

Low dimensional systems, nanostructured materials, and nanomagnetism

2 - 1 – B3LYP/cc-pVTZ study on the growing pattern of small Al/P clusters

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Semiconductors formed by group 13/15 elements have growing importance due to the potential application in the preparation of thin films for electronic devices [1]. The interest in the study of AlN atomic clusters is based on the fact that the application in thin films requires a profound understanding of properties at atomic level as well as the growing pattern followed by the aggregates.

Results obtained for clusters up to five atoms are reported, with emphasis on the growing pattern followed for the aggregates. Al/P aggregates were studied with tools from density functional theory (DFT); using the B3LYP hybrid exchange and correlation functional [2], with cc-pVTZ triple- ζ basis functions [3], as implemented in the Gaussian 03 program [4]. Equilibrium geometries were obtained starting from the AlP dimer and adding up aluminium and phosphorus atoms to grow the aggregates. The increase in the binding energy per atom was used to evaluate the growing. The preferred growing pattern was found to be AlP (³A) - AlPP (²A) - PAIPP (³A) - PPAIPP (²A). Molecular electrostatic potentials (MEP), spin densities and charges derived from electrostatic potentials were calculated to get a quantitative picture of the whole process. It is found that Al-P clusters tend to grow following a non planar pattern, preferring zones in which MEP's are negative and where unpaired electrons are located.

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2 - 2 – Theoretical study of the structural, electronic and magnetic properties of small Molybdenum clusters and their reactivity towards H₂ adsorption and dissociation

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Small neutral and ionic Mo_N clusters, with N = 2-6, are studied within the framework of the density functional theory (DFT) [1]. After an extensive test of several exchange and correlation functionals, it is found that the BLYP one [2] provides the best results for some selected properties of atomic Mo and Mo₂. In all cases, the basis functions used are of triple-zeta quality with polarization functions. The calculations are carried out with the ADF program [3-5]. Geometries of isolated clusters are optimized without symmetry constraints. The electron spin multiplicity is also considered as a variable during optimizations. Eigenvalues of the hessian matrix are determined to confirm that the optimized structures are indeed minima on the potential energy surface of the aggregates and not saddle points. For the most stable clusters of every size, the interaction of the hydrogen molecule with different possible sites are investigated. Special emphasis is laid on those sites being able to dissociate the molecule.

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2 - 3 – Thermoelectric effects in the (111)-FCC Al surface coupled to an interacting quantum dot

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We study the thermoelectric transport properties through the (111)-FCC Al surface coupled to a gate-defined quantum dot (QD). The local density of states (DOS) for the surface have been calculated using the Quantum-EXPRESSO package, which calculates the electronic-structure properties within Density-Functional Theory, using a Plane-Wave basis

set and pseudopotentials. The calculations were carried out with a (1×1) slab of five atomic layers. We obtain the surface Green's function (GF), linked to the (111) -FCC Al plane, using that surface DOS. The interaction between the QD and the surface is described employing the Anderson impurity model (AIM), in the frame-work of the Atomic Approach [1]. The localized state in the AIM is linked with the QD, considering finite U electronic repulsion inside it, the surface is associated with the continuous states in the model. The thermoelectric transport coefficients were obtained by the Keldysh non-equilibrium GFs technique with the Onsager relation in the linear regime automatically satisfied [2]. We compute the thermopower S , linear thermal conductance K , linear electric conductance G and the thermoelectric figure of merit Z , for all the regimes of the system, as function of the QD energy and the temperature T . Our results are similar to the obtained for a quantum wire with a side coupled QD [3,4] and for metallic surfaces with Kondo absorbed impurities (G results) [5]. We discuss the possibility of practical applications of the system in mesoscopic cooling process, based in the results of the ZT product.

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2 - 4 – Magnetic and structural properties of $Co_{1-x}TM_x$ (Fe, Cr and Mn) nanoparticles

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In the last years metal nanoparticles have drawn much attention because of their potential for development in building ultrahigh density hard drives, devices for biomedical applications and chemical sensing [1,2]. Therefore, for that materials can to have applications is necessary a good control of well-defined size, geometry and surface chemistry effects for minimize coalescence between the particles. In this sense several synthesis process (chemistry and physics) have

been extensively investigated. In this work we have studied the structural and magnetic properties of $Co_{1-x}TM_x$ (Fe, Mn and Cr) nanocrystalline alloys using X-ray diffraction and magnetic measurements. The nanocrystalline alloys were obtained chemical route via co-thermolysis of metallic acetylacetonate precursor in oleylamine surfactant/phenylether at low temperature ($TS \approx 250^\circ C$). X-ray diffraction results and Rietveld refinement analysis show for samples with concentrations lower than 20% of TM, the crystalline structure is similar to the cubic structure of the Co with average size of 5 nm. Magnetizations measurements as function of field show that the particles present to be soft magnetically. Zero-Field-Cooling and Field-Cooling magnetization curves suggest that the surface anisotropy prevail at low temperature and the systems are strongly interacting and same for samples disperse on the polymeric matrix. Transmission Electronic images would be shown to verify the morphology and size distribution of the nanoparticles. (CNPq)

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2 - 5 – Fe-based bulk metallic glass plates with Y and Gd addition

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Fe-based bulk metallic glasses (BMG) have been developed since 1995 and achieve an interesting combination of physical and mechanical properties. While conventional metallic glasses require rapid solidification with a cooling rate of about 10^6 K/s, BMGs can be formed at cooling rates between 1 and 100 K/s, leading to the possibility of casting much thicker objects. At first, Fe-based BMGs were developed with the purpose of obtaining very good soft ferromagnetic properties owing to the structural isotropy of the material (high Fe content alloys in Fe-B-Si system). However, during the last decade, researchers were able to prepare these materials with less Fe content, so that they become paramagnetic at room temperature. These materials were named structural amorphous steels (SAS) [1]. There were then obtained SASs with a maximum thickness of 16 mm, very high strength, high hardness and excellent corrosion resistance, but highly brittle. The aim of this work is to present our recent studies on amorphous alloys with composition (at%) $Fe_{48}Cr_{15}Mo_{14}C_{15}B_6Gd_2$ (A) and $Fe_{48}Cr_{15}Mo_{14}C_{15}B_6Y_2$ (B1). Copper-mold injection

casting in air atmosphere was used to obtain plate samples with a fix thickness of 2 mm and variable lengths between 10 and 20 mm. In order to evaluate the possibility of commercial application of the material, 56% (wt) of B1 alloy was replaced with commercial AISI430 steel and was cast into rods of 2 mm diameter (B2). The structure and microstructure of the obtained samples was studied by means of optical microscopy, X-ray diffraction and scanning electron microscopy. DSC measurements showed a glass transition temperature of 856 K for alloy A and 841 K for alloy B1, and an onset crystallization temperature of 887 K for alloy A and 885 K for alloy B1. Furthermore, the hardness of the alloy was measured by means of nanoindentation tests and was found to be around 13 GPa for both alloys. The role of Y and Gd on the formation of the glassy phase under adverse casting conditions including air atmosphere and the partial replacement of pure elements with commercial steel will be discussed.

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2 - 6 – Synthesis and characterization of Co_3O_4 Nanoparticles with addition of organic precursor

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In the last years several methods to synthesize nanostructured materials have been extensively explored to control the size, size distribution and morphology. Considerable interest in these properties is related to the good control in the physical properties that these materials can present. Besides of these properties, in particular, the magnetic nanoparticles (NP's) need to be in monodisperse suspensions. The head of this high demand is related to the new physical and chemical properties that arise in these materials with a decrease in their size compared to in bulk form. Thus, it is essential to search for methods of synthesis that produce nanoparticles with controlled size and morphology. In this paper we have use co-precipitation to synthesize Co_3O_4 NP's at low temperature, controlling the growth with the addition of an organic precursor (OP) to study the structural and magnetic properties. The nanoparticles were synthesized at temperatures of 80°C for 72h and 200°C for 3h with and without addition of OP. Results of X-ray diffraction together Rietveld refinement confirmed the formation of single crystalline phase for all samples. The results show that the crystallite average size of the resulting products ranges between 47

and 54nm for samples without addition of OP and a mean of 19nm for samples with OP, respectively. Results of Scanning Electron Microscope show particles with spherical morphology and sizes consistent with those obtained with the Scherrer formula trough values extracted by Rietveld refinement. Preliminary measures of magnetization as a function of applied field at room temperature, show a superparamagnetic behavior. Measurements of magnetization in SQUID magnetometer will be held to a more wide characterization of the magnetic behavior of the samples.

2 - 7 – Monte Carlo simulation of Geometrical Influence on Magnetic Properties of Ferromagnetic Nanotubes

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A computational model was developed for describing magnetic properties of ferromagnetic nanotubes. They were based on the Monte Carlo method with nearest neighbors interaction employing Metropolis dynamics. Magnetization per magnetic site, magnetic susceptibility, ferromagnetic energy and specific heat were computed for nanotubes with square and hexagonal unit cells. These properties were simulated varying parameters as the system size, temperature, and anisotropy; also an external magnetic field was taken into account. The dependence on the exchange parameter of the nanotubes geometrical appearance was also discussed. A strong influence on the magnetic properties, especially the Curie temperature because of the difference in the interactions density of the nanotubes was observed.

2 - 8 – Superparamagnetic nano magnetites forming oriented structures in elastomer composites

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Structured magnetoelastic composites are promising materials for its applications in field sensitive devices, such as field-modulated inductances and sensors of magnetic field and pressure. The central aspect is that smart materials can be obtained by combining the magnetic properties of fillers nanoparticles with the elastic characteristic of a hosting elastomeric polymer matrix, particularly when anisotropy is induced in the composite. In the present work the preparation and characterization of structured composites is presented, using nanoparticles of magnetite as fillers and polydimethylsiloxane (PDMS) as the elastomer matrix. The strategy for obtaining structured magnetoelastomers was preparing the magnetite-PDMS mixture before casting and then curing the mixture in the presence of a uniform, and relatively intense, magnetic field.

Magnetite nanoparticles were prepared by the coprecipitation method, dissolving stoichiometric amounts of the precursors (Fe(II) and Fe(III) chlorides), in acid media, which was added to a basic solution at controlled pH and temperature. The precipitation of dark brown nanoparticles occurred immediately. The obtained material was magnetic, with superparamagnetic behavior at room temperature (determined by Vibrating Sampling Magnetometer, VSM). XRD pattern was compatible with magnetite structure, while SEM images shown particles of 15 nm average size.

Mixtures of magnetite-PDMS at defined proportions were placed for curing inside a cylindrical mould, which is part of a designed device that allows curing the samples at a given temperature in the presence of an applied magnetic field, while rotating the sample at constant speed. Formation of chains (needles) of magnetite aggregates, oriented in the direction of the applied field, appears after polymerization. Chains as long as 1.5 mm length and 40 microns diameters were observed, which are composed by aggregation of particles with individual sizes about 20 nm. Anisotropic effects are under quantification at present, both for the magnetic and elastic properties, by VSM, SQUID and texture analysis(1).

It is remarkable that the anisotropic composite is obtained using superparamagnetic particles, while for the case of cobalt-iron oxides, structured composites were obtained when using ferromagnetic nanoparticles only.

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2 - 9 – Nickel ferromagnetic nanoparticles of different sizes in anisotropic magnetoelastomer materials

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Magnetoelastomers are dispersions of magnetic particles into an elastomer polymer matrix [1,2]. These materials combine magnetic and elastic properties in the same material. In this work, nickel ferromagnetic nanoparticles were synthesized, following Sidhaye et al [3]. The syntheses were performed at different concentrations and temperatures (up to 60° C) in order to explore their influence in the properties of nanoparticles. The X-ray powder diffraction patterns indicate that the formation of Ni nanoparticles is favored at low concentration of reactants and at room temperature. As the concentration of reactants and the temperature of synthesis are increased, formation of hydroxides and oxides nanoparticles of Ni(II) and Ni(III) is observed. SEM images show a significant decrease in the particle size when both the concentration of reactants and temperature of synthesis are increased. VSM (Vibrating Sample Magnetometer) measurements are in good agreement with the results of XRD and SEM. First, in the case of nanoparticles synthesized at room temperature and low concentrations of reactants, a ferromagnetic behavior is observed. Moreover, a saturation magnetization of about 40 emu/g is obtained. Second, with other synthesis conditions, a marked decrease of the saturation magnetization is observed, due to the presence of hydroxides/oxides of Ni(II) and Ni(III). Composites of PDMS (poly-dimethylsiloxane) and nanoparticles synthesized at room temperature were prepared. In the absence of an external magnetic field during curing, composites of uniform distribution of nanoparticles are observed in SEM images. On the other hand, when curing is performed in the presence of an external magnetic field, formation of macroscopic needles oriented along the direction of the magnetic field is observed. Those needles were also observed by SEM, being wider when preparing

composites with nanoparticles with higher saturation magnetization. Finally, the composites were characterized by VSM and texture measurements. From those results it is concluded that the material have both magnetic and elastic anisotropy.

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2 - 10 – Nanostructured ZnO layer fabrication by pulsed electrodeposition for morphology control

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ZnO electrodeposited layers have properties strongly dependent on their morphology. Their applications are directly linked to the obtained properties. On this paper a fabrication method based on pulsed electrodeposition is presented with good results on final morphology control. The samples are fabricated over ITO sputtered glass substrates. Process optimization is guided through AFM analysis of the nucleation stage according to different pulse train designs. SEM characterization and electrochemical techniques allow the evaluation of the morphology and the properties obtained. Optical properties characterization allows a bandgap measurement correlated to the obtained morphology through the Tauc plot.

2 - 11 – Study of Al-doped Zinc Oxide nanocrystalline powders subjected mechanical milling

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The interest in new materials of nano-sized scale for applications in industry, medicine and other fields has led to research in the many ways of producing them with good efficiency and trying to improve the quality of the final products. Of the many techniques of obtaining nanomaterials, mechanical ball-milling has the virtues of being efficient in producing large

amount of material, obtaining incorporation of doping material into the main structure and/or creating blends, alloys, non-equilibrium phases and oxide-reduction reactions, etc. This is of particular importance in the study of semiconductors, like ZnO, whose electrical/optic/other properties can be ameliorated with doping of metals or metal-oxide substances. The aim of this article is to study the final products of milling ZnO powders doped in different proportions (5, 10 and 30 at%) with Al powder. We have used X-ray diffraction (XRD) for following the structural ZnO changes. We have observed that under certain circumstances ZnO can be reduced in milling with Al without obtaining alumina. XRD patterns corroborate the incorporation of aluminum into the wurtzite ZnO structure. Ternary oxides of the form $Zn_{1-x}Al_xO$ are obtained in all samples subjected to 16 hours of milling time. Avoiding the reduction of ZnO in mechanical milling with Al is a question of low doping fraction and large milling duration.

2 - 12 – Ab initio study for ultrathin Fe films onto MnAs

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Recent magnetic anisotropy measurements of Fe thin films epitaxially grown on MnAs/GaAs(001) [Phys.Rev. B 82,094423 (2010)] show that Fe films are magnetically decoupled from the MnAs substrate at low temperatures. This unexpected behaviour motivated us to tackle this system by means of first principles calculations.

We compute the magnetic interaction of Fe ultrathin films onto a MnAs slab taking into account different possible interfaces between them. Our calculations suggest that the Fe magnetic properties are independent of the magnetic configuration of the MnAs substrate and that interfacial effects seem to play an important role in the decoupling mechanism.

2 - 13 – Gas Sensing Properties of Nanostructured MoO₃ Thin Films Prepared by Spray Pyrolysis

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Molybdenum oxides are extremely interesting from a chemical point of view because of their wide exploitation in both, catalytic and industrial processes of

industrial relevance. In recent years, a strong research effort has been made for developing gas sensors based on these materials. In this work, thin films of molybdenum trioxide (MoO_3) were deposited on common glass using the chemical spray pyrolysis technique. A $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}\text{H}_2\text{O}$ solution 0.1M was used as precursor one. The influence of substrate temperature on the crystallographic structure, surface morphology and electrical behavior of MoO_3 thin films was studied. MoO_3 can exist in two crystalline forms, the thermodynamically stable orthorhombic α - MoO_3 and the metastable monoclinic β - MoO_3 phase. XRD-spectra showed a growth of α - MoO_3 phase percentage as substrate temperature increases from 450K up to 700K. Films deposited in the 500-600K range have a clearly porous surface structure of nanometer order as can be seen in SEM images. Changes up to six magnitude orders were observed in MoO_3 thin films electrical resistance when films temperature varied from 100K up to 500K. The sensing property of these MoO_3 films was also studied. The sensitivity was investigated in the temperature range 160K and 360K for H_2O and CO gases. Both of them are of reducing nature. In all studied cases sensitivity decrease slowly as film temperature is raised. At room temperature the sensitivity changes from 15 up to 70 depending on substrate temperature. The sensitivity for CO gas was found to be lower than that of H_2O .

2 - 14 – Dynamic coercivity of Mo-doped FINEMETs

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Over the past decades, there has been an important interest in nanocrystalline soft magnetic materials due to their attractive magnetic properties compared with conventional crystalline alloys. These materials are suitable for a wide range of applications at ac field such as transformer cores, inductive devices, sensors, etc. and, therefore, it is important to know their frequency dependence of their magnetic properties.

In previous works, the structure and some magnetic properties of a series of FINEMET-type alloys with a partial replacement of Nb by Mo has been studied including: i) the magnetostrictive behaviour of the series, ii) a thorough analysis of the phase transformations occurring during the crystallization process of the alloys and finally, iii) the estimation of amorphous and crystalline phases' fractions, chemical compositions and contributions in the magnetization of the sample.

It is the aim of the given contribution to present a study of the frequency dependence of the coer-

civity in as-quenched (amorphous) and isothermally annealed (nanocrystalline) samples of composition $\text{Fe}_{73.5}\text{Si}_{13.5}\text{B}_9\text{Nb}_{3-x}\text{Mo}_x\text{Cu}_1$ ($x = 0, 1.5$ and 3 ; Mo0, Mo1.5 and Mo3, respectively). Although the general form of the curves coercivity vs frequency is the same for all ribbons, a clear distinction in the values was observed between the amorphous and the nanocrystalline samples. Moreover, a molybdenum-content dependence of the dynamic coercivity was seen.

2 - 15 – Magnetic coupling and exchange-bias on multilayers with CoFe_2O_4 as pinner layer

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Multilayered films composed by two decoupled ferromagnetic thin layers separated by a non-magnetic (NM) spacer layer are the basic architecture of spin valve devices and magnetic random access memories (MRAM). The decoupling can usually be obtained by different methods, one of them is the use of a synthetic antiferromagnet (such as $\text{Ir}_{20}\text{Mn}_{80}/\text{Co}/\text{NM}/\text{Ni}_{81}\text{Fe}_{19}$) [1]. The natural CoFe_2O_4 ferrimagnet is a suitable candidate for its use as pinner layer for these systems grown by pulsed laser deposition technique [2]. We prepared $\text{CoFe}_2\text{O}_4(340\text{nm})/\text{FM}(50\text{nm})/\text{NM}(5\text{nm})/\text{FM}(50\text{nm})$ multilayered films (NM = AlO_x and TiO_2 , FM = Fe and $\text{Ni}_{80}\text{Fe}_{20}$) by pulsed laser deposition (Nd-YAG, $\lambda = 355$ nm). The films were grown on a $\langle 100 \rangle$ Si substrate. The structural properties of the samples were analyzed by X-ray diffraction and scanning electron microscopy. At low temperature (50K), a good coupling between free and pinned FM layers was observed only for $\text{CoFe}_2\text{O}_4/\text{Fe}/\text{TiO}_2/\text{Fe}$. For both multilayers with FM = $\text{Ni}_{80}\text{Fe}_{20}$, it was observed a vertically biased cycle that is originated in uncompensated magnetic moments at the interface between CoFe_2O_4 and pinned $\text{Ni}_{80}\text{Fe}_{20}$ layers. Moreover in these samples, ZFC and FC measurements show a monotonically decrease with T, fact that also reinforces this hypothesis.

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2 - 16 – Synthesis and Magnetic Properties in Fe₂O₃ Nanorod obtained using chelating agent

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Much attention has been gained on the magnetic nanomaterials by researchers from various fields such as physics, medicine, biology, and materials science due to their multifunctional properties such as small size, superparamagnetism and low toxicity [1]. In this work Fe₂O₃ nanopowders were synthesized in nanoscale dimensions by co-precipitation method on the addition of a chelating agent. X-ray diffraction and Rietveld refinement analysis results added to the magnetism results show that the addition of organic precursor in the synthesis influence significantly on the control particles sizes distribution. Transmission and scanning electron microscopy images show that the particles change your shape from 5 nm for faceted particles and 8x30 nm² for nanorods to depend of the agent chelating concentration. These results also show a preferential growth in 110 crystalline plane for nanorod. Therefore for samples prepared without organic precursor present average size of 75nm and temperature-dependent field cooling magnetization showed that there was Morin transition, in which indicate a large particle size distribution. ZFC-FC magnetizations curves show that samples obtained at low temperature present a superparamagnetic behavior with blocking and irreversibility temperatures around 95 and 135K, respectively, which increase with increasing of synthesis temperature. Moreover, we have found that the presence of chelating agent in the synthesis inhibited the coalescence effect (CNPq, FAPITEC-SE).

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2 - 17 – Raman characterization of bulk ferromagnetic nanostructured graphite

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Despite the fact that in the last 20 years have regularly appeared reports with experimental verification of the presence of ferromagnetism in pure carbon materials, still exists skepticism about this phenomenon being intrinsic. Previously, we presented a method for modifying pristine graphite in order to obtain ferromagnetic graphite at room temperature. This method is relatively easy to implement and economically affordable, which makes it particularly interesting for technological applications. Such materials could be used in magnetic imaging in medicine, communications, electronics, sensors and/or catalysis. In this work Raman spectroscopy was used to characterize bulk ferromagnetic graphite samples. The G:D band intensity ratio, the position of the 2D band and the presence of a band around 2950 cm⁻¹ showed a high degree of disorder in the modified graphite sample, with a significant presence of exposed edges of graphene as well as a high degree of attached hydrogen atoms.

2 - 18 – Electronic properties of NbS₂ and TiS₂ low dimensional structures.

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Transition metal dichalcogenides are well known because of their laminar structure, weakly bound through van der Waals interactions. Due to their technological applications in catalytic processes the bulk structure of many of them has been widely studied in the last 30 years. Some of them, such as NbTe₂ and TiSe₂, show superconductivity and, due to this, have been the subject of intense study. In 2004 Novoselov *et al* achieved to isolate not only graphene but also other bidimensional crystals, among them monolayers of some dichalcogenides [1]. These bidimensional crystals preserve their monocrystallinity under normal ambient conditions, keeping the crystal structure of the bulk. In this contribution we study the magnetic and electronic properties of 2D monolayers of NbS₂ (metallic in 3D) and TiS₂ (semimetallic in 3D) and the presence and characteristics of edge states of quasi 1D stripes of different widths cut out of these layers.

[1] K.S. Novoselov, D. Jiang, F. Schedin, T.J. Booth, V.V. Khotkevich, S.V. Morozov and A.K. Geim, PNAS 102, 10451 (2005)

2 - 19 – FESEM and GIXRD characterization of nanostructured NiCr thin films

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The application of NiCr thin films is widely well established in several microelectronic applications due to its relative large resistivity, more resistant to oxidation and a low temperature coefficient of resistance (TCR). These interesting properties of NiCr thin films show a strong dependence on their preparation conditions, i.e. the deposition environment and subsequent annealing treatments.

In this case, NiCr thin films were deposited by RF magnetron sputtering on a Si/Si₃N₄ substrate using a 3-inch Ni/Cr (80/20 %wt) alloy target. The thickness for each sample was 50 nm. Annealing treatments were subsequently performed at three different temperatures during 6 hours at 400, 600 and 800 °C in air and N₂ ambient, respectively. These temperatures were chosen in order to appreciate the change of the crystal size and the surface composition of the thin films according with the recrystallization temperature. In this work, the appreciation of the three stages in the annealing process of a NiCr metallic alloy in a nanostructured scale is aimed. The annealing process is split in three stages: recovery, recrystallization and grain growth, respectively. To observe this effect, surface composition of each sample is determined. It is also studied, how the crystal growth in N₂ ambient was formed and stabilized due to the suppression of oxidized substance on the film surface. Crystallographic structure as well as interatomic spacing of this nanocrystalline material is also characterized.

The characteristics of these films such as crystal structure and changes of microstructure are analyzed as function of annealing temperature and atmosphere conditions. In this work, surface composition and crystallography of the samples are determined by means of field emission scanning electron microscopy (FESEM/EDAX) and X-ray diffraction in the grazing incidence mode (GIXRD) methods, respectively.

Comparisons of structural and crystallographic properties of the nanostructured RF sputtered NiCr thin films under the variation of annealing conditions will be presented on final paper.

2 - 20 – Electron Spin Resonance studies of Magnetic Ions (Er³⁺, Yb³⁺ and Mn²⁺) Diluted in Ag Nanoparticles

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Ag nanoparticles doped with Er are of particular interest in industry of photonics, due to the remarkable enhancement of the Er³⁺ photoluminescence intensity. In this paper we describe the synthesis of nanoparticles doped with Re = Er³⁺, Yb³⁺ and Mn²⁺, by reducing the AgNO₃ and oxides of transition ions. We have performed the structural characterization and the study of the magnetic properties of these ions (concentration = 5%) diluted in colloid Ag nanoparticles. Electron Spin Resonance experiments indicate that magnetic ions are located in the matrix cubic in the AgRe. The exchange interaction, $J_{fs}\mathbf{S}_f\cdot\mathbf{s}$, between the Re localized magnetic moment and the host's conduction-electrons has no effect on the ESR data, in contrast to bulk system.

2 - 21 – Electronic Structure of TiO₂ and related nanostructures for Dye Sensitized Solar Cells

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The dye sensitized solar cell (DSSC) is an emerging alternative for the production of electricity from solar energy. It is based on a junction between a n-type wide gap semiconductor and a p-type light absorbing material. The selected material for the first one, in most cases, corresponds to TiO₂ nanoparticles, while the second one consists on an organic or inorganic dye. The open-circuit voltage generated in the cell corresponds to the difference between the Fermi level of the electron in the solid and the redox potential of the electrolyte used in order to regenerate the dye molecule. Thus, the electronic structure, and in particular the band gap of the n-type nanoparticles, influence the efficiency of the cell [1]. In this work we present structural and electronic properties study for bulk polymorphs of TiO₂, and related nanostructures simulated by slabs. All of them are based on: Rutile, Anatase and Monoclinic TiO₂(B). We report band gaps and surface energies, discussing the geometrical reconstruction in each case. TiO₂(B) is included due to experimental results, in which it appears during the thermal annealing of H₃Ti₃O₇ nanostructures obtained by hydrothermal synthesis [2], which

was also verified by our group. Since there is no much work on this polymorph nanostructure, our findings could contribute to the state of art of TiO₂ for DSSC purposes. The simulations were performed using the DFT-GGA, using SIESTA code [3], Quantum Espresso [4] and WIEN2k [5]. SIESTA calculations were used for the structural optimization of bulk and slab models. After this surface energy were determined by Quantum Espresso, which adopts a plane-wave basis set. Finally, for the bulk structures, we performed all-electron-full-potential-plane-wave code WIEN2k, in order to apply the recent modified-Becke-Johnson exchange potential + LDA-correlation [6], which allows better estimation for band gaps, closer to experimental ones. The comparison between these models is also based on the corresponding band gaps, and surface energy [7-8].

[1] M. Grätzel, *Journal of Photochemistry and Photobiology C: Photochemistry Reviews* 4, 145 (2003)
 [2] Y. V. Kolen'ko et al, *J. Phys. Chem. B* 110, 4030 (2006) [3] Soler, J. M. et al, *J. Phys.: Condens. Matter* 14, 2745 (2002) [4] Giannozzi, P. et al, *J. Phys.: Condens. Matter* 21, 395502 (2009) [5] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2 [6] F. Tran, and P. Blaha, *Phys. Rev. Lett.* 102, 226401 (2009). [7] O.V. Prezhdo et al, *Progress in Surface Science* 84, 30 (2009). [8] M. Casarin et al, *ACS Nano* 3 (2), 317 (2009).

2 - 22 – Density Functional Theory applied to the study of Au atom and dimer on MgO(001) surface

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The most important catalytic reactions in the chemical industry are those that take place on metals, mainly transition metals. However, some metal oxides have electronic and physical properties that can induce catalytic properties of metals. Among the wide variety of oxides available for the application in catalytic systems, magnesium oxide has particularly been used in both theoretical and experimental basic research due to its apparent structural simplicity and facility of synthesis. It has been found that the most important properties of the MgO are directly or indirectly related to the presence of defects, particularly of defective points. The most important defects in magnesium oxide are those created by oxygen vacancies. It is well known that defects not only can act as catalytic

centers for chemisorption of small species but also as nucleation centers for growing metal clusters and can modify the catalytic activity of these adsorbed metal particles via the metal-support interaction at the interface. In the present work, we carried out a systematic study using Density Functional Theory (DFT) to analyze the adsorption energy and chemical reactivity of one Au atom and the Au₂ dimer on regular site and neutral oxygen vacancies (Fs sites) of MgO(001) surface. The molecular electrostatic potential (MEPs) have been used to determine how the reactivity of a particular site on MgO(001) surface changes during the adsorption of Au_n (n=1-2). Our results indicate that the neutral oxygen vacancies is more reactive than regular sites of MgO surface and does not promote dimerization of gold.

2 - 23 – Anisotropy and relaxation processes of uniaxially oriented CoFe₂O₄ nanoparticles dispersed in PDMS

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When a uniaxial magnetic field is applied to a non-magnetic dispersive medium filled with magnetic nanoparticles, they auto-assemble into thin needles parallel to the field direction, due to the strong dipolar interaction among them. We have prepared in this way magnetically oriented nanocomposites of nanometer-size CoFe₂O₄ particles in a PDMS polymer matrix, with 5 and 10 % w/w of magnetic particles. In this work, we present the characteristic magnetization and magnetic relaxation curves measured with applied magnetic fields forming an angle α with respect to the needle direction. In both experiments, a small magnetic anisotropy is present. We show that the magnetic viscosity (calculated from the logarithmic relaxation curves) as a function of α presents a minimum at $\alpha=0$, indicating slower relaxation processes associated with this configuration of fields. The results seem to point out that the local magnetic anisotropy of the nanoparticles is oriented along the needles, resulting in the macroscopic magnetic anisotropy observed in our measurements.

2 - 24 – On Local Temperatures for Quantum Driven Systems and Heat Flow

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We introduce thermometers to define the local temperature of an electronic system driven out-of-equilibrium by local AC fields. We also define the effective temperature in terms of a local fluctuation-dissipation-relation. We show that within the weak driving regime these two temperatures coincide. We also discuss the behavior of the local temperature along the sample. We show that it exhibits spatial fluctuations following an oscillatory pattern. We also show that the local temperature is the correct indicator for heat flow and its use allows for a generalization of the Wiedemann-Franz law.

2 - 25 – Magnetization reversal in Ni and Co nanowire arrays: simulations and measurements

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The study of magnetic nanostructured systems is a topic that attracted considerable interest due to their interesting physical properties and potential technological applications. In particular, highly ordered arrays of magnetic nanowires produced inside the pores of anodic alumina membranes by electrochemical deposition have been the focus of intense research. Different groups have investigated the stable magnetic configurations as a function of the aspect ratio of the magnetic cylinders, the reversion mechanisms of the magnetization in nanowires, the influence of magnetostatic interactions among nanowires, and in general, the behavior of the magnetic properties as a function of different parameters.

In this work, we perform a study of the magnetic properties (reversal mode, coercivity and remanence) as a function of the angle existing between the applied field and the nanowire axis through micromagnetic simulations and measurements. Arrays of Ni and Co nanowires have been prepared by electrodeposition into nanopores of alumina membranes which were prepared from an ultra pure aluminum foil by the two-step anodization technique. The morphological characterization of this system was performed by Transmission Electron Microscopy (TEM) which reveals an ordered hexagonal structure. Magnetic properties were studied in a Vibrating Sample Magne-

tometer (VSM) with the external magnetic field applied at different angles. The magnetization reversal has been investigated using the three-dimensional Object Oriented MicroMagnetic Framework software (OOMMF). In this work we investigate the magnetic properties of Ni and Co nanowires characterized by 1 μm of length and 25 nm of radii. In order to study the effect of the magnetostatic interactions between the wires, we have simulated a hexagonal cell of seven nanowires with a 100 nm center-to-center distance. We have used the exchange coupling $A = 30 \times 10^{-12}$ J/m ($A = 9 \times 10^{-12}$ J/m) and saturated magnetization $M_s = 5.2 \times 10^5$ A/m ($M_s = 4.9 \times 10^5$ A/m) for Co (Ni) nanowires. Besides, we have used a size mesh of 5 nm in which magnetization is free to rotate in three dimensions. In all the cases the damping constant is 0.5. The magnetostatic interaction between the nanowires reduces the coercivity, in contrast to the remanence which is not affected. Finally, the simulation results are compared with the measurements at Ni and Co nanowire arrays.

2 - 26 – Study of the magnetic properties of Ni granular films

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In this work, we perform a study of the magnetic and morphological properties of the granular $\text{Ni}(\text{SiO}_2)$ films which were prepared in a magnetron co-sputtering system, with the transition metal and SiO_2 (or Ag) targets mounted on two separate guns. The glass substrates were rotated during sputtering, to ensure composition uniformity. The metal volume fraction was controlled by the relative sputtering rates, and then determined by energy-dispersive X-ray spectroscopy using a Philips EDAX XL30 on films deposited in the same run on Kapton. The samples deposited on Kapton were used for magnetic measurements. The morphological characterization of this system was performed by Transmission Electron Microscopy (TEM) and High Resolution Transmission Electron Microscopy (HRTEM) which reveal a structure with extremely fine dispersion of Ni metal nanoparticles embedded in an insulating matrix. Magnetic properties were studied in a Superconducting Quantum Interference Device (SQUID) and a Quantum Design MPMS XL7 system in the temperature range 5-300 K showing that these Ni nanoparticles are superparamagnetic.

In order to have a more detailed picture of the magnetic characteristics of this system at 5 K, we have performed a detailed magnetic characterization by means

of First Order Reversal Curves (FORC) and FORC diagrams. The major hysteresis loops, delineated by the outer boundaries of the FORCs, correspond exactly to the hysteresis curves of the sample. The Ni nanoparticles show a regular hysteresis loop with a coercivity of 850 Oe at 5 K, in contrast with the superparamagnetic hysteresis loop at 300 K. In the FORC diagram of the sample at 5 K one can observe the presence of a narrow ridge centered around 0 Oe, that is the reversible component of the magnetization, and only one narrow ridge along the coercivity axis corresponding to the irreversible component of magnetization, this ridge is peaked at 817 Oe, near the major hysteresis loop coercivity value of 850 Oe. This pattern is characteristic of a set of noninteracting single-domain particles as is expected for this sample. Finally, the distribution of coercivity of the FORC diagram at 5 K is related to the size distribution of the Ni nanoparticles.

2 - 27 – Microwave absorption behavior of a polyaniline magnetic composite in the X- band

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The development of nanosized materials is a subject of considerable interest both for understanding of the fundamental properties of magnetic materials, and for new technological applications. Polyaniline (PANI) / Fe₃O₄, Fe₂O₃ composites with conducting, magnetic and electromagnetic properties were successfully prepared with various amounts of Fe₃O₄, Fe₂O₃. The samples were characterized structurally by scanning electron microscopy and x ray diffraction and magnetically with a vibrating sample magnetometer. In order to explore microwave-absorbing properties in X-band, composite nanoparticles were mixed with an epoxy resin to be converted into a microwave-absorbing composite. Microwave behavior with different Polyaniline (PANI) / Fe₃O₄, Fe₂O₃ ratio (9, 14 and 18%w/w) were studied using a microwave vector network analyzer from 7.5 to 13.5GHz. Absorption increases when sample ratio increases for a constant thickness of 2 mm. Magnetite contents increase sample absorption. Preliminary results on samples prepared under a moderate magnetic field are presented.

2 - 28 – Four terminal resistance of an interacting quantum wire with a back-scattering impurity.

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We investigate the behaviour of the four-terminal resistance R_{4pt} in an interacting quantum wire described by a Luttinger liquid in the presence of a single impurity within the wire. Results are discussed at zero and finite temperature, as well as the effects of the relative magnitudes of the coupling parameters involved in the system.

2 - 29 – Graphene on epitaxial ferroelectric BaTiO₃: an atomistic study

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The exceptional electrical properties of graphene have made it a promising material for device applications, such as field effect transistors. However its intrinsic high mobility can be degraded when it is supported on a dielectric substrate, as the widely used SiO₂, due to the substrate surface properties. Recently it was reported that graphene mobility increases when SiO₂ is replaced by a ferroelectric material, which is characterized by a reversible nonvolatile electric polarization. Here we study the interaction of a graphene nanodot with the film surface of the prototypical ferroelectric BaTiO₃ using atomistic modeling through Molecular Dynamics simulations performed at room temperature. The ferroelectric film is under bi-axial compressive strain presenting a tetragonal (001)-oriented phase, and domains with electric polarization pointing towards and inwards the surface. Binding energies for graphene dots of different sizes depending on the polarizations and boundaries of the domains are reported.

2 - 30 – Adsorption of Mn and V on BN nanotubes: a theoretical study

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Boron nitride nanotubes (BNNts) have extraordinary chemical and physical properties that suggest a large number of nanotechnological applications. In particular, the study about adsorption of transition-metal atoms on BNNts is interesting for the changes that it produced in nanotube's properties. Previous studies have found that transition-metal atoms like V, Mn and Cr are adsorbed on the walls of BNNts and cause a net magnetic moment ($4.39 \mu_B$ with an atom of V, $4.99 \mu_B$ with Mn y $4.08 \mu_B$ for the Cr) [1]. These results suggest their use on spintronics and molecular electronic. By means of calculations based on Density Functional Theory (DFT) within ultrasoft pseudopotential approximation [2], we study the adsorption of atoms of Mn and V on (8,0) zigzag and (5,0) arm-chair BNNts. In each case, we found adsorption energies of most stable configurations (0.04 eV for Mn and 0.47 eV for V). This, in contrast with previous results reported by Wu et. al. (0.4 eV for Mn and 0.83 eV for V) [1]. In this work, we study changes in electronic properties of systems (band structures, densities of states and charge densities) produced by the adsorption. This study reveals important aspects about potential bonds on external walls of BNNts.

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2 - 31 – Characterization of Platinum clusters through chemical reactivity descriptors and vibrational spectroscopy: a theoretical study .

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Metallic clusters have been the object of many studies, due to the novel properties that they present at

bulk level. Transition metal clusters have been studied for its potential use as catalysers and in the production of electronic nanodevices. In particular, platinum clusters are used as catalysers in chemical industry, in CO, NO reduction and play an important role in fuel cells to produce energy from Hydrogen, as an alternative source of clean energy. Theoretical computations by means of density functional theory (DFT) were performed to study structural evolution, electronic properties and vibrational spectroscopy of Pt_n ($n=2-13$) clusters. Here we present the characterization of such clusters through global reactivity descriptors, chemical potential, chemical hardness and electrophilicity index, computed using vertical electronic affinities and ionization potentials. Our results show that platinum clusters tend to stabilize in high spin configurations, as reactivity and size increase. All computations were performed with B3PW91 exchange and correlation functional and Gaussian 03 suite of programmes.

2 - 32 – Large surface anisotropy in Fe-doped NiO nanoparticles

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Nanoparticles (NP's) have been subject of several studies due to the new properties that these materials present when crystallite size is reduced. In case particular of the magnetic nanoparticles, your properties are modified when NPs have size lower than 10 nm [1]. These magnetic properties are related to the finite size effects and/or high surface/volume ratio [1,2]. Besides the interface effects can present magnetic properties different of the superparamagnetic behavior observed in these systems. Surface and interface driven properties play a dominant role in all applications of magnetic nanoparticles [2]. In this sense, the main challenge is the control of the size, size distribution and morphology of NP's. In this work, we have used the co-precipitation method [3] to obtain $Ni_{1-x}Fe_xO$ nanoparticles with different particle sizes and doping concentrations ($1\% \leq x \leq 10\%$) in the presence of organic precursor to study the magnetic and structural properties. X-ray diffraction (XRD) results show that all samples present NiO cubic crystallographic phases without presence impurities phases. Our analysis XRD using Rietveld refinement and Scherrer equation show a decreasing in the particle size as function of synthesis temperature and of the doping amount. ZFC-FC magnetization curves carried out on a superconducting quantum interference device (SQUID) magnetometer point out a non-homogeneous distribution of particle size and a large surface effect for 10% Fe-doped samples at low temperature region. We believe that this behavior can be associated to the bro-

ken exchange bond resulting of freezing of disordered surface spins caused by Fe ions.

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2 - 33 – CT-AFM Electrical Transport Studies in Patterned Silver-Mesoporous Titania Nanocomposite Thin Films

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The unique electronic, optical catalytic and chemical properties of metallic nanoparticles (NP) embedded in oxide thin films represent a great promise for advanced applications such as nanoelectronics, bioanalysis and optoelectronics. For the development of NP-based electronics, it is desirable to engineer three-dimensional arrays of metal nanoparticles that can be used as highly controlled wires, circuits and/or electrodes. Embedding NP within thin films permits to exploit their properties derived from size or confinement and protect them from the environment. Mesoporous thin films (MTF) provide restricted chemical environments and grant accessibility to ions or molecules due to their controlled pore size domains, constituting ideal matrices for metallic NP inclusion. In this work, we explore the 3D electronic conductive properties of patterned nanocomposites formed by TiO_2 MTF loaded with Ag NP by the Photocatalysis-Assisted Mesopore Patterned Array (PAMPA) lithography procedure previously *developed*¹ We performed conductive tip atomic force microscopy (CT-AFM) measurements to study for the first time the localized electrical properties of the NP-MTF patterned nanocomposite, A remarkable conductivity dependence on the film mesostructure and metal NP loading was observed, confirming a three-dimensional current flow throughout the nanocomposite.

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2 - 34 – Characterization structural, morphological and optoelectrical of Bi_2S_3 thin films grown by co-evaporation

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This work presents results concerning the synthesis and characterization of polycrystalline n-type Bi_2S_3 thin films. The films were grown by a chemical reaction of their precursor elements which are co-evaporated on a soda-lime glass substrate, and later will be used as an buffer layer in solar cells based in Cu_3BiS_3 . The effect of the preparation conditions on the optical, morphological and structural properties, as well as on the electrical conductivity (σ) was studied through spectral transmittance, X-ray diffraction (XRD), atomic force microscopy (AFM) and σ versus T measurements, respectively. The results revealed that, independently of the deposition conditions, the films grow only in the orthorhombic Bi_2S_3 bismuthinite phase. It was also found that the Bi_2S_3 films present an energy band gap E_g of about 1.38 eV, regardless of the thickness of the samples. It was also found that the electrical conductivity of the Bi_2S_3 films is affected by the transport of free carriers in extended states of the conduction band as well as for variable range hopping transport mechanisms, each one predominating in a different temperature range

2 - 35 – Impurity-assisted chain creation in transition-metal break junction experiments studied from first principles

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In the last few years, one-dimensional systems were experimentally realized as suspended monoatomic chains in mechanically controllable break junctions (MCBJs). In these experiments the chains under consideration are not at their equilibrium interatomic distance due to mechanical stress. Using first-principles calculations, we extended a stability and producibility

criteria for chain formation to zig-zag and dimerization and applied it successfully to Cu, Ag, Au, Ir and Pt atomic chains.

It has been shown experimentally that oxidization of chains can trigger the formation of significantly longer chains. The improvement of our model for chain formation enables us to take a detailed look into impurity assisted chain formation, where zig-zag bonds can play an important role. In particular we focus on O, N, C and H assisted noble metal as well as magnetic Ir and Pt chains. For simplicity, we assumed that the presence of impurity atoms in experiments results in ..M-X-M-X... (M:metal, X:impurity) chain structure in between the metal leads.

2 - 36 – Synthesis and characterization of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3/\text{SiO}_2$ core-shell nanoparticles

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$\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x=0.22, 0.3$ and 0.33) nanoparticles (NP) were synthesized using liquid-mix method, starting from metallic nitrates and adding citric acid to obtain cation complexes and ethylenglycol to polymerize. The powder obtained after a thermal treatment at 700°C was dispersed in isopropyl alcohol and SiO_2 coated using the Stöber method. An aqueous ferrofluid of $\text{La}_{0.78}\text{Sr}_{0.22}\text{MnO}_3$ (0.6mg/ml) and gels from $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x=0.3$ y 0.22) NP and oil-wax gel (Gelwax®) were prepared. X Ray diffraction analysis, scanning and transmission electron microscopy, infrared spectroscopy and magnetic measurements were used to characterize the samples.

The thermal response of a ferrofluid containing $\text{La}_{0.78}\text{Sr}_{0.22}\text{MnO}_3$ (NP) suspended in aqueous solution of chondroitin 6-sulfate sodium salt (3mg/ml), and a gel containing $\text{La}_{0.75}\text{Sr}_{0.3}\text{MnO}_3$ NP were studied, while exposing the samples to a RF magnetic field (41 kA/m, 260kHz). The temperature vs. time curves were recorded and the gel's Specific Loss Power (SLP) was obtained from the initial slope of such curves. SLP values around 3W/g were obtained. The relationship of SLP to the variable AC field was studied.

The order temperature of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x=0.22$ and 0.33) NP, was determined by Magnetic-Thermo-Gravimetry, leading values of about 334K and 368K, respectively. From the comparison of ac susceptibility measurements on coated and uncoated samples ($x=0.33$), the thickness of the SiO_2 layer was estimated to be of the order of 4 nm. M vs H curves have a

Langevin-like shape, however displaying a small coercivity of about 30 Oe ($x=0.22$). From these curves magnetic cores of 14 to 21 nm diameter were estimated.

2 - 37 – Charge localization in Co doped Ceria with oxygen vacancies

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The search and development of novel materials, ferromagnetic beyond room temperature, is currently a subject of intense work with the driving force of its potential technological applications. In this regard, Cerium oxide with diluted magnetic impurities is a natural candidate for spintronics as it offers a good integrability with the current electronic devices. However, this material still poses several questions being the main one to find a widely acceptable explanation for the observed room temperature ferromagnetism. There is experimental evidence supporting the idea that the free electrons left behind by oxygen vacancies localize themselves in specific Cobalt and Cerium atoms, changing their oxidation states ($\text{Co}^{4+} \rightarrow \text{Co}^{2+}$ and $\text{Ce}^{4+} \rightarrow \text{Ce}^{3+}$, respectively) and turning the Cerium atoms into magnetic ones. The study of this charge localization is crucial to approach an understanding of the magnetic properties in these materials. Using the framework of the density functional theory, we study the relative stability of different Oxygen vacancies and we show that they tend to locate close to the Co impurities. In addition, we address the issue of charge localization in these materials for different concentrations of both Co impurities and Oxygen vacancies.

2 - 38 – Structural and magnetic properties of FeGa alloy grown as thin film

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The FeGa (iron gallium) alloy has the particularity of being magnetostrictive, i.e., it modifies its lattice parameter when its magnetic state is changed. This property allows us to think about possible applications

in the field of nanotechnology, due to the possibility of controlling the magnetism of devices without applying external magnetic fields. The previous studies have been made on FeGa bulk; however, future applications, as nanodevices, require that FeGa were grown as thin films.

The samples studied are epitaxied $\text{Fe}_{1-x}\text{Ga}_x$ thin films (grown by MBE) with x from $\sim 10\%$ to $\sim 30\%$ and different thickness. X-ray diffraction shows that there is a coexistence of two crystalline phases, one of which is tetragonal and whose base and height ratio increases monotonically with the Ga concentration. The other phase is cubic and its lattice parameter also increases with Ga concentration. We have also determined the thickness of these samples by small angle x-ray reflectometry.

We have performed the magnetic characterization of these samples by mean of magnetometry and ferromagnetic resonance. The results show changes in the magnetic structure as a function of the Ga concentration and the film thickness. When $x > 0.2$ the in-plane uniaxial hard axis turns from the $[0-11]$ direction to $[100]$. Furthermore, when the film thickness is varied, changes in anisotropy directions are observed, indicating the strong influence of the interface magnetic structure on the magnetic behavior of the film.

2 - 39 – “p”-orbitals’ mediated magnetic interaction: the case of Mn chains

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Molecular layers grown on metallic surfaces constitute adequate substrates to study the nature of mediated magnetic interactions. The case of Mn chains deposited on a copper nitride molecular monolayer grown on $\text{Cu}(001)$ has already been addressed in the literature, both, theoretically as well as experimentally. Different deposition sites for the chains have been considered appearing clear differences in the mechanisms which give rise to the magnetic ground state. In this contribution, we are interested in the role played by different “p” orbitals in the mediation of magnetic interactions among Mn atoms. We consider, thereafter, Mn chains deposited on $\text{Cu}(001)$ with $\frac{1}{4}$ monolayer Oxygen and $\frac{1}{4}$ monolayer Nitrogen coverage, which build non reconstructed surfaces with (2×2) unit cells, and perform calculations within the frame of Density Functional Theory.

2 - 40 – A ferromagnetic resonance study of Fe/MnAs bilayers: magnetic anisotropies and interlayer coupling

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In this work we present a ferromagnetic resonance (FMR) study of Fe/MnAs bilayers epitaxially grown on GaAs (100). Important Fe/MnAs interface effects are observed, i.e., the very weak exchange coupling between Fe/MnAs, and the addition of uniaxial anisotropy terms to the free energy density of the iron layer. Moreover, the general appearance of the FMR iron spectrum is highly temperature dependent. The resonance field, linewidth, and intensity of the Fe line are strongly altered in the alpha-beta phase coexistence region of the MnAs layer, where a severe drop of the resonance field is simultaneously observed. A complementary chemical profile analysis of the sample shows an important intermixing at the Fe/MnAs interface, which arises as a crucial factor for the understanding of the magnetic behavior of this system

2 - 41 – Influence to the spatial conformation of NT functionalized with different polymers according to their electronic distribution.

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The purpose of this work is to study the influence to the spatial conformation of a polymer grafted onto multi-walled carbon nanotubes (MWCNT) according to the differing electronic distribution of the polymer's repetitive unit. It is known that polymers with aromatic rings interact with the nanotube through pi-pi stacking interactions, tending to wrap the MWCNT and propitiating a better dispersion of them in a solvent with affinity to the polymer or in the polymer itself, leading to a composite material with well dispersed MWCNT. On the other hand, if trying to anchor the MWNT to one of the phases of a block copolymer, it would be more efficient to have the MWCNT functionalized with a polymer that does not wrap the nanotube, thus allowing the anchorage by means of inter-diffusion of the polymer into the block with more affinity to it. In this work, we made a graft-from functionalization using as monomers: 4-vinylpyridine (monomer with an aromatic substituent) and acrylonitrile (monomer with a non aromatic, where the substituent is a nitrile group). The functionalization efficiency was studied by spectroscopic and thermal technique. The spacial conformations of the polymer around carbon nanotubes were studied by high resolution transmission electron microscopy (HRTEM). It was seen, in both cases, polymer wrapping the NT. However, for polymers with aromatic rings, this effect is predominant, while with polyacrylonitrile derivates what can be seen is polymer wrapped onto itself and bound to the MWCNT's wall.

2 - 42 – Influence in the optical response of the addition of multiwalled carbon nanotubes in films of epoxy resin and azobenzenes.

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Among many others, one of the applications of multi-walled carbon nanotubes (MWCNT) is to immerse them in a polymer matrix since new mechanical, electrical or thermal properties could be induced into the polymer. Azobenzene and its derivatives are widely known for undergoing a photoisomerization process when illuminated with light of the proper wavelength. When added to a hosted matrix, these nonlinear optical materials may give rise to certain degree of anisotropy when exposed to linear polarized light. The photoinduced trans-cis-trans cycles of these kinds of molecules end up when their dipole moment is normal to the polarization axis of the light. Maximum anisotropy is thus reached when molecules are all aligned in that direction and there is no coupling

with the electrical field of light. When the exposure light is turned off, some degree of anisotropy is lost. Moreover, anisotropy is totally lost when illuminating with circular polarized light. The fact that anisotropy loss occurs limits the capability of using these materials in data storage, optical switching or holographic recording and making this characteristic still a challenging subject of study. We recently demonstrated that MWCNT interact with an azobenzene derivative, Disperse Orange 3 (DO3) via π - π stacking interactions [1]. In this sense, it could be expected that MWCNT interacting with DO3 molecules partially inhibit the molecules trans-cis-trans cycles. Therefore a change in the rate of induced anisotropy as well as in the relaxation rate or in the percentage of anisotropy losses could also be expected. In this work, we studied the optical response of epoxy resin films filled with MWCNT non-covalent functionalized with DO3. Also films of epoxy resin and DO3 without MWCNT were done in order to see the effect of MWCNT in these films. We found that in the case of films containing MWCNT the process of reaching the maximum anisotropy is slower that the obtained for films without them. The anisotropy loss process is also different in both films indicating that a higher anisotropy would remain in the film with MWCNT.

[1] Díaz Costanzo, G.; Ledesma, S.; Mondragón, I.; Goyanes, S. J. Phys. Chem. C, 2010, **114** (34), pp 14347-14352

2 - 43 – Production of carbon nanotubes: influence of the catalyst on the yield

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Multi-wall carbon nanotubes (MWCNTs) were synthesized by chemical vapor deposition (CVD) on catalytic iron nanoparticles dispersed in a silica matrix, prepared by sol gel method. This work explores the influence of the variables of synthesis that rules the sol to xerogel transition on the catalytic activity of the iron nanoparticles. In particular, the variation of both iron precursor and hydrolysis-condensation catalyst agent on the matrix structure, and its influence on the yield of carbon nanotubes growth was studied. The

silica precursor utilized was tetraethyl-orthosilicate. As metal precursor, it was used iron (III) nitrate or iron (III) chloride. The hydrolysis-condensation catalysts used were hydrochloric, nitric or hydrofluoric acids. The sols were dried at two different temperatures in air (25 or 80°C) and then treated at 450°C for 10h. The catalyst was characterized by XRD and TPR. The xerogels were introduced into the CVD chamber and reduced in a hydrogen/nitrogen (10% v/v) atmosphere at 600°C. MWCNTs were formed by deposition of carbon atoms from decomposition of acetylene at 700°C. The samples were characterized by XRD, TGA, SEM and TEM. After calcination at 450°C, each system acquired different crystalline structure and degree of crystallinity. MWCNT yield was notably dependent on the Fe-matrix synthesis conditions, in spite that all the other variables (as Fe/Si ratio, gas flow, temperature, etc) were identical. The most active catalyst was that prepared with HF dried at 25°C, and the less active was that prepared with HNO₃. Carbon nanotubes displayed a diameter of about 25-40nm and several micron lengths. The growth mechanism of MWCNTs is base growth mode for all catalysts. The differences in MWCNT yield are discussed in terms of crystalline and iron nanoparticles sizes.

2 - 44 – Influence of filler alignment in the mechanical and electrical properties of carbon nanotubes/epoxy nanocomposites

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Current and projected markets for carbon nanotube based polymer composites are aimed at the exploitation of the high electrical conductivity of carbon nanotubes coupled to their unique geometry. Due to the low filler loading fractions required, the mechanical properties and the surface finish of the composite matrix can be maintained. In previous studies we have shown that the use of random disperse multi-wall carbon nanotubes (MWCNT) as a conductive filler in an epoxy matrix leads to an electrical conductivity exceeding 10^{-6} Sm^{-1} , sufficient for anti-static applications, at filler concentrations as low as 0.4 wt%. The present work investigated the influence of an alternating current (AC) electric field on dispersions of

MWCNT in an epoxy matrix during curing. The expectation was that an aligned network would form if the aggregation process was guided in this way, and that interesting anisotropic electrical conductivities and mechanical properties might emerge. The composite materials are disks of 30mm diameter and 3.6mm of thickness. The matrix is diglycidyl ether of bisphenol-A with isophorone-diamine as hardener and MWCNT with weight percentage between 0.04 and 0.2 wt% were used as filler. An AC electric field (250 ACV; 50 Hz) along thickness was applied before and through curing. The AC electric current through the sample, in the thickness direction, was measured during the whole cure cycle. The evolution of the electrical conductivity shows that MWCNT alignment begins at ambient temperature but goes to saturation during the gelification process (50 min at 60°C for this epoxy system). This result, novel in the literature, allows optimizing the time and the temperature during which is necessary to apply the electric field to achieve the maximum possible alignment. The DC conductivity was measured after cure cycle. The percolation threshold was around 0.06 wt% of MWCNT content with a conductivity of $1.4 \times 10^{-5} \text{ Sm}^{-1}$, this is one order less in the filler content than the composite with MWCNT dispersed at random. The Rockwell hardness of the nano-composites decreases but the wear resistance increases for both aligned and random MWCNT networks. The hardness fall is stronger for the composites with the aligned network. This could be explained by a “crack initiator” behavior of the carbon nanotubes due the weak interaction between nanotube wall and resin.

2 - 45 – Nanostructures titanium films grown with a plasma immersion ion implantation and deposition system: influence of the bias voltage on the crystalline structure

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Titanium films have been widely investigated in the last years because of their importance in a large variety of technological applications. Ti coatings have been employed as interlayer on steel to improve adhesion of hard coatings based on titanium compounds or to allow the diffusion of carbon from DLC coatings. Ti coatings on titanium alloys have been proposed to im-

prove the biocompatibility of the alloy, since a pure titanium barrier layer prevents harmful substances such as aluminum or vanadium from leaching into biological tissues. Methods based on plasmas, such as magnetron dc sputtering and vacuum arcs, have been employed to obtain titanium films. Plasma immersion ion implantation combined with deposition (PII&D) using cathodic arcs as plasma sources is a technique that has demonstrated to be useful for the fabrication of nanostructure coatings. Applying PII&D a substrate is immersed into the plasma plume produced with a cathodic arc and is biased with high-voltage pulses. When the high negative potential (typically many kilovolts) is on, a plasma sheath forms around the workpiece and ions are accelerated towards the surface and implanted. While the bias is off, ions condense on the surface resulting in the deposition of a coating or a film. The use of high voltage pulses to bias the substrate allows to obtain denser films and to relax internal stress improving the adhesion, tribological and mechanical properties. In this work the characteristics of Ti coatings on steel and on copper substrates obtained with a PII&D system were analyzed. The films were deposited varying the pulse amplitude from 2 to 12 kV, with a pulse frequency of 200 Hz and locating the substrate at two distances from the cathode, 20 and 40 cm. The film structure was studied by glancing-angle X-ray diffraction (GA-XRD). The morphology was observed with an atomic force microscope. Significant changes in GA-XRD spectra with the bias voltage were observed indicating important modifications on the film structure produced by the implantation of high energy ions.

2 - 46 – Magnetic states of Co- and Fe impurities on graphene

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We present ab-initio calculations of the stability and electronic structure of graphene mono- and bilayers systems. We study the magnetic behavior of Co and Fe impurities, substitutionally introduced in graphene monolayers, and substitutional and interstitially in bilayers. The behavior is completely different in each case. Particularly the stability of the graphene bilayer is pretty enhanced by the introduction of these impurities. We analyze the dependence of magnetic moments on Co-C or Fe-C distances, and on external applied electric field.

2 - 47 – Vortices in magnetic nanodots

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Nanodots of magnetic materials may present magnetic vortices in their ground state configuration. These are flux closure structures, with the magnetic moments generally confined to the plane, except at their cores[1]. Vortices in nanodots have many potential applications, such as magnetic memories (VRAM's) and spin transfer nano-oscillators (STNO's). The characteristics of these vortices, including the vortex core size can be controlled to suit these applications. This can be achieved making use of the interface interactions in multilayers, e.g., using a stack of Co/Pt bilayers[2]. The magnetization of the vortex cores can be inverted through the application of static, rotary, or pulsed magnetic fields; polarized currents have the same effect. Manipulation of the sign of the core magnetization is required for the application of nanodots as memory elements, or oscillators. In the present work we show recent results obtained with micromagnetic simulation of static and dynamic properties of vortices in magnetic multilayers.

[1] Guslienko J. *Nanosc. Nanotech.* **8**, 2745 (2008)

[2] Garcia et al. *Appl. Phys. Lett.* **97**, 022501 (2010).