

Invited Talks

1 – Magnetism under the microscope

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Unraveling complex magnetic structures of magnets with nano-scale dimensions is a true challenge. The spin-polarized scanning tunneling microscopy (SP-STM) and spectroscopy (SP-STs) has a great potential of becoming a unique tool in the frontier field of nanomagnetism addressing and manipulating the magnetism down to the spatial limit. In this contribution an overview is presented of complex magnetic structures in ultra-thin films. A focus is on magnetically frustrated systems [1]. Based on a simple model of the SP-STM/SP-STs [2] we give arguments and evidence that the SP-STM operated in the constant-current mode is a powerful tool to investigate complex atomic-scale magnetic structures [3] and that the spectroscopy mode is ideal to look at magnetic structures at the mesoscopic length scale. We discuss the contrast formation of the STM signal due to spin-polarized tunneling between an antiferromagnetic tip and magnetic sample and how the spin-orbit dependence in the tunneling cross section can be used to detect magnetism using a conventional non-magnetic tip [4]. The results are underpinned applying density functional theory to a range of magnetic systems in low-dimensions and the results are compared to experiments [5].

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2 – Lattice disorder and magnetism in selected *f*-electron intermetallic compounds

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Real materials can have real differences with ideal systems. For instance, non-Fermi liquid (NFL) behavior was initially thought to be due to chemical disorder, since the first such materials were all substituted. Although several nominally well ordered NFL's have been discovered and extensively studied, the effect of disorder on the magnetic properties of *f*-electron intermetallic systems remains poorly understood. I will present the case from an experimental, local structure point of view, reviewing our work on the nominally disordered UCu_{5-x}Pd_x and CeRhRuSi₂ systems, the nominally ordered U₃Ni₃Sn₄ and Ce-based 115 systems, and present the unusual case of the Ce-based Laves phase compounds CeAl₂ and CePt₂ in nanoparticles.

3 – Giant spin/lattice coupling in multiferroics

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Ferroelectric and magnetic materials have been a time-honored subject of study and have led to some of the most important technological advances to date. Magnetism and ferroelectricity are involved with local spins and off-center structural distortions, respectively. These two seemingly unrelated phenomena can coexist in certain unusual materials, termed multiferroics. Despite the possible coexistence of ferroelectricity and magnetism, a pronounced interplay between these properties has rarely been observed. This has prevented the realization of multiferroic devices offering such functionality. We will discuss newly-found, extraordinary coupling between spin and lattice degrees of freedom in a certain class of multiferroics. For example, in the multiferroic TbMn_2O_5 , we have discovered a highly reproducible electric polarization reversal and permanent polarization imprint that are both actuated by an applied magnetic field.

4 – Two fluid model of the Kondo lattice

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It is possible to view the temperature evolution of the Kondo lattice as the condensation of Kondo centers into a heavy electron liquid below a low temperature coherence temperature. This will be presented in the context of the CeMIn_5 ($\text{M}=\text{Co}, \text{Rh}$ and Ir) group of heavy Fermion materials, and shown to account for a number of the unusual low temperature properties.

5 – Structural and magnetic aspects of nanocrystalline alloys

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During the last 15 years, great attention was devoted to understand the origin of excellent soft magnetic properties of nanocrystalline alloys, since the discovery of Finemet by Yoshizawa et al. These materials which are obtained by a subsequent annealing of the amorphous precursor consist of nanocrystalline ferromagnetic grains embedded in an amorphous matrix. We report in this presentation first on the thermodynamic aspects allowing the nanocrystalline state to be understood. Then we discussed the structural and microstructural modeling of these two-phase alloys on the basis of different experimental techniques. Both the macroscopic and local magnetic properties are finally reported for the different varieties of nanocrystalline alloys. The origin of the soft magnetic properties are discussed on the basis of random anisotropy models while the local magnetic properties are compared to some numeric computer simulation predictions.

6 – Tailored electronic states for magnetoelectronics

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The rapidly growing field of magnetoelectronics (spintronics) is based on the manipulation of spin currents instead of charge currents. Examples are the use of giant magnetoresistance (GMR) in magnetic sensors, of tunneling magnetoresistance (TMR or JMR) in magnetic random access memory (MRAM), magnetic semiconductors, and magnetic doping. This overview will cover the spin-dependent electronic states that underlie these phenomena and various methods for mapping them.

7 – Fluctuating field model for conduction electron spin resonance in graphite

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We outline a theory for conduction electron spin resonance (CESR) in highly oriented pyrolytic graphite (HOPG). The fundamental approximation is to treat the spin-orbit interaction as an effective field. In this approach, the shift in the g-factor, which is associated with the mean value of the field, is related to the orbital susceptibility of the electrons. The linewidth comes from fluctuations in the effective field caused by the scattering of the electrons. The theory is used to interpret our CESR measurements.

8 – The effect of dipolar interactions on the magnetic properties of granular magnetic systems

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Studies of magnetic nanoparticle systems have attracted much interest in the last few years owing to their fundamental interest and technological applications. In particular, the correlation of parameters such as size, morphology, crystalline structure, and shape of the particles with the resulting magnetic properties has been thoroughly investigated, but many open questions remain to be answered. Up to now there it is not clear how the dipole-dipole interactions can affect the macroscopic magnetic response of the system. Many different, often conflicting models have been applied to explain the experimental data on interacting magnetic nanoparticle systems. One of the main approaches considers the interparticle interactions through a change of the energy barriers of isolated particles [1]. This approach corresponds to replacing a genuine many-body effect with a single-particle description; it is therefore no more than a simplified representation of a much more complex, and qualitatively different situation. On the other hand, a second approach takes into account collective phenomena [2], but the predictions of such a model seem to contradict several experimental results. Consequently, there has been a considerable discussion about the existence of significant collective effects in magnetic nanoparticle systems, and several speculations regarding a spin-glass-like phase at low temperatures on dipole-dipole interacting systems. With the inclusion of dipolar interactions the problem becomes complex and it is usually solved by means of some approximation. One of the most used methods to investigate the role of interactions has been Monte Carlo simulations. Also, novel phenomenological approaches have proposed analytical models that take explicitly into account the correlation arising from the dipolar interactions on nearly superparamagnetic systems [3]. As a matter of fact, the lack of close-to-ideal samples (with controlled grain size, shape, etc.) hindered more systematic experimental studies. In turn, the absence of perfectly reliable experimental data did not allow a consistent comparison with theoretical models and/or computer simulations. In this work, a brief review on the existing models will be given, and new experimental results on sets of sputtered and chemically grown nanocrystalline samples will be shown. Systematic studies as a function of grain size, distance among magnetic entities will be analyzed through the different theoretical models, demonstrating the great

importance of dipolar interactions on the magnetic properties of granular systems.

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9 – Magnetic Order and Fluctuations in Cuprate Superconductors

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The magnetic properties of the copper oxide class of materials has been of central interest since the early days of high T_C superconductors. The parent materials are two-dimensional antiferromagnetic insulators, but the magnetism persists into the superconducting realm and may be the origin of the pairing. Early indications were that long range order was suppressed in the doping regime where superconductivity occurs, but recent experimental and theoretical results indicate that spin-density-wave order can coexist with superconductivity, and may be the closest competing ground state. Neutron scattering results for the composition and field dependence of the magnetic order in both hole-doped and electron-doped cuprate superconductors will be reviewed, and recent results presented.

10 — Novel collective magnetic relaxation phenomena in manganites: an spin-glass behavior?

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In this talk we address many of the fundamental open questions regarding the glassy behavior of the magnetic/electronic phase segregated state in rare earth perovskites. In particular, ac/dc magnetic relaxation experiments support that the collective effects (memory, ageing, etc.) are due to interparticle interactions, rather than the double-exchange vs. superexchange competition. We have performed a careful study of the non-linear susceptibility in the critical region, and the critical exponents derived will be discussed and contrasted with those of conventional spin-glasses and concentrated quenched ferrofluids. We will propose here that the phase segregated state constitutes a sort of self-generated assembly of magnetic particles in which the magnetic interaction introduces collectivity among the clusters. Moreover, the strength of the interactions can be tuned by composition and/or magnetic field, through the control of the size and concentration of the magnetic clusters. We believe that these results are general and should be applicable to other systems close to a first order electronic transition similar to the one described here, like cobaltates, etc.

11 — Magnetic Aerogels

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Silica aerogels are sol-gel derived nanostructured materials which exhibit accessible internal porous structures. Due to their high porosity they present very low densities ($\rho = 0.04 - 0.6 \text{ g/cm}^3$) and high specific surfaces. These materials are thermally insulating and optically transparent with low dielectric constant. Their various potential applications have recently been increased by locating nanosized magnetic particles into the internal porous structure [1,2,3]. Development of magnetic aerogels with specific properties, prepared by chemical sol-gel routes, requires the determination of their basic phase compositions and nanostructures, their dependence on process parameters and starting materials, and the study and interpretation of their magnetic response. In this contribution we present an overview of the work done recently in this area and discuss our results for iron oxide/silica nanocomposites with nominal mass iron concentrations $\text{Fe/Si} = 0.4$ [4]. From these results a picture emerges in which nanosized iron oxide particles are most probably located inside the aerogel nanopores isolated from each other. Actual iron concentrations were found to be lower than nominal ones. Different approaches have been applied to derive the magnetic dynamic response of the system from ac susceptibility measurements which allowed us to determine characteristic relaxation times and energy barrier distributions within an improved degree of confidence. par—

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12 – Non-Fermi liquid behavior and coexistence of ordered phases induced by nested Fermi surfaces

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The nesting of the Fermi surfaces of an electron pocket and a hole pocket separated by a wavevector \mathbf{Q} interacting via a repulsive potential gives rise to itinerant antiferromagnetism. The order can gradually be suppressed by mismatching the nesting and a quantum critical point (QCP) is obtained as $T_N \rightarrow 0$. The renormalization group flow is studied by eliminating the fast degrees of freedom close to the ultraviolet cut-off, leading to a strong coupling fixed point [1]. In the paramagnetic phase the system follows a Fermi liquid picture with a renormalized temperature dependent effective mass. The specific heat γ coefficient and the uniform magnetic field susceptibility increase on a logarithmic scale when the temperature is lowered. The effective mass diverges at the critical point signaling the breakdown of the Fermi liquid. The system is also unstable to singlet and triplet superconducting fluctuations [2]. A strong magnetic field changes the nesting condition favoring one of the spin components, so that a phase with spin- and charge-density waves and a ferromagnetic component can coexist [3]. The QCP also strongly renormalizes the electron-phonon coupling, the phonon spectrum, and the thermal expansion. The results are discussed in the context of non-Fermi-liquid behavior observed in some heavy fermion compounds [4].

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13 – Molecular magnets: bolometers and microwaves emitters

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In my talk I will review the possibility to use high spin molecular magnets as both detectors and emitters of electromagnetic radiation in the range of microwaves. Molecular magnets show magnetic bistability due to the magnetic anisotropy barrier between the spin up and spin down states. The occurrence of this strong uniaxial anisotropy yields double degenerate ground states in zero field and a set of excited levels in the microwave - infrared range. I will start describing an experimental method for quick, high resolution determination of the resonant frequencies of any resonator based upon the variation of the equilibrium magnetic moment for a magnetic sample inside. In particular I will show examples using several resonant devices like coils and cavities in which we place a sample made of molecular magnets. The main result refer to the remarkable observation of sharp peaks in the equilibrium magnetization and the ac susceptibility for the resonant frequencies of these devices. I will also discuss the case of the quantum dynamics of crystals of molecular magnets inside a resonant cavity. In particular I will discuss the results showing that crystals of molecular magnets exhibit enhanced magnetic relaxation when placed inside a resonant cavity. This result may be interpreted as an indirect existence of the emission of coherent radiation from the crystals. When this radiation matches the cavity modes is re-absorbed giving rise to the enhancement of the magnetic relaxation. The last topic in my talk will be the detection of the electromagnetic radiation emitted in the demagnetization process of molecular magnets. In our experiments we have used InSb bolometer to detect the radiation and we have clearly established that the rapid inversion of the total magnetic moment of the sample made of a set of single crystals of molecular magnets is accompanied by the detection of a voltage drop in the bolometer.

14 – Magnetic Interactions in arrays of self-assembled nanomagnets

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In the interdisciplinary field of nanoscience, an enormous effort is being focused to synthesize and study ordered assemblies of nanoscaled materials. Such materials are intrinsically interesting to study their collective properties, and for technological applications [1]. An overview on particular arrays of magnetic nanowires and nanoparticles is here presented.

Magnetic nanowires have been synthesized into self-assembled arrays of nanopores of alumina membranes by controlled two-step anodisation processes and subsequent filling of pores by electrodeposition. They form densely packed arrays of wires with hexagonal symmetry, and tailorable geometrical characteristics: a) wire diameter (15 to 80 nm), b) lattice parameter (65 and 105 nm), c) ordering degree (crystalline domain size), and d) wire length (typically within the order of 1 micron [2]. Arrays structure and geometry are characterised by HRSEM, AFM, and RBS. Studies of collective magnetic behaviour are mainly focused on properties of the arrays as a function of the mentioned geometrical characteristics by VSM magnetometer, while individual magnetic state of nanowires is evaluated by MFM.

On the other hand, magnetic nanoparticles are prepared by colloidal syntheses [3], at the presence of organic acids as stabilising agents to prevent precipitation and coalescence [4]. Their highly monodispersity and the surfactant coating enable their self-ordering into close-packed assemblies of nanoparticles. Self-organised CoNi and FePt nanoparticle arrays have been synthesized and structurally and magnetically characterised. Square, hexagonal close-packed and (pseudo)-honeycomb organizations and spherical superstructures have been found. The collective magnetic behaviour has been studied as a function of temperature (4 to 300 K), particle size (4 to 10 nm), and interparticle distance (2 to 5 nm).

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15 – Surface-core intraparticle interactions in nanoparticles

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The surface/volume ratio is large in nanoparticles (e.g. for ~ 3 nm nanoparticles, approximately 70% of atoms are in the surface), and consequently surface effects play an important role in determining their magnetic behaviour. In amorphous single domains the shape anisotropy affects the core magnetic moment and the surface anisotropy is originated only by the spin-orbit coupling of each surface ion. As it is expected, all surface effects are enhanced (e.g., an enlargement of the disordered shell) and amorphous nanoparticles give us a chance to study this effect under a different point of view. Magnetization measurements in ~ 3 nm amorphous nanoparticles are presented where surface effects and intra-particle interactions are significant. Interparticle interaction effects on the surface magnetic order are also discussed.

Talks

16 – Electronic structure of the negative charge-transfer materials Sr_3FeMO_7 ($M = \text{Fe}, \text{Co}, \text{Ni}$)

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The Ruddlesden-Popper series $\text{Sr}_3\text{M}_2\text{O}_7$ have transition metal ions M in a tetravalent state. The structure resembles 2 SrMO_3 perovskite layers stacked between a SrO rock-salt layer. The crystal structure of $\text{Sr}_3\text{M}_2\text{O}_7$ is tetragonal with a space group given by $I4/mmm$. The $\text{Sr}_3\text{M}_2\text{O}_7$ compounds are semiconductors with (thermally) activated carriers. The low temperature region is characterized by a weak activation, whereas the high temperature region presents a larger activation. The electrical conductivity of Sr_3FeMO_7 increases in the series from $M = \text{Fe}$ to Ni . There are few comparative studies of the electronic structure of these compounds. This information is needed to understand the origin of their physical properties. We studied the electronic structure of substituted Sr_3FeMO_7 with $M = \text{Fe}, \text{Co}, \text{Ni}$. The experimental technique used in the study was $M\ 2p$ X-Ray Photoelectron Spectroscopy (XPS). The charge-transfer satellites in the spectra were analyzed using cluster-model calculations. The Sr_3FeMO_7 samples were prepared by an acetic acid based gel route. The oxygen content of the samples was determined by iodometric titration. The XRD analysis indicated that the samples were single phase. The XPS spectra were taken using a commercial VG-ESCA system. The samples were scraped to remove surface contamination. The spectra were collected using $\text{Al } K\alpha$ radiation and the energy resolution was 1 eV. The cluster-model was solved using the configuration interaction method. The parameters of the model are: the charge-transfer energy Δ , the Coulomb repulsion U , the core-hole potential Q , and the $p-d$ transfer integral T_σ . The ground state and final state are expanded in terms of charge-transfer configurations, and the core-level transitions are calculated within the sudden approximation. The analysis of the spectra shows that these materials are in the negative charge-transfer regime. The ground state is dominated by the $3d^n\bar{L}$ configuration (where \bar{L} denotes an O $2p$ hole in the oxygen band). The results are similar to those found in the related SrMO_3 and Sr_2MO_4 compounds. The band gap of these compounds is caused by the relatively large value of T_σ . The lowest lying excitations are $3d^n\bar{L} + 3d^n\bar{L} \rightarrow 3d^n + 3d^n\bar{L}^2$, and consequently the band gap is of the $p-p$ type. The weight of the $3d^n\bar{L}$ configuration in the ground state of Sr_3FeMO_7 increases from $M = \text{Fe}$ to Ni ; this helps to explain the observed increase in the conductivity of the series from Fe to Ni .

17 – Current-induced effects in $\text{La}_{0.275}\text{Pr}_{0.350}\text{Ca}_{0.375}\text{MnO}_3$ single crystals

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DC electrical current-dependent resistance and pulsed current-voltage characteristics as a function of temperature are reported on mixed valent Mn oxide based $\text{La}_{0.275}\text{Pr}_{0.350}\text{Ca}_{0.375}\text{MnO}_3$ single crystals. We find that the low temperature regime of this material is strongly current dependent. For small current densities ($\sim 10 \mu\text{A}/\text{cm}^2$), the metal insulator transition related to the low temperature enlargement of the ferromagnetic fraction is not observed down to 10 K. Higher current densities causes a large decrease of the resistance, which is temperature dependent and exhibits memory effects. Our results are interpreted within a scenario of strong competition between charge and ferromagnetic ordering.

18 – Magnetic behavior of icosahedral Pd clusters

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We study the magnetic properties of free-standing Pd clusters of some selected sizes with icosahedral structures which are obtained as the most stable ones using the Embedded Atom Method from an uniform relaxation of different geometrical configurations. The spin-polarized electronic structure and related magnetic properties of those optimized geometries were calculated by solving self-consistently a spd tight-binding Hamiltonian. The magnetic moments obtained in our calculations present an step-like dependence as a function of the exchange parameter. We discuss the results in comparison with previous calculations for fcc Pd clusters and with recent experimental findings.

19 – Doping in FeMo

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The measurement of an appreciable increase in the Curie temperature of double perovskites of the type $\text{La}_x\text{Sr}_{2-x}\text{FeMoO}_6$ with electron doping [1,2] poses a question mark on the ‘traditional’ models of the electronic structure of these materials [3-5]. Substitution of the divalent chalcogenides by trivalent rare earths presumably increases the number of carriers and produces a rise of the Curie temperature of a few degrees per per cent of rare earth. Most theories based on a high correlation at the Fe orbitals predict a lowering of T_c with electron doping contrary to experiment. The picture proposed by Tovar *et al.* on the other side based on a mean field argument predicts an increase of T_c proportional to the density of states at the Fermi level. We discuss the implications of these experimental facts on the different models and propose different experiments that could shed some light on the matter.

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20 – Dynamic Effects on the Magnetoconductivity of Quasi One-Dimensional Single Crystals

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We study in this work the appearance of transient magnetoconductivity peaks in quasi-1D $\text{Ca}_3\text{Co}_2\text{O}_6$ single crystals. Steady state transport in these crystals has shown Variable Range Hopping conductivity with a temperature-induced crossover between 1D (intra-chain) and 3D transport. This appears along with the opening of a Coulomb gap in the d bands and with the ferromagnetic intra-chain ordering [1]. From the high field resistivity vs. temperature analysis, we inferred a field-induced suppression of this Coulomb gap responsible for a large decrease in resistivity. The magnetoresistance thus obtained from pulsed fields is rather large, negative and monotonic, and comes superimposed by large peaks in the conductivity. The observed magnetoconductivity peaks are linked to the rate of change of the magnetic field, and are also magnetic-history dependent. We initially attributed this effect to the magnetocaloric effect [1], as seen in various thermomagnetic materials [2]. This,

however, does not explain the observed appearance or suppression of one of the conductance peaks according to whether the sample was previously taken to higher fields or not. The application of a rapidly variable magnetic field can be equivalent to thermodynamic quenching if the rates of energy transfer are comparable. As our pulsed field can change at rates as high as 500T/s, and having in mind the mobility of the electrons as opposed to that of atomic interdiffusion, we can indeed have a “magnetic quench” of the system. Based on the model of electronic phase-separation for manganites and other oxides [3], we propose that the magnetoconductivity peaks should be an equivalent to the properties of materials undergoing spinodal decomposition, as in metastable alloys or mixtures. The proposed mechanism would have the segregation of the two electronic states producing, for some quenching conditions, a percolative state of the conducting phase that translates into a plunge of the resistivity. This is supported by the direct relation between the position of the peaks and the rate of change of the magnetic energy transfer, even for cases where only one peak is observed. This is also in full accordance with the observation that the peaks in conductivity occur at the fields where the steps in magnetization are observed.

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21 – Spintronics and Edge States in Semiconducting heterostructures

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In many transport experiments in two dimensional electron gases (2DEG) with a transverse magnetic field, including quantum hall effect and transverse magnetic focusing, edge states play a central role. The possibility of building quantum point contacts and quantum dots (QD) at the edge of 2DEG, that couple with edge states, opens new opportunities for the fast developing fields of spintronics. We first analyze focusing experiments including the effect of spin orbit interaction and show how polarized currents are generated. Then we show how the effective non-local exchange interaction between QD’s mediated by edge states can be tuned with a small magnetic field. The proposal is based precisely on the possibility of focusing the electrons that interact with one quantum dot onto the other by the action of the external field. When the cyclotron radius is commensurate with the inter-dot distance, the spin-spin interaction is largely amplified and may increase a few orders of magnitude.

22 – Switching field of partially exchange-coupled particles

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The magnetization reversal of partially exchange-coupled particles is studied in detail. The starting point is the observation of a complicated phenomenology in the irreversible susceptibility and FORC distribution functions of Ba hexaferrite samples obtained by means of different sintering conditions. Several peaks in the FORC distribution functions were identified and associated with clusters with different number of particles. The switching fields of these clusters were related to an effective anisotropy constant K_{eff} that depends on the number of particles in the cluster. K_{eff} is linked to the exchange-coupled volume between two neighboring particles and as a weighted mean between the anisotropy constants of the coupled and uncoupled volumes. By using the modified Brown's equation $\alpha_{\text{ex}} = 0.322$ is obtained.

In order to interpret these results, the switching field of a two-particle system with partial exchange-coupling is studied. It is assumed that the spins re-orientation across the contact plane between the particles is like a Bloch wall. The energy of the system is written in terms of the fraction of volume affected by exchange coupling and the switching fields for both particles are calculated. At small interaction volume each particle inverts its magnetization independently from the other. As the fraction of exchange-coupled volume increases, cooperative effects appear and the two particles invert their magnetization in a cooperative way.

The proposed model allows to interpret for the first time the empirical factor α_{ex} in terms of physical arguments and also explain the details observed in the FORC distribution function.

23 – Electric field induced metal insulator transition in $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ thin films

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In this work, the electrical behavior of polycrystalline $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ thin films, deposited by pulsed laser deposition (PLD) on (100) Silicon substrate, is reported and discussed. The electric resistance of the manganite films, with thickness between

37 to 100 nm, was measured as a function of temperature for different applied electric fields. A metal-insulating transition at around 150 K is found, which is field and thickness dependent. At low temperature we found that the conductivity of the films is non-Ohmic and moderate electric fields results in resistivity switching to metaestable low-resistive states. The experimental results, shown in this work, put in evidence that the fraction of FMM regions remains constant when electric fields are applied. Then, the responsible of the MI transition and of the conduction behavior at low temperatures in $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ thin films is the appearance of connective paths produced by the enhance mobility of the carriers activated by the electric fields.

24 – Influence of the interface on the magnetic anisotropy of CoCu granular alloys

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Granular alloys composed of magnetic clusters embedded in metallic non-magnetic matrices display the giant magnetoresistance (GMR) phenomenon, that is, their electrical resistance decreases notably under an applied magnetic field. We have studied $\text{Co}_x\text{Cu}_{100-x}$ ($x = 5, 10, 15, 20$) melt-spun granular ribbons in the as-quenched state and annealed at increasing temperatures from 400 to 650°C. Due to the immiscibility between Co and Cu, the annealing induces the precipitation of both, thus clusters of the minority element (Co) appear embedded in the matrix formed by the majority one (Cu). The microstructure of the samples plays a decisive role in the GMR response, as has been extensively studied [1], the most influencing factors being the size, size-distribution, concentration and interfacial roughness of the magnetic clusters. Previous studies on the CoCu granular alloys show that the increase of the interfacial roughness due to the slight miscibility of Co and Cu appearing above $\approx 500^\circ\text{C}$ induces the sudden drop of the GMR observed above this annealing temperature [2]. In this work we have focussed on the influence of the Co clusters interfaces on the magnetic response of the samples. In this way, we have calculated the effective anisotropy constant as a function of the Co clusters size from the fitting of the zero field cooling - field cooling curves. As expected from previous studies on nanogranular systems [3], the effective anisotropy increases towards the fcc Co bulk one ($2.6 \times 10^5 \text{ J/m}^3$) as the cluster diameter increases. Finally, we have correlated the effective anisotropy to both the anisotropy in the core and in the surface of the magnetic clusters, as a function of the cluster diameter, and obtained a surface anisotropy of $3.8 \times 10^{-1} \text{ mJ/m}^2$, what is an indication of the important contribution of the surface atoms to the net anisotropy.

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25 – Applying Synchrotron Light Techniques to Strongly Correlated Electron Systems

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Strongly correlated electron systems are presently one of the main frontiers of condensed matter physics, continuously generating phenomena of strong scientific and technological interest, such as high temperature superconductivity in cuprates and colossal magnetoresistance in manganites. The high complexity of such systems has demanded increasing sophistication on both theoretical and experimental approaches, and, not rarely, synchrotron light techniques have been employed. In this presentation, I will discuss some of the experimental studies being performed in strongly correlated systems at Laboratório Nacional de Luz Síncrotron (LNLS), Campinas, Brazil. These include magnetic x-ray diffraction on the intermetallic compound Gd_2IrIn_8 , probing the Re $5d$ magnetism in the bulk $A_2\text{FeReO}_6$ ($A = \text{Ca}, \text{Ba}$) double perovskites, as well as a search for tiny structural distortions associated with orbital ordering phenomena in these compounds. These preliminary results evidence the great potential that the open facilities installed at the LNLS offer to the study of strongly correlated electron systems.

26 – Magnetic Normal Modes in Nanoparticles

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We present a method via which the magnetic normal modes of a ferromagnetic particle can be calculated. The method is a hybrid of micromagnetic simulations and a “dynamical matrix” approach similar to that used for vibrational studies. We use the method to calculate the normal modes of an Fe parallelepiped and compare our results with the modes recently extracted using a pure micromagnetic simulation approach. The results of the two approaches are in excellent agreement and the pros and cons of the two methods are discussed. We present information on standing waves with wavevector perpendicular to the applied field and also on a family of modes localized at the particle ends.

27 – Static and dynamic properties of phase separated rare earth manganese oxide based compounds

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The tendency of some manganese-based oxides with perovskite like structure to display phase separation, i.e. submicrometric coexistence of ferromagnetic (conductive) and charge ordered (insulating) regions, is a challenge issue of the physics of the strongly correlated systems. The existence of phase separated states strongly affects macroscopic properties, as magnetization and electric transport. At the microscopic level, the delicate balance between the free energies of the coexisting phases gives rise to interesting effects, as slow relaxation, rejuvenation, and abrupt step transitions. We summarize some recently obtained data on polycrystalline samples of some manganites: half doped $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$, B site doped $\text{La}_{0.5}\text{Ca}_{0.5}(\text{MnFe})\text{O}_3$, and A site doped $(\text{LaPr})_{0.625}\text{Ca}_{0.375}\text{MnO}_3$. For the last mentioned compound, results obtained on nanotube structures will be also presented. We focus our attention on both static and dynamic properties (memory effects, abrupt changes in magnetization) related to the phase separated nature of these compounds.

28 – Quasiparticle excitations in a frustrated antiferromagnet

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We have studied the dynamics of a single charge in a triangular antiferromagnet. Using a charge-magnon effective Hamiltonian we have computed the quasiparticle wave function taking into account multi-magnon contributions in the self consistent Born approximation. We have found qualitative differences between the electron and the hole doped cases regarding the structure and the own existence of the quasiparticle excitations. Such differences are due to the subtle interplay between magnon-assisted and free hopping mechanisms. We conclude that the conventional quasiparticle picture can be broken by geometrical magnetic frustration without invoking spin liquid phases.

29 – Magnetic alterations produced by rare earth doping in Y_2BaCuO_5

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In the literature, the magnetic ordering of compounds of the series R_2BaMO_5 ($R = Y$ or rare earth and $M =$ transition metal) are reported to occur at different temperatures. In addition, discussions about the cause for the dimensional changes observed in the array of the magnetic moments of some members of the series are still taking place. In this work we report on results obtained by doping the green phase Y_2BaCuO_5 with Dy. We discuss the change in the 2-D to 3-D magnetic array, the shift on the ordering temperature from 27 K to 16 K experienced by Y_2BaCuO_5 when doped with 1 at.% and 5 at.% Dy, and compare these results with experimental evidences from other systems. We discuss the effect that the R-doping might have on the electronic structure of the Cu ions involved in the superexchange pathways.

30 – Vortex matter in the presence of a minimally ordered mesh of defects: crossover in vortex dynamics

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Vortex matter in the presence of a minimally ordered mesh of defects is the central subject of a study which we have been conducting in different superconducting systems [1-7]. The present contribution includes results on some selected samples of Mg -deficient MgB_2 [3]; on specimens of filamentary Nb embedded in a Cu matrix [4]; on $YBCO$ films with arrays of columnar defects [5]; as well as in some tridimensional disordered Josephson junction arrays of Nb [6] and $YBCO$ [7] produced using specially developed routines. The studied samples have in common a characteristic microstructure consisting of two coexisting subsystems, one being the superconductor itself, and the other a linking matrix: Mg -deficient insulating clusters in MgB_2 ; Cu in Nb/Cu ; nanoin-dented columns in $YBCO$ films; and intergrain material in Nb and in $YBCO$ Josephson arrays. These systems were not selected at random, but in view of their uncommon characteristic of exhibiting a narrow distribution of weak-link critical currents, revealed by independent methods. Most of these systems exhibit a threshold temperature, T^* , at which the vortex dynamics changes abruptly, as revealed by a crossover in the time evolution of magnetization, from steady to relaxing. This crossover is also uncovered by the AC-susceptibility which, below T^* , becomes dependent on the amplitude of the excitation field. Magnetic and transport measurements allowed for the identification of T^* with the onset of the weak-linkage between superconducting regions. Of course, this is a major reason for the careful selection of samples for the present study, as T^* for standard granular specimens varies substantially throughout the volume and the feature discussed here is simply hidden in bulk measurements of such 'regular samples'. We have also detected that T^* evolves as a function of an externally applied magnetic DC field, so that $H^*(T)$ is a relevant boundary in the phase diagram, across which the vortex dynamics is modified as a result of the interaction between vortex matter and its neighboring mesh of defects. There is interesting physics to learn from the study of this boundary, not only for its universal character of being exhibited by different classes of superconductors, but also for the experimental evidence that there might be a scaling law behind it.

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31 – Monte Carlo study of the bulk magnetic properties of magnetite

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Within the framework of a three dimensional Ising model with nearest neighbor interactions, and using a Metropolis algorithm for equilibrium and energy minimization, we compute the canonical ensemble averages for magnetization, magnetic susceptibility and specific heat of pure magnetite Fe_3O_4 . In the model, atoms are distributed on an inverse spinel structure for which competitive interactions coming from antiferromagnetic Fe3+A-Fe3+A, Fe3+A-Fe3+B, Fe3+A-Fe2+B couplings and Ferromagnetic Fe3+B-Fe3+B, Fe3+B-Fe2+B, Fe2+B-Fe2+B bonds (where A and B labels refer to tetrahedral and octahedral sites respectively) are taken into account. Results of the simulation allow obtaining information about the way as every sublattice contributes to the magnetic critical properties of the system as a function of temperature.

32 – Magnetic polaron and Fermi surface effects on the ESR Spin-Flip scattering of EuB_6 above $T_c \approx 15$ K

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The spin-flip scattering between conduction and $4f^7 \text{Eu}^{2+} (^8S_{7/2})$ electrons in the paramagnetic phase of EuB_6 ($T \geq 2T_c \simeq 30$ K) is studied by means of electron spin resonance (ESR) at various frequencies. The single Dysonian resonance observed in all the cases suggests a *metallic* environment for the Eu^{2+} ions and is consistent with the semimetallic character of EuB_6 . The ESR at high field, $H \simeq 12.05$ kG ($\nu \simeq 33.9$ GHz), shows isotropic g -value and an anisotropic line width with cubic symmetry. This anisotropy arises from a non-trivial exchange interaction between the spins of Eu^{2+} and the conduction states in the *hole* and *electron* pockets at the X points of the Brillouin zone. The

low-field, 1.46 kG (4.1 GHz) and 3.35 kG (9.5 GHz), ESR line widths are unexpectedly broader and have a smaller anisotropy than at high field (12.05 kG). This unconventional narrowing of the line width at higher fields is indicative of a homogeneous resonance and is a microscopic evidence for a strong reduction in the electronic spin-flip scattering by magnetic polarons.

33 – Morphological and magnetic characterization of nanowires and nanotubes based on manganites oxide

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A morphological and magnetic study of sub-micrometric nanostructures of a manganese oxide based compounds is presented. Nanowires of 50 and 100 nm and tubes with external diameters of 200 nm and 800 nm were synthesized. Scanning Electron Microscopy with EDS microanalysis (SEM) and Transmission Electron Microscopy (TEM) allowed to characterize the morphology and microstructure of these nanostructures. The walls of the nanotubes are composed of on average 40 nm grain size particles and they are quite uniform on the micron scale length. The small grains are present a random crystalline orientation, as it is confirmed by diffraction experiments in the TEM. Magnetization measurements and hysteresis loops are presented and discussed based on magnetic interaction between the grains, anisotropy considerations and reversal magnetization mechanisms. Work done in collaboration with J. Curiale, H.E. Troiani, H. Pastoriza, A.G. Leyva and P.Levy.

34 – Effects of Zn and Ni doping on the properties of hematite obtained from mixed metal oxinates

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Hematite, $\alpha\text{-Fe}_2\text{O}_3$, is an important iron oxide, which has been the subject of intensive research for a long time. Recently, increasing efforts are devoted to the search for new methods of preparation, with emphasis in the doping. A new method of synthesis of Al doped hematites has recently appeared in the literature. In the present investigation, we apply this method in the study of the changes produced in the structural and magnetic properties of hematite upon 5 at. % Zn and 5 at. percent Ni substitution. The method is based upon the combustion process of mixed metal oxinates. Thermogravimetric curves show that the decomposition proceeds in an overweigh loss formed at least by two stages in both types of metal oxinates; the weigh loss is related with the formation of probably CO_2 , N_2 and H_2O , and a solid residue. X-ray diffraction and Mössbauer spectroscopy show that the solid residue of the thermally treated Fe-Zn oxinates is hematite and franklinite, whereas it is Ni-hematite and trevorite in the case of Fe-Ni oxinates. Changes in the cell parameters, the saturation hyperfine fields, the Morin and Néel temperatures are observed. These effects are due to the fact that the magnetic behavior of hematite depends on the presence of the dopant, vacancy sites and lattice distortion.

35 – Detecting new Quantum Critical Point related effects on Ce magnetic systems

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Detailed experimental studies in the proximity of Quantum Critical Points, QCP, are scarce because only a few antiferro- or ferro-magnetic phase boundaries, $T_{N,C}(x, p)$, can be unambiguously traced for at least one decade of temperature as a function of concentration x or pressure p . In the former case, the three Ce-systems: $\text{CeIn}_{3-x}\text{Sn}_x$; $\text{CePd}_{1-x}\text{Rh}_x$ and $\text{CeCu}_{6-x}\text{Au}_x$, where $T_{N,C}(x)$ was traced down well below 10% of the original $T_{N,C}$ values, i.e. $< 0.1T_{N,C}(x = 0)$, a ground state transformation is observed at $x^* \approx 1/2x_{cr}$, being x_{cr} the concentration of the critical point where $T_{N,C}(x) \rightarrow 0$. Apart from the typical specific heat temperature dependence: $C_m/T \propto \ln(1/T)$, new QCP related effects are observed in their thermal properties within the $x^* < x < x_{cr}$ region. They are: i) a change from the negative curvature of $T_{N,C}(x)$ to a linear x dependence, ii) a nearly constant value (i.e. independent of x) of C_m/T at $T = T_{N,C}$, iii) a scaling of $C_m/T(T)$ with $\Delta T = T - T_{N,C}(x)$ and iv) an increase of the zero point entropy, $S_0(x)$, if the total $S_m = R \ln 2$ entropy for a doublet Ce ground state is taken as a constant. In the case of $\text{CeIn}_{3-x}\text{Sn}_x$, the computed values for $S_m(T)$ and internal energy, $U_m(T)$, for $T > T_N$ correspond to those of simple quadratic antiferromagnetic 2D-layers predicted by standard models, as reminiscence of the CeIn_3 (3D) magnetic structure. Furthermore, dynamic effects are detected in dissipative AC-susceptibility signal, χ'' , of ferromagnetic $\text{CePd}_{1-x}\text{Rh}_x$. As $x \rightarrow x_{cr}$ there is an increasing dependence on the frequency of the AC-excitation-field of the temperature of the $\chi''(T)$ maximum together with an extra contribution arising at $T \rightarrow 0$, while the χ'_{AC} signal remains unchanged. Consequences on the Free Energy evolution within the $x^* < x < x_{cr}$ region and implications of the $S_0(x)$ contribution are discussed.

36 — Magnetic properties of semiconductor-based heterostructures

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The comprehension of the magnetic properties of hybrid nanostructures, built of magnetic and semiconducting materials is crucial for the design of spintronics devices. The magnetism of these structures lay on the magnetic coupling across semiconducting barriers, the magnetism at the ferromagnetic(FM)/semiconductor(SM) interfaces and the bulk and interface anisotropies of the magnetic layers. Ferromagnetic resonance spectroscopy (FMR) is one of the most used tool to study the magnetic properties of films and multilayers. The dependence of the resonance frequencies on the energy density of the samples, provides us the essential parameters that describe the magnetic properties of the structures. This technique is sensitive to very small amount of material and is capable to identify magnetic ions in different environments and materials with different anisotropies. Our work is focused on the study of the magnetic coupling and magnetic anisotropies of FM/SM structures, based on FMR experiments. In this talk, I will present some recent results obtained in different semiconductor-based hybrid heterostructures.

37 — Magnetic properties of Nanowires

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The magnetic properties of arrays of magnetic nanowires are analyzed using both an analytical approach and Monte Carlo method. The role of the interaction in the hysteresis curve of Ni-nanowires with mean diameter of $\approx 30\text{nm}$ and lengths of 4000nm is discussed. The hysteresis behavior in 2D hexagonal lattices, can be explained using both non interacting model as well as a model which takes into account the interaction among the wires. Due to the large length to diameter ratio in the individual wires the dipolar approximation breaks down when treating the magnetostatic interactions among them, because of the higher order multipoles. These multipolar terms have the main effect of reducing the effective interaction between neighboring wires. The internal magnetic structure of an individual nanowire during the reversion is also analyzed using scaled Monte Carlo technique.

38 — Hysteresis of systems with random competing interactions

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We begin by motivating the talk with the report of magnetic measurements of magnetic hysteresis for perovskites randomly doped with Ce atoms: A step-like hysteresis cycle is found for very weak fields (under 50 Oe) when high resolution experiments are performed. The possibility of random competing interactions in such system is discussed. Then we move onto the proposal of a simple Ising Hamiltonian retaining the most important features of such system: ferromagnetic and antiferromagnetic interactions, anisotropy and randomness. Then a Monte Carlo simulation is started showing that some of the features of the experiment are reproduced: steps at low-field values, no return-point memory, temperature dependence. Consequences of these observations are discussed.

Posters

Magnetic Oxides and CMR

1 - 1 – Thermopower of an intermediate valence model of $\text{Ti}_2\text{Mn}_2\text{O}_7$.

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In this work we calculate the thermopower of $\text{Ti}_2\text{Mn}_2\text{O}_7$, together with its static resistivity and dynamical conductivity. The appearance of colossal magneto resistance (CM) in this system has stimulated many recent studies of the pyrochlore family of compounds ($\text{A}_2\text{B}_2\text{O}_7$). This material is ferromagnetic and with enormous negative magneto resistance in the region of the ferromagnetic transition ($T_c \sim 121\text{K}$), but the double exchange (DE) model of Zener does not explain the CM in this material. Like the In pyrochlore, $\text{Ti}_2\text{Mn}_2\text{O}_7$ has a very high T_c , but its metallic conductivity cannot be explained by doping. According to several recent band calculations, the material is expected to be “half metallic”, with the conductivity driven at low temperatures within one of the spin directions only. We employ the intermediate valence model of Ventura and Alascio (Phys. Rev. B **56**, 14533 (1997)) to describe the electronic structure and transport properties of $\text{Ti}_2\text{Mn}_2\text{O}_7$. Two magnetic configurations describe the $3d$ orbitals of Mn, hybridized with a conduction band associated to the Ti, and in the present work we write the model Hamiltonian employing Hubbard operators, and reformulate a previous treatment by Foglio and Figueira (Phys. Rev. B **60**, 11361, (1999)) to obtain approximate one-electron Green’s Functions (GF) for the model. We have calculated the spectral densities derived from these GF at different temperatures, both with and without magnetic field. We have employed these GF to obtain the thermopower, together with the static and the dynamic conductivity of this compound for several values of the system parameters. A qualitative agreement was obtained with the thermopower measurements of H. Imai et al. (Phys. Rev. B **62**, 12190, (2000)), as well as with the measurements of static resistivity of Y. Shimakawa et al. (Phys. Rev. B **55**, 6399, (1997)) and the experimental results of optical conductivity of Okamura et al. (Phys. Rev. B **64**, 180409, (2001)).

1 - 2 – Photoemission spectra and band structure calculations of CaRuO_3 and SrRuO_3

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CaRuO_3 is a paramagnetic metal while SrRuO_3 is a ferromagnetic metal with $T_C = 165\text{K}$. This is surprising because these materials have similar electronic and crystal structures. The origin of the different magnetic properties in CaRuO_3 and SrRuO_3 is not yet understood. There are few comparative studies of the electronic structure of these compounds. We studied the electronic structure of the CaRuO_3 and the SrRuO_3 compounds using photoemission spectroscopy (PES). These results were compared to DOS obtained from LDA band structure calculations. The CaRuO_3 and SrRuO_3 samples were prepared using the standard solid state reaction method. The PES spectra were measured at the PGM beamline in CAMD. The photon energy was 40 eV and the energy resolution was 50 meV. The samples were scraped *in situ* with a diamond file to remove surface contamination. In a first approximation, the PES spectra reflect the occupied electronic states in the valence band. The spectra present a strong structure with broad peaks around 5 and 10 eV; this structure is attributed mainly to the O $2p$ band. In addition, the spectra present also a weaker feature just below the Fermi level, between 0 and 2 eV; this feature is ascribed mostly to the Ru $4d$ band. The presence of a Fermi edge in the Ru $4d$ band region confirms that these materials are metallic. The relative intensity of the Ru $4d$ feature in SrRuO_3 this peak is slightly larger than in CaRuO_3 ; this difference might be related to the differences in the magnetic properties of these compounds. The DOS were calculated using the standard LMTO method. For simplicity, the DOS were calculated in the pseudocubic crystal structure. For CaRuO_3 , it was calculated the non-magnetic solution, using $a = 0.384\text{ nm}$. For SrRuO_3 , it was calculated the ferromagnetic solution, with $a = 0.392\text{ nm}$; the calculated magnetic moment was about $\mu = 0.9\mu_B$. The DOS were calculated using 220 irreducible \mathbf{k} -points in the Brillouin zone. The linearization energies E_ν were floated to the center of gravity of the occupied bands. The calculation gives a metallic solution for both CaRuO_3 and SrRuO_3 , with a relatively large DOS derived from the Ru $4d$ band at the Fermi level. The structure between 2 and 8 eV corresponds to the O $2p$ band. In the region between 5 and 8 eV, the O $2p$ states are heavily mixed with Ru $4d$ states; whereas in the region between 2 and 5 eV, the O $2p$ states are mixed with neighbouring O $2p$ states. The Ru $4d$ band in SrRuO_3 shows a clear splitting at the Fermi level between the spin-up and spin-down sub-bands.

1 - 3 – Magnetoresistive memory in phase separated $La_{0.5}Ca_{0.5}MnO_3$

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We have studied a non volatile memory effect in the mixed valent compound $La_{0.5}Ca_{0.5}MnO_3$ induced by magnetic field. In a previous work, we have shown that the response of this system upon application of H strongly depends on the temperature range, related to three well differentiated regimes of phase separation (submicrometric coexistence of ferromagnetic and non ferromagnetic regions) occurring below 220 K. In this work we compare memory capabilities of the $La_{0.5}Ca_{0.5}MnO_3$ compound, determined following two different experimental procedures for applying H, namely zero field cooling or field cooling the sample. Magnetization and transport data are reported. No memory was observed above 200 K due to the mostly paramagnetic character of the system and below 70 K due to the freezing of the relative fraction volumes. Magnetic field can irreversibly determine the phase fraction following both procedures in the 200 - 70 K range. The actual volume and distribution of phases determines main features of this memory effect. Below the charge ordering temperature ($T_{co} \approx 150$ K), the field cooling procedure depicts higher sensitivity to magnetic field changes. However, above this temperature both procedures exhibit similar features. These results are analyzed and discussed within the PS scenario.

1 - 4 – Characterization of the charge-order to ferromagnetic crossover behaviour in $(La_{1-y}Pr_y)_{0.5}Ca_{0.5}MnO_3$

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The study of manganese perovskites, particularly those in which there is a competition and coexistence of charge order insulator (COI) and ferromagnetic metallic (FMM) states, has received a lot of attention recently. In these perovskites, a change of the ionic radius in site A (r_A) modifies the structural parameters, which strongly affect the physical properties of these compounds. We present magnetization measurements in large-grain ($\approx 5 - 7 \mu m$) ceramic samples of the family $(La_yPr_{1-y})_{0.5}Ca_{0.5}MnO_3$ with $Y = 0, 0.15, 0.3,$

0.5, 0.7, 0.85, and 1.0. In the extreme $Y = 1$ the sample undergoes first a ferromagnetic (FM) transition near $T_C = 255$ K, a charge-order (CO) transition near $T_{CO} = 205$ K and an antiferromagnetic (AF) transition near $T_N = 150$ K. While T_N remains essentially constant through the series, T_C decreases rapidly and T_{CO} increases on decreasing Y . The crossover of T_C and T_{CO} determines a critical tolerance factor ($t_c = 0.975$) consistent with previous reports on other systems with the same Mn^{3+}/Mn^{4+} ratio. For tolerance factors $t \sim t_c$ we observe phase separation between FM and CO of varying degree depending on Y and disappearing only for $Y \lesssim 0.15$. For certain compositions, where the COI state is stabilized at low temperatures, it can be partially removed by the application of a magnetic field. We discuss the role of $\langle r_A \rangle$ and disorder in the phase separation of these systems.

1 - 5 – Study of memory effects in manganite thin films trilayers

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Memory effects reported on mixed valent Mn based oxides (manganites) exhibiting intrinsic coexistence of phases with dissimilar properties, i.e. metallic and insulating ones, are induced producing changes of the phase fraction with external parameters, i.e. magnetic field, hydrostatic pressure, X ray illumination. In these compounds, submicrometric domain formation is caused by the presence of an intrinsic elastic energy landscape, where strain effects play a major role. Thin film trilayers, consisting of a phase separated manganite sandwiched between two homogenous ferromagnetic manganite electrodes, were grown by laser ablation and patterned by optical lithography, with the aim of investigating electric transport through the phase separated layer. The material chosen to be the middle layer of these trilayers was $La_{1-x}Ca_xMnO_3$ (with $0.40 \leq x \leq 0.50$ Ca doping) because thin films of this compound, grown on $NdGaO_3$, exhibit coexisting phases states, as a consequence of strain effects. Within this framework, the main focus of our investigation is the study of the role of spatial confinement on memory effects on the current perpendicular to plane configuration as a function of the applied magnetic field and electric current, for different areas of the trilayers (from 5×5 to $20 \times 20 \mu m^2$). We report here some preliminary results.

1 - 6 – Phase competition study in the $\text{L}_{0.5}\text{A}_{0.5}\text{MnO}_3$ system by ESR

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The $\text{L}_{0.5}\text{A}_{0.5}\text{MnO}_3$ perovskite, with L = rare earth and A = alkaline earth, have a fixed ratio $\text{Mn(IV)} / \text{Mn(III)} = 1$, but it is possible to cross from localized to itinerant electronic behavior by varying the mean size of the L and A ions and consequently the geometric tolerance factor, t . The phase diagram (T vs t) reveal the existence of a critical tolerance factor $t_c \sim 0.975$ that separates both states (F. Rivadulla *et al.* Phys. Rev B **66**, 174432, 2002). Several phases compete at t_c due to the existence of charge as well as orbital ordering and the formation of Zener polarons. For $t < t_c$ a classical charge order phase occurs below $T_{CO} \sim 230$ K and antiferromagnetic CE-type order is stabilized at $T_N \sim 160$ K. For $t > t_c$ the charge order is suppressed and a ferromagnetic metallic phase occurs below $T_C \sim 230$ K and for lower temperatures ($T < 160$ K) Zener polaron ordering in an antiferromagnetic CE-type phase was founded. In this work we present an ESR study of the competing phases at the crossover from localized to itinerant behavior. The changes in the linewidth, g -factor and ESR intensity as a function of the temperature for the different tolerance factor were studied. The ESR spectrum at room temperature consist of a single lorentzian line centered at $g = 2.020(5)$. This line shows some structure below T_{CO} , for the samples with $t \approx t_c$. The linewidth shows a change of behavior at the different transition temperature according to the different exchange interactions present in each phase. We compare and discuss the different antiferromagnetic phases present at both sides of t_c .

1 - 7 – Magnetic phases coexistence in CMR manganites: ESR evidence

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The coexistence of magnetic phases in colossal magnetoresistent (CMR) manganites is a characteristic found in this family of compounds. We study this phenomenon in hole doped samples of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ by means of Magnetization measurements and Electron Spin Resonance (ESR) technique. In this paper we present results on the $x = 0.25$ compound

where clear evidences of phase coexistence were found. In the paramagnetic (PM) regime, well above 250 K, the ESR spectrum consists of a single lorentzian line centered at $g = 1.99$. The linewidth, ΔH_{pp} , depends on the temperature and a continuous narrowing is observed when T decreases. This is an indication of the ferromagnetic (FM) character of the spin-spin interactions originated in the double exchange model proposed for CMR manganites. As in other magnetic compounds we fit this dependence to $\Delta H_{pp}(T) = [C/(T\chi(T))]\Delta H_\infty$ where C is the Curie constant, $\chi(T)$ is the dc susceptibility, and ΔH_∞ is the limiting value of the linewidth at very high T . The ESR resonance splits below 250 K and a second resonance, of FM character, is present with a T dependent resonance field (H_r). When T decreases, H_r diminishes for the FM line while the PM line remains centered at a constant H_r . At the same time, a continuous transference of intensity, from the PM line to the FM one, takes place. We observe the coexistence of both, PM and FM lines, down to 220 K. In this extended range of coexistence (250 K - 220 K) the magnetization shows also a peculiar behavior. We will describe together both experiments (Magnetization and ESR) and we will compare the results with those obtained in other compounds of the series.

1 - 8 – Cationic ordering in $\text{Sr}_2\text{FeMoO}_6$ prepared by a new chemical route

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We report a novel technique to produce ultrafine crystallites ($< 50\text{nm}$) of $\text{Sr}_2\text{FeMoO}_6$ at relatively low temperatures. Powders that were fired at an above 850°C for two hours have almost a single-phase structure. However, longer annealing time can improve cationic ordering and consequently its saturation magnetization. Several thermal conditions were tried to get samples with differing amounts of disorder. Mössbauer spectra (MS) at room and low temperatures (RT and LT) and magnetic measures of these samples were performed. MS spectra at RT for all samples show broad and complicated absorption lines, reflecting the effect of multiple metal neighbor environments on the magnetic field of iron ions although the LT spectra has better resolution. The three magnetic sextets were assigned to Fe atoms whose first neighbours have well-ordered Mo environments, disordered Mo environments, and Fe ions in B' sites with six Fe neighbors. The magnetization data also shows a significant reduction of the saturation magnetic moment (RT) with decreasing annealing temperature. These results indicate that there is a correlation between the defect concentration and the magnetic properties.

1 - 9 – Magnetism and structure of $\text{Zn}_{1-x}\text{Co}_x\text{O}$ thin films

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This work is focused on the study of magnetic and structural properties of Co-doped ZnO films. These diluted semiconductors are expected to be ferromagnetic at room temperature and thus they would be used as electrodes in semiconductor-based magnetoresistive devices. Transparent and electrically conductive Co-doped ZnO thin films were deposited by pulsed laser deposition on Si_3N_4 buffered Si and (h00)-sapphire substrates. Two series of samples with different Co concentration (0.5% and 0.15%) were grown. Within each series, the thin films were grown at different substrates temperatures, T_S , varying between 200°C and 400°C, in order to study the effect of microstructure on the magnetic properties of this material. The crystalline structure of the samples was analysed by X-ray diffraction (XRD). The XRD patterns showed that the films deposited on $\text{Si}_3\text{N}_4/\text{Si}$ are strongly textured in the c-axis direction, while the ones grown on sapphire have a (h00)-preferred orientation. Simulations of the XRD patterns indicate that the Co ions replace the Zn in the ZnO wurtzite structure. The lattice parameters of the structure depend on the Co concentration, following the Vegard's law. EDX analysis indicate that the Co is homogeneously diluted in the samples, keeping the nominal composition of the ceramic target. The change of the samples morphology with T_S has been studied with AFM. The temperature and field dependence of the magnetization were measured to study the ferromagnetic order of the films. The magnetization curves indicate the coexistence of single-domain ferromagnetic clusters with small multidomain ferromagnetic zones. Low-temperature magnetic resonance experiments are under progress to complement the previous results and give further information about the Co ions environment.

1 - 10 – Different coexistence regimes in $\text{La}_{0.325}\text{Pr}_{0.300}\text{Ca}_{0.375}\text{MnO}_3$

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The mixed valent Mn oxide based $\text{La}_{0.325}\text{Pr}_{0.300}\text{Ca}_{0.375}\text{MnO}_3$ compound exhibits intrinsic phase coexistence in a wide range of temperatures (70K;T;230K) In that range, time relaxation in magnetization and transport properties display an unexpected temperature dependence, suggesting the presence of different coexistence regimes. While above $T=120$ K relaxations reveal a decrease in the amount of the ferromagnetic phase preformed at higher temperature, below $T=120$ K the data suggest an increase in their amount. Also around 120 K, a change in the temperature dependence of the metamagnetic field is observed. In this work these experimental results will be discussed within the framework of the three phases (ferromagnetic, charge ordered and strain induced charge distorted) coexistence scenario previously addressed by others authors.

1 - 11 – Mössbauer study of mechanical alloyed Fe-doped TiO_2 compounds

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Recent advances in the spintronic technology have stimulated considerable interest in ferromagnetic semiconductors with high Curie temperature for the development of innovative spintronic devices. In this work, we have studied the local environment surrounding magnetic impurity atoms of Fe-doped TiO_2 compounds obtained by mechanical alloying. The atomic content of Fe ranged from 5 to 15 % and the milling conditions (time of milling, atmosphere, mill and container) were varied in order to study the dependence of the resulting phases with such variables. The obtained alloys were study by Mössbauer effect spectroscopy and X-ray diffraction. X-ray diffraction of the precursor TiO_2 shows a predominant polycrystalline anatase structure accompanied by some minority rutile features. In Fe-doped milled samples anatase feature disappears leaving the sample to be majority rutile, metallic Fe and Ilmenite. The relative amount of these phases varies with the milling conditions. Mössbauer spectroscopy shows that doped samples contain Fe atoms in Fe^0 (metallic), Fe^{+2} and Fe^{+3} states. In this work the correspondence between the different Fe oxidation states and the resulting phases will be discussed.

Nanostructured materials, GMR, TMR and GMI

2 - 1 – Electron spin resonance and magnetic properties of superparamagnetic particles of $Y_3Fe_5O_{12}$ prepared by sol-gel method

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We present Electron Spin Resonance (ESR) and magnetic properties of superparamagnetic $Y_3Fe_5O_{12}$ nanoparticles. The powder samples were prepared by the sol-gel method. Varying the temperature and the time of the thermal treatments, we obtain sets of particles with different average size between 45 to 450 nm. X-ray diffraction were used to check the phase formation, and to determine the mean crystallite sizes from the linewidth X-ray peaks using the Scherrer relation. These sizes were confirmed by Transmission Electron Microscopy. The magnetic properties show an important diminution of the magnetization due to the increases surface/volume contribution. For the smaller sizes, practically $\frac{1}{3}$ of the magnetization is lost by the surface. The magnetic field coercivity temperature behaviour indicates that those samples with sizes less than the critical value ($D \leq 190$ nm) are in a superparamagnetic blocking state. The ESR data of the sample with an average size of 57 nm, confirm this state below $350\text{ K} \leq T_C = 550\text{ K}$ (The Curie temperature). Data of the magnetic resonance field, linewidth and intensity of the ESR spectra are presented and estimations of anisotropy and dipolar energies are discussed.

2 - 2 – Ferromagnetic resonance in FePt-Au self assembled arrays of nanoparticles

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Self assembled arrays of magnetic nanoparticles have attracted considerable interest due to their potential application as media for ultra high density

magnetic recording. Chemically produced FePt particles have an average size of 3.5 nm and crystallize in a disordered FCC phase. The ordered high anisotropy $L1_0$ phase can be obtained if the sample is annealed at temperatures above 550 C. Recently it was shown that the addition of small amounts of Ag or Au reduces the order-disorder transition temperature by $\sim 150\text{ C}$ [1]. These particles can be slowly evaporated on top of a silicon substrate forming a nearly perfect hexagonal array. Magnetic measurements suggest that the distribution of anisotropy energies is very large [2]. We have made ferromagnetic resonance measurements in as-made and annealed (30 min. at 450 C) $Fe_{46}Pt_{46}Au_8$ self assembled arrays of nanoparticles. For the as-made sample we have observed an isotropic angular behavior when the external field is rotated from the in-plane to the out of plane direction, indicating that the demagnetizing field and the anisotropy are very small. Annealed samples are anisotropic, both the resonance field and the linewidth change when the field direction is rotated. From the angular variation of the resonance field we have obtained the effective anisotropy constant $K_z \sim 8 \cdot 10^6\text{ emu/cm}^3$. The angular dependence of the linewidth is compatible with large variations in the effective field coming either from fluctuations of the magnetization M or the anisotropy K_z . Measurements of the resonance field and the linewidth as a function of temperature will be also presented.

[1] S. Kang, D. E. Nikles and J. W. Harrell, Nano Letters **2**, 1033 (2002).

[2] S. Kang, D.E. Nikles and J.W. Harrell, J.Appl.Phys. **93**, 7178 (2003).

2 - 3 – Structure and magnetic properties of $La_{2/3}Sr_{1/3}MnO_3/CaMnO_3$ multilayers.

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In this work, we present structural and magnetic characterization of trilayers composed of ferromagnetic and metallic electrodes and antiferromagnetic insulator barriers. Our samples alternate $La_{2/3}Sr_{1/3}MnO_3$ with $CaMnO_3$ layers. These compounds have similar lattice parameters, so we expect an excellent matching of the different layers along the structure. Ferromagnetic manganites such as $La_{2/3}Sr_{1/3}MnO_3$, are optimal materials to use as electrodes in tunnel junctions due to their large spin polarization as well as their chemical stability in air. To get a first insight of this system, we fabricated multilayers

of $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3/\text{CaMnO}_3$ (LSMO/CMO) by sputtering, using (100) SrTiO_3 and (100) MgO substrates. X-ray diffraction patterns show that the structure is strongly textured in the (100) direction when grown on SrTiO_3 , regardless of which material is first deposited onto the substrate. A different result is found on the same system grown on MgO : when the bottom layer is CaMnO_3 , the structure grows in the (110) orientation while it grows in the (100) direction when the bottom layer is $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$. These results allow us to select the crystal orientation of the multilayer by introducing a buffer layer of CMO or LSMO. The composition of the samples has been controlled by EDAX and the layers topography analysed by AFM. Magnetic coupling of the ferromagnetic layers across the antiferromagnetic spacer is being studied with magnetization and ferromagnetic resonance measurements.

2 - 4 – Magnetic properties of electrodeposited ZnO-Fe granular films

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Among the several techniques currently used to prepare ZnO films and their nanosized heterostructures, the electrodeposition is one of the most attractive because it is a low-cost technique with the possibility of large-scale production even on substrates of complex shapes. In this work, we report the successful preparation of ZnO-Fe granular films using the electrodeposition from aqueous sulfate solutions. ZnO-Fe films were cathodically deposited from aqueous solutions containing reagent grade 1 mmol/L zinc sulfate and different concentrations of ferrous sulfate (from 0.001 to 10 mmol/L Fe) directly on p-type (001) Si wafers with resistivity of 10 $\Omega\cdot\text{cm}$. The ZnO-Fe films with thickness of 2-4 nm were grown at 300 K at a cathodic potential of -0.9 V for 1 h. Magnetization measurements as a function of temperature were carried out combining zero-field cooling (ZFC) and field cooling (FC) routine with an applied magnetic field of 500 Oe and temperature changes of 2 K/min. No contaminants were found by X-ray Photoelectron Spectroscopy analyses and no intermediate compound formation such as $\text{Zn}_{1-x}\text{Fe}_x\text{O}$ or iron oxides were observed by X-ray Diffraction and Transmission Electron Microscopy analyses, except $\text{Zn}(\text{OH})_2$ precipitation for higher Fe concentration. The hydroxide formation and local pH factor enhancement is described by the imbalance of the following reaction: $\text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- \rightarrow 4\text{OH}^-$ in the sulfate solutions with their soluble species and ions. The scan in the anodic

direction reveals significant dissociation effect where $\text{Zn}(\text{OH})_2 \rightarrow \text{ZnO} + \text{H}_2\text{O}$ and metallic zinc reoxydized to ZnO or directly to Zn^{2+} is likely occurring at the cathode since $\text{Zn}(\text{OH})_2$ and metallic Zn presence are negligible in ZnO films grown from acidic sulfate solutions. The magnetization curves suggest the existence of an assembly of magnetic particles with quite large size distribution. Thus, even at room temperature superparamagnetic relaxation does not occur. The field dependence of the magnetization is characteristic of a fine particle magnetism. However, the hysteresis loops do not exhibit a zero remanent magnetization M_r and coercive field H_c as required by an assembly of a non-interacting single-domain particles even at room temperature. The fitting of the magnetic data to a conventional Langevin function is investigated taking explicitly into account the magnetic moment calculation from the particle size distribution experimentally determined by transmission electron microscopy analyses.

2 - 5 – Magnetic and chemical aspects of $(\text{GaSe})_{1-x}\text{Fe}_x$ granular films.

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In this work we investigated the $(\text{GaSe})_{1-x}\text{Fe}_x$ [20nm]/GaSe[6nm]/GaAS(111)B grown in a hybrid molecular beam epitaxy system equipped with Reflection High-Energy Electron Diffraction (RHEED) and X-ray Photoelectron Spectroscopy (XPS) facilities. According to XPS analyses, the $(\text{GaSe})_{1-x}\text{Fe}_x$ epilayers with Fe concentration of 7at.% and 17at.% could be obtained by using GaSe deposition rates of 1.1nm/min and 0.55nm/min under growth temperatures ranged between 550 K and 660 K. XPS analyses reveal the presence of metallic Fe, while X-ray diffraction analyses confirm the formation of lamellar GaSe with no evidence of intermediary compounds formation. Magnetization measurements were performed using a SQUID magnetometer from 5K to 300K. In plane magnetization versus field curve for the sample grown at 650K (1,1nm/min) shows a hysteretic behavior with a small remanence 12,7% (32,2%) the saturation magnetization and coercive field of about 230 Oe (40 Oe) for the measurements performed at 5K(300K), respectively. The hysteresis cycles were deconvoluted in three parts:(i) non-interacting monodomain particles exhibiting superparamagnetic

(SPM) behavior, (ii) interacting and/or larger particles exhibiting a ferromagnetic (FM) response, and (iii) diamagnetic (DM) component associated with the GaAs substrate and GaSe epilayer. Taking into account all these contributions, a SPM behavior could reasonably be described by a Langevin function of an assembly of particles with average diameter sizes of 5.12 nm and saturation magnetization of ~ 1710 G. Magnetic irreversibility associated with the branching of field-cooled (FC) and zero-field-cooled (ZFC) curves suggest the existence of a SPM behavior with a large size distribution of magnetic particles. A blocking temperature is estimated as 137 K, which gives metallic Fe particles with diameter of 12 nm if magnetocrystalline anisotropy constant of bulk Fe is assumed. Cathodoluminescence (CL) measurements show the presence of an energy bandgap of $E_G = 1.8$ eV, indicating a semiconducting behavior of the GaSe matrix for different grown conditions even if disorder effects are observed associated with the incorporation of iron.

2 - 6 – Magnetic order in amorphous $(\text{Fe}_x\text{Nd}_{1-x})_{1-y}\text{B}_y$ nanoparticles

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We present magnetization measurements on $(\text{Fe}_x\text{Nd}_{1-x})_{1-y}\text{B}_y$ ($0 \leq x \leq 1$) amorphous nanoparticles (~ 7 nm) obtained by chemical reduction. Samples were characterized by XRD, TEM and light scattering measurements. Our results show a sharp change in the saturation magnetization and the coercivity with the Nd composition. This is an evidence of the disorder induced by the Nd that breaks the strong exchange between the Fe atoms. The noninteracting system dynamic is studied by dispersing the powder sample in a non-magnetic matrix. The $M(T)$ measurements show a clear difference for different sample concentrations.

2 - 7 – Surface and local anisotropy effect in the magnetic order of Fe-Co-B nanoparticles

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Nanoparticles of 3 nm $(\text{Fe}_x\text{Co}_{1-x})_y\text{B}_{1-y}$ ($0 \leq x \leq 1$, $y \approx 0.4$) were synthesized by chemical route. XRD and TEM measurement show the amorphous

nature of the samples. Size distribution was characterized by light scattering measurement. Magnetization vs. magnetic field measurement at room temperature show hysteresis loop for all composition typical of blocked single-domains. Cohesive field, remanent and saturation magnetization as function of composition exhibit a minimum at $x = 0.15$. This behavior is related to the composition of the different local anisotropy associated to Fe and Co ions.

2 - 8 – Magnetic characterization of the mechanically induced thermite reaction between Fe_2O_3 and Al

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Composites of the type $\text{Fe}_x(\text{Al}_2\text{O}_3)_{100-x}$ with compositions in the range $0.4 \leq x \leq 60$ have been studied by several groups due to interesting technological possibilities. Here we investigated the mechanically induced thermite reaction between hematite (Fe_2O_3) and aluminium. In this reaction the final phases, Al_2O_3 and Fe, are formed by an in situ chemical reaction in which Al reduces the oxide and simultaneously reduces the metal. This exothermic, non-gradual, reaction proceeds in a well-defined milling time (the ignition time). The resulting iron-alumina composition is well above the percolation limit (i.e. $x > 60$) as a consequence of initial stoichiometry requirements to favor the reaction occurrence. The experimental techniques used to characterize the evolution of the system with milling time have been: X-ray diffractometry (XRD), Transmission Electron Microscopy (TEM), Magnetometry (at room temperature and 5 K) and Mössbauer Spectroscopy (at room and N_2 liquid temperature). After reaction, Fe particles of nanometer size in a crystalline Al_2O_3 matrix have been formed, as seen by XRD. At longer milling times, a rather wide particle-size distribution, around 20 nm, was observed by this technique. Mössbauer spectra were constituted of both paramagnetic and ferromagnetic contributions. The paramagnetic contribution was associated with small grains of superparamagnetic Fe and hercynite (FeAl_2O_4), whereas the magnetic component was associated to larger iron grains (i.e. > 20 nm). Saturation magnetization, coercivity field and remanent magnetization rapidly reached a stationary value with milling time. A correlation between the microstructural characteristics of the sample and its magnetic properties is proposed.

2 - 9 – Magnetic properties of Co nanoclusters electrodeposited on alumina.

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Magnetic properties of magnetic nanostructured structures, such as nanodots, prompt much attention due to their potential applications in the high-density magnetic recording industry. Recent works have been demonstrated the feasibility of the ordered arrangements of magnetic nanodots in the surface of the anodized alumina with self-assembled nanocavities arrays. The anodization process of aluminum in a solution of oxalic acid 0.3 mol/L at 40 V during 6 hours produces an alumina layer (γ - Al_2O_3) with a self-arranged pattern of nanopores. The removal of the porous alumina with an aqueous solution of 1.8% H_2CrO_4 and 6% H_3PO_4 (in volume) at 60°C for 21 hours leads to a very thin alumina layer with shallow cavities with a nanometer size. The electrodeposition of the cobalt onto nanopatterned alumina was made using a potentiodynamic method (one cycle from -400 mV to -800 mV versus Ag/AgCl) from an aqueous sulfated solutions containing 1 mmol/L Co. A conventional cell with three stationary electrodes, containing a reference electrode of Ag/AgCl, a platinum disk as counter electrode, and a alumina plate of 3 cm^2 as working electrode were employed. Cyclic voltammograms and chronoamperometric analyses were accomplished to obtain a partial filling of the nanocavities in a such way that a non-percolating arrangement of Co nanoclusters is formed. The alumina patterning and Co islanding were studied by Scanning Electron Microscopy and Atomic Force Microscopy in the contact mode. After the chemical removal of the porous alumina, the etched alumina surface presents an ordered arrangement of shallow cavities with radius of approximately 32nm spaced by ≈ 75 nm. X-ray Photoelectrons Spectroscopy were accomplished for chemical characterization of the alumina surface and Co electrodeposits. Within the sensitivity limit of 1%, no contamination were found, while a clear metallic character of Co is observed. X-ray diffraction analyses reveal a polycrystalline character of cobalt dominated by (0002), (01 $\bar{1}$ 0) and (01 $\bar{1}$ 1) Bragg reflections of a hexagonal close-packed structure. Perpendicular magnetic anisotropy were found at room temperature. A comparison between magnetization curves with magnetic field applied in plane and out of the plane and ageing effects are discussed.

2 - 10 – Magnetic study of $Fe_{65}Ni_{20}Nb_6B_9$ nanocomposite alloys

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The alloy $Fe_{65}Ni_{20}Nb_6B_9$ was obtained from the elemental constituents in a high-energy planetary ball mill, this sample was later thermally treated at 873 and 900 K in order to obtain the equilibrium phases. They were studied by ^{57}Fe Mössbauer effect spectroscopy (ME), X-ray diffraction (XRD), ac-susceptibility and SQUID. The as-prepared nanocrystalline alloy consists primarily of metastable bcc α -Fe(Ni) nanocrystals as seen by XRD and ME. The treated samples consist of a mixture of bcc (ferromagnetic) and fcc (paramagnetic) phase. All the hysteresis loops (at 5 and 300 K) present low remanence and coercivity. Saturation is not reached in treated samples even in fields as high as 5 T. In all samples both the Zero-Field-Cooling and Field-Cooling magnetisation, as well as susceptibility curves show a superparamagnetic feature, with a maximum between 50 and 100 K. This feature is caused by nanometric-sized magnetic particles. The huge difference between blocking and irreversibility temperatures indicates a wide size distribution. Presence of a bulk magnetic phase cannot be discarded. The relationship between the frequency dependence of the ac-susceptibility, magnetic behaviour and microstructure will be discussed.

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2 - 11 – Structural and magnetic study of nanostructured $(\text{Fe}_{79}\text{Mn}_{21})_{80}\text{Cu}_{20}$ alloy synthesized by ball milling

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Iron-Mn based alloys show considerable promise for technological applications. Its physical properties can be modified by the incorporation of miscible or immiscible alloying atoms such as Si or Cu. Since the high-energy ball milling technique allows synthesizing phases far from the equilibrium and very defective nanostructures, our research project is devoted to the study of nanoparticles obtained by this process in the Fe-Mn and Fe-Mn-X (with X=Si, Cu) systems. In particular, the present work is focused in the $(\text{Fe}_{79}\text{Mn}_{21})_{80}\text{Cu}_{20}$ composition. Accurate amounts of elemental Fe, Mn, Cu powders were high-energy-ball-milled during 15 hours using a vibratory miller. The sample characterization was performed by X-ray diffraction and transmission electron microscopy (TEM). The magnetic behavior of the particles was analyzed by means of Mössbauer spectroscopy, dc-magnetization and ac-susceptibility measurements. X-ray diffractograms revealed that *fcc* is the prevailing phase, although a tiny amount of the *bcc* phase is also present. A dispersion of nanoparticle sizes was detected using TEM. The dark field technique revealed that isolated nanoparticles were constituted by smaller regions (average size 10 nm) with different crystalline orientation among them. The thermal dependence of both the magnetization and susceptibility data were interpreted in relation to the present phases and the influence of the particle size distribution. The Mössbauer spectra were fitted to a component belonging to the antiferromagnetic *fcc* phase, in addition to a paramagnetic signal. The thermal evolution of these spectra showed that the ordering of the antiferromagnetic γ -FeMn phase occurs at about 180 K, while the other component remains in a paramagnetic state even at the lowest temperature achieved. Finally, the influence of the nanostructured and disordered nature of the present phases on the magnetic behaviour was discussed.

2 - 12 – Magnetic behavior of Co clusters embeded in a zeolite matrix

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A medium pore zeolitic material with MEL structure modified with Co cations was synthesized. It was characterized by Atomic Absorption, X-ray diffraction, Fourier transformed infrared and BET. The Co ions were introduced by ionic interchange in liquid phase followed by different thermal treatments. The magnetization M and/or magnetic susceptibility χ were measured after zero field cooling, together with magnetization as function of the applied magnetic field for several constant temperatures between 4.2 and 30 K. No blocking temperature was detected and a pure superparamagnetic behavior was obtained. M vs. T and χ vs. T were adjusted by Brillouin and Langevin functions obtaining the same results in both cases. Curve fitting gave an effective moment of $100 \mu_B$ for the cases under study. The results are analyzed in terms of the possible cluster structure that may appear.

2 - 13 – X-ray Absorption Fine Structure study of nanostructured Fe-Au alloys

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Mechanical alloying has demonstrated its ability to form metastable alloys [1]. In previous works, the fabrication of Fe-Au nanostructured alloys by mechanical alloying has been reported [2]. Magnetic and magnetotransport properties compatible with a model of nanosized iron particles immersed in an Au matrix has been observed. Particularly intriguing has been the question of the structural state of these iron particles, because the X-ray diffractograms shows only broad peaks at angles near the reflections of the bulk Au, with no evidence of bulk α -Fe peaks. X-ray Absorption Fine Structure (XAFS) technique has the advantage of the atom selectivity, which allows us to investigate the neighborhoods of the iron and gold atoms separately. The magnetism of fcc-Fe is very sensitive to structural changes, and small variations of the lattice parameter lead to different phases and spin moments.

So, useful information for explaining observed magnetic and magnetotransport properties of these alloys can be obtained through such study. We measured XAFS at the XAS station of LNLS (National Synchrotron Light Laboratory, Campinas, Brazil) in a set of $\text{Fe}_x \text{Au}_{100-x}$ ($15 \leq x \leq 30$) alloys produced by mechanical alloying [3]. Measurements were done at the Fe K edge (7112.0 eV) and at the Au L_3 edge (11918.7 eV). X-ray Absorption Near Edge Structure (XANES) spectra obtained from the absorption spectra from both edges was studied using a powerful analysis method, the Principal Component Analysis (PCA) [3], which has been recently used for the study of XANES data. PCA results of our data shows clearly that the Fe has two differentiated neighborhoods, both different from the bulk α -Fe and fcc-Fe, in agreement with the idea of iron-rich nanoparticles embedded in an Au-based matrix. For the case of Au we have found two neighborhoods too, different of the bulk pure phase.

LMS acknowledge the help of FAPESP (Brazil). Research partially supported by LNLS – National Synchrotron Light Laboratory, Campinas, Brazil

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[2] L. M. Socolovsky, F. H. Sánchez and P. H. Shingu; Physica B: Physics of Condensed Matter **320**, 149-152 (2002). L. M. Socolovsky, F. H. Sánchez, P. H. Shingu; Journal of Magnetism and Magnetic Materials **226-230**, 736 (2001).

[3] M. Fernandez-García, C. Marquez-Alvarez and G. L. Haller; J. Phys. Chem. **99**, 12565-12569 (1995).

2 - 14 – Effect of milling speed on Fe/SiO₂ system prepared by mechanical alloying

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A mixture of 50 % wt Fe in SiO₂ was ball milled for an extended period of time in a closed vial. A planetary ball mill (Fritsch Pulverisette 5) with hardened stainless vials and balls was used. Abrasion of the mill inevitably causes contamination of the sample. Based on measurement of the Cr content in the sample we estimate a low contamination level. X-Ray diffractometry was used to obtain information about nanocrystalline structure. SEM analysis were performed to investigate the structural morphology of the samples. The ultrafine grain structures of the samples consist of magnetic nanocrystallites embedded in a residual ferromagnetic amorphous matrix. Large coercivities were found in nanostructured Fe/SiO₂ granular materials prepared by mechanical milling. This behaviour was also reported in nanostructured Fe/SiO₂ materials prepared by sputtering [1]. The ferromagnetic

nanostructured alloys have been studied on the basis of the random anisotropy model (RAM) [2], where the effective magnetocrystalline anisotropy $\langle K_i \rangle$ is deduced by considering an assembly of ferromagnetically coupled grains with magnetocrystalline anisotropies oriented at random.

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[2] Hernando A., Vasquez M., Kulik T., Prados C.. Phys. Rev. B **51**, 3581 (1995).

2 - 15 – Magnetic and structural characterization of new nanostructured systems.

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This work focuses on the search of new magnetic materials for magnetoelectronic applications. We present an investigation of the magnetic and structural properties of Fe/SC/Fe trilayers with SC: Si and FeSi and barrier thickness varying between 2nm and 10nm. The samples were deposited by dc and rf sputtering on (111) Si single-crystalline substrates. A silicon top layer is deposited onto the structures to prevent the oxidation of the top electrode. X-ray diffraction patterns show that our samples are strongly textured in the [110] direction. We have investigated the magnetic properties of the trilayers through magnetization and ferromagnetic resonance (FMR) measurements. FMR spectra allow us to identify the different magnetic components of the trilayers, including silicides formed at the Fe/SC interfaces. The angular dependence of the resonance modes has been studied in the out-of-plane geometry. From the analysis of this variation we have deduced the magnetic anisotropy of the system. In addition to the shape anisotropy we have measured a small out-of-plane uniaxial anisotropy, arising from the magnetic/non magnetic interfaces. Transport measurements are under progress.

2 - 16 – Ferromagnetic resonance in Co(*x*)-SiO₂ (1 – *x*) granular films

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We have studied the magnetic behavior of heterogeneous Co-SiO₂ granular films as a function of the Co volume concentration, *x*, and the temperature, *T*. Films, with *x* in the range 0.18 to 0.62, were prepared using rf sputtering from a mosaic target. Samples thickness was approximately 100 nm. We have used ferromagnetic resonance at X-band ($\nu = 9.4$ GHz) and Q-band ($\nu = 34$ GHz) to characterize the magnetic response of the films. In the whole studied *x*-range we

have observed a main absorption signal associated to the uniform precession of magnetic moments. We also have observed an additional absorption above a critical concentration ($x_c = 0.37$) that could be associated to a surface resonance mode. In the present work we discuss the linewidth behavior of the ferromagnetic modes as a function of x and the temperature dependence of the resonance field. We have observed that annealing of the films at moderate temperatures produced irreversible changes in the film microstructure. Using the surface inhomogeneity model we deduced that the two surfaces are affected in a different way during the annealing process.

2 - 17 – Magnetic polymers of maghemite $\gamma\text{-Fe}_2\text{O}_3$ and polyvinyl alcohol

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The particles synthesized and dispersed in aqueous medium can be trapped in different solid matrices keeping their dispersion rate. The oxide/polymer mass ratio determines the average distance between the particles existing in the sol. Ultrafine magnetite particles were prepared in aqueous solution of polyvinylalcohol (PVA) with a technique "in situ" to at concentrations up to 40 g dm^{-3} . The average diameter particles were minor than 10 nm. Adsorption of PVA on the surface of maghemite was examined by infrared spectra and thermogravimetry analysis. The mode of agglomeration and dispersion of the particles were different depending on the properties of polymers in the solvent. The dispersions of the magnetite particles prepared at 2% and 3% were more stable than the dispersions of 0.5% and 1%. The dispersion and agglomeration of the particles were different in the aqueous solution at 4% because the magnetite particles were of an small diameter. Magnetic and dielectric properties of these composites are evaluated.

2 - 18 – Magnetotransport properties of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ bicrystalline films: influence of magnetic field orientation

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Bicrystalline substrates are ingenious devices appropriate to investigate the basic mechanisms of the low field magnetoresistance (LFMR) in manganese

films, by isolating an unique artificial grain boundary (AGB). We report on magnetoresistance measurements performed on $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x = 0.67, 0.75$) films grown on SrTiO_3 bicrystalline substrates of 24° misorientation angle. The films, with a thickness of 1200 nm were deposited by dc sputtering at a substrate temperature of 760°C . The orientation of the substrates were determined by x-ray diffraction measurements performed at room temperature in a four-circle diffractometer. The analysis of x-ray diffraction patterns obtained for specific positions of the sample in conventional powder diffractometer suggests that the films grow textured along the (001) direction. The in-plane resistivity measurements were carried out in patterned films. A Wheatstone bridge has been patterned on the samples using electron lithography and Ar ion milling. The device is built up with two sets of identical arms, each of which consists of n tracks of micrometric width. The grain boundary is crossed by two of the four bridge arms, and thus the output voltage gives a direct measurement of the resistivity across the AGB [1]. By varying the width of the tracks between $2-20\mu\text{m}$ it is possible to investigate the role played by the magnetic domains near the AGB. We have measured the LFMR across the AGB as a function of the angle ϕ between the magnetic field and the AGB. The angular dependence of the magnetoresistance was correlated with magnetization measurements performed in a vibrating sample magnetometer at $T = 85 \text{ K}$. We discuss our results in terms of the magnetic anisotropy of the samples.

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2 - 19 – Taming the giant magnetoresistance of noncollinear LaMn_2Ge_2

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Many family of materials containing manganese exhibit a rich variety of magnetic ground states. In particular, the intermetallic ternary compounds of the type RMn_2X_2 ($\text{R} = \text{Ca}, \text{La}, \text{Ba}, \text{Y}$ and $\text{X} = \text{Si}, \text{Ge}$), crystallizing in the ThCr_2Si_2 structure, show a large variety of collinear and noncollinear magnetic ground states depending on R and X. The key parameter responsible for the different magnetic configurations is the change of Mn-Mn distance. In this contribution we focus our analysis on LaMn_2Ge_2 which shows a complex magnetic phase diagram. At high temperatures

this compound is a purely collinear antiferromagnet (AFM), showing a ferromagnetic (FM) stacking of AFM (001) planes. At low temperatures it presents a noncollinear magnetic structure with the Mn's magnetic moments ordered in a conical arrangement and FM coupling along the c-axis. However, the most interesting feature of this material is that it shows an inverse giant magnetoresistance [1] (GMR) and is therefore a good candidate for studying the dependence of the band structure contribution to the GMR on the different magnetic configurations of this naturally layered compound. A qualitative understanding of the GMR effect in this material should be possible due to its coherent electronic structure: Changes in the electronic structure as a function of magnetic order lead to changes in the Fermi surface, in the Fermi velocities and thereafter in the conductivity tensor. The calculation of the GMR effect requires the energy bands as inputs and are computed by means of the FLEUR code, an implementation of the FLAPW method.

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2 - 20 — Phase stabilization and magnetic response of nanocrystalline copper ferrite

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Ferrites physical properties may be altered by stabilization of either the tetragonal or cubic form, which depends on the cationic distribution. In this work, nanocrystalline copper ferrite obtained by coprecipitation was high-energy-milled during different periods of up to 12 hours. The samples were characterized by small and wide angle x-ray scattering experiments. Mössbauer and magnetic measurements, reveal a superparamagnetic behavior at room temperature. The superparamagnetic limit shifts to higher temperatures as the sample is milled. The 10 h milled sample shows only copper iron spinel (D=13 nm) in its metastable cubic phase. The strain reduction and the increment of the crystallinity observed in this sample can be related to the raise of blocking temperature and mean magnetic moment per grain determined from magnetic and Mössbauer data. The thermal stability of this sample was studied by combined in-situ real time SAXS and WAXS experiments as function of temperature from ambient to 723K. WAXS results show a progressive improvement in the ferrite crystallinity, by increasing the grain size and decreasing

the strain level. The SAXS responses present an exponential behavior, $I(q) = Kq^{-\alpha}$ that depart from a Porod's law at low q , this indicating polydispersity or crystallites surface roughness. To better disclose the influence of particle size distribution dynamic light scattering experiments were also performed.

2 - 21 — Synthesis and characterization of manganese oxide based nanotubes

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A method for obtaining hollow cylindrical structures of a mixed valent manganese oxide based compound in the nanometer range is reported. The pore wetting of sacrificial porous substrates technique was used. Plastic templates with pores ranging 0.2 to 1 micron were employed, and the liquid precursor was allowed to freely wet their inner walls. During ulterior thermal treatment processes the binary oxide $\text{La}_{0.325}\text{Pr}_{0.300}\text{Ca}_{0.375}\text{MnO}_3$ is formed and the template is destroyed. Self standing tubes were obtained with walls formed by around 30 nm sized grains, their overall geometry being determined by the pores. A variety of techniques (scanning and transmission electron microscopy, scanning probe microscopy) allowed to fully characterize the microstructure and morphology of these tubular structures. Tubes with external diameter 800 nm have wall thickness around 150 nm and length around 4 to 5 microns.

2 - 22 — Surface electronic structure of Co thin films on Cu(111)

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There has been some controversy regarding the STM spectra of Co overlayers on Cu(111). Some recent experiments find a peak 0.4 eV below the Fermi energy [1,2], at the onset energy of the Cu(111) surface state, while previous ones found two peaks, one 1 eV below the Fermi level and another 0.5 eV above it [3]. To address this problem we have performed a parametrized tight binding calculation of a Cu(111) slab with two Co layers on each surface. The basis set contains s , p and d orbitals and also extra s orbitals

near the surface to include the effect of spill over. Our results for the local density of states at the site of the extra s orbital and at the Co surface site reproduce the feature at -0.4 eV, which also appears in pure Co slabs, and is therefore not related to the Cu(111) surface state.

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2 - 23 – Tunnelling through a semi-conducting spacer: complex band predictions versus thin film calculations.

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The phenomenon of spin dependent tunnelling handles with spin-dependent transport effects, which may become in the near future of major technological importance. Spin tunnelling magnetoresistance, usually called tunnelling magnetoresistance (TMR), is the dependence of tunnelling current between ferromagnetic electrodes separated by a non-conducting barrier on the relative orientation of the magnetic moments of the side electrodes. Mavropoulos *et al.* have shown that tunnelling through insulators can be understood in terms of metal-induced gap states and that the framework to investigate them is the complex band structure of the insulator in the gap region, which are obtained from a bulk calculation and are independent of the characteristics of the electrodes [1]. The energy band corresponding to complex values of the k vectors are called complex bands, and the corresponding eigenstates decay exponentially into the barrier and constitute the evanescent states responsible for tunnelling. In this work we compare, using a simple semiconducting tight-binding model system, the limitations of the tunnelling predictions coming out of complex band calculations with the output of calculations done for the same semiconducting spacer but of finite width, and sandwiched by metallic electrodes. We study the spacer width effect and consider the influence of interfacial roughness.

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2 - 24 – Chitosan based ferrimagnetic membrane

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Chitosan is a biopolymer that comes originally from chitin which is normally found in crustacean shells. It is produced by the deacetylation of chitin under high temperatures [1]. Chitosan is used as an adsorbent in the removal of a large variety of metals, aromatic species, organic and inorganic acids from polluted water. In this work, we have as objective the study of the physic properties of the new chitosan-nickel ferrite membrane. The nickel ferrite ($NiFe_2O_4$) powder used in this work was prepared by a new sol-gel route [2]. The average crystallite size as determined by x-ray diffractometry was about 67 nm. By mixture of chitosan (Sigma) with acetic acid at pH 3, a solution of 10 mg/mL was obtained where $NiFe_2O_4$ powder was added. After this, the solution was spread over an acrylic plate and dried at low temperature and humidity. The membrane formed was about 0.25 mm thick with 3%/wg of $NiFe_2O_4$ powder. X-ray results of the $NiFe_2O_4$ powder and a blend of *Chitosan/NiFe₂O₄* show agree well with the powder diffraction files obtained in ICDD 86-2267. All the peaks of *Chitosan/NiFe₂O₄* are broad due to the formation of the undesired undulate surface which produces peaks at different Bragg angles but still have the $NiFe_2O_4$ pattern, which demonstrates, therefore, that the $NiFe_2O_4$ powder remains stable even when mixed with chitosan. The behavior of magnetization vs magnetic field suggests that the blend is a soft ferrimagnetic material. The saturation magnetization (SM) was about 17 emu/g for field of 50 kOe, which corresponds to 35% of the value obtained with $NiFe_2O_4$ powder [2]. The presence of chitosan contributed with the reduction of SM. The adsorption behavior of this material towards Hg(II), Cu(II) and Zn(II) was investigated by and isothermal microcalorimetric technique. The exothermic enthalpy changes in the sequence $Cu > Hg > Zn$ shows the high potential of the *Chitosan/NiFe₂O₄* to remove the metals and that the interactions at solid/liquid interface are enthalpically favorable. The presence of $NiFe_2O_4$ in the chitosan is fundamental because its recover can be done by an electromagnet.

[1] E. Khor and L. Y. Lim, *Biomaterials* **24**, 2339 (2003).

[2] M. N. B. Silva, J. G. S. Duque, D. X. Gouveia, J. A. C. Paiva and M. A. Macedo, *Japan Journal Applied of*

Physics, submitted (2003).

2 - 25 – Finite size effects and spin transitions in ball-milled FeMnCu nanostructured alloys

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FeMnCu alloys were prepared by high-energy ball milling over a wide range of grinding times from 15 minutes up to 72 hours. Magnetic properties were followed by means of vibrating sample magnetometry, magnetic susceptibility and Mössbauer spectroscopy. By using a Rietveld structural analysis of high resolution X-ray diffraction data, lattice parameter and grain size correlations with magnetization and coercive force were also carried out. Results revealed a strong microstructural dependence of the magnetic properties with the grain size resembling a finite size-driven magnetic transition at a critical crystallite value of around 8.5 nm. This behavior is endorsed by a partial low-spin to high-spin transition at a critical unit cell volume of around 50 Å³ at 77 K attributed to strong local variations of the interatomic spacing according to Mössbauer results. Finally as concerns to temperature behavior, samples exhibited a freezing temperature at around 61 K ascribed to the presence of interacting CuMn and FeMnCu clusters.

2 - 26 – Study of anisotropy induced in CoFeSiB amorphous ribbons by solidification in magnetic field using Giant Magnetoimpedance measurements.

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Recently a method to induce magnetic anisotropy by applying a dc magnetic field during the melt spinning process has been developed [1]. Using this method $\text{Co}_{69}\text{Fe}_4\text{Si}_{15}\text{B}_{12}$ amorphous ribbons were melt spun with a 0.07T dc magnetic field applied transversely to the ribbon axis. The same composition was melt spun in identical technological conditions but without applied field in order to establish

a comparison between the results. In both cases ribbons of 0.015 mm thick and 0.4 mm wide were obtained and were cut to 90 mm length to perform magnetic measurements in samples of the same geometry. The magnetoimpedance was used as a tool to investigate the effectiveness of this method to induce magnetic anisotropy. Hysteresis loops were also measured showing the very soft magnetic properties of this kind of alloys (coercivity lower than 0.1 Oe and saturation field lower than 1 Oe). The magnetoimpedance effect was measured in function of an external dc field (-90 to 90 Oe) and an exciting current (intensity of 10 to 100 mA and frequency of 0.1 to 15 MHz) for both kinds of ribbons. In both cases magnetoimpedance response to the external field showed a general shape of single peak curves, but in the case of the ribbon made with the applied magnetic field there is a slight double peak structure superimposed on it. The maximum value of the GMI ratio is almost the same for both samples in the studied range but sensibility increased significantly in sample obtained with the applied field. From the analysis of the magnetoimpedance effect we can study the induced magnetic anisotropy. Magnetoimpedance demonstrates to be a fine instrument to detect small changes of anisotropies and evaluate surface anisotropy, and it is a good technique to be employed in very narrow ribbons where other techniques are ineffective or unfeasible.

[1] Tejedor, M., García, J. A., Carrizo, J., Elbaile, L., Santos, J., Appl. Phys. Lett. **82**, 937 (2003).

2 - 27 – Magnetic and crystal structure refinement in $\beta\text{-FeO}(\text{OH})_x\text{Cl}_{1-x}\cdot n\text{H}_2\text{O}$ nanoparticle

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Applied field Mössbauer spectrometry and X-ray diffraction analysis have been used to refine the magnetic and crystal structures of synthetic akaganeite nanoparticles. Samples were prepared by thermal hydrolysis of FeCl_3 solutions at 70°C during 48 hours according to the literature. Additionally, the products were characterized by thermogravimetric and magnetization measurements, and infrared spectroscopy. All techniques demonstrate the purity of the synthetic samples. Crystal structure refinement using the Rietveld method shows that the symmetry is monoclinic (C2/m:b3) with $\mathbf{a} = 10.5238(6)$ Å, $\beta = 3.0343(1)$ Å,

$c = 10.5415(6)$ Å and $b = 90.110(6)^\circ$. The average particle size is estimated at about 46(6) nm. The monoclinic symmetry points to the existence of two distinct iron octahedral sites, which is also confirmed by the Mössbauer spectra in the paramagnetic state. However, detailed computer analysis of both zero field and in-field Mössbauer spectra suggest the presence of four non-equivalent iron sites. The physical origin of these different components in the magnetic region is discussed in this paper.

2 - 28 – Magnetic studies of melt spun NdFeAl-C alloys

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Alloys with compositions $\text{Nd}_{60-x}\text{C}_x\text{Fe}_{30}\text{Al}_{10}$ ($x = 0, 1, 5$ and 10) were processed by melt spinning at a tangential speed of 5 m/s. The as cast ribbons were characterized by X-ray diffraction (XRD), Mössbauer Effect (ME) spectroscopy, room temperature demagnetization curves at different field rates and Thermomagnetic (TM) analysis. XRD patterns show the presence of broad halos and sharp peaks in correspondence with the expected existence of an amorphous structure embedding crystalline particles. The crystalline particles were identified as mainly dhcp-Nd for $x=0$, dhcp-Nd /fcc-Nd for $0 < x < 10$, and iron carbides for $x = 10$. ME spectra of all the samples, show strong evidence of the presence of Fe in crystalline magnetic phases as well as in a paramagnetic one. The crystalline phase was identified as a μ -type (or A1) metastable phase, which has been reported to have a large anisotropy field $\mu_0 H_A > 8\text{T}$ and a saturation polarization of 0.85 T [1]. The magnetic measurements display an increase of coercivity and remanence with the C concentration, this is in agreement with the Mössbauer results that show an enlargement of the abundance and average hyperfine field of the μ -type phase. A correlation exists between the amount of μ -type phase and the hysteresis behavior; it is proposed that small crystals of this phase should confere the hard magnetic properties to these alloys.

[1] B. Grieb, E.-Th. Henig, G. Martinek, H. H. Stadelmaier and G. Petzow, IEEE Trans. on Magn. **26**, 1367 (1990).

2 - 29 – Nanoscopic transformations and GMR in bulk nonequilibrium CuCo alloys

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The nanostructural transformations of $\text{Cu}_{1-x}\text{Co}_x$ ribbons ($x = 0.05, 0.10, 0.15$ and 0.20) for isochronous thermal annealing with different final temperatures were investigated using Transmission Electron Microscopy (TEM) and compared with the temperature dependence of the resistivity and the giant magnetoresistance (GMR). The microstructural grains of the ribbons in the "as-made" samples have average sizes of 1 μm , most of them presenting a lamellar spinodal decomposition therein, whose wavelength changes monotonically with the nominal Co content, from 41 nm for $x = 0.05$ to 54 nm for $x = 0.20$. The observation of increasing modulation for larger Co content agrees well with our isothermal simulation of the spinodal decomposition occurring in these samples by using a Cahn-Hilliard diffusion equation. Some nuclei due to precipitation of nearly pure Co are also present in the segregation process. They appear mostly in the samples with higher Co contents and the size of such crystallites increases sharply as the Co content increases. These precipitates appear in well-defined crystalline directions and have sizes that, for the case $x = 0.20$, can be comparable to the size of the structural grains. All samples investigated present GMR, and some features in the magnetotransport behaviour are linked to changes in the nanostructures, which are seen either with the annealing or with the variation of Co content. The fact that the maximum in the saturation value of the GMR is observed for $x = 0.10$, where most of the Co is distributed in the spinodal phase, establishes a positive correlation between GMR and spinodal decomposition. This is not explained by existing transport theories for these GMR materials.

2 - 30 — Sintering of $\text{Fe}_{0.912-x}\text{Mn}_x\text{Al}_{0.075}\text{C}_{0.01}\text{Cu}_{0.003}$ alloys with $x = 0.412$ and 0.162

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Powders of $\text{Fe}_{0.912-x}\text{Mn}_x\text{Al}_{0.075}\text{C}_{0.01}\text{Cu}_{0.003}$ alloys, with $x = 0.412$ and 0.162 , were obtained after a ball milling process during 10 hours period using a 4:1 ball mass to powder mass ratio. These powders were compacted and later sintered in hydrogen atmosphere at 900, 1000, 1100, 1200 and 1300 °C during periods varying from 2 to 48 hours. X-ray diffraction results of the milled powders showed the coexistence of the elements and a ternary Fe-Mn-Al fcc phase. Mössbauer spectra of these samples were fitted with two hyperfine field distributions, one with low fields (fcc phase) and other with high fields (Fe with some impurities of Mn and Al atoms). After sintering at 900 and 1000 °C during short times (2 and 4 hours), the samples with $x = 0.412$ showed the austenitic structure but low sinterability, while the $x = 0.162$ sample showed the bcc and fcc phases. For longer periods (48 hours) at 1200 °, few pores were observed, proving a significant sample sintering but accompanied with a decreasing sample density due to vaporization of some elements from the alloy surface.

Hard and soft magnetic materials

3 - 1 - Study of structural and magnetic properties of B-rich RE-Fe-B nanocomposite ribbons

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Nanocomposite magnets constitute novel magnetic systems, with interesting properties originating from the exchange coupling between hard and soft magnetic phases. They are also named “exchange-spring” magnets. B-rich nanocomposite RE-Fe-B magnets (RE: Rare Earth) have reasonable magnetic properties, low production cost and greater corrosion resistance than that observed in conventional RE magnets. In previous works, we found a dilution of RE atoms in the structure of boride phases with a diminution of coercive field, as compared with similar B-rich Nd-Fe-B nanocomposite ribbons. This result can be attributed to a decrease in the magnetocrystalline anisotropy when the majorities of Ce and La atoms dilute in those structures. In this work, we present a systematic study of the structural and magnetic properties of (MM_x, Nd_{1-x})_{4.5}Fe₇₇B_{18.5} ribbons (MM: Mischmetal, $x=0.25, 0.5, 0.75$ and 1.00). Their crystallisation kinetics is analysed using differential scanning calorimetry and the nanocrystalline phases are characterised by means of X-ray diffraction and Mossbauer effect spectroscopy. Finally, the dependence of their magnetic properties on x is discussed, emphasising the magnetocrystalline anisotropy variation originated by structural changes.

3 - 2 - Magnetic properties and Structural evolution of FINEMET alloys with Ge addition

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The influence of Ge addition on the devitrification process of FINEMET alloys into nanocrystalline structure has been examined. Fe_{73.5}Si_{13.5-x}Ge_xNb₃B₉Cu₁ ($0 \leq x \leq 13.5$) ribbons were obtained by the melt spinning technique. The structure of partially crystallized alloys was investigated by X-ray diffraction (XRD) and Differential Scanning Calorimetry (DSC). Hysteresis loops of the ribbons after heating at increasing temperatures, T_A , up to full devitrification of the amorphous precursors into a nanocrystalline state were performed to study the magnetic properties of the different alloys.

3 - 3 - Gadolinium-nickel ferrites prepared from metal citrates precursors

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A series 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 final solids. Six samples with overall composition $NiFe_{2-y}Gd_yO_4$, $y=0.00; 0.04; 0.05; 0.10; 0.12$ and 0.15 , were prepared by the auto-combustion method. After combustion, the gel directly transformed into single-phased, nano-sized Ni ferrite particles for $y < 0.05$. For samples with $y > 0.05$, the substituted ferrite and an orthorhombic phase, $GdFeO_3$, are observed. Mössbauer spectra and the Rietveld simulation for all samples allow the determination of Gd-for-Fe substitution in the magnetic phase. Ferrite-cell parameters indicate that the maximum substitution is accomplished in $y = 0.05$. Samples with $y > 0.05$ show a decrease in cell parameters indicating a smaller degree of substitution followed by an increment in the formation of $GdFeO_3$. Magnetic measurements indicate an enhancement of the magnetic permeability for increasing Gd-for-Fe substituted ferrites.

3 - 4 - Thermal stability of magnetic microstructures in Nd₆₀Fe₃₀Al₁₀ melt spun alloys

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The glass forming Nd₆₀Fe₃₀Al₁₀ alloy processed by melt spinning exhibits hard magnetic properties. For a relatively wide range of quenching rates, a single magnetic phase behavior is observed at room temperature, with coercivities between 0.1T and 0.4 T. As the quenching rate decreases, the hard magnetic properties improve and the thermal stability of the resulting magnetic microstructure -as measured by the reciprocal of the mean fluctuations field H_f - decreases. The hysteresis and thermal relaxation properties observed for different cooling rates are discussed on the basis of domain wall movement in a ferromagnetic matrix in which small, highly anisotropic clusters develop as the quenching rate decreases.

3 - 5 – Mechanical spectroscopy studies of partially amorphous $\text{Nd}_{60}\text{Fe}_{30}\text{Al}_{10}$ alloys

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The hard magnetic properties of melt spun $\text{Nd}_{60}\text{Fe}_{30}\text{Al}_{10}$ alloys are attributed to a major matrix nominally amorphous for X-ray diffraction. This matrix is actually found to be composed by two metastable nanosized (~ 5 nm) phases with different structures, compositions and intrinsic magnetic properties. This composite matrix phase is investigated for the first time by mechanical spectroscopy techniques (dynamic elastic modulus and internal friction measurements) in a wide temperature range (50 K - 450 K). The as cast microstructure irreversibly changes during annealing above 330K, leading to a large modulus recovery accompanied by a reduction in the internal friction level. A relatively large relaxation effect is observed near 290 K, evidenced by a narrow Debye-type internal friction peak with the corresponding step in the elastic modulus; this peak is stable under thermal cycling between 330K and 200 K but is affected by aging 11 h. at 330K and practically vanishes after heating to 450 K. Another internal friction peak is observed at about 240 K which has associated an anomalous modulus effect; in this temperature range, the elastic modulus exhibits heating/cooling hysteresis, which strongly depends on the extreme temperatures of the thermal cycle as well as on the number of cycles performed. These first results concerning transitory and relaxation effects in these melt spun alloys are analyzed and briefly discussed.

3 - 6 – The $\langle 12 \rangle$ -AF transition of UNi_2Si_2 : Heisenberg model, bi-quadratic interactions and the mean-field approximation

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We study a lattice of localized magnetic moments by means of a Heisenberg model with bilinear and bi-quadratic interactions and a local anisotropy field. As temperature T is varied the system may undergo transitions between different magnetic structures. The free energies of these structures are evaluated in a mean-field approximation which takes into account

the variation with T of the orientations of the local moments and the probability distribution of the magnetic states at a reference site. As an application of this formalism we find that the sequence of the magnetic structures of UNi_2Si_2 with increasing T can be explained if a suitable set of values of the interaction constants is assumed.

3 - 7 – Composite of polyaniline containing iron oxides

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A composite of polyaniline (PANI) containing iron oxides with nanometer size was prepared by a chemical method. Polymer adsorption on the surface of magnetite particles was investigated. The electrical and ferromagnetic properties of the composites were measured as a function of the concentration of KOH during polymerization. The conductivity of the composites at room temperature decreases with the increase of the concentration of KOH. For the basic preparation conditions, the resulting $\text{PANI-Fe}_x\text{O}_y$ composite can be attracted by a magnet at room temperature and shows an insulating behaviour.

3 - 8 – Electrical permittivity of Ni and NiZn ferrite-polymer composites

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Electrical and magnetic properties of polymers, well known for their insulating properties, may be improved by adding various functional fillers. Polymer-ferrite composites have been a subject of recent extensive research. Electric and magnetic properties of such composites depend on the size, shape and amount of added filler in general. When polymer-ferrite composites particularly are used as electromagnetic wave absorbers and EMI shielding materials, it is very important to explain the variation of permeability and permittivity in the measured frequency ranges. In this paper epoxy-Ni ferrite composites and epoxy Ni-Zn ferrite composites were used. The effects of the volume fraction and particle size of ferrite on the frequency dispersion characteristics of the complex permittivity and permeability are studied.

3 - 9 – Properties of $\text{Fe}_{60}\text{Mn}_{10}\text{Al}_{30}$ alloys milled with Nb

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$\text{Fe}_{60}\text{Mn}_{10}\text{Al}_{30}$ alloys were prepared by mechanical alloying adding Nb. Nb was added in two ways: first by substituting the tree components as $(\text{Fe}_{60}\text{Mn}_{10}\text{Al}_{30})_{95}\text{Nb}_5$ and $(\text{Fe}_{60}\text{Mn}_{10}\text{Al}_{30})_{90}\text{Nb}_{10}$ and milling during 12 hours; and second substituting Al by Nb as $\text{Fe}_{60}\text{Mn}_{10}\text{Al}_{20}\text{Nb}_{10}$ and milling during 12, 26 and 36 hours. All samples were studied by X-ray diffraction, Mössbauer spectrometry, Differential Scanning Calorimetry, Thermo Gravimetry and magnetic measurements (hysteresis cycles) at room temperature. The Nb substitution induces the presence of a hexagonal Fe_2Nb phase in the alloys, in addition to the bcc FeAlMn alloy phase. Both, the lattice parameter and the mean grain size of the bcc phase decrease when the Nb content increases and the amorphous character increases when milling time increases. The obtained Mössbauer spectra show a decreasing magnetic component with broad lines and an increasing broad paramagnetic component when the Nb concentration increases or the milling time increases. The spectra were then fitted by means of a hyperfine field distribution and a quadrupolar splitting distribution, respectively. It is concluded that the magnetic character of Fe-Mn-Al alloy decreases with the Nb substitution or with the increase of milling time. Also, the amorphous character increases when Nb and milling time increase.

3 - 10 – Extended Heisenberg Hamiltonian for LaMn_2X_2 (X=Si,Ge) using an *ab-initio* parametrization

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The compounds RT_2X_2 (R = rare earth, T = transition metal, X = Ge, Si) exhibit a great variety of magnetic structures and of temperature-driven transitions between them. A phenomenological study of the behaviour of each of them requires a Hamiltonian containing the interactions between the localized moments. On the other hand, one can find the energy of different configurations by *ab-initio* calculations, and thereby obtain the values of the interaction constants

appearing in the Hamiltonian. Once the Hamiltonian is known one can calculate the free energy of different magnetic structures at different temperatures T, finding possible phase transitions between them.

Here we consider LaMn_2Ge_2 and LaMn_2Si_2 . The ground state magnetic structure of both compounds is of the "conical" type (ferro and helicoidal arrangement for the *z* and *xy* components, respectively). For increasing T, LaMn_2Ge_2 undergoes successive transitions: first to a purely helicoidal, then to an antiferro with moments in the $\pm x$ direction. LaMn_2Si_2 has a similar behaviour, with a canted structure (ferro ordering for the *z* components and antiferro for the *x* components) instead of the helicoidal structure. At high T the moments are totally disordered in both compounds.

We assume a model Hamiltonian with bilinear and bi-quadratic interactions, for which the interaction constants are obtained by *ab-initio* calculations. The free energies of the above mentioned configurations are then evaluated in a mean field approximation (MFA). The observed phase sequence can be obtained for both compounds.

3 - 11 – Crystallisation kinetics of B-rich Mischmetal-Fe-B nanocomposite ribbons

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In a previous article [1], it was reported that $\text{Nd}_3\text{Fe}_{79}\text{B}_{18}$ melt-spun and subsequently crystallised nanocomposite ribbons had a coercivity value $H_c = 200$ kA/m. After the controlled annealing, it was found that $\text{t-Fe}_3\text{B}$ and $\alpha\text{-Fe}$ had precipitated containing a dilution of Nd atoms in the boride structure. This fact promoted a magnetic hardening of $\text{t-Fe}_3\text{B}$ phase due to an increase of its magnetocrystalline anisotropy. It was concluded that B-rich nanocomposite ribbons with a composition of $\text{RE}_{2.5}\text{Fe}_{79}\text{B}_{18.5}$, are at the onset of the RE content range which would promote their magnetic hardening. In this work, the Mössbauer thermal scan analysis method [2] was employed to follow the crystallisation kinetics of $\text{MM}_{2.5}\text{Fe}_{79}\text{B}_{18.5}$ (MM: Mischmetal) and the results were compared with those obtained by other techniques, such as thermomagnetic measurements and differential scanning calorimetry. The evolution of the crystalline phases fraction (in this alloy, Fe_2B and $\alpha\text{-Fe}$) was also determined by Mössbauer spectroscopy performed during isothermal annealing at 550 °C.

[1] B. X. Gu, J. Magn. Magn. Mat. **263**, 332-336 (2003).

- [2] P. Mendoza Zélis, G. Pasquevich, F.H. Sánchez, N. Martínez y A. Veiga. Phys. Lett. A **298**, 55-59 (2002).

Magnetic properties of High Tc Superconductors

4 - 1 – Metastability of static configurations of the vortex lattice in YBCO crystals

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Memory effects in the dynamic response of the vortex lattice (VL) in type II superconductors and its relationship with the controversial peak effect, have attracted a great interest for a long time. In the last years, these features have been observed in YBCO single crystals, with the dc magnetic field tilted away from the twin planes and were related with robust dynamical states characterized by different degrees of mobility. Recently, we reported that the previous dynamical history of the VL can modify not only its dynamic response, but can even modify its static properties as well. In the present work we study with ac susceptibility techniques the stability of the different static configurations by sensing the effective ac penetration depth in the linear Campbell regime. We report history dependent effective pinning potential well curvatures. Interestingly, we observe that the more pinned VL configuration is not the more stable.

4 - 2 – Dynamical properties of vortex lines in BSCCO single crystals under uniaxial pressure

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In order to understand which is the influence of anisotropy on the dynamics of vortex lines in high temperature superconductors, we have applied uniaxial pressures parallel to the c-axis of BSCCO (2212) single crystals, reducing the interplanar spacing of the CuO₂ superconducting planes. Using the pseudo DC flux transformer technique, we have studied the sensitivity of the TAFF regime to the anisotropy of the sample. We have been able to obtain information related to the correlation of the vortex lines along the sample's thickness. Our results indicate that the correlation length in the c direction can be effectively increased with pressure, modifying the dissipative behavior of vortex lines in the liquid regime.

Low dimensional magnetism

5 - 1 – Structural properties and magnetism in bimetallic CoRh nano-clusters

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The structural and magnetic properties of free-standing bimetallic Co_nRh_m ($n \sim m \sim 55$) nanoparticles were studied. We performed a local structural optimization starting from clusters with Rh-bulk distances and three different symmetries: cubo-octahedral, icosahedral, and hexagonal close-packed. For each symmetry, two types of chemical ordering were considered: a) segregated phase (a Rh rich core with an external Co shell), and b) alternate layering alloyed. The geometrical results show that the most stable structures are those with hcp symmetry. In general it was found that the clusters in the segregated phase have lower energies than the corresponding alloying case. The bond length of all optimized clusters are smaller than the initial ones, in good agreement with the recent experiment (*Phys. Rev. Lett.* **89**, 037203 (2002)). The calculations of the electronic structure and related magnetic properties were done by self-consistently solving an unrestricted *spd* tight-binding Hamiltonian. In the layered alloying clusters, the magnetic moments at rhodium (cobalt) sites are enhanced (diminished) in reference to the segregated phase case. Nevertheless, the total average magnetic moment per atom does not sensitively depends on the two types of chemical ordering here considered. Comparison with the experimental report and the available theoretical calculations in the literature is done.

5 - 2 – Electrodeposition of Fe/Au(111) ultrathin layers with perpendicular magnetic anisotropy

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Electrodeposition (ED) of ultrathin magnetic layers and multilayers is an emerging topic, with the observation of giant magnetoresistance (GMR) [1] and the perpendicular magnetic anisotropy (PMA) [2], which is of interest for data storage. One important advantage of ED is an easy control of the growth parameters by varying the potential and the solution composition. This work investigates the magnetic and structural properties of ultrathin electrodeposited Fe/Au(111) layers. The magnetic state was characterized using in-situ (i.e. in the electrolytic environment) alternating gradient force magnetometer (AGFM) and in-situ polar magnetic optical Kerr effect (PMOKE). The AGFM experimental set-up enables to probe both the perpendicular and parallel components of magnetization from the very initial stages of the metal growth. Hysteresis loops were also recorded in-situ. Results show that Fe films are ferromagnetic at room temperature, down to 1 ML and that the easy axis of magnetization is normal to the surface below $t^* \sim 2$ ML. The value of t^* depends however on the outer interface, since the magnetization takes the in plane orientation upon deposition of a copper layer on top of the iron film. Complementary to magnetic measurements, in-situ STM, shows that Fe films grow in a layer by layer fashion. Ex-situ EXAFS, after capping with a Cu layer, indicates that the film is fcc Fe(111) in initial stages and becomes bcc Fe(110) above 2-3 ML. Results will be discussed in terms of anisotropy of magnetization and compared with results obtained with similar structures produced by others techniques, such as MBE and PLD.

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[2] J.L. Bubendorff et al., Phys. Rev. B **56**, R7120 (1997).

5 - 3 – Ferromagnetic resonance in amorphous nanoparticles

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The results of the ferromagnetics measurements (FMR) on noninteracting amorphous nanoparticles systems $(\text{Co}_{0.25}\text{Ni}_{0.75})_{65}\text{B}_{35}$ (CNB2) and $(\text{Fe}_{0.26}\text{Ni}_{0.74})_{50}\text{B}_{50}$ (FNB2) in a temperature range of 10 - 300 K are reported. The high temperatures results show symmetric lineshapes that indicate a low value of effective anisotropy. When cooling these samples, the lineshapes lose their symmetric behavior indicating light prolate particles. Decreasing temperature we observe an increase of the total linewidth and the spectra intensity. Around 60 K in CNB2 (\approx 40 K in FNB2) we observe a marked fall on the resonance field. On further cooling, an intensity maximum appears and at 10 K it falls notably. In CNB2 we observe a nonuniform behavior of the linewidth and the resonance field below 40 K. Previous magnetics measurements on these systems indicate large surface effects in the same temperature region. This picture, together with simulations, permit us to explain interpret this FMR behavior.

5 - 4 – Thermodynamic properties of the spatially anisotropic triangular antiferromagnet

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We study finite temperature properties of the spatially anisotropic Heisenberg antiferromagnet on a triangular lattice. In order to fulfill Mermin Wagner's theorem we impose a zero magnetization condition in the spin waves theory. We compute the specific heat, the static structure factor, and the uniform static susceptibility as a function of both frustration and temperature. Motivated by experimental studies of NMR on organic superconductors, we calculate the relaxation time T_1 and analyze the interplay between pressure and magnetic frustration. We also discuss the validity of a localized spin model to describe the magnetic phase of the κ pattern of organic superconductors.

5 - 5 – Magnetic properties of nanotube structures

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With the discovery of carbon nanotube structures, a new class of materials with a reduced dimensionality has been introduced. A great deal of progress has been made in the research of carbon nanotubes due to their technological applications, such as nanoelectronic devices, probing tips, electron emitters, etc. The nanotubes are made of coaxial graphene cylinders. Each cylinder can be visualized as the conformal mapping of a two-dimensional honeycomb lattice onto its surface with a diameter as small as some angstroms. The tubule is usually characterized by two integers (n,m) specifying the circumference vector in an unrolled planar graphene sheet. The tubule geometry is given uniquely by the (n,m) indices. Band-structure calculations predict that the (n,m) indices determine its electronic properties. For example, (n,n) or armchair tubes are metals, while (n,0) or zigzag tubes are metals if n is a multiple of 3, or semiconductors otherwise. Experimental results show that structural parameters, such as, diameter, helicity, and number of concentric cylinders, strongly influence the electronic properties of carbon nanotubes. It has also been showed that the presence of a magnetic field strongly affects the magnetic susceptibility. Among various forms of carbon nanotubes, the single-walled nanotube has attracted much attention because of its unique structural and electrical properties. A recent experiment has reported the production of a stable armchair (2,2) tubule. In this work, we have considered nanotube models of armchair (2,2) and zigzag (4,0) with one p orbital per atom. Here we have studied the magnetic thermodynamic properties of these models using a single Hubbard model at half-filling. In these calculations we have used the grand canonical quantum Monte Carlo method. We used a discrete Hubbard-Stratonovich transformation to convert the problem into one of free particles interacting with a time-dependent Ising field, together with an exact updating algorithm for the fermions Green's function for computing the relative weights of the Ising configurations. We have studied lattices of up to 64 sites. We calculate the temperature dependence of the magnetic susceptibility and the spin-spin correlation functions. Our results show that all studied systems at low-magnetic field posses antiferromagnetic short-range correlation. The calculated magnetic susceptibility, subtracting the diamagnetic contribution, is strongly temperature dependent at low-field as well as at high-field, but exists an intermediate critical magnetic field in which the susceptibility is almost temperature independent. Our results show the temperature and field dependence of the magnetic susceptibility of the considered nanotube models in very good qualitative

agreement with the experimental data for a mixture of nanotubes of different diameters.

5 - 6 – Thermodynamics of the one-dimensional Hubbard model with next-nearest-neighbor hopping

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The Hubbard model is frequently used in the scientific literature to investigate the properties of magnetic materials and superconductors, because it considers the strong electronic correlation that happens in magnetic systems characterized by itinerant electrons. For one-dimensional systems, Lieb and Mattis have proven that the ground state is unmagnetized for any real and particle-symmetric but otherwise arbitrary interaction. This theorem applies to a single band in one dimension, provided that the hopping is only between nearest neighbors and the interaction involves only densities. Since both conditions are fulfilled in the Hubbard model, its ground state in $d=1$ cannot be ferromagnetic. In principle, the Hubbard model is obtained from an extreme truncation of a more general Hamiltonian describing interacting electrons in a solid. Only the on-site interaction and one relevant band are kept. Recent studies suggest that the inclusion of next-nearest-neighbor hopping in the model favors the long range magnetic ordering. Contributing for a better understanding of the phenomenon, we have used the method of small cluster exact diagonalization and the grand canonical quantum Monte Carlo method in order to study the temperature dependence of the specific heat, spin average value, magnetic susceptibility and correlation functions. We have obtained a magnetic correlation phase diagram for different values of t_2/t_1 (relative magnitude of the next nearest neighbor hopping to the nearest neighbor hopping) of the linear lattice. In the limit of a non interacting electron system we have calculated the density of electronic states for a linear lattice. Our results have shown that the inclusion of the t_2 causes the appearance of ferromagnetic correlation regions in the diagrams obtained for a linear lattice which do not appear when $t_2 = 0$. In the density of states, the additional hopping ($t_2 \neq 0$) causes a breaking in the characteristic symmetry of the lattice studied here. Therefore we have verified the importance of the application of the Hubbard model with this new hopping term to the study of ferromagnetic systems that presents the electron itinerancy as a main characteristic.

5 - 7 – Specific heat at the magnetic order transitions in $\text{RbFe}(\text{MoO}_4)_2$

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The material $\text{RbFe}(\text{MoO}_4)_2$ (RFMO) is a rare example of a nearly two-dimensional Heisenberg antiferromagnet on a triangular lattice, in which the $S=5/2$ Fe^{3+} ions interact via oxygen superexchange paths. The in-plane exchange integral J is much larger than the vertical inter-plane exchange integral J' , and diagonal inter-plane interactions J'_1 and J'_2 . In absence of magnetic field, the material experiences a transition to an incommensurate antiferromagnetic order along the c -axis at 3.6 K, due to the diagonal interplanar interactions, forming a stacked 120° structure. As magnetic field is applied in the ordered state, the different interactions yield a rich variety of magnetic ordered phases, with the material entering first into a commensurate magnetic order in plane and out of plane, then into an incommensurate order along the c -axis. We measured the specific heat as a function of the temperature of a RFMO single crystal by means of a microcalorimetric technique in applied magnetic fields up to 15 T. Different peaks were observed, corresponding to the different magnetic order transition. The specific heat anomalies and transition temperatures are in agreement with a Neutron Scattering experiment. We found that the upper transition to the paramagnetic state decreases in increasing fields, and extrapolates to zero temperature at an approximate field of 18 T. Other results and implications will be further discussed at the presentation.

5 - 8 – Magnetic studies of Dy-doped Y_2BaCuO_5

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We report the effect that doping Y_2BaCuO_5 with Dy has on its two dimensional (2D) magnetic structure. Pure samples at both ends of the series, as well as samples doped with 1%, 5%, 10% and 25% dysprosium, have been characterized using X-ray diffraction, and AC susceptibility together with neutron diffraction studies on the 1% and 5% samples, which were used to measure the magnetic ordering at low temperatures. In addition, the data obtained with up-to-date detectors and better analytical techniques, will allow us to resolve the magnetic structure of Y_2BaCuO_5 , which, in spite of the published results, still has some ambiguities. The results show that 1% Dy is enough to disrupt the 2D magnetic ordering turning it into a 3D array. The low dysprosium concentration indicates that the 3D ordering is achieved without the existence of a rare earth magnetic sublattice. The discrepancy between the parameters obtained by the Curie-Weiss fittings of the real part of the AC susceptibility and the neutron diffraction results, shows that the exchange mechanism deviates from the mean field model for all dysprosium concentrations.

5 - 9 – Magnetic properties of bimetallic Ni-Pd nanoclusters

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We study the dependence of the magnetic properties of Ni-Pd nanoclusters (Ni cores coated by Pd atoms) on size and relative composition. We consider Ni-Pd clusters having closed shell cubo-octahedral structure with an increasing Ni core. The electronic and magnetic properties are calculated with a parametrized Hubbard Hamiltonian within the unrestricted Hartree-Fock Approximation. We show that, depending on the relative composition, the Pd coating can give rise to an enhancement of the average magnetic moment of the Ni core. This enhancement ends when there is a mixing of both Ni and Pd atoms on the surface.

5 - 10 – Magnetic properties of Ni-Rh clusters in the Ni-rich region

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We study the magnetic properties of bimetallic Ni-Rh 55-atom clusters in the Ni-rich region as function of the Rh composition. The minimum energy structures are taken from Molecular Dynamics simulations by using empirical potentials (in the Second Moment Approximation). We then calculate the electronic and magnetic properties of these structures by using a Tight-Binding Hamiltonian. The magnetic solutions were found resolving a Hubbard-like Hamiltonian within the unrestricted Hartree-Fock Approximation. Bulk parameters and Andersen's exponential law for the dependence of hopping on distance are taken into account. We obtain that a little number of Rh atoms considerably modifies the average magnetic moment (μ) depending not only on the positions of the Rh atoms (either on the surface, middle, or central shell) but also on their relative positions. The μ curve corresponding to the minimum energy structures show a minimum for 3 Rh atoms and then there is an enhancement of the μ up to 6 Rh atoms, leading to μ values even higher than the corresponding to the pure Ni cluster.

5 - 11 – Real Space Electronic Structure Calculations using a Multi-level Method

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An object oriented code to solve the Density Functional Theory (DFT) equations in real space was developed. The eigenproblem that appears in the selfconsistency iteration was treated by using the Rayleigh Quotient Multigrid (RQMG) method. The code was tested by performing all-electron electronic structure calculations for isolated atoms and small molecules. The use of local mesh refinements to improve resolution near the nuclei is discussed.

Semiconductors, anomalous rare-earths and other magnetic materials

6 - 1 — Theoretical study of the independent temperature resistivity of *s-p* and rare-earth impurities diluted in transition hosts: A two band model

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In this work, we study the temperature independent resistivity of *s-p* impurities and rare-earth impurities diluted in transition hosts, using a *T*-matrix formulation in a two-band hybridized system. We consider that the conduction is entirely performed by the *s*-electrons and the screening of the charge difference induced by the impurities is made by the *d*-electrons. In particular, within our picture, one has the possibility of separating *d-d* impurity induced scattering effects from *s-d* impurity induced scattering. We take into account the translational symmetry breaking and therefore a non local charge potential is obtained, which can be self-consistently calculated *via* an extended Friedel sum rule. The effect of volume difference between impurity and host elements is also considered in the calculation.

6 - 2 — *ab initio* study of structural, electronic, and magnetic properties of magnetic impurities in rutile TiO₂.

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Integrating spin functionality into otherwise non-magnetic materials has become a highly desirable goal in the last years. In particular, dilute magnetic impurities in semiconductors and oxides (DMS) produce novel materials appealing for spintronics and optoelectronics [1,2]. While most of the DMS have Curie temperatures much lower than room temperature, this is not so for Co-doped rutile and anatase TiO₂ [2,3]. However, many questions remain regarding the location of Co in the host lattice and the underlying

microscopic mechanism of long-range magnetic order. In this contribution we present a set of density-functional-theory-based calculations in the systems R_xTi_{1-x}O₂ (R = Mn, Fe, Co, Ni). The calculations were performed with the WIEN97 implementation [4] of the full-potential linearized-augmented-plane-wave (FP-LAPW) method, assuming that the magnetic impurities substitutionally replace the Ti ions. The calculations were performed considering different dilutions and distributions of the impurities. The effects of the structural relaxations induced by the impurities in the host-lattice on the magnetic properties and the tendencies to ferromagnetism or antiferromagnetism are discussed and compared with previous calculations and experiments.

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6 - 3 — Electronic structure of *fcc*-FeX (X = C, N) alloys

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The *fcc* Carbon and Nitrogen Fe alloys are widely used for the production of cast irons and steels when critical temperatures range and cyclic thermal conditions, corrosives atmospheres, etc., are the working conditions of the material. The solid solution phase, usually referred to as austenite, has attracted considerable attention, in connection with the modelling of thermodynamic properties, the prediction of phase diagrams, the diffusion controlled reactions and the martensitic phase transitions. Chemical activity data and Mössbauer spectroscopy have been traditionally used to check the different models and simulations developed to determine the solute distribution. The electronic properties have been also subject

of great interest since they are intimately correlated to the solute distribution and crystal structure of the alloys. A systematic comparison of the hyperfine parameters obtained by Mössbauer spectroscopy and by full-potential linear augmented-plane wave (FLAPW) method will give a more accurate picture of the solid solution. We present here the density of states, magnetic moments, isomer shifts, and hyperfine magnetic fields obtained by FLAPW assuming Fe_8X and Fe_4X structures and the Mössbauer data.

6 - 4 – Residual resistivity of n -d impurities diluted in noble hosts

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We discuss the temperature independent resistivity of nd ($n=3,4$) transition metal impurities diluted in Cu host, using a T -matrix formulation in a single band model. We take into account the translational symmetry breaking and therefore a non local charge potential is obtained. The effect of volume difference between impurity and host elements is also considered in the calculation. Our numerical results describe quite well the available experimental data.

6 - 5 – The Rashba effect on a double-barrier spin polarizer

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The Rashba effect on a double-barrier spin polarizer is considered using a formalism that produces accurate results with little computational effort. In previous articles we proposed a spin polarizer consisting of a well made of a dilute magnetic semiconductor (DMS) enclosed by two non-magnetic barriers. In the absence of Rashba effect, the magnetization of the well produces totally polarized electronic levels separated by 0.15 eV. The highest steady magnetic field obtained in a laboratory could not produce a Zeeman splitting so big. As a consequence the calculated currents are almost totally polarized. The Rashba spin-orbit Hamiltonian produces a spin flip. Therefore the levels at the well have not well defined spin polarization and

the currents are less polarized. The device presented here would be useful for spintronics because there are DMS ferromagnetic at room temperature. Our tight-binding Hamiltonian, including the Rashba term, is

$$\mathcal{H} = \mathcal{H}_K + \mathcal{H}_P + \mathcal{H}_E + \mathcal{H}_M + \mathcal{H}_{h-i} + \mathcal{H}_{h-h} + \mathcal{H}_R.$$

The first term is the kinetic energy. \mathcal{H}_P describes the double-barrier profile and the third term represents the electric field due to the applied bias. The magnetic \mathcal{H}_M , the hole-impurity \mathcal{H}_{h-i} and the hole-hole \mathcal{H}_{h-h} terms are included in the mean field approximation. The profile and the charge distribution are calculated self-consistently. By using a decimation formalism, all these terms are treated exactly. Finally, the Rashba term \mathcal{H}_R is very small. Therefore it is treated using second order perturbation theory. The calculation confirms that the Rashba effect on the currents is of second order. Consequently the resulting depolarization is very small.

6 - 6 – First order phase transitions in spin-glass models with manifold paramagnetic solutions

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Paramagnetic and one-step replica symmetric breaking spin-glass solutions of a p -spin glass model in the presence of a transverse field are studied in the neighborhood of the phase transition curve. Two qualitatively different regions are found in the phase diagram. For a transition temperature higher than a certain value T^* , the phase transition is of second order, otherwise the phase transition is of first order with latent heat. It is shown that T^* signals a point in the phase transition curve where an unstable paramagnetic solution appears. A discussion about the order of phase transition in related spin-glass models like the random energy model and the random orthogonal model is presented.

6 - 7 – AC susceptibility in $Y_{1-x}\text{Tb}_x\text{Co}_2$ compounds

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AC susceptibility measurements, as a function of temperature and frequency, have been carried out in $Y_{1-x}\text{Tb}_x\text{Co}_2$ ($0.1 \leq x \leq 0.9$) compounds to investigate the magnetic phase transition. It is known that YCo_2 exhibit very strongly enhanced Pauli paramagnetism while TbCo_2 order magnetically by inducing a

magnetic moment on the cobalt and displays a second order phase transition at 230 K. We show that in the studied compounds a change in the order of the phase transition from first order to second order appears at around $x = 0.4$. The increase in the order temperature with *Tb* concentration is analyzed and discussed in the framework of the Inoue- Shimizu model.

6 - 8 – Crystal growth, structural and magnetic properties of the MnNb_2S_4 semiconductor

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We have prepared magnetic semiconductors through a novel direct melting method of homogeneous elements in which the crystal structures are similar to materials grown by other techniques. The semimagnetic MnNb_2S_4 show an hexagonal type structure with the presence of a second crystalline phase. A ferromagnetic transition was observed at 50K, with an significant increasing of the magnetization in the orderly phase. In the paramagnetic state the measures show two different magnetic moments, which corresponding to two Curie temperature, to $T_c=50\text{K}$, the magnetic moment is 0.67 Bohr magnetons, while to $T_c=21.5\text{K}$ the magnetic moment is 0.77 Bohr magnetons, this values could be associated to the different crystalline phases

6 - 9 – Spectral properties of the CeM_2Si_2 compounds ($M=\text{Ru}$, Rh and Pd).

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We study the spectral properties of the tetragonal series CeM_2Si_2 with $M=\text{Ru}$, Rh and Pd applying two mixed techniques, LDA+U and LDA+NCA. LDA+U method introduces an *ad-hoc* term into the LDA functional that accounts for the strong correlations of the *4f* states. This method corrects the position of the *4f* state with respect to LDA. We analyse the obtained results in terms of *4f-4d* hybridization. The second mixed technique solves the Anderson impurity model within the *non crossing approximation* (NCA) using as input the hybridization function $\Gamma(\varepsilon)$ calculated from first principles (LDA). The calculated spectral functions of the three systems under study are compared with photoemission spectra taken from the literature. The low energy spectral properties reflect the experimental sequence of Kondo temperatures within the series, result that could be obtained just because the $\Gamma(\varepsilon)$ function contains the detailed information of the crystal environment. LDA+NCA proves to be a valuable tool to study highly correlated Cerium compounds.

Magnetic and structural experimental techniques. Instrumentation

7 - 1 – Effect of temperature on the ferromagnetic resonance of $\text{Ni}_{50}\text{Fe}_{50}$ thin films

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We report on the effect of temperature on the ferromagnetic resonance (FMR) spectra of $\text{Ni}_{50}\text{Fe}_{50}$ thin films sputtered on Si (001) wafers. The FMR field and linewidth were studied as a function of the ferromagnetic layer thickness, t , and temperature, T . The data are interpreted in the framework of a phenomenological model that includes in- and out-of-plane uniaxial anisotropy fields. The main effect of temperature on the magnetic properties of these films is to induce a surface anisotropy that pushes the magnetization out-of-plane. The temperature dependence of the resonance field is explained assuming the magnetic anisotropies varying as m^3 , where $m=M(T)/M(0)$ is a reduce magnetization and $M(T)$ follows the law $(1-CT \exp(-E/KT))$, where E proportional T_c is the energy gap of the spin wave spectrum, and TC being the Curie temperature. The resonance field as a function of temperature show a transition temperature separating two different ferromagnetic regimes. At lower temperatures a new magnetic transition is observed in thinner films. The temperature behavior of the FMR linewidth reflect the same features as the resonance field, indicating that both parameters have the same origin.

7 - 2 – Thermomagnetometric measurements obtained using an adapted thermogravimetric analysis device

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In this contribution we present thermomagnetometric measurements (on FINEMET, steels, Nd-Fe-Al ribbons, and some pure metals) taken with a thermogravimeter equipment (TG) adapted as a thermomagnetometer. The adaptation was carried out placing a permanent $\text{Nd}_2\text{Fe}_{14}\text{B}$ -based magnet below the oven of the balance, which provides a magnetic field induction B of approximately 50mT and a gradient dB/dz of about 23 mT/cm at the sample position.

During heating (or cooling) the mass registered with the thermobalance varies because the magnetic force is modified due to changes of the sample magnetization. Then, the magnetic behavior can be monitored. With this modification of a conventional TG, curves of Zero-Field-Cooling and Field-Cooling magnetisation have been obtained for Nd-Fe-Al and other materials, which are similar to those obtained with other magnetometer devices. The relation between the resulting curves with the magnetic behavior and structural changes of the present phases and microstructure will be discussed.

7 - 3 – Magneto-optical imaging in commercial audio tapes

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Magneto-optical imaging has become a powerful technique for the measurement of local magnetic fields. The technique consists in measuring the rotation in the light polarization plane when light travels through a sensitive garnet (Yttrium Iron Garnet, YIG). The plane rotation is a function of the local magnetic field at which the garnet is exposed. As a test of the technique, we have studied commercial audio tapes, in which computer generated functions were directly recorded with a tape recorder. We present a study of the magnetic field generated by the different periodically magnetized tapes (e.g. square, cosine, triangle and sawtooth waveforms) for different frequencies and amplitudes. Observations are described modelizing the magnetized tapes as an array of coaxial circular coils where the current in each coil reproduces the recorded functions.

7 - 4 – Hyperfine field temperature dependence of Fe_3Si from Mössbauer thermal scans

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Mössbauer thermal scans combined with a new data analysis methodology has been proved to be a valuable technique to determine a cuasi continuous dependence of the magnetic hyperfine field with temperature. This demonstration was achieved by studying an antiferromagnet compound in which Fe atoms locates at a unique crystallographic site [1]. Here a more complex situation is addressed in the case of the ferromagnetic $\text{bcc} - \text{Fe}_3\text{Si}$ compound where Fe atoms

occupy two crystallographic sites. The Fe_3Si conventional Mössbauer spectrum consist of two sextets which became, at the Curie temperature of 852 K, an asymmetric line due to the two unresolved singlet lines of each Fe site. Thermal scans were performed at various distinct Doppler energies. Transmission at a fix Doppler velocity vs. temperature shows a well defined minimum when a Mössbauer line position shift to the chose velocity due to temperature increase. Fitting procedure for the Mössbauer absorption without the usual thin absorber approximation will be discussed. From this model and assuming other parameters as second order Doppler shift temperature dependence known the hyperfine field temperature dependence is obtained.

[1] P.Mendoza Zélis, G. Pasquevich, F.H. Sánchez, N. Martinez, A. Veiga, Physics Letters A **298**, 55-59 (2002).

7 - 5 – Evidences of the stability of magnetite on a soil from Northwestern Argentina by Mössbauer spectroscopy and Magnetization measurements

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Numerous studies on basalt derived soils (Ultisols, Oxisols and Alfisols) from Northwestern Argentina and Brazil have shown the conspicuous presence of magnetic material. Recently and with the aid of Mössbauer spectroscopy magnetite was found to be pedogenically unstable weathering to maghemite. However in an Ultisol from Misiones, Argentina magnetite was found in all size fractions. The study at different depths is a first step towards the understanding of the stability of the magnetite in these soils. In this study the magnetic fraction of the Bt22 horizon (105-155 cm depth) of a claylay red Ultisol from the subtropical forest of Misiones, Argentina was studied by X-ray diffraction, saturation magnetization σ_s , optical microscopy and Mössbauer spectroscopy. Saturation magnetization for the whole sand fraction (wsf), the non magnetic (nmsf) and the magnetic fractions (msf) are 10.79, 16.92 and 1.50 JT⁻¹Kg⁻¹ respectively. Mainly quartz, ilmenite, Al substituted hematite, magnetite-maghemite, and goethite are found. Magnetite-maghemite contents are high, being magnetite predominant in the msf. Results are compared with those of from the upper B1 horizon (10-35 cm depth) of the same soil, in which a lower (wsf) σ_s value, and higher values of (msf) σ_s and of ($\sigma_{s(msf)} - \sigma_{s(wsf)}$) values were measured. These results confirm the stability of magnetite in this soil

contrasting with other results on soils from neighboring areas

7 - 6 – Multi-modal bridging ligands to engineer molecular magnets

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Dicarboxylates are versatile tools useful in the design of polynuclear complexes with interesting magnetic properties. The ability of the carboxylate bridge to mediate significant ferro- or anti-ferromagnetic interaction accounts for their use. Depending on the length of the dicarboxylate chain $[O_2C(CH_2)_nCO_2]$ a large variation in coordination behaviors, which can coexist, can be obtained. Coordination ways include chelating, bidentate-bridging or chelating-bridging modes, which allows for the formation of polymeric arrangements of different dimensionalities. Rare earth metals are attractive as metal centers for their high coordination number, which help construction of magnetically interesting coordination polymers that also exhibit other attractive and advantageous properties, such as optical activity, and thermal stability. In this study, we report two Nd adipates, $[Nd_2(O_2C(CH_2)_4CO_2)_3(H_2O)_4] \cdot 6H_2O$ (**I**) and $Nd_2(O_2C(CH_2)_4CO_2)_3(H_2O)_4 \cdot 2H_2O$ (**II**). The x-ray analysis of **I** shows infinite chains, form by Nd-O-Nd bridges alternating with Nd-O-C-O-Nd bridges while in the structure of **II** two different Nd-O-Nd bridges build the chain. The influence of the coordination sphere, bridging units and coordination and hydration water on the AC magnetic susceptibility of both compounds is discussed.

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