnetic field change are found. Using magnetocaloric effect and specific heat data the magnetic entropy changes ΔSmag are estimated for all studied samples. The temperatures of magnetocaloric effect maximums are close to room temperatures. The maximal value of MCE observed for $La_{0.8}Ag_{0.15}MnO_3$ manganite and is equal to ΔS=5.7 J/kg K at magnetic field change of ΔH=2.6 T. The relations between technologies of a sample preparation and thermal and magnetic properties are analyzed.

1 - 8 – Half-metallic behavior and electronic structure of Sr_2CrMoO_6 magnetic system

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Complex perovskite materials with the $A_2BB'O_6$ formula have been recently studied because of their peculiar magnetic and electronic properties. The origin of magnetism in the double perovskite Sr_2FeMoO_6 brought these properties again into discussion. Recently a new interaction mechanism was proposed by Sarma [1], according to this mechanism the hybridization of 3d and 2p levels of Mo with the 3d Fe levels are responsible for the half-metallic behavior of Sr_2FeMoO_6. We report here on LAPW ab initio calculations within the Spin Local Density Approximation (SLDA) to DFT for another double perovskite, namely, Sr_2CrMoO_6. Our results show that this is also a half-metallic system. We correlate our results with an extension of the recent model proposed by Sarma to explain the conduction mechanism in this compound.

[1] D.D. Sarma, Sugata Ray, Chem. Sci. **113**, 515 (2001).

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1 - 9 – Nanostructuration and pressure effects on manganites

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We have measured the pressure sensitivity of magnetic properties on $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ nanostructured powders. Samples were synthesized following a microwave assisted denitration process and a final heat treatment at different temperatures to control the grain size of the samples. A span in grain diameters from 40 nm to 1200 nm was obtained. Magnetization curves as a function of temperature and hysteresis loops were measured following different thermomagnetic histories. AC susceptibility as a function of temperature was also measured at different hydrostatic pressures (up to 1 GPa) and for different frequencies. Our results indicate that the nanostructuration plays a role of an internal pressure, producing a structural deformation with similar effects to those obtained under an external hydrostatic pressure.

1 - 10 – Electronic and magnetic properties of the charge disproportionated perovskite $YNiO_3$

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Transition metal oxides are currently a high interesting topic due to the strong connection among their structural, electronic and magnetic properties. In particular, the metal-insulator transition in some of them have been the subject of an intense debate in the last years. Recently, it has been observed that the perovskite $YNiO_3$ presents simultaneous metal-insulator and structural transitions. This structural transition generates two kinds of Ni atoms with different charges and magnetic moments. Up to now, there were no theoretical work that was able to reproduce this magnetic structure. In this work, we study several possible magnetic configurations using *ab initio* calculations by analyzing their total energies and electronic properties.

1 - 11 – Mössbauer and FP-LAPW study of Fe-doped TiO_2 and SnO_2

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During the last years the study of transition metal-doped TiO_2 and SnO_2 semiconductors has become a topic of interest, not only because of the many current industrial applications of these materials, as for example in catalysis, but also because of their potential use in spintronic devices.

There is a great deal of new experimental and theoretical work on these TM-doped systems (TM= Mn, Co, Fe, Ni, Cu), focused on their magnetic properties. In the case of Fe doping, Mössbauer studies were performed in order to elucidate the local atomic structures associated to the observed interactions. Despite the several reports published on quadrupole splitting data, a unique consensus on the hyperfine parameters associated to Fe substitutional in the rutile structure has not been achieved yet. Several questions remain open concerning the Fe location in the host structure, and/or the short range order around impurities, as well as the assignment of the observed hyperfine interactions.

In 2002 we demonstrated the capability of the ab initio full potential linearized augmented plane waves (FP-LAPW) method to predict the hyperfine parameters at impurity sites. Following this approach, in this work we present a comparative experimental Mössbauer spectroscopy and theoretical FP-LAPW calculations of the hyperfine parameters at Fe impurity in the rutile phase of TiO_2 and SnO_2.

1 - 12 – Magnetic behavior of one-dimensional cobaltite $Sr_xBa_{1-x}CoO_3$ ($x < 0.5$)

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The system $BaCoO_3$ has recently received considerable attention because of their interesting magnetic properties [1,2]. These are related to its uncommon crystalline structure, which consists in hexagonally ordered chains of CoO_6 face-sharing octahedra, running along the c direction. The Co-Co distance along this axis is much shorter than between the chains, giving the structure a strong 1D character, while the triangular arrangement of these chains gives rise to the hexagonal structure. The isoelectronic substitution of Ba by Sr decreases the separation between the chains, changing the magnetic interactions. The hexagonal crystalline structure remains up to doping levels of 0.5.

Recent experiments on this system showed a competition between antiferromagnetic and ferromagnetic interactions [1,2]. However, theoretical studies [3,4] suggest the ground state is formed by ferromagnetic droplets of a nanometric size embedded in a non-ferromagnetic matrix, which is the signature of intrinsic nanoscale phase separation.

In this work, for further understanding the magnetism of $Sr_xBa_{1-x}CoO_3$, dc and ac magnetic susceptibilities at low applied fields as a function of temperature were measured. Powders with x ranging 0.1-0.5 were prepared by a citrate technique, using thermal treatments under high oxygen-pressure. dc susceptibility curves show a clear maximum, which appears at lower temperatures for higher applied fields. This behavior is typical for a fine-particle magnetic system with a blocking temperature, T_B. ac susceptibility measurements confirm this magnetic response and also provide information about the thermal relaxation of the ferromagnetic clusters. The effect of doping with Sr on the phase separation phenomenon is discussed.

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1 - 13 – Effects of cation disorder due to Ca substitution on the physical properties of layered cobaltites $Y(Ba_{1-x}Ca_x)Co_2O_{5.5}$

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The family of layered perovskites $RBaCo_2O_{5+\delta}$ (where R is a rare earth element) shows extremely rich structural, electronic and magnetic phase diagrams due to the presence of the 3d-transition element cobalt. These compounds are oxygen non-stoichiometric ($0 < \delta < 1$) which allows the cobalt cation to adopt different oxidation states depending on the oxygen content. Particularly interesting are compounds where Co ions have an average 3+ valence ($\delta = 0.5$). At this composition a structural arrangement of oxygen leads to the so-called 212 superstructure due to the ordering of Co atoms with two different oxygen coordinations (pyramids and octahedra). Moreover, the spin state of each Co atom is dependent on its coordination and can take the values S=0, 1 and 2. In the present work we report on the effects of a partial substitution of Ba with the smaller cation Ca in the cobaltite $YBaCo_2O_{5.5}$. We have synthesized the compounds $YBaCo_2O_{5.5}$, $YBa_{0.95}Ca_{0.05}Co_2O_{5.5}$ and $YBa_{0.9}Ca_{0.1}Co_2O_{5.5}$ by solid state reaction to obtain policrystalline samples. We characterized its physical properties using various experimental techniques within the 5-500 K temperature range, which include neutron diffraction, magnetic measurements, thermoelectric power and resistivity experiments. We have found the magnetic properties to be strongly affected by the cationic disorder. The addition of Ca was found to destroy the antiferromagnetic long-range order, stabilizing ferromagnetic correlations, although with an important degree of frustration. A model for ferrimagnets was applied to the susceptibility data which allows to discuss on the possible spin states of the Co atoms at low temperature.

1 - 14 – Structural and magnetic properties of $La_{0.75}Sr_{0.25}MnO_3$/ $LaNiO_3$ superlattice

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In this work we present a study of the structural and magnetic properties of $La_{0.75}Sr_{0.25}MnO_3/LaNiO_3$ (LSMO/LNO) multilayers. With this purpose, we have grown $[LSMO_{t1}/LNO_{t2}]_n$ multilayers on crystalline (100) $SrTiO_3$ (STO) substrates by dc sputtering. The superlattices consist on n bilayers LSMO/LNO being t1 and t2 the thicknesses of LSMO and LNO, respectively.

We performed a morphological and structural characterization of the samples by X-ray diffraction spectroscopy (XRD). We found that the LSMO and LNO layers grow textured in the [100] direction. The surface's roughness of the samples has been studied by Atomic Force Microscopy (AFM). The roughness at the interfaces, the lattice parameters of the films and layer's thicknesses (t1 and t2) of the

superlattices, were determined by fitting the theta-2theta XRD patterns at high-angles considering the kinematical model in the Suprex program [1].

The angular dependence of the remanent magnetization was measured at different temperatures in order to deduce the anisotropies of the samples. The experimental data were analyzed assuming a free energy density of the samples that includes cubic magnetocrystalline anisotropy, uniaxial and shape anisotropies deduced for the single LSMO layers studied as references. The results for ferromagnetic LSMO layers show a cubic magnetocrystalline anisotropy (Kcub$<$0) and a uniaxial anisotropy oriented along one of the crystalline axes of the perovskite structure in the plane of the film [2].

We also studied the shape of the magnetization loops for different LNO's thickness t2.

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1 - 15 – Iron oxide - silica aerogel nanocomposites

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Magnetic properties of iron oxide particles hosted in silica aerogeles pores were studied by means of magnetization, a.c. susceptibility and transmission electron microscopy. The nanocomposite gels were prepared by Sol-Gel method The precursors: TEOS or TEMOS and $Fe(NO_3)_3.9H_2O$, for two nominal composition given by the mass quotient Fe/Si equal to 0.3 and 0.54, were submitted to hydrolysis and condensation reactions in water and Methanol. Some gels were dried at supercritical conditions and others at atmospheric conditions (xerogel). The a.c. susceptibility $\chi(T)$ displays a broad peak which shift to large temperatures by increasing the a.c applied field frequency, indicating that the particles ensemble behaves as a superparamagnet. The presence of interactions depends on composition. Temperature magnetization dependence for the sample cooled without applied field also indicates a maximum associated to a blocking temperature. Although room temperature Mössbauer Effect spectrum of some aerogels consist of a doublet fitted with superparamagnetic maghemite parameters, microscopy indicates no crystallinity. Interrelation between synthesis parameter, structure and magnetic behavior is discussed

1 - 16 – Mechanosyntesis of Fe doped SnO_2 nanoparticles

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In the last years, research on magnetic nanostructures has been the subject of a number of works. Samples obtained by mechanosynthesis offer the possibility to study size-dependent magnetic phenomena related to the existence of clusters or particles of nanometric scale. Furthermore the obtained heterogeneous magnetic nanostructure can give rise to different magnetic behaviors, such as spin glass, cluster spin glass or superparamagnetism. In this work we focused on the structural and magnetic characterizations of Fe-doped rutile SnO_2 prepared by mechanical alloying. Samples, with 5, 7 and 10 % at of Fe (SnO_2 + Fe_2O_3), were characterized by X-ray diffraction (XRD), Mössbauer effect spectroscopy (ME), ac-susceptibility and magnetization measurements. After 10 h of milling no traces of the precursor α-Fe_2O_3 were observed by XRD. Three paramagnetic interactions corresponding to Fe in +2 and +3 valence states are observed in the Mössbauer spectra of all samples. AC-susceptibility measurements indicate a magnetic behavior intermediate between those of a cluster spin glass and of a system of superparamagnetic interacting particles. The room temperature magnetization curves display the typical superparamagnetic behavior in agreement with the ME results.

1 - 17 – Study of the local structures and their thermal evolution in a HfO_2-20 mol% CaO film

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A film of HfO_2-20 mol % CaO prepared by sol-gel has been grown onto Al_2O_3 by dip coating. The film is investigated by using Differential Thermal Analyses (DTA-TGA), X-ray diffraction (XRD) as a function of annealing temperatures and the Perturbed Angular Correlation (PAC) technique in temperature and after annealing. XRD and DTA experiments were performed in air and PAC measurements in air and vacuum. XRD on the as-prepared material shows a cubic structure and in agreement PAC results exhibit mainly a cubic hyperfine interaction. After annealing at 850^oC the monoclinic phase appears and turns to be predominant upon cooling from 1000^oC. PAC results, in

progress, will be compared with the XRD and DTA thermal evolution. A comparison with results obtained in other calcia stabilized hafnia ceramics will also be carried out.

1 - 18 – Electric and magnetic characterization of $metal/La_{0.7}Ca_{0.3}MnO_3$ interfaces

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Resistive switching and rectifying current-voltage characteristics were recently reported on many complex oxide-metal junctions [1,2], and also on all-oxide heterojunction devices [3,4]. Within an intriguing scenario dominated by complex oxides, these effects have been undoubtedly related to the role of the metal-oxide interface.

In order to study the electrical transport properties of a single mixed valent manganese oxide-metal interface, Kelvin bridge type devices were fabricated from $metal/La_{0.7}Ca_{0.3}MnO_3$ thin films. Different metals (Au, Ag and Ti) were deposited in-situ on $La_{0.7}Ca_{0.3}MnO_3$ films, epitaxially grown on NdGaO3 substrates by pulsed laser ablation. Devices were obtained by standard microfabrication techniques.

The geometry tested permitted 4 probe resistance measurements of the devices, each containing a single interface that was a few square microns in area.

We present the electrical transport characteristics of this interface as a function of temperature and magnetic field.

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1 - 19 – Study of the correlation between electrical and magnetic properties of phase separated manganites using a General Effective Medium approach

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We have performed electrical resistivity and DC magnetization measurements as a function of temperature, on polycrystalline samples of phase separated $La_{5/8-x}Pr_xCa_{3/8}MnO_3$ (x = 0.3). We have used the General Effective Medium Theory to obtain theoretical resistivity vs. temperature curves corresponding to different fixed ferromagnetic volume fraction values, assuming that the sample is a mixture of typical metallic - like and insulating manganites. By comparing this data with our experimental resistivity curves we have obtained the relative ferromagnetic volume fraction of our sample as a function of temperature. This result matches with the corresponding magnetization data in well qualitative agreement showing that a mixed phase scenario is the key element to explain both the magnetic and transport properties in the present compound.

1 - 20 – Magnetic interactions in high-energy ball-milled $(NiZnFe_2O_4)/(SiO_2)$ system

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The system $Ni_{0.5}Zn_{0.5}Fe_2O_4/SiO_2$ was subjected to high-energy ball-milling, with the milling time varying between 1h and 200 h, at room temperature. The samples were obtained by milling the precursor powders in stoichiometric proportions. The as-milled powders were then isothermally annealed for 1 h at temperatures between 673 K and 1273 K, under air and argon atmospheres, respectively. X-ray diffraction, TEM and vibrating sample magnetization were used for structural characterization. As milling proceeds, a complex microstructure develops with small hematite crystals mixed with NiO, ZnO and SiO_2 particles and very small NiZn ferrite clusters. These magnetic clusters reach a mean size of $\sim$10 nm after 160 h of grinding. The apparition of the NiZn ferrite phase leads to an increase in both, the maximum and the remanent magnetization. Also, a gradual decrease of the coercive field is observed which may be attributed to the superparamagnetic behavior of these small crystals and to a gradual rupture of hematite agglomerates taking place during grinding. The high temperature treatments remove the hematite grains from the powder and promote the growth of NiZn ferrite grains to reach mean sizes of $\sim$ 20 nm. For treatments in oxidizing atmosphere the major phases are SiO_2 and NiZn ferrite, while for annealing in Ar a new phase appears, fayalite, which has a canted antiferromagnetic spin arrangement at room temperature. This explains the lower maximum magnetization observed in the powders annealed one hour at 1273 K in an Ar environment.

These results are interpreted considering the different magnetic phases obtained, their crystal sizes and their mutual interactions, which are found to strongly depend on the milling time, and also on the temperature and atmosphere of the final heat treatment.

1 - 21 – Ising spin glass state in $Fe_{0.5}Ni_{0.5}TiO_3$ polycrystal

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The Ising spin glass $Fe_{0.5}Ni_{0.5}TiO_3$ has been studied by dc/ac susceptibility as well as Mössbauer spectroscopy measurements. The data show a transition from a paramagnetic to an antiferromagnetic state at $T_N = 116$ K and an Ising spin-glass behavior is observed below $T_{sg} = 60$ K. At $T < T_{sg}$, the in-phase component of the ac susceptibility, $\chi'(T)$, becomes frequency dependent and, the out-of-phase component of the susceptibility, $\chi''(T)$, emerges. The ^{57}Fe Mössbauer spectra of the powder sample above T_N are quadrupole splits doublets with rather narrow lines at room temperature and for $T < T_N$ are broad patterns typical of disordered systems.

1 - 22 – Electronic and structural properties of Sr_2YSbO_6

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The electronic and structural properties of Sr_2YSbO_6 (SYSO) perovskite material were predicted by means of *ab initio* calculations of band structures and density of states. The calculations were carried based on the DFT–LAPW method with the Wien2k computer code. As result, for the ground state, the compound has been found insulator material, which is agree with experimental results. In addition, we have determined the optimal structure for the SYSO by energy–volume calculations using $Fm3m$ (225) and $I4/mmm$ (139) space groups. We found the $Fm3m$ with the lesser value of minimal energy. Furthermore, we have performed a comparative study between structural properties predicted (with DFT) and the structural ordering (experimental) found by Rietveld analysis on XRD pattern of SYSO. Previously, we have reported this material as a potential substrate material for deposition of $YBa_2Cu_3O_{7-\delta}$ (YBCO) superconductor films, due to its favorable characteristics [1]: chemical stability of SYSO with YBCO; good lattice matching and no degradation of superconductor transition temperature of YBCO due to interaction with SYSO.

[1]O. Ortiz Diaz, *et. al.*, *Mod. Phys. Lett. B*, **18** 1035–1042 (2004)

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1 - 23 – Magnetic properties of Cu/Mn/O powders obtained by controlled high energetic ball milling

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The $Cu_xMn_yO_z$ system shows a variety of magnetic and electrical conductivity properties depending on the x, y and z values. Yang et al. [Yang, S. G. et al. Appl. Phys. Lett. 83, 3746 (2003)] have found that $Cu_{1-x}Mn_xO$ (for $0.05 < x < 0.15$) prepared by co-precipitation methods presents ferromagnetic properties below 80K, while $CuMn_2O_4$, synthesized following the same route, exhibits a canted antiferromagnetic behavior with a Néel temperature of about 30 K. Taking into account that the preparation way and crystallite size influence the properties of the systems of the binary oxides powders, Cu/O [Bianchi.A. et al. Report do LNLS 2003, 131-132 (2004) and references therein] and Mn/O [Bianchi.A. et al. Report do LNLS 2004], we have produced, by controlled high energetic ball milling (HEBM) (up to 48 hs) of mixtures of CuO and α-Mn_2O_3 in the ratio 1/3, and studied powders of Cu/O/Mn. Selected samples were annealed at 400K during different times. All the prepared samples were characterized by x-ray diffraction and their magnetic behavior was studied from AC susceptibility measurements performed in the range 14 to 300K. Ball milled samples susceptibility curve shows a broad peak centered in 32K and increase in magnetic response as function of milling time. Thermal treatments of the 36h ball milled sample induce an increase in the magnetic response and a shift in the susceptibility maximum towards higher temperatures. These results can be rationalized as due to the stabilization of the $Cu_{1.5}Mn_{1.5}O_4$ phase.

1 - 24 – Relaxation of substitutive atoms in manganites $La_{2/3}Ca_{1/3}MnO_3$, $La_{2/3}Sr_{1/3}MnO_3$ and $La_{2/3}Ba_{1/3}MnO_3$

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In previous works we have made internal friction (IF) and elastic shear modulus (G) measurements on several manganites containing substitutional atoms at the place of La, in the temperature range 100-500 K, showing the existence of one anelastic relaxation at around 400K. Confirming this hypothesis the 400K peak is absent in the system LaMnO3. The 400K peaks have the following

activation energies:(3.77±0.5)eV for $La_{2/3}Sr_{1/3}MnO_3$, (4.6±0.1) eV for $La_{2/3}Ba_{1/3}MnO_3$ and (5.4±0.6)eV for $La_{2/3}Ca_{1/3}MnO_3$. Their IF maxima and their relative modulus variation ($\Delta G/G$) are the followings: a) IFmax: (0.146±0.05), (0.166±0.05) and 0.170±.02); and b) $\Delta G/G$: (0.035±0,005), (0.066±0.005) and (0.840±0.005), for $La_{2/3}Ca_{1/3}MnO_3$, $La_{2/3}Sr_{1/3}MnO_3$ and $La2/3Ba_{1/3}MnO_3$ respectively. The mechanism associate to those 400 K IF peaks are related to a Zener relaxation (1) of the cations that ocuppied the same crystallographic site. A pair of these substitution cations are induced to move to another equivalent crystallographic site and then come back, by the sinusoidal applied stress, in our case with a frequency of 1Hz. The magnitude of the relaxation strength Δ (taken from $\Delta G/G$) and the IF peak height increase with the substitutional atom radii. The atomic radii of the substitutional atoms are 1.26 Å, 1.39 Å and 1.56 Å for Ca, Sr and Ba respectively. The intensity of the relaxation Δ depends on the derivative of the distorsions introduced by the substitution atom respect to the applied stress. It depends also of other parameters (as the lattice parameter and the activation volume). In consequence, when the substituting atoms are greater, the IFmax and the $\Delta G/G$ are also greater.

1 - 25 – Colossal Magnetoresistance study in the manganite $La_{1-x}Sr_xMnO_3$

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$La_{1-x}Sr_xMnO_3$ manganites with $0.0 < x < 0.5$ were prepared by a citrate method with controllable content of *Sr* according to inductively coupled plasma - atomic emission spectrometry (ICP-AES) and with perovskite structure according to x-ray diffraction (DRX). For the present work we have utilized $x = 0,2$. The sample was compacted and sinterized into a disc shape. Metallic electrodes were placed on it in order to measure electric resistance variations as a function of the temperature in the presence of an external magnetic field . The measuring range went from 0 to $1,3\,T$ for external magnetic field and from 87 to $330\,K$ for temperature. The experimental results showed a Colossal Magnetoresistance (CMR) value of 50% near $300\,K$. An increment in the critical temperature of approximately 20K in the presence of a $1,3\,T$ magnetic field has been seen. Resistivity and Hall effect measurements of the remaining doping level values are currently being carried out, as well as ac resistometry measurements in order to detect weak-order phase transitions.

1 - 26 – Microstructural and magnetic studies on nanocrystalline Fe/SiO_2 composites

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Nanocrystalline Fe_2O_3 / SiO_2 has been synthesized with various grain sizes by high-energy ball-milling, with the milling time varying between 1 h and 340 h. The precursor powders, iron and SiO_2, were milled at room temperature under specific milling conditions. Structural changes were followed by X-ray diffraction analysis, TEM and magnetization measurements after various milling times. As milling proceeds, a complex microstructure develops with small iron crystals mixed with Fe_3O_4 cluster and SiO_2. These magnetic clusters reach a mean size of ∼7 nm after 180 h of grinding. After 220 h of milling, XRD analysis identified a mixture of Fe_2O_3 / SiO_2 and Fe_3O_4 / SiO_2 phases. Iron as well as other phases were not detected. Before nucleation of the Fe_3O_4 phase the crystallites of Fe phase were reduced to a minimal size. A similar behavior was observed before nucleation of Fe_2O_3 phase. Therefore, it appears that before nucleation of the new phase, it is necessary to reduce the size of the crystallites of the starting phase to some critical value. After 280 h of milling, it was found that complete transformation of Fe/SiO_2 to Fe_2O_3/SiO_2 is possible during milling in an air atmosphere under appropriate milling conditions. The temperature dependence of the magnetization investigated under zero field cooling (ZFC) and field cooling (FC), measured applying a DC field of 100 Oe, gave further confirmation of superparamagnetism specially in the powders milled in the range of 160- 220 h. The sharp maximum of the ZFC and the splitting between ZFC and FC curves just above of this maximum indicate a narrow particle size distribution. These results are interpreted considering the different magnetic phases obtained, their crystal sizes and their mutual interactions, which are found to strongly depend of the milling conditions.

1 - 27 – Three-peak Behavior in Giant Magnetoimpedance Effect in Amorphous $Fe_{73.5-x}Cr_xNb_3Cu_1Si_{13.5}B_9$ Alloy Ribbons

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A systematic study of the giant magnetoimpedance (GMI) effect in amorphous magnetic $Fe_{73.5-x}Cr_xNb_3Cu_1Si_{13.5}B_9$ alloy ribbons with x = 0, 2, 4, 6, 8, and 10 is presented. The complex impedance in these compounds was measured for applied fields from -80 to 80 Oe at room temperature, via the so-called four probe technique. H was applied parallel to the AC driving current along the longitudinal direction of the ribbons. The frequency of the AC driving current ranged from 0.5 to 20 MHz, while its amplitude was kept at 1 mA (rms value). Depending on the frequency, the experimentally observed GMI curves exhibit two types of behavior, namely single-peak (SP), and two-peak (TP). These behaviors depend on the relative contributions of domain wall motion and magnetization rotation processes to the

circular permeability, u = uwall + urot [1-3]. We emphasize the appearance of a three-behavior in GMI curves. It occurs between SP and TP behaviors. The mechanics leading to the three-peak behavior are discussed.

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1 - 28 – The electronic and magnetic properties of Ni_3Fe and $NiFe_3$ alloys

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Electronic structure calculations of the ordered ferromagnetic and paramagnetic transition metal alloys $NiFe_3$ and Ni_3Fe are performed using the full-potential linearized augmented plane wave method . We find that $NiFe_3$ and Ni_3Fe exhibit strong ferromagnetism . The magnetic moments for the Fe and Ni atoms are in good agreement with experimental values. It should be noted that in both Ni_3Fe and $NiFe_3$ alloys the Fermi level lies near the peak that is located in the valley between the two main DOS peaks

1 - 29 – Magnetic behavior of Ca_2BWO_6 (B=Co,Ni) double perovskites

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The discovery of colossal magnetoresistance (CMR) properties in hole-doped manganese perovskites has stimulated the enthusiasm of solid-state chemists and physicists. As basic features, a CMR material must exhibit a semi-metallic, spin-polarized conductivity and experience a ferromagnetic (FM) ordering at Curie temperatures, TC, as high as possible, ideally well above room temperature (RT). It is now well established that Curie temperatures of mixed-valence manganites (based upon LaMnO3 perovskite) cannot be increased above 400 K by any chemical substitution. However this temperature is overcome in the some members of the family of double perovskites of composition A2B´B´´O6 (A = alkali earths, B´, B´´ = transition metals) proposed as half-ferromagnets (best described as ferrimagnets). These are an alternative to manganites.

The revival of interest in this family was triggered by a report on Sr_2FeMoO_6, demonstrating that in the electronic structure only minority spins are present at the Fermi level; this material was shown to exhibit intrinsic tunneling-type magnetoresistance (MR) at RT. The ferrimagnetic structure can be described as an ordered arrangement of parallel Fe^{3+} (S = 5/2) magnetic moments antiferromagnetically coupled with Mo^{5+} (S = 1/2) spins. The occurrence of MR properties is a common feature in other members of the $A_2B´B´´O_6$ family. The A = Ca and Ba analogues of the Sr_2FeMoO_6 were also found to exhibit semimetallic and ferrimagnetic properties. The CMR has also been induced in phases with B´ = Co, as the recently reported in Sr_2CoMoO_6 upon chemical reduction, via topotactical removal of oxygen atoms.

Because satisfactory results have been obtained with $A_2B´B´´O_6$ double perovskites, have given our attention to phases Ca_2CoWO_6 and Ca_2NiWO_6. They were studied in the sixties and forgotten for more than 30 years. Recently these phases have been studied by Martínez-Lope and col. with data of neutron powder diffraction. These crystalline structures were reported as monoclinic perovskite and antiferromagnetic TN = 36 K and TN = 56 K for the Co and Ni, respectively.

We have chosen to study the magnetic properties of Ca_2CoWO_6 and Ca_2NiWO_6 for several reasons. In this work these compounds are characterized by XRD on a well-crystallized samples and their monoclinic distorted structure is confirmed by Rietveld methods. A new study is presented starting from macroscopic magnetic in order to corroborating the magnetic structure obtained previously by ND data and to confront with previous magnetic data.

Low dimensional and nanostructured materials

2 - 1 – Magnetic properties of $NiFe_2O_4$ nanoparticles produced by a new chemical method

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We have investigated the anomalous magnetic properties of nickel ferrite ($NiFe_2O_4$) nanoparticles (NP´s) obtained through a new route chemical, in which has been on the use of sucrose as chelating agent [1]. X-ray diffraction (XRD) confirms that $NiFe_2O_4$ NP´s with inverse spinel structure is already formed at 300^{o}C, and present average size 11 nm. Magnetic measurements point out that hysteresis loops remain in a non-saturated state at fields up to 20 kOe. Besides, an irreversible behavior of the high field ZFC-FC moment are found as well. The effective magnetic moment per molecule evaluated from hysteresis loops at magnetic field of 20 kOe is smaller than 2B/molecule as it should be expected in $NiFe_2O_4$ (CNPq, FAPESP, CAPES).

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2 - 2 – The influence of the pressure and temperature on the light emission of the ZnO

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A proteic sol was prepared dissolving zinc nitrate in filtered coconut water (cocos nucifera) with a concentration of 0.5 mol/dm^3. Afterwards the sol was heated to 100^{o}C for 24 h and then submitted to calcination at 1000^{o}C for 24 h in air, in order to completely oxidize the salts. Then, the final product was quenched back to room temperature. The crystalline phase of the powder was consistent with standard XRD pattern to the JCPDS 36-1451. The powder was pressured at 1 ton and a ZnO pellet was obtained. The emission spectrum was recorded in a spectrofluorimeter under excitation at 200 nm. The powder showed two large peaks around 470 and 600 nm, which is typical for the ZnO nanocrystal. However, for the pellet, it has been observed a structure of narrow peaks in the same region. The interpretation for this behavior is that, after pressure and calcination procedures, the luminescent site is submitted to a stronger crystal field than in the powder sample, and a more crystalline structure is achieved. This is an indication that the combination of pressure and temperature can become possible to get emission characteristic kind of monocrystal.

2 - 3 – Phase Diagram and Tricritical Magnetic properties of mixed bond Ising systems investigated by use of Monte Carlo and the effective-field theory

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The phase transition of a random mixed-bond Ising ferromagnet on a cubic lattice model is studied both numerically and analytically. Analytical studies on Mixed-bond Ising model by using renormalization group technique predict the existence of reentrant magnetism in a certain range of values of the competition parameter α. This phenomenon typically is found in systems presenting spin glass phase, for instance Eu_pSr_{1-p}. We seek the existence of the reentrance by means of Monte Carlo simulations. In this work, we use the Cluster algorithms de Wolff and of Glauber to simulate the dynamics of the system. We obtained the thermodynamic quantities such as magnetization, susceptibility, and specific heat. Critical temperatures were estimated of the maximum of the susceptibility and with these values we made the phase diagram T_C vs. p for different α values. Our results were compared with those obtained using a new technique in effective field theory that employs similar probability distribution within the framework of two-site clusters.

2 - 4 – Phase Diagram and Tricritical Behavior of an Ising Metamagnet Model in a Trimodal Random Field

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Monte Carlo simulation was used to determine the phase diagram of a metamagnet Ising model in the presence of a random and uniform magnetic field. The model consists of a spin-$1/2$ metamagnet in which the nearest neighbor and next nearest neighbor spin interactions are antiferromagnetic ($J_1 < 0$) and ferromagnetic ($J_2 > 0$), respectively. We used a bimodal probability distribution for the random magnetic field. We have calculated the staggered

magnetization and the fourth-order Binder cumulants in order to obtain the critical points. The phase diagram in the uniform field versus temperature plane presents continuous and first-order transition lines. The phase diagram of an Ising metamagnet in an uniform and random magnetic field is studied using effective field theory. The phase diagram presents tricritical behavior and reentrance phenomenon for determined values of the random magnetic field above a certain critical value. The reentrance phenomenon is due to the competition between the other interactions (ferromagnetic, antiferromagnetic, uniform magnetic field) and the random magnetic field.

2 - 5 – The interplay of the lateral Fano anti-resonances and the Kondo effect in the low temperature regime of a side-coupled quantum dot

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We study the electronic transport through a quantum wire (QW), described by a tight-binding linear chain, with a side-coupled quantum dot (QD), here modeled by the Anderson impurity model. Contrary to the earlier work [1] where we describe the lateral Fano anti-resonances employing the X-boson approach [2], here we employ the atomic approach [3] that describes the Kondo effect in a very precise way. To study the interplay of the lateral Fano anti-resonances and the Kondo effect we change the position of the chemical potential across the conduction band and when it is located at the edge of the conduction band, very close to the conduction Van-Hove singularity we observe the effect of the lateral resonance over the Kondo peak in the low temperature regime. We obtain the conductance with a strong Fano anti-resonance in the low temperature regime. The calculated density of states (DOS) shows that this behavior is associated to a many-body renormalized QD resonant level $\tilde{E_f}$ at the edge of the conduction band (CB) strongly hybridized with the Van-Hove singularity of the one-dimensional density of states of the lead. We present results for the density of states and the conductance.

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2 - 6 – Determining superconducting parameters from the analysis of magnetization fluctuations for the $CaLaBaCu_3O_{7-\delta}$ superconductor

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In this work we report analysis of magnetization fluctuations for the $CaLaBaCu_3O_{7-\delta}$ superconductor system. We describe a procedure for extracting the penetration depth and the coherence length parameters from the magnetization, as a function of applied magnetic field, M(H) data. Second critical magnetic field Hc2 was else obtained. This procedure takes the vortex fluctuation into account. The data of the magnetization excess is analyzed for different values of temperature, in the interval of 65 to 73 K. For several magnetic fields we observed a crossover in the magnetization curves at the temperature value T*=72.12 K. We calculated the data of magnetization excess from curves of M as a function of lnH. This procedure was performed by using the recipe of Bulaevskii, Ledvij and Kogan (BLK) [1] for polycrystalline samples of $CaLaBaCu_3O_{7-\delta}$. We notice that the values for these superconducting parameters are in agreement with reports for other high temperature superconductors [1,2].

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2 - 7 – Coupling between structural and chemical phase transitions during Sb/Si(111) adsorption

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The kinetic and thermodynamic properties of adsorption and desorption of onto Si(111) surface are analysed by mass spectrometry and ab-initio calculations. It is found that when Sb coverage exceeds a critical value (in the submonolayer range) Sb/Si(111) undergoes a site transition from ternary towards on top site. This structural transition is associated to a spectacular change of the character of the - effective interactions from repulsive at low coverage towards attractive at the monolayer completion. Introducing such site-dependent interactions in a Monte-Carlo simulation enables us to simulate the adsorption-desorption isotherms. The so-obtained isotherms are compared to the experimental ones and the corresponding simulated structures are discussed in terms of coupling between structural and chemical phase transition.

2 - 8 – Polaron Variable Range Hopping in $TiO_{2-\delta}(-0.04 \leq \delta \leq 0.2)$ Thin Films

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Thin films and nanostructures of TiO_2, a wide band gap semiconductor, have been studied for application as a gate insulator for MOS device applicatioms. Despite its diverse technological applications, the charge transport in TiO_2 is also of considerable interest from the perspective of fundamental physics. The TiO_2 exhibits strong electron-phonon coupling, resulting in low room temperature electron mobility. Although progress was already made studying electrical and optical properties of crystalline TiO_2 in rutile or anatase phase[1], the understanding of the conduction mechanisms in this material, with regard to the growth conditions, is still incomplete and challenging.

In this work, the mechanisms of electrical conduction in $TiO_{2-\delta}$ $(-0.04 \leq \delta \leq 0.2)$ have been investigated. The films were prepared by the rf-diode reactive sputtering of a titanium target in O_2+ Ar gas mixtures and changes in δ were achieved by varying the O_2 flow rate (FO_2) and the substrate temperature. The electrical transport properties were investigated by measuring the conductivity as a function of temperature between 20K and room temperature, and correlated with structural and compositional studies.

A higher resistivity was observed in samples with less percentage of anastase phase $TiO_{2-\delta}$ film ($\delta = -0.04$)in comparison with sample rich in anatase phase. At the temperatures ranges between 200 and 290 K approximately the best fit to the experimental data for three samples was obtained assuming a dependence $\sigma = ALn(T_o/T)^{1/4}$ characteristic of adiabatic variable range hopping[2]. At low temperature, between 17K and 200K, the activation energy decrease. Hopping distance and hopping energy, between 3 nm and 48 nm and between 96 and 18 meV respectively were calculated by assuming the localization length a to be equal to the inverse of the effective Bohr radius.

The nature of electron transport is probably determined by electron-phonon interaction and the small values of the hopping distance suggest that carrier is a small polaron [3]. The estimated polaron radius are comparable to the lattice spacing . We suggested that the conduction mechanism in the samples studied in this work is adiabatic small polaron hopping for the temperature range measured. This is not in agreement with the works of Hassan et al. [4] where the authors suggested a non-adiabatic hopping conduction.

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2 - 9 – Monoatomic metallic wires : structure, electric transport and normal modes

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A traditionally idealized textbook example, the atomic linear chain, has recently become an actual system that can be explored experimentally. The formation of atomic chains several (up to 7-8) atoms long has been achieved in recent years using experimental techniques like scanning tunneling microscope and mechanically controllable break junctions [1]. In both cases, evidence has been found of chain formation in the last stages of pulling an atomic contact for certain metallic elements like Au, Pt and Ir.

At low voltages (zero-bias conductance), these atomic chains exhibit interesting properties. Recent experimental results indicate the presence of conductance oscillations with period $\sim 2a$ (a being the interatomic distance) after averaging over many realizations of the chain [2]. While in the case of Au the oscillations are superimposed to an almost constant background of the order of the quantum of conductance $G_0 = 2e^2/h$, in the case of Pt the mean value of the conductance exhibits a continuous decrease from ~ 2.5 to $\sim 1.0G_0$. For Ir chains the conductance varies between ~ 2.2 and $\sim 1.8G_0$ with a less clear oscillatory behavior.

On the other hand, the dependence of the conductance with the applied voltage shows that transport in these wires is non-dissipative up to a threshold of several meV, which corresponds to the energy of the vibrational normal modes of the chain [3].

In this work, we present our calculations of the electronic structure and conductance of atomic chains of 5d elements like Au, Pt and Ir. We show that, in addition to the even-odd parity oscillations characteristic of Au, conduction channels associated with the almost full d bands in Pt and Ir give rise to longer periods which could be observed in sufficiently long chains. The results for short chains are in good agreement with recent experimental measurements [4].

We will also show, preliminary results obtained from molecular dynamic simulations using a tight-binding Hamiltonian [5]. For Au, we will present computer simulations showing the formation and compression of atomic wires. We report the atomic processes involved in the formation and crush of the atomic chains, the evolution of the conductance and the normal modes of vibration.

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2 - 10 – FORC analisys in the hysteretic behaviour of boron-rich nanocomposite Nd-Fe-B ribbons

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In recent years, permanent magnet industries and materials scientists have focused their efforts to the development of nanocomposite materials, as well as to the study and modelisation of their magnetic response. Also named exchange-spring magnets, they exhibit interesting properties, such as remanence enhancement, moderated to high coercivities and theoretically expected energy products as high as 8 GJ/m^3 . This properties are due to exchange coupling between a hard and a soft magnetic phases at nanometric scale. In the case of boron enriched alloys, the selected nanostructure is obtained from amorphous precursors after a thermal annealing. Their magnetic response is highly dependent on the precipitated phases.

In this work, we produced amorphous ribbons with the composition $Nd_{4.5}Fe_{72}Co_2Cr_3Al_1B_{17.5}$, employing the melt-spinning technique. The ribbons were submitted to different thermal treatments at 685, 710 and 735 ^{o}C, for 10 min.

Their crystallisation, kinetic and precipitated phases, were determined by means of differential scanning calorimetry (DSC), Mössbauer effect spectroscopy (ME) and X-ray diffraction (XRD). The presence of a solid solution α-(Fe, Co), for lower annealing temperatures, was recognized from ME spectra. For the sample treated at 735 ^{o}C, it was detected α-Fe rather than any evidence of that solid solution. The magnetic properties of annealed ribbons were analyzed by means of their FORC distributions. The mentioned structural modification promoted a sharp peak near the origin in the $h_c - h_u$ plane. Other changes among FORC distributions of different samples will be discussed in terms of observed interactions and structural modification.

2 - 11 – Internal magnetic order of the sample $(Fe_{0.85}Nd_{0.15})_{0.60}B_{0.40}$

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We have synthesised and magnetically characterised $(Fe_{0.85}Nd_{0.15})_{0.6}B_{0.40}$ amorphous nanoparticles ($\sim$7 nm). The $(Fe_{0.85}Nd_{0.15})_{0.6}B_{0.40}$ alloy, very well known because its technological applications, shows several anomalies which consist in an evident reduction of the saturation magnetisation and coercive field for this particular sample compared to its neighbouring compositions. We studied both dispersed and powder samples, the dispersed one (in a non-magnetic matrix) let us study the intrinsic magnetic order inside the nanoparticle, whereas the in the powder one the particles interact among them and the internal order is somehow frustrated. The observed anomalies seem to vanish for temperatures higher than RT and are present in dispersed and powder samples. Coercive field follows the magnetic moment tendency confirming that the anysotropy is mainly due to the shape of the particles [(1)]. We associate this behaviour with a spin reversal inside the particle for this composition which tends to reduce the magnetic moment of the particles, leading to the observed decreasing of saturation magnetisation and coercive field relative to the values of the neighbouring compositions

2 - 12 – Time Reversal Mirror and Perfect Inverse Filter in a Microscopic Model for Sound Propagation

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Time reversal of quantum dynamics can be achieved by changing the sign of the Hamiltonian, as in the Loschmidt Echo experiments in NMR [1]. However, this global procedure, dubbed a “hasty Loschmidt daemon”, has an efficiency which is limited by chaos and disorder. In contrast, for classical sound waves, the Time Reversal Mirror (TRM) [2] has proved being very robust precisely for those cases. This procedure, called “stubborn Loschmidt daemon”, consists of a persistent injection of wave function amplitude at the periphery of the region we want to control and would work in a quantum system [3]. However, the theory behind this stability is not yet developed. As a first step, we introduce a simple model for one-dimensional sound propagation where dissipation and inhomogeneity are achieved by coupling an impurity oscillator to a chain of oscillators [4]. Perfect time reversal requires a procedure, the Perfect Inverse Filter (PIF), where the signals detected at the control points are processed to account for memory effects. In order to ensure numerical stability in the solution of the many-body dynamics, we develop a procedure based on the Trotter-Suzuki algorithm used for quantum dynamics [5]. We show that PIF procedure corrects the imperfections of the TRM that manifest when the initial state is built up from an inhomogeneous spectrum. This leads to substantial qualitative and quantitative improvements of the reversal quality when this system is used as an “acoustic bazooka”[6].

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2 - 13 – Surface anisotropy and exchange interaction of Co nanoparticles embedded in a Cr_2O_3 matrix

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We study the effect of the exchange interaction at the interface of Co nanoparticles embedded in an antiferromagnetic Cr_2O_3 matrix. The samples were prepared by two methods: from chemical precipitation and from solid state reaction follow by a calcination in an Ar_2/H_2 atmosphere. From the first method the samples consist in $\sim$ 6 nm Co nanoparticles embedded in $\sim$ 200 nm Cr_2O_3 matrix. From the second method the obtained $\sim$ 6 nm Co nanopaticles are embedded in $\sim$ 80 nm Cr_2O_3 nanoparticles. Both systems present exchange bias effect when are cooling applying a magnetic field thought the matrix antiferromagnetic transition temperature T_N=308 K. We found that the exchange field depends on the cooling field and the temperature. The maximum exchange field was observed cooling the sample with an applied field of 2000 Oe. We compare these results with the magnetic behavior of Co nanoparticles dispersed in a diamagnetic Al_2O_3 matrix.

2 - 14 – Hysteretic current – voltage characteristics in rf-sputtered $TiO_{2-\delta}$ (-0.04 $\leq \delta \leq$ 0.2) thin films

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Resistive switching in transition metal oxide films, such as TiO_2,attracts great interest for a possible application in nonvolatile memory devices due to low required current for switching compared to phase change memories. In this work, we have measured the current - voltage characteristics and voltage vs. time response at room temperature in $TiO_{2-\delta}$ (-0.04 $\leq \delta \leq$ 0.2) thin films fabricated by the reactive rf-sputtering of a Ti target in Ar and O_2 mixtures. The films were deposited on ITO buffered glass substrates. Copper wires were soldered on the top surface of the film and on the ITO bottom electrode using Indium. A hysteretic and asymmetric response is found in the current - voltage curves that were measured for different ranges of current and voltage. Resistance transients evolutions are also measured for current or voltage constant excitation. For those transients, long time constant (on the order of the minutes) were found.The hysteresis in the IV curves are discussed on the basis of the charge trapping/detrapping process at the interfaces and changes in the carrier density. This density changes affect the degree of the band bending at the electrode-semiconductor interface and hence the IV characteristics. The resistance changes are related to the carrier trapping levels induced by the voltage pulses. Electrical transport and photoconductivity characterizations of these films that are expected to yield further insight into the resistive switching phenomenon will be described.

2 - 15 – Quantum pumping for fermions in a ring

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We study transport properties of fermions in a ring geometry and in contact to fermionic reservoirs and time dependent scatterers. We use the Schwinger-Keldysh closed time path formalism to treat the interactions that drive the system away from equilibrium. For the case of two forward scatterers oscillating harmonically with phase lag δ, we obtain an analytical expression for the transmission coefficient, exact up to second order in the amplitude of the barriers. We discuss the phenomenon of quantum pumping in this context.

2 - 16 – The effect of electron-phonon interaction on a carbon nanotube with an adsorbed molecule

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We present theoretical results on the effect of vibrational modes of adsorbed molecules on the transport properties of carbon nanotubes.

Due to the one-dimensional nature of the carbon nanotube, it is expected that a scattering mechanism modifies its conductance. Recently was shown experimentally[1] the effect of a vibrational-electronic interaction in single-wall carbon nanotubes (SWCNTs).

On the other hand a SWCNT coated with metal nanoparticles facilitates the adsorption of organic molecules. The use of biomaterials with carbon tubes has also provided different routes of using the complex systems as biosensor devices. Also, spin polarized transport may be achieved by adsorbing transition metal on the walls of nanotubes.

Vibration states induced by the adsorption of different atoms or molecules may be calculated. How quantized vibration modes may affect the electron transport through a single molecule has been discussed in the literature, taking into account that charging effects on the molecule plays an important role on the conduction.

Here we consider a single molecule attached to one of the atoms laid at the carbon tube wall and investigate the changes in the electronic density of states and electronic current.

The electronic system is described using a single $\pi\pi$-band within a tight-binding approximation. A single optical phonon mode is considered coupled to the electrons through the Fröhlich interaction. The present theoretical description in the Fock space[2], maps the system into a set of coupled one-dimensional tubes, each one associated to a particular number of phonons. The system is solved using the Keldysh Green function formalism. We show that, even being the electron-phonon interaction much smaller than the electronic hopping, it could lead to important changes in the transport properties. This is a clear consequence of the quasi one-dimensional nature of the carbon nanotube structure.

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2 - 17 – Structural and magnetic characterization of the $Fe_{73.5}Ge_{15.5}Nb_3B_7Cu_1$ alloy

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In this work, we studied the magnetic and structural properties of the $Fe_{73.5}Ge_{15.5}Nb_3B_7Cu_1$ alloy. Nanocrystalline ribbons were obtained from controlled crystallization of amorphous material made employing the melt spinning technique. The structural evolution of these alloys was studied using X-ray diffraction (DRX) and Differential Scanning Calorimetry (DSC) and these results were correlated with their magnetic properties at different annealing temperatures. Magnetic Saturation for the sample annealed at different temperatures was measured in a Physical Property Measurement System (PPMS) at room temperature. Coercivity was obtained using a low frequency fluxometric method by applying an axial field on the sample and collecting the induced signal in a secondary compensated pick-up coil. The magnetic environment of the Fe in the annealed alloy at 723K was obtained by Mössbauer Spectroscopy. From these data the magnetic contribution of the nanocrystals to the alloy was estimated.

2 - 18 – Amorphous and nanocrystalline fraction calculus for the $Fe_{73.5}Si_{3.5}Ge_{10}Nb_3B_9Cu_1$ alloy

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We studied the relationship between the saturation magnetization (Ms) of the $Fe_{73.5}Si_{3.5}Ge_{10}Nb_3B_9Cu_1$ alloy and its nanocrystalline structure. Amorphous ribbons obtained by the melt spinning technique were heat treated for one hour at different temperatures. The optimal heat treatments that led to the formation of a homogeneous structure of Fe_3(Si, Ge) nanocrystals with a grain size around 11 nm embedded in an amorphous matrix were performed at 813K. We calculated the magnetic contribution of the nanocrystals to the heat treated alloy using a lineal model. On the other hand, saturation magnetization (Ms) of the nanocrystalline and of the amorphous alloys were measured. From experimental data and using the theoretical calculus we obtained the amorphous and crystalline fraction of the heat treated ribbons.

2 - 19 – Effect of the Cu concentration on the magnetic properties of mechanically alloyed FeMnCu system

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Magnetic nanoparticles materials are one of the topics under research, especially due to the production of a large variety of new structures with interesting physical properties. The investigation and improvement of these properties can lead to the discovery of novel magnetic materials with potential applications in new technologies. In order to get deeper into the knowledge of the nanoestructurated metallic systems, allowed powders of $(Fe_{79}Mn_{21})_{1-x}Cu_x$ (x = 0.2, 0.25 and 0.3) were prepared by milling the elemental species in a horizontal vibrating device with steel balls and vial, under Ar atmosphere during 15 h at 33Hz. The analysis of structural properties was carried out using X-ray diffraction (XRD). Measurements of AC-susceptibility, zero field cooling-field cooling (ZFC-FC) and M vs H cycles were also performed to obtain a magnetic characterization of the samples. The XRD results show only the presence of FCC-phase for the three concentrations. The AC-susceptibility curves show the existence of a characteristic temperature T_c which shifts to lower temperatures with the increase of the Cu content. The irreversibility of magnetic properties has been studied as function of the applied field to the ZFC-FC curves. The hysteresis loops, recorded at several temperatures, can be reproduced using three contributions, two magnetics and one non-magnetic. These results provide evidences for a highly disordered magnetic system with spin-glass-like behavior.

2 - 20 – SnO_2 nanostructures on top of a silicon nitride surface

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Films of SnO_2 have been used for gas sensing obtaining very low limit detection of CO, ethanol, hydrogen and other gaseous contaminants. Recently it has been reported a single square shaped SnO_2 nanotube gas sensor to ethanol (1). Several advantages like higher active surface area, flexibility in surface modification for chemically or biologically selective catalysis, accelerated transport of gas/liquid and drastically enhanced electrical transport properties have been reported. A SnO_2 nanotube sheet sensor has also been characterized (2). SnO_2 nanotubes have been synthesized using a polycarbonate template method (3-5). The precursor solution was obtained dissolving $SnCl_2.2H_2O$ in deionized water, adding acetic acid, small portions of metallic tin powder and 30% hydrogen peroxide were added slowly. The templates were filled using a syringe filter device and were treated at 600°C during 10 minutes. The SnO2 nanostructures onto silicon nitride surface were obtained attaching the filled template to the surface and performing the same thermal treatment. The material was characterized by X-ray diffraction analysis and scanning electron microscopy. Electrical characterization is in progress.

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2 - 21 – Measurement of mesoscopic High-Tc superconductors by micro-oscillators

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In mesoscopic samples, when the size of the sample is comparable to the characteristic lengths of the system, appear news and very interesting properties. To measure this kind of samples it is necessary to have instruments sensible enough to detect its signals. Our intention is to study the different vortex phases present in mesoscopic high Tc superconductors measuring them we use micro oscillators. We place our sample on the oscillator and we detect variations in its resonant frequency and in its quality factor, these variations are produced by changes in the magnetic properties of the sample. In this work we study how we can use micro oscillators as magnetometers. In particular, we present the response of an oscillator when a disk of BSCCO (2212) of 12 microns of diameter and 2 microns in high is placed on it and a magnetic field perpendicular to the disk is applied. We discuss our results based in the existence and contribution of inter and intra layer currents.

2 - 22 – Photoconductivity Decay in RF-Sputtered Nanocrystalline $TiO_{2-\delta}$ (-0.04 $\leq \delta \leq$ 0.2) Thin Films

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TiO_2 is a wide bandgap semiconductor ($\sim 3.2\ eV$) that finds many potential applications, such as in spintronics, photovoltaic conversion, degradation of pollutants, microelectronics, photonics, chemical sensors, actuators, and more. The photoconductivity is very important for the characterization of electrophotonic devices, since it relates to crucial factors such as photon-charge carrier conversion, photocarrier radiative or non-radiative recombination, and the distribution of electronic states that participate in theses processes. In this contribution, we have measured the photoconductivity (PC) and its time decay in vacuum and at the room temperature in nanocrystalline $TiO_{2-\delta}$ (-0.04 $\leq \delta \leq$ 0.2) thin films fabricated by the reactive rf-sputtering of a Ti target in Ar and O_2 mixtures. The bandgap of these films, as determined by UV-visible transmittance measurements, varies within the 3.18 a 3.34 eV range. PC was measured by exciting the films using a commercial LED whose emission is peaked at $h\nu = 3.1\ eV$ and spectral width is $\sim 5\%$.

Different PC values are obtained depending on thin film sample preparation conditions; the PC to dark conductivity ratio varies between ~ 1 and $\sim 10^4$. In all cases, the photocurrent decays very slowly (many hours to days) when the light source is switched off.

In general, the data can be satisfactorily analized by assuming that PC decay is due to thermal emission of holes from traps, which in turn are due to disorder and defect-related subgap states. The energy distribution of these traps is taken as a free functional in a fitting procedure where the PC decay is calculated numerically. Different trap energy distributions are considered, such as single peaked at known defect level energies in TiO_2, disorder-related exponential tail, or mixed type distribution. The experimental results and their analysis provide a new potential way of linking measured structural and morphological properties of the films with subgap and deep electronic states that govern phototransport in these and similar systems.

2 - 23 – EPR and Magnetic Susceptibility of Vanadium Oxide Multiwall Nanotubes

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The recent synthesis of inorganic oxide nanotubes opens a promising area for applications in nanoelectronic. In particular, the vanadium oxides attracted much attention as example of typical oxides with a Mott metal-insulator transition. The ratio V^{3+}/V^{4+} plays an important role determining the electronic properties of the material. In this work we present a characterization of a hybrid nanocomposites constituted by vanadium oxide (V_2O_5 and VO_x) / Polymer. The tubes were synthesized by sol-gel method followed by hydrothermal treatment. The different reduction process, used to form the Polyaniline (PANI) or Hexadecylamine (Hexa) templates, introduces changes in the oxidation states of the V ions. The nanostructures were confirmed by Transmission Electron Microscopy observing a multiwall tubular symmetry and the amounts of vanadium atoms, presents in each sample, were determined by neutron activation analysis. Electronic Paramagnetic Resonances (EPR) and dc-magnetic susceptibility were performed as a function of temperature comparing the properties of vanadium oxides nanotubes with the V_2O_5 bulk material. A Curie paramagnetic behavior and a temperature independent contribution to the magnetic susceptibility were detected in all the cases. The EPR spectrum taken at room temperature is a single line of approximately 100 Oe of linewidth and a g-value of ≈ 1.96, with a weak superstructure due to hyperfine structure (hfs). Both experiments in the nanotubes confirm that a small fraction of the V atoms are in the V^{4+} state and the hfs observed is due to the interaction between the nuclear (^{51}V - I = 7/2) and the electronic (S =1/2) of the V^{4+} ions can detected.

2 - 24 – Photoluminescence and Band Edge Absorption Shift from ZnO thin films

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Zinc Oxide is a versatile semiconductor whose main characteristics are its high bandgap energy (3.1 - 3.4 eV), exciton binding energy (60 meV) and different photoluminescent (PL) bands: band edge blue emission, and intraband green and orange-red [1]. The first two PL bands previously mentioned were extensively studied, while the last orange-red one has not been so widely addressed [2]. On the other hand, the uncertainty of its bandgap energy has been assigned to the influence of a shallow donor state, which makes the bandgap energy determination dependent on the measurement process [3].

In nanocrystalline electrodeposited ZnO thin films the measured values of absorption edge depends on film thickness [4], deposition temperature [5], and doping [6]. For example, deposition temperature induces energy shifts due to nanocrystalline size effects [5]. Also the PL depends on nanocrystallite shapes [2]. The electrodeposited samples show a strong orange-red band which is studied in the present work. The PL spectra has a width on the order of 100 nm peaked between 610 to 640 nm. These peaks are correlated with the band edge absorption, which depends on the sample preparation conditions. The absorption coefficient is indirectly obtained from diffuse reflectance measurements [7].

The most important feature of the below bandgap luminescence is that its peak position follows the shift of the band edge absorption for all samples studied. Moreover, the PL spectra slightly shift to the high-energy region when cooling down to 20 K by means of a cryostat. This suggests the PL is originated in a transition from a band or shallow state to an intrinsic deep state. When comparing the low temperature PL with the similar behavior of ZnO samples showing room temperature green emission, the shallow state nature of the emission is confirmed.

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2 - 25 – Complex Fano factor in an Aharonov-Bohm Ring with a Quantum Dot

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When a quantum dot is embedded in a branch of an Aharonov-Bohm ring it is possible to observe quantum interference between the resonant pathway through the quantum dot and the direct channel. As consequence the conductance shows a characteristic asymmetric line shape as a function of the gate or bias voltage. Fano [1] proposed this interference in a general system: a discrete energy level

embedded in a continuum energy state with a coupling between these two states. Then, a resonant state arises around the discrete level, and a transition from an arbitrary initial state occurs through two interfering configurations, one directy through the continuum and the other through the resonance. The transition probability around the resonance energy has the form $(e+q)^2/(1+e^2)$, with $e=(\varepsilon-\varepsilon_0)/\Gamma_0$, where ε_0 and Γ_0 are the energy and the width of the resonance, respectively. The factor q, known as the Fano's asymmetry factor q, gives a measure of the coupling and strength between the continuum state and the resonance state.

Later on, it was shown [2] that the interference gives rise to an antiresonance, i.e., a zero in the transmitance, which, besides yielding the characteristic asymmetric line shape, has a strong sensitivity to magnetic flux. This is because it depends on a phase difference that is controlled by magnetic field. Hence, the observed oscillations in the conductance result from the displacement of the antiresonances. The description of this phenomenon required the use of a parameter q as a complex number [3].

In this work, we introduce a simple Hamiltonian model from which a complex q factor is analitically obtained. Besides allowing the exploration of the parameter regime for symmetric and asymmetric resonance shapes.

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2 - 26 – Conductance distributions of 1D-disordered systems in a strong out of equilibrium regime

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In this work we calculate the conductance distributions $P(G(V,T))$ of a one-dimensional disordered wire at finite temperature T and bias voltage V in an independent electron picture. We obtained the $P(G(V,T))$ as a result of performing an specific number of autoconvolutions with the well known equilibrium conductance distributions $P(G(V=0,T=0))$. The number of autoconvolutions depends on T and V. Strong effects of finite T and V on the conductance distribution are observed and well described by our theoretical analysis, as we verified by performing a number of numerical simulations of a one-dimensional disordered wire at different temperatures, voltages, and lengths of the wire. We have also studied the conductance distributions of a one-dimensional disordered ring threaded by a magnetic flux that varies linearly in time. The system is connected to a particle reservoir which induces inelastic scattering processes and produces a non vanishing dc-current.

2 - 27 – Magnetic properties of Lanthanide(III) Succinates

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In the last decade a great effort has been devoted to investigate the main physicochemical properties of materials constructed from metal cations and organic multifunctional anions, known as hybrid materials. They can build up open structures with pores of different sizes and supramolecular assemblies of varied dimensions. In particular when the building constituents of hybrid materials are dicarboxylate anions and Ln(III) cations, because of the various coordination modes of dicarboxylates with the Ln(III), structures with different framework that might display interesting magnetic properties can be obtained. With the main purpose to rationalized the influence of the crystal structure on the magnetic response of Ln(III) ions [where Ln= Nd, Eu, Gd, Dy, Ho, and Er] we present and discuss here the observed magnetic susceptibility behaviors as a function of the temperature, in the range of 2-300K, of two Ln(III) succinates: $Ln_2[O_2C(CH_2)_2CO_2)_3(H_2O)_4].6H_2O$ and $Ln_2[O_2C(CH_2)_2CO_2)_3(H_2O)_2].H_2O$, which show inorganic LnO_2 networks of different dimensionality.

2 - 28 – Synthesis and characterization of nanostructured cobaltite - based oxides for cathode of solid - oxide fuel cells

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Cobaltite - based oxides are at the present time one of the materials most widely used as cathode for intermediate temperature solid - oxide fuel cells. A significant increase of the specific area of the cathode can be achieved by preparing structures on the nanometric scale. Nanocrystalline tubular structures of several compositions of these oxides were synthesized by denitration, using polycarbonate porous templates, microwave irradiation and a further calcination at 800°C. The shape and size of the tubes are determined by the characteristics of the template pores. The subsequent thermal treatment is needed to obtain the desired crystal structure. The resulting products were studied by means of X ray diffraction and electron microscopy techniques.

2 - 29 – Relation among grain size, tube to wire crossover and wall thickness for manganite nanoparticle assembled nanostructures

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Nanoparticle assembled into nanostructures of manganese perovkite oxides for different compositions and diameters have been synthesized following a template assisted method. In this paper we discuss the relation among geometrical, structural and nanostructural parameters observed when synthesizing $La_{0.66}Sr_{0.33}MnO_3$, $La_{0.66}Ca_{0.33}MnO_3$ and $La_{0.325}Pr_{0.300}Ca_{0.375}MnO_3$ manganite based complex oxides. For all compounds studied, obtained nanostructures are composed by an assembly of small (some few tenths of nanometers) grains. They form nanotubes above some threshold diameter of the template, and nanowires below it. Here we focus on the correlation among grain size, the diameter at which the tube to wire crossover occurs, and the corresponding wall thickness. We show that the threshold for this tube to wall crossover depends on the specific compound. Moreover, we present evidence from Transmission Electron Microscopy observations which allow a rationalization of several phenomena implicated in the synthesis process.

2 - 30 – MD simulations of films from C_{60} molecules deposited on Ge

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Molecular dynamics simulations have been used to investigate the microscopic processes of the growth of carbon thin films obtained from the collision of C_{60} molecules on germanium substrates. The Tersoff potential has been employed to describe the atomic interactions. Some properties of the films have been studied as a function of the deposition energy (from 10 up to 1000 eV): density of the films, width of the interface region, coordination number of C and Ge atoms, radial and angular distribution functions and vibrational density of states. Results have been correlated to those obtained on silicon by similar methods. The simulations show that the structural and dynamical properties of the films depend on deposition energy, in agreement with previous results on Si substrates [1,2]. For low deposition energies, the molecules preserve their identity, while at high energies the films resemble amorphous carbon ones. For the studied energies, the simulated interface thickness is larger in germanium substrates than in silicon ones. Special attention has been focused onto the interface region, since poor adherence of the films to the substrate has been experimentally observed.

The local stresses have been analyzed. For films deposited at energies above 500 eV, a high percentage of five- and six-coordinated atoms (mainly Ge atoms) have been observed in the interface region, showing that this is a highly stressed material. Annealing of the samples up to 2500 K shows a conversion of four- to three-coordinated C atoms (graphitization), but minor changes in the Ge atoms coordination.

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2 - 31 – Structure and magnetic properties of Cu-10 w.% Co alloys processed by twin roller melt spinning

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Nanostructured magnetic Cu-10 w.% Co alloys displaying giant magnetoresistance have been prepared by ultra rapid solidification, using the twin roller melt spinning technique. This solidification procedure is known to promote a more uniform microstructure as compared with that obtained in single wheel spinning devices.

The structural properties of ribbons processed at tangential wheel speeds between 5 m/s and 23 m/s, in the as cast state and after heat treatments at temperatures below 700 °C, are investigated by X-ray diffraction techniques; the magnetic properties are characterized by J-H loops measurements and the electric resistance measured as a function of temperature and the applied magnetic field.

The J-H loops in as cast samples can be described by the sum of a superparamagnetic component involving small clusters of pure Co with sizes below the detection limit of X-ray diffraction, and a soft ferromagnetic contribution which is likely to arise in the matrix. The X-ray spectra are consistent with a Cu matrix exhibiting a spinodal like Co profile.

Isothermal annealing above 600°C results in the formation of larger Co cluster; these changes are accompanied by an improvement in the apparent coercivity and in the polarization attained at a maximum field of 1.5 T.

Magnetoresistance effects are observed in as cast samples solidified at 23 m/s and completely disappear after a treatment of 1 h at 650C.

2 - 32 – Low dimensional and alloying effects on the magnetic properties of Co-Rh and Ni-Rh nanostructures

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Low dimensional effects enhances the magnetic properties of Co and Ni nanostructures and gives rise to magnetic order in the case of Rh. We study the evolution of the magnetic properties of Co-Rh and Ni-Rh nanostructures (free-standing monolayers and wires) on Rh content (x). As it is well known, Rh is non magnetic in bulk, but shows magnetic order as free-standing monolayer and nano-wire, being $1.03\mu_B$ and $0.26\mu_B$ their corresponding magnetic moments, calculated by using the $ab-initio$ Wien-2k code. In the case of $Co_{1-x}Rh_x$ and $Ni_{1-x}Rh_x$ wires, the evolution of the Rh magnetic moment is similar for both cases, being enhanced with respect to pure Rh wire value and reaching the largest values at x=.5 ($1.36\mu_B$ and $1.31\mu_B$ respectively). If $x > 0.5$ all the magnetic moments fall. If $x < .5$ the Co and Ni magnetic moments reach values larger than the corresponding pure wire and than their saturation magnetic moments. When alloying with Co or Ni, Rh enhances its magnetic moment with respect to the pure Rh wire in the case of mixed wires.On the other hand Rh magnetic moments of mixed monolayers are not enhanced.

2 - 33 – 3D Invariant Embedding Model for Backscattering Electrons Applied to Materials Characterization

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Most of the microscopes used in nanoscience and nanotechnology are electronic ones. They operate based on the interaction of an electron beam with the substances present in the sample. As the electrons of the beam penetrate within the sample they are scattered, giving rise to backscattered electrons, secondary electrons, absorbed electrons and X-rays spectra (characteristic and continuum). The working principle of the different kinds of electronic microscopes depends on which of these "signals" (one or many) are detected and analyzed. Theoretical and experimental study of the backscattered electrons are prticularly valuable in several fields. For instance, backscattered electrons are used in approaches to estimate the absorption correction factor in quantitative microanalysis, in reflection electrons energy loss spectroscopy, and in theories of bremsstrahlung production. Also its applications in scanning electron microscopy (SEM) and in film thickness determinations are of great importance. In particular, SEM represents a high-performance method of investigating structures and devices in the nanometer scale.

Theoretical study of the electron transport in microscopy may be dealt with in the general framework of linear transport theory. The traditional treatment makes use of the Boltzmann transport equation to describe the electron distribution into the sample, but the resulting integral-differential equation is hard to solve when those experimental conditions usual in quantitative microanalysis are taken into account[1]. A different way of approaching this issue was recently outlined, namely the so-called Invariant embedding approach to Microanalysis (IEAM), which yields analytical expressions from a simple 1D model, and have shown a good performance in the interpretation of experimental data[3]. In this work, the results of a 3D model used to describe the fraction of backscattered electrons, together with its energy and angular distributions, will be reported. This 3D model is the result of improvements in the IEAM. Comparisons with experiment show that the theoretical results follow the general trend of experimental data, when parameters (such as atomic number, energy of the impinging electrons and tilted angle) are changed.

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2 - 34 – Spin state dynamics during thermal annealing in semiconductor quantum dots

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Motivated by recently obtained experimental evidence of spin-splitting modulation by thermal processing in self-assembled semiconductor quantum dots, we report a systematic theoretical study of their electronic properties once subjected to different thermal annealing times. The experimental characterization has been simulated by a multi-band theoretical analysis. The effects of thermal processing on the magnetic properties of the system have been fully understood. The annealing time tuning of important electronic and optical properties has been characterized both qualitatively and quantitatively. The discussion highlights the correlation between band structure parameters and external factors that effectively affects the magnetic properties of the system. An applied magnetic field has been combined with changes of the quantum dot size and variations of the chemical composition induced by thermal annealing. They have proven to be key factors for the manipulation of spin-states in the quantum dots. The variations of the effective Landè g-factor expected in the experimental results have been theoretically con-

firmed as caused by the peculiar band structure dependence on quantum dot size and geometry. This study is based on a multiband calculation of the electronic structure of $CdSe/Cd_{1-x}Zn_xSe$ quantum dot subjected to an external magnetic field. The theoretical model combines the effect of confinement, chemical composition and interband coupling within the same mathematical framework. The effect of thermal processing has been simulated by changing the system parameters according to the experimental measurements. During the process of annealing, the relation between life-times of each given parameter will define the time-evolution of the optical response. The theoretical model has confirmed the qualitative trends of the experimental observations. The analysis of the thermal processing and its thermodynamics has proved to be a tool for the tuning of magnetic properties such as the effective Zeeman splitting detected optically. The ability to control the microstructure of semiconductor nanocrystals using thermal annealing provides opportunities for creating novel devices, and can be generalized to other substrates or other synthesis techniques.

2 - 35 – Conductivity fluctuation and superconducting parameters of the $YBa_2Cu_{3-x}(PO_4)_xO_{7-\delta}$ material

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Synthesis of the $YBa2Cu_{3-x}(PO_4)_xO_{7-\delta}$ superconducting material by the standard solid state reaction is reported. DC resistivity measurements reveal the improvement of the critical temperature (Tc) when substitution of phosphate in the Cu sites is performed. A bulk Tc = 97 K was determined by the criterion of the maximum in the temperature derivative of electrical resistivity. This is the highest Tc reported for the $YBa_2Cu_3O_{7-\delta}$ family. Structure characterization by means the x-ray diffraction technique shows the crystalline appropriated distribution of PO_4 into the CuO_2 superconducting planes. In order to examine the effect of phosphates 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 that reported on $YBa_2Cu_3O_{7-\delta}$, but an enhancement of the Gaussian fluctuation regimes was experimentally detected as a result of introduction of phosphates in the crystalline structure. 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.

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2 - 36 – Magnetic behavior across intergranular regions

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By using the variational principle for the Gibbs free energy, based on the Bogoliubov inequality, the magnetic properties of disordered systems with competing interactions are studied. In our model we immplement periodic boundary conditions stressing on how the number of first nearest neighbors can modify the magnetism. Concerning the competing interactions, we have considered those values corresponding to the ternary system Fe-Mn-Al. This system exhibits magnetic phases as the spin glass behavior arising from atomic disorder, bond competition and the dilutor effect of aluminium atoms. In this work we compute the magnetization per site and the magnetic susceptibility as a function of temperature, for different values of the coordination number. Results reveal an increase of the Curie temperature with the number of first nearest neighbors, as well as the existence of a minimum critical coordination number below which the system becomes paramagnetic. The present work is applied to elucidate the magnetic behavior at atomic level in intergranular regions characterized by a high degree of structural disorder.

2 - 37 – *Ab initio* electronic structure calculations for Mn linear chains deposited on CuN/Cu(001) surfaces

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Understanding the electronic and magnetic properties at atomic scale is essential for possible applications in spintronic. It has become a reality nowadays to use scanning tunneling microscopy (STM) to manipulate and probe magnetic nanostructures.

In a recent experimental work, STM has been used to study the interactions between manganese atoms lying in

linear chains, ranging from 1 to 10 atoms, on thin insulating islands of CuN(001) deposited on Cu(001). Analyzing the spectroscopic results with a nearest neighbor Heisenberg model Hamiltonian the authors obtain the value of the exchange interactions between manganese atoms. They also show that the coupling strength depends on the deposition sites of the Mn atoms (N or Cu). In this contribution we perform ab initio calculations for different arrangements of infinite Mn chains on CuN in order to

2 - 38 – Static and dynamic magnetic properties of MnAs

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One of the most interesting topics in MnAs grown as thin films respect to the bulk is the coexistance of alpha and beta phases. Up to 313K, MnAs bulk presents a ferromagnetic hexagonal structure (alpha phase). At this temperature a magneto-structural transition occurs and beyond 313K the beta phase, which is orthorombic and no magnetic, is set. In MnAs thin films, these two phases coexist in a certain range of temperature and it is well known that the coexistance is selforganized when MnAs is grown over GaAs(100), while it is disordered over GaAs(111). However, the reason of the appearence of the beta phase below 313K is not well understood yet.

In order to get a deeper understanding of the nucleation of the beta phase, we have performed magnetometric measurements and ferromagnetic resonance (FMR) experiments as a function of temperature in MnAs grown over GaAs(111) and GaAs(100) and MnAs powder. The static measurements was done in a SQUID magnetometer and the FMR spectra was taken at different frequencies (9, 33 and 94 GHz).

From the results we clearly see the differences between the bulk and thin films, mainly, through the behavior of coercive field and the FMR spectra. We observe the appearence of the beta phase at 200K, but its growth remains almost freeze up to 273K. At this temperature, the amount of beta phase increases rapidly up to the end of the phase coexistance.

Dilute magnetic semiconductors and semiconducting heterostructures

3 - 1 – Composition influence on surface morphology and optical properties of nanocolumnar ZnO films

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ZnO nanocolumnar films were prepared by electrodeposition (ED) on polycrystalline conductive ITO covered glass. The films where grown introducing different nature dopants (Mg, H, N, etc.), in order to follow the evolution of optical and structural properties. The optical properties of these films were studied by means of photoluminescence spectroscopy (PL) and the structural properties by scanning electron microscopy (SEM) and X-ray diffraction (XRD). The size and surface-volume ratios of the ZnO columns depend mainly on the growth parameters such as current density, deposition rate and temperature of the deposition bath. All type of films were annealed at 300°C in order to improve the crystal order, because preliminary results indicate that the 300°C annealing step causes a homogenisation of the surface morphology.

3 - 2 – Structural and magnetic properties in mechanically alloyed $Zn_{1-x}Co_xO$ semiconductor powders

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Thin films and nanostructured thin films of the transparent magnetic semiconductor alloy Zn_{1-x} Co_xO has been extensively studied due to its attractive properties for optoelectronic and spintronic applications. However, the mechanism responsible of such singular ferromagnetic behaviour is not yet well understood. The object of this work is the preparation and structural and magnetic characterization of $Zn_{1-x}Co_xO$ powders. Our purpose is to investigate the basic properties on bulk materials in order to contribute to the comprehension of the magnetic character in these semiconductors. The samples were obtained by mechanical alloying the binary oxides ZnO and CoO at different concentrations and milling times. The cation substitution was verified by X−ray diffraction. The magnetic properties were evaluated by field-cooled and zero-field-cooled magnetization measurements.

3 - 3 – Structural and magnetic studies on $GeSe_2 - Se$ (Fe) diluted magnetic semiconductors

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The $GeSe_2 - Se$ system presents an extensive glass forming composition range by the melt quenching technique. The interest on these materials is due to the ease to be conformed as films, their stability and resistance to water and corrosive media and the possibility to control their physicochemical properties by adding a third element even in a low concentration. The binary glasses, as well as the crystalline phases, are semiconductors with a band gap above 2eV.

The fundamental structural unit of pure chalcogen glasses is based on a single atom, therefore the short range order is rather straightforward and Se coordination number is n=2. For binary glasses the situation is more complex. Their structure consists of tetrahedral units centered on the tathogen, e.g. $GeSe_{4/2}$. Ge coordination number is n=4. In GeSe2-Se system glasses Ge centered tetrahedra are connected by Se bridges whereas in glasses with higher Ge fraction the tetrahedra are either corner sharing or edge sharing. Crystalline $GeSe_2$ has a layered structure formed by chains of tetrahedra whereas crystalline Se is formed by Se chains.

$Ge_{0.25}Se_{0.75}$ and $(Ge_{0.25}Se_{0.75})_{0.995}Fe_{0.005}$ glasses have been obtained and analyzed by different techniques. Their structure was characterized by X-ray diffraction whereas the presence of Fe was utilized as a probe to study the short range order of the structure by means of Mössbauer spectroscopy. The magnetic behavior was characterized employing SQUID-VSM magnetometers. After crystallization Se and $GeSe_2$ were identified in X-ray diffraction patterns. The crystallization products were analyzed and DC magnetization was measured as a function of temperature and magnetic field from 5K to 300K on witness $(GeSe_2)_{0.995}Fe_{0.005}$ and $Se_{0.995}Fe_{0.005}$ evidencing ferromagnetic behavior.

3 - 4 – First-principles calculation of structural properties of $Sc_{1-x}In_xN$ compound

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We have studied the structural properties of $Sc_{1-x}In_xN$ compound in sodium chloride and wurtzite structures using first-principles total energy calculations. The effect of composition on lattice constants , bulk modulus and cohesive energy in the equilibrium volume was investigated for the two structures. Deviations of the lattice constants fron Vegard's law and the bulk modulus from linear concentration dependence were observed for the sodium chloride and wurtzite structures. The relative stabilility of the sodium chloride and wurtzite structures it changes for an approximate concentration of In 50%.

3 - 5 – The wide-gap of $Sc_{1-x}In_xN$ compound: a comparative theoretical study among the approaches GGA and EV-GGA

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The wide-gap of $Sc_{1-x}In_xN$ compound were investigated using the Linearized Augmented Plane Wave (LAPW) method as implemented in the wien2k code. We used density functional theory with the Generalized Gradient Approximation (GGA) and the Engel-Vosko GGA formalism to calculate the band structure at equilibrium volume for each *In* concentration in the sodium chloride and wurtzite structures. We have studied the effect of composition on wide-gap of compound in sodium chloride and wurtzite structures. The origins of gap bowing in sodium chloride and wurtzite structures of ternary compound, have been explained in detail. The band structure calculated by GGA and EV-GGA for the compound in sodium chloride (or wurtzite) structure were similar, however the value of bandgap was wider with EV-GGA.

3 - 6 – EXAFS study of the local environment of impurities in doped TiO_2 thin films

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Diluted magnetic semiconductors (DMS) are attractive materials because they combine two properties: semiconductivity and magnetism. For their practical applications, ferromagnetic semiconductors are required to have a high Curie temperature. From the discovering of room temperature magnetism in Co-doped anatase TiO_2 thin films many research groups have focused on doping TiO_2 with transition metals. These results have motivated intensive experimental and theoretical studies on the structural and electronic properties of these materials. However, due to intrinsic complexities, many questions remain regarding the underlying microscopic mechanism of long-range magnetic order. Carrier induced interaction between the magnetic atoms was first suggested as the important ingredient underlying ferromagnetism in III-V based DMSs. Subsequent reports have raised concerns about the initially suggested intrinsic nature of ferromagnetism in these materials, due to the possibility of ferromagnetic metal clustering under different growth conditions. Furthermore, it has been suggested that strong interaction between Co and vacancy moments in Co-doped TiO_2 plays a key role for the explanation of its high Tc. In order to clarify the role of impurities in the presence of magnetism it is crucial to determine the local environment of magnetic or non magnetic impurities. In this work we present an EXAFS (extended x-ray absorption fine structure) characterization of the local environment of M (Co, Ni, Cu or Zn) in anatase TiO_2 doped thin films. The films were deposited on $LaAlO_3$ (001) substrate by Pulsed Laser Deposition using a Nd:YAG laser. They were transparent, strongly textured (showing only the (001) reflections of the anatase structure) and ferromagnetic at room temperature. We did not found presence of metallic clusters in any case. The oxidation state is +2 and the local coordination of oxygen is similar to MO (CoO, NiO, CuO or ZnO) but, except in the Cu case, the similarity with these oxides only exits in the short range scale.

3 - 7 – About the magnetism in pure SnO_2 and TiO_2 oxides thin films

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Recently, interesting results were reported showing room temperature ferromagnetism on pure TiO_2, HfO_2, SnO_2 and In_2O_3 oxide films[2, 3, 4] and also in films doped with non-magnetic impurities [5]. They assume that defect, especially oxygen vacancies could be the reason of the observed magnetism. The saturation magnetization is in all cases in the order 20-30 emu/cm3 and the magnetic moment (in films deposited on $LaAlO_3$ with a surface of 0.5x0.5 cm_2) in the order of 105 emu. In this work we present a study of the magnetic properties of pure SnO_2 and TiO_2 thin films deposited on $LaAlO_3$ by pulsed laser deposition (PLD) that result ferromagnetic at room temperature. We explore the influence of deposition, cleaning of the films previous to the magnetic measurement and substrate treatment conditions on the presence of magnetism in these samples. The samples were characterized by X-ray diffraction (XRD) and magnetometer measurements performed using a SQUID.

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Spintronics

4 - 1 – Tunneling magnetoresistance of Fe/ZnSe (001) single-and double-barrier junctions as a function of interface structure

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In this contribution, we calculate the spin-dependent transport through Fe/ZnSe (001) simple and double magnetic tunnel junctions[1], of the type Fe(inf.)/ZnSe(n)/Fe(inf.) and Fe(inf.)/ZnSe(n)/Fe(m)/ZnSe(n)/Fe(inf.), respectively. Fe(inf.) are semi-infinite electrodes and n, m are thicknesses. The electronic structure of the junctions is modeled by a second-nearest neighbors *spd* tight-binding hamiltonian parametrized to *ab initio* calculated band structures, while the conductances and the tunneling magnetoresistance (TMR) are calculated within Landauer's formalism expressed in terms of Green's functions.

The calculations are done at zero bias voltage and as a function of energy, for junctions with a given n value and variable m. We show and discuss how the insertion of Fe layers in between the ZnSe spacer modifies the electronic structure of the junctions and, consequently, their spin-dependent transport properties[1-3], focusing on the effect of the in-between Fe layers on the k//-dependence of the conductance.

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4 - 2 – Anisotropic magnetoresistance in $La_{0.75}Sr_{0.25}MnO_3/LaNiO_3$ trilayers

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Ferromagnetic manganites are interesting compounds to be used in magnetorresistive devices due to their half-metallic character. Moreover, there are a large number of compounds with the same crystalline structure but different magnetic and electric properties. $La_{0.75}Sr_{0.25}MnO_3$ (LSMO) is ferromagnetic and metallic below its Curie temperature and $LaNiO_3$ (LNO) presents Pauli paramagnetism and is metallic. For this study we grew metallic trilayers LSMO/LNO/LSMO on (100) $SrTiO_3$ single crystalline substrates, aiming to the fabrication of giant magnetoresistance (GMR) devices.

In a previous work [1], we studied the magnetic coupling between the LSMO layers in these samples. Once the samples were magnetically characterized, we performed in-plane electric transport measurements. In-plane GMR is weak and so other effects contributing to the low-field magnetoresistance should be carefully taken into account in analyzing the measured data. The anisotropic magnetoresistance (AMR) is an effect that depends on the angle between the magnetization and the electrical current, and its magnitude is important in manganite films. We studied the AMR on reference LSMO thin films and LSMO/LNO/LSMO trilayers. We found that the general features of the AMR observed in LSMO films appear in trilayers. The differences in the shape of the magnetoresistance curves of the trilayers, in comparison to that of the LSMO films are attributed to the GMR effect.

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4 - 3 – Structural magnetic and electric characterization of $Sr_3M_2ReO_9$ (M= Cr, Fe)

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The search of new materials with colossal magnetoresistant (CMR) includes some members of the family of double perovskites $A_2BB'O_6$ (A= alkali earths and B, B'= transition metals). These, as an alternative to perovskite manganites, have been proposed as half-metallic ferromagnets with T_C's well above room temperature. These transition metals oxides have a "double" crystalline structure because they have, in an ideal order, the M ions alternated in two different B site. The interest in this family was triggered by a report on Sr_2FeMoO_6, demonstrating that in the electronic structure only minority spins are present at the Fermi level. This material exhibits magnetoresistance (MR) at room temperature, which has also been observed for double perovskites containing other transition metals than Mo, such as A_2FeReO_6 (A= Ca, Sr, Ba). In the present work we present magnetoresistance, hysteresis loops, magnetization and electrical resistivity as a function of temperature from a new chemical composition of these oxides: $Sr_3M_2ReO_9$ with M= Cr or Fe. Their crystallographic formula can be written like $Sr_2[(M)_{2a}(M,Re)_{2b}]O_6$, being the site 2b occupied by $\frac{1}{3}$ of M ions and $\frac{2}{3}$ by Re ions, turning it one in a double Perovskite with intrinsic disorder in the 2a and 2b crystallographic B sites.

Highly correlated systems

5 - 1 – Valence band and core-level spectra of metallic and insulating V_2O_3: Cluster model calculations with nonlocal screening channels

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We have studied the electronic structure of metallic and insulating V_2O_3 using a cluster model with non-local screening channels. The calculation reproduces both the valence band and the core-level photoemission spectra, showing a good agreement with the experiment. The calculation of the metallic phase included a coherent screening channel from a delocalized state at the Fermi level. The valence band of metallic V_2O_3 presents a coherent structure at the Fermi level and an incoherent feature at lower energy. The coherent peak in the spectrum is attributed to the coherent screened $3d^2\underline{C}$ state, whereas the incoherent part is mostly due to the ligand screened $3d^2\underline{L}$ state. The poorly screened $3d^1$ state, which corresponds to the lower Hubbard band, appears at much lower energies. The core-level spectrum presents a similar spectral distribution. The higher energy structure is related to the coherent screened $\underline{c}3d^3\underline{C}$ state, whereas the main peak in the spectra is due to the ligand screened $\underline{c}3d^3\underline{L}$ state. Finally, the lower energy feature, which corresponds to the charge-transfer satellite, is mostly formed by the poorly screened $\underline{c}3d^2$ state. The insulating calculation included a typical Hubbard screening channel from a neighboring V^{3+} ion in the structure. The coherent screened state $3d^2\underline{C}$ ($\underline{c}3d^3\underline{C}$) in the insulating valence band (core-level) is replaced by the Hubbard screened state $3d^2\underline{D}$ ($\underline{c}3d^3\underline{D}$). The Hubbard state appears at lower energy and the resulting transfer of spectral weight opens the insulating band gap. The calculation shows that the incoherent feature contains considerable $O2p$ character, whereas the coherent structure contains almost pure $V3d$ weight. The photon energy dependence of the valence band spectra can be mainly attributed to the relative $V3d - O2p$ cross section. The V_2O_3 compound can be classified as a strongly hybridized $V3d - O2p$ Mott-Hubbard system, where the $O2p$ orbitals have to be considered explicitly.

5 - 2 – Crystal Field effects of Eu^{2+} in LaB_6

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Electron Spin Resonance (ESR) of Eu^{2+} ($4f^7$, S = 7/2) in $La_{1-x}Eu_xB_6$ x = 0.0025 single crystal show, for the localized Eu^{2+} magnetic moment, an anresolved dysonian resonance with anisotropic linewidth. It is shown that the anisotropy of the Eu^{2+} ESR linewidth indicates that the ions sense a cubic crystal field of positive fourth order crystal field parameter, b_4. This is in agreement with the general behaviour found for the S ground state of Eu^{2+} and Gd^{3+} in any cubic metallic host.

5 - 3 – The one-dimensional asymmetric Hubbard model at partial band filling

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We study the one-dimensional asymmetric Hubbard model through the White's density matrix renormalization group technique at the density n=0.8. The asymmetric Hubbard model describes a correlated system where the hoppings of electrons depend on their spin. The charge structure factor and the density expectation value of heavy electrons were calculated as a function of the hopping and the repulsive on-site interaction. We found that the ground state displays phase separation for strong coupling and the critical hopping tc=0.6 separates the density wave state and the phase separation one. This result generalizes the found one in the Falicov-Kimball model, which is a particular case of the asymmetric Hubbard model.

5 - 4 – Magnetic properties of Y-doped highly frustrated pirocloro $GdInCu_4$

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The study of frustration magnetic phenomena has been the focus of intense and interesting research in solid state physics because the spin fluctuations derived from a frustrated magnetic state is believed to give rise to fascinating physics phenomena such as, quantum fluctuations, spin glass, Non-Fermi-Liquid (NFL) and even non-conventional superconductivity. In this work, we have investigated the physical properties of Y-doped single crystals of highly frustrated $GdInCu_4$. We report results of powder X-ray diffraction, and temperature dependent DC magnetic susceptibility, ESR and heat capacity. We will discussed how the effects of dilution and disorder introduced by the Y-doping affects the frustrated long-range antiferromagnetic order setting it at the Neel temperature (T_N) and also the strong short range magnetic correlations taking place above T_N.

5 - 5 – The exhaustion problem in the periodic Anderson model: Optical and transport manifestations

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We study the optical and transport properties of the periodic Anderson model (PAM), within the X-boson approach. The exhaustion problem is studied, we compute the optical conductivity, the electrical conductivity and the low energy part of the photoemission spectroscopy, for the heavy fermion Kondo regime (HF-K) of the PAM. We obtain the evolution of physical properties as function of the conduction electron occupation number n_c, the results shows a supresion of the Drude peak in metallic situations with the drop of n_c, two frecuency scales arise in the optical conductivity, linked with the optical direct-gap and the frecuency value where is manifest the Drude peak at low values for n_c. We compute the spectral weight transfer and the validity of the optical sum rule in a low value of n_c as temperature function.

5 - 6 – Study of the quantum phase transition to a nematic and an hexatic Fermi fluid

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We study a two-dimensional Fermi fluid by means of bosonization. We discuss Pomeranchuk instabilities of the Fermi surface of this system. In particular, we are interested on the quantum critical behavior of the transition from a Fermi fluid to a nematic and to an hexatic state which break spontaneously the rotational invariance of the Fermi liquid. The nematic phase was recently observed in half filled quantum Hall systems and it was proposed as a candidate to the "normal state" of high T_c superconductors. On the other hand, the hexatic phase can be understood as a melted Wigner crystal, therefore justifying the study of its competition with the nematic and the isotropic phase. We carefully study the phase diagram for the isotropic/nematic/hexatic quantum phase transition evaluating in particular the dynamics of the collective modes that could be observed in scattering experiments.

5 - 7 – Ferromagnetic resonance study in $Pr_{0.5}(Ca_{1-x}Sr_x)_{0.5}MnO_3$, with $0.10 \leq x \leq 0.75$

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We study the competing phases at the crossover from localized to itinerant electronic behaviour in the system $Pr_{0.5}(Ca_{1-x}Sr_x)_{0.5}MnO_3$, with $0.10 \leq x \leq 0.75$. The tolerance factor (t) of the samples change from 0.973 to 0.985 and present the localized to itinerant transition at the critical value t_c = 0.975, wich correspond to x=0.2. The study was performed by Q-band (35 GHz) electron spin resonance experiments. At room temperature the samples show a single Lorentzian line centered at g=2.020 (5). Instead, at low temperature all the samples present a ferromagnetic resonance line (FMR) coexisting with a paramagnetic absorption. For x=0.15 the FMR absorption is observed below $T_C \approx 200$ K. This transition shifts to higher temperatures when the tolerance factor increases and for x=0.75, $T_C \approx 260$ K. The FM phase change from a minority phase, when $x<0.2$, to a majority one, for $x>0.2$. We fit the temperature dependence of the ESR spectra considering a FM phase with uniaxial anisotropy that coexist with a PM phase. We have found that the anisotropy field of the FM phase increases when the tolerance factor decreases.

5 - 8 – Signatures of a quantum dynamical phase transition in a 3-spin system in presence of a spin environment

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Recently we observed an environmentally induced quantum dynamical phase transition in the dynamics of a two spin experimental swapping gate [J. Chem Phys. **124**, 194507 (2006)]. There, the exchange of the coupled states $|\uparrow,\downarrow\rangle$ and $|\downarrow,\uparrow\rangle$ gives an oscillation with a Rabi frecuency $b/\hbar$ (the spins coupling). The interaction, $\hbar/\tau_{SE}$ with a spin-bath degrades the oscillation with a characteristic decoherence time. We showed that the swapping regime is restricted only to $b\tau_{SE} \gtrsim \hbar$. However, beyond a critical interaction with the environment the swapping freezes and the system enters to a Quantum Zeno dynamical phase where relaxation decreases as coupling with the environment increases. The critical point depends of the anisotropy relation of the system-environment interaction quantified as the ratio between Ising and XY terms. Here, we solve the quantum dynamics of a two spin system coupled to a spin-bath within the density matrix formalism and we compare the results with our previous work. Then, we extend the model to a three interacting spins system where only one is coupled to the environment. Here, beyond a critical interaction the two spins not coupled to the environment oscillate with the bare Rabi frequency and relax more slowly. This effect is more pronounced when the anisotropy of the system-environment interaction goes from a purely XY to an Ising interaction form.

5 - 9 – Volume effects on the crystal-field splittings of CeZ (Z=Sb,Te)

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Among the Cerium compounds, the monochalcogenides CeY (Y=S,Se,Te) as well as the monopnictides CeX (X=P,As,Sb,Bi) show very interesting physical properties. In particular the heavier ones (CeSb,CeBi and CeTe) have a very small crystalline electric field splitting and are highly sensitive to applied hydrostatic pressure. In this contribution we study pressure effects on the values of the crystal-field splittings (Δ_{CF}) of CeSb and CeTe and compare with experimental results for the $CeSb_{1-x}Te_x$ alloys (chemical pressure). We calculate the splittings using a mixed procedure which combines *ab initio* calculations with a many body technique.

5 - 10 – The completeness problem in the impurity Anderson model

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With the recent development of the nanoscopic technology, the impurity Anderson model (AIM) was experimentally realized in quantum dot devices [1]. In the limit of infinite electronic repulsion one can obtain several Green's functions approximations by the equation of motion method (EOM) incorporating the Kondo effect through a di-gamma function (cf. reference [2]), and at least qualitatively they provide an adequate tool to describe the Kondo effect. However, these approximations present several drawbacks: they are no longer valid as the temperature decreases below the Kondo temperature, because the logarithmic divergence of the di-gamma function makes the spectral density at the chemical potential to vanish. Further drawbacks are that the Friedel sum rule and the completeness in the occupation numbers are not fulfilled. In this work we present a critical discussion comparing the results of this class of di-gamma GF with other GF that satisfy both the completeness and the Friedel sum rule, i.e. those obtained by the slave boson and by the X-boson mean field approach [3] as well as those obtained by the atomic approach [4], recently developed by some of us. We present results for the density of states, for the Friedel sum rule and for the completeness.

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[4] T. Lobo, M.S. Figueira, and M.E. Foglio, Braz. J. of Phys. **36**, 397 (2006).

5 - 11 – *Ab initio* and experimental study of Ta-doped In_2O_3 semiconductor

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Ab initio calculations based in the Density Functional Theory have shown to be very accurate to describe structural and electronic properties of oxides semiconductors doped with diluted metallic impurities. Therefore these calculations are a powerful tool in the interpretation of experiments in which, e.g., the assignment of hyperfine interactions are rather difficult. In this work we present an *ab initio* and a new experimental Perturbed Angular Correlation (PAC) study of the In_2O_3 semiconductor doped with Ta impurities. The theoretical study has suggested in this case a reinterpretation of old experiments and to perform a "cleaner" new experiment. In_2O_3 pellets with high purity and crystallinity were implanted with $^{181}Hf(\rightarrow {}^{181}Ta)$ ions at the ISKP accelerator of Bonn (Germany) and measured at La Plata with a high time-resolution and efficiency spectrometer. Magnitude and symmetry of the electric-field gradient (EFG) tensor were determined at room temperature after each step of an annealing series in air (1 h at 673K, 1 h at 1073K, 6 hs at 1273K, and 1 h at 1373K). Two monochromatic EFGs were found with the population expected by a homogenous distribution of the probes in both cationic sites C and D free of defects of the bixbyite structure (f_C/f_D=3). These results were compared with those obtained in previous experiments done on samples chemically prepared and on implanted thin films with different initial degrees of crystallinity, in which four interactions were necessary to account for the spectra and the cation site probe population was inverted. The electronic structure calculations were carried out with an impurity dilution of 1:12 using the WIEN97 implementation of the FP-LAPW method. The calculations were carried out for the neutral (Ta^0) and charged (Ta^{2+}) state of the impurities, and compared with PCM calculations and the old and new experimental results. From the excellent agreement between the new experiment and the FP-LAPW predictions the neutral state of the impurity could be determined and a correct assignment of the hyperfine interactions in all the experiments were done.

General Field Theory applications

6 - 1 – Entanglement in quantum dissipative Ising spin system

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We study the behavior of entanglement estimators on chains of a few quantum Ising spins coupled to the environment by means of Monte Carlo simulations. We describe the environment by a quantum thermal bath composed by independent quantum harmonic oscillators following the formulation of Feynman and Vernon for dissipation. The simulations run on an equivalent (1+1)-D classical spin lattice through a Suzuki decomposition. We analyze the ground state value of the von Neumann entropy and the concurrence of our spins system for different couplings with the quantum bath and different strengths of a transverse magnetic field.

Soft Condensed Matter

7 - 1 – Parametric Resonance for NLSE solitons trapped by an external time-dependent harmonic potential

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The dynamics of nonlinear solitary waves is studied by using the model of nonlinear Schrödinger equation (NLSE) with an external harmonic potential. The model allows one to analyse on the general basis a variety of nonlinear phenomena appearing both in Bose-Einstein condensate in a magnetic trap, whose profile is describe by a quadratic function of coordinates, and in nonlinear optics, physics of lasers, condensed matter physics and biophysics. It is shown that exact solutions for a quantum-mechanical particle in a harmonic potential and solutions obtained within the framework of the soliton adiabatic perturbation theory are completely identical. This fact not only proves once more that solitons behave like particles but also that they can preserve such properties in different traps for the which the parabolic approximation is valid near the potential energy minima. The assumed adiabatical dynamics of the NLSE soliton in a parabolic trap and the mathematical analogy with the parametric resonance in oscillatory systems, allow one to consider more complicated processes appearing in the time-dependent harmonic potential. We show the possibility of the appearance of a soliton parametric resonance when the amplitude of soliton oscillations in the trap exponentially increases with time. To verify this conclusion, we performed numerical calculations in the framework of the NLSE model with varying in time harmonic potential for a broad range of variations of parameters. We show that the exact analytical solutions of the problem can be found by using the Miura transformation of the soliton theory. These novel solutions open up the possibility to control the dynamics of solitons in the traps. New effects are predicted, which are called the reversible and irreversible denaturation of solitons in a nonstationary harmonic potential.

7 - 2 – Electronic conductivity of the composite epoxy-cobalt

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The resin epoxy is quite used in the composite form in several sections of the industry, such as: motoring, building site, aerospace, petroleum and gas. In this work, we intended to do a study of the electronic properties of the resin epoxy-cobalt, with the objective of making possible its applicability in electronic devices. Sample of epoxy resin cured with polymercaptan was mixed with cobalt(II) chloride hexahydrate in the reason in mass 1:1. It was formed a dark red composite that was deposited in a glass sheet forming a layer 200 μm of thickness. After the hardening, the composite was dipped in an aqueous solution of sodium borohydride for reduction of Co(II) for Co(0) (metallic cobalt). Measures of ray-X indicated the presence of the chloride of cobalt soaked by epoxy resin, however it was not possible the detection of the metallic cobalt due to the size nanometric of the particles. Using the method of four tips of Van der Pauw, it was obtained the resistivity to room temperature. The measured value was of 0.05 Ohm.cm, indicating a change in the electronic conductivity of insulating for conductor. Measures of resistivity are being achieved in function of the temperature and the concentration of cobalt chloride, with the intention of determining the temperature and the minimum concentration for the transition insulating-conductor.

7 - 3 – Electron spin resonance study of $Y_{1-x}Ca_xMnO_3$

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We present an electron spin resonance (ESR) studies in the series $Y_{1-x}Ca_xMnO_3$ for $0 \leq x \leq 1$. As a consequence of the small ionic radio of the rare earth, this compound present a very distorted perovskite structure, therefore a long range ferromagnetic order is never reach. The extreme compounds $YMnO_3$ and $CaMnO_3$ are G-type antiferromagnets with $T_N = 44K$ and $123K$ respectively. Because to the ESR contribute only the resonant species the transition temperatures can be better resolved than in the DC magnetization measurements. Therefore the ESR measurements allow us to determined the charge order transition temperature (CO) that present a maximum at x = 0.5 (T_{CO}= 290 K). The Néel temperature was determined for all the series, and a spin glass transition $T_{SG} \sim 40K$ was observed for intermediate doping. In all the studied cases the linewidht of the ESR resonance, in the paramagnetic region, can be fitted by the expression $[\chi_0(T)/\chi(T)]\Delta H_{pp}(\infty)$, where the first factor is the ratio of the Curie susceptibility to the measured susceptibility and the second factor is a temperature independent constant.

Development of Experimental and Computational techniques

8 - 1 – Non-periodic pseudo-random numbers used in Monte Carlo calculations

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The generation of pseudo-random numbers is one of the interesting problems in Monte Carlo simulations, mostly because the common computer generators produce periodic numbers. The use of simple chaotic systems, as the well known logistic map to generate the pseudo-random numbers allows one to develop Monte Carlo simulations with bigger number of systems. As the numbers are non-periodic, but their obtention is deterministic, the calculations can be proved to be repetitive before running bigger models. We studied and analyzed a set of numbers, using the statistical methods, standard and more sophisticated, to prove the set is non periodical up to 10^{13} numbers. After the test with classical applications, as the simple 2-D or 3-D Ising models, we applied the numbers to solid state problems, using both non-quantum and quantum Monte Carlo methods, with excellent results.

8 - 2 – Mössbauer Magnetic Scans: experimental setup and data analysis

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In this work Mössbauer Magnetic Scans (MMS) technique is addressed. The experimental set-up and new results are discussed. The measurement of the Mossbauer transmission at a fixed Doppler energy while the sample is subjected to an a.c. external magnetic field allows magnetic hysteresis mechanisms to be studied. In a previous work [Phys B, 384 (2006) 348] a 20 μm NANOPERM ribbon was studied and the feasibility of the MMS technique was demonstrated. However, these previous results could not be satisfactorily explained with standard analysis models, presumably because of the saturation and polarization absorption phenomena, which are important in the case of thick absorbers.

Therefore, a simpler system was chosen in order to elucidate the physics underlying the data analysis procedure. A sputtered film with a thickness lower than 1 μm and a 12 μm sheet, both of α-Fe, were studied. The dependence of the relative absorption of the spectral lines with a magnetic field (Hmax= 6.3 kA/m) applied parallel to the sample and perpendicular to the gamma ray was determined.

For the film, the line intensities magnetic field dependence was in agreement with the predictions of the thin absorber approximation. In this case, the magnetic moments orientation dependence on the magnetic field can be modeled.

For the analysis of the 12 μm sheet results, the thin absorber approximation was not adequate, therefore the exact expression for the Mössbauer absorption was used.

In conclusion, we found that the MMS technique allows the study of magnetic hysteresis mechanisms. With the available analysis procedures, quantitative information can be retrieved in the case of thin absorbers, while for thick ones, data analysis through the exact expression is under progress.

8 - 3 – Time Evolution of Multiple Quantum Coherences in NMR

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In multiple quantum NMR, individual spins become correlated with one another over time through their dipolar couplings. In this way, the usual Zeeman selection rule can be overcome, and forbidden transitions can be excited. Experimentally, these multiple quantum coherences (MQC) are formed by the application of appropriate sequences of radio frequency pulses to the system during a time τ; thus creating Hamiltonians that force the spins to act collectively.

A basic bidimensional experiment to follow the development of MQC involves four periods each one characterized by a time variable: preparation (τ), evolution (t_1), reconversion or mixing (τ) and detection (t_2).

^{1}H spin coherences of even order up to 32 were excited in a polycrystalline sample of ferrocene $(C_5H_5)_2Fe$ and their evolutions studied under different conditions: (a) under the natural dipolar Hamiltonian, $\mathcal{H}_{dip}$(free evolution) and with $\mathcal{H}_{dip}$ cancelled out by (b) magic echoes or (c) with the MREV8 sequence. It is interesting to note that coherences of order six are excited at $\tau \leq 120$ μs indicating that the excitation has already gone out of the five member ring at that time. Besides, the results show that when cancelling $\mathcal{H}_{dip}$ the coherences decay with characteristic times ($\tau_c \approx 120$ μs) which are more than one order of magnitude longer than those under free evolution ($\tau_c \approx 10$ μs). In addition it is observed that with the MREV8 sequence, the larger the order of the coherence (larger number of correlated spins) the faster the speed of degradation, as it happens during the evolution with $\mathcal{H}_{dip}$ (Krojanski H. and Suter D. in *Phys. Rev. Lett.* 2004 **Vol.**93 **N**3 090501). In contrast, this is not observed when $\mathcal{H}_{dip}$ is cancelled out by the magic echoes sequence. In this case, the characteristic time of degradation of the coherences of different orders is approximately constant ($\tau_c \approx 150$ μs).

8 - 4 – Magnetism in $Y_{1-x}Tb_xCo_2$ compounds

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YCo_2 exhibits a very strongly Pauli paramagnetism and undergoes a first-order metamagnetic transition under an external field (exceeding a certain critical value), $TbCo_2$ orders ferrimagnetically and the magnetic phase transition is of second order. The magnetic phase transition of pseudo-binary Laves phases $Y_{1-x}Tb_xCo_2$ (R= rare earth), previously studied by perturbed angular correlation measurements (PAC)[1] and a.c susceptibility[2] has been investigated with d.c magnetization measurements. Susceptibility data was in agreement with a scenario of gradual change from l-type shape to a more symmetric character. PAC measurements have reflected a gradual change in the jump of the 3d magnetization of Co subsystem at T_c, clearly indicate first order for x less than 0.3 in agreement with Inoue-Shimizu model. Although these and other previous studies show that the magnetic transition change from first to second order as x increases, the critical concentration for the change is still a subject a controversy. In order to complete previous studies, d.c magnetic measurements were carried out using various protocols: ZFC and FC (10 Oe and 1000 Oe) magnetization temperature dependence and applied field magnetization dependence. The measurements were performed over the same samples used in cited references. The new results will be contrasted with previous ones.

[1] [M. Forker *et. al.*, J. Phys.: Condens. Matter **18** (2006) 253.

[2] A.F. Pasquevich *et. al.*, Physica B. **354** (2004) 357.

8 - 5 – Bimagnetic trilayer Ni/Amorphous/Ni with applications as magnetoelastic temperature sensors

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Recently, bimagnetic trilayers $M/Am/M$, where Am is an Fe rich amorphous ribbon and M another magnetic material have been proved to be very good candidates as nuclei of minicoils used as sensing elements for magnetoelastic temperature devices. As temperature is modified, mechanical stress is induced due to differences in thermal expansion coefficients, and given the magnetostrictive character of the layers, it produces changes of the trilayer permeability and inductance.

When M and Am are characterised by opposite sign magnetostriction the ac response of minicoil inductance (L) to tempertaure changes (ΔT) is enhanced. This allows us the choice of M and Am with thermal expansion coefficients differences of the order of no more than about 10 &percnt and therefore the possibility of working under smaller stresses (longer useful life of the trilayer) and the attainment of a conveniently linear L vs ΔT dependence.

Due to these attractive features, we have further characterized the field response of $Ni/Am/Ni$ minicoils prepared by Ni electrodeposition on both sides of a positive magnetostriction $20\mu m$ melt-spun $FeSiB$ amorphous ribbon. Both Ni layers were nominally identical, also with thicknesses of about $20\mu m$. The coil inductance was studied as a function of the longitudinal magnetic field produced by a dc current through the coil, for several temperatures between 18 and 75^oC, under a testing 100 Hz ac current. Percent inductance-field responses of about 0.36 and 0.81 Oe-1 were measured at 18 and 75^oC, respectively. Change of inductance response with temperature was of about 0.26 and 0.07 C-1 under dc fields of 0 and $10Oe$, respectively. Inductance dependence with frequency f was also determined at RT, being of about 1.64 and 3.72% $(logf)^-1$ under dc fields of 0 and 10 Oe, respectively. These results will be discussed along with an interpretative simple physical model.

8 - 6 – Vibrational Spectra of para-nitroaniline

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The fast and efficient response of molecular materials have made them promising candidates for a number of nonlinear optical (NLO) applications. NLO effects such as second harmonic generation (SHG) are sensitive to the structure of the molecules as well as their assembly pattern. Push-pull chromophores are a class of molecules that feature an electron-donating group and an electron-accepting group connected by a conjugated pi-system. These molecules possess large nonlinear optical responses. Two resonance forms can be written for the electronic structure of a push-pull chromophore: a neutral structure having zero or small formal charges on the donor and acceptor groups, and a zwitterionic form. These two structures are often taken as basis states, whose linear combinations compose the two lowest-energy electronic eigenstates, with the ground state being predominantly the neutral form. p-nitroaniline is the prototypical push-pull system but the centric nature of its crystal structure inhibits macroscopic NLO response. Samples prepared by crystallization under an intense static electric field of 200 kV/m have shown NLO response. No single crystal suitable for X-ray diffraction has been obtained and powder X ray diffraction did not show evidence of space group modification. These findings led to a research on the possible influence of the internal vibrational degrees of freedom on the

observed NLO behavior. Vibrational spectra of crystalline powders with and without NLO response were obtained at different temperatures. The results are analyzed on the basis of ab-initio and DFT calculations on monomers and clusters and data of picosecond anti-Stokes resonance Raman spectroscopy found in the literature.

8 - 7 – Magnetic properties of non-oriented grain (NOG) electrical steel

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The anisotropy of the magnetic properties of a low-carbon aluminium-killed non-oriented grain (NOG) electrical steel were studied. The studied steel presented a grain size of 11 um. Permeability, core losses, remanence and coercivity were analyzed in Epstein test frame cut at 0^o, 30^o, 45^o, 60^o, 75^o and 90^o from the rolling direction. Orientation distribution function (ODF) were determined from X-ray pole figures. Magnetic flow density was measured at the magnetic field strength of 2500 A/m (B_{25}) and 5000 A/m (B_{50}) as a function of the angle to the rolling direction. These magnetic fields are sufficiently high so that most of magnetization process is rotation controlled. B_{25} and B_{50}, as a function of angle to the rolling direction, show a minimum between 30^o and 60^o indicating a texture more unfavorable to magnetization at this direction than parallel and perpendicular to rolling. Hysteresis curves for all the samples were measured with a maximum induction of 1.5T and the losses were determined as the internal area of these curves. Coercive force continuosly increased as the angle varied from 0^o to 90^o, whereas remanence decrease.

8 - 8 – Magneto optic imaging of domain walls in a Bi doped YFe ferrite

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Magneto optic imaging consists in the measurement of the Faraday rotation angle of linearly polarized incident light as it passes through a sensitive garnet (YIG Yttrium Iron Garnet) placed over the sample. Considering the anisotropy, exchange and magnetostatic energies both in the Bloch walls as in the Neel tails and the contribution of an applied magnetic field, it is possible to describe the ”zig-zag” walls that separate domains with opposite in-plane magnetization. We have observed that the size of the walls grows as the spatial derivative of the parallel field component, B//, decreases. We have studied the evolution of these domain walls as we force the change in sign of B// to shorter length scales, from hundreds to a few microns. We describe how we have controlled the change in sign of B// and we analyze images that evolve from ”zig-zag” walls to much more complex closed domain structures.

Structural and magnetic properties of intermetallic compounds

9 - 1 – Structural and thermal properties on Cu−Hf−Ti ternary metallic glasses

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Cu−based ternary metallic glasses are promising for practical applications since they joint together interesting mechanical properties like strong glass−forming ability, high strength, ductility and low cost. It was observed that composition and variety of constituents improve some of the above properties against others. In particular, for the Cu−Hf−Ti system, Ti addition increases the thermal stability of the alloy. In this work we study the thermal stability on melt−spunn Cu−Hf−Ti ribbons at different Ti content by differential scanning calorimetry (DSC). The short range order evolution with annealing treatments was also investigated by means of perturbed angular correlation (PAC). The results for the starting alloys indicate that the short range order can be described by a dense random packing of atoms (DRP). The electric field gradient (EFG) behavior with alloy composition is comparable to that previously observed in binary and multicomponet Zr and Hf−based amorphous alloys.

9 - 2 – A first-principles model for electron-capture "after-effects" in ^{111}Cd: In_2O_3

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The temperature dependence of the electric-field gradient (EFG) tensor at ^{111}Cd impurity sites in oxides with the bixbyite structure has been intensively studied by means of the PAC technique in the last twenty years. In these systems two reversible behaviors have been observed apparently depending if the cation has closed electronic shells (such as in Sc, In, and Y) or if it has incomplete shells as in the case of the rare earths: time-dependent ("dynamic") hyperfine interactions and static interactions variable with temperature were found, respectively. In_2O_3 doped with ^{111}In (which decay to ^{111}Cd by Electron Capture) is the prototype of the first behaviour. In this work we report DFT electronic structure calculations at Cd impurities located at both cationic sites C and D of the In_2O_3 semiconductor, performed with the FP-LAPW method with a dilution of 1:32. We studied the EFG at both cationic sites for different charge states of the impurities, and these results were found to be in excellent agreement with the experimental values. A model based in changes of the occupation of impurity gap energy levels localized near the top of the valence band is proposed to described the origin of the experimentally observed dynamic interactions in this impurity-host system.

Index