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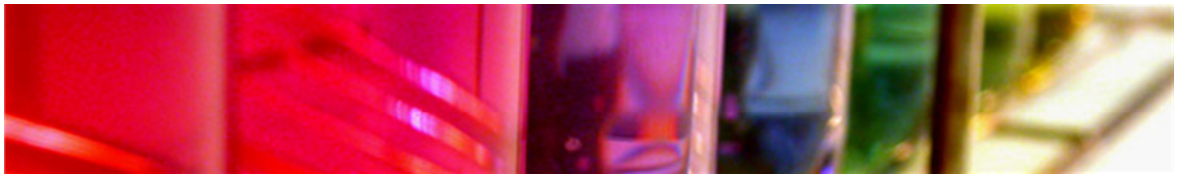

6-8 de Febrero de 2008

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5ª Reunión del Grupo Especializado de Física de Estado Sólido (GEFES)

SANTIAGO DE COMPOSTELA

Facultad de Química

6-8 Febrero 2008

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Single human Rad50/Mre11 protein complex bound to a DNA molecule.
Image size 100 nm x 100 nm
Moreno-Herrero et al. Nature. 437, 440-443 (2005).

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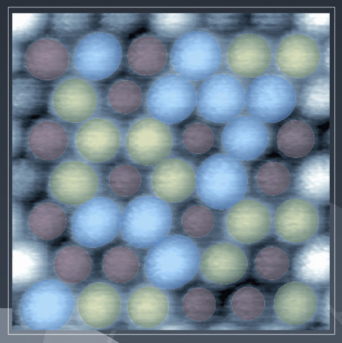

Atomically resolved topographic image of a surface alloy made up of silicon (red), tin (blue) and lead atoms (green) blended in equal proportion on a Si(111) substrate.
Image size 4.3 nm x 4.3 nm
Y.Sugimoto et al. Nature 446 64-67 (2007)

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PROGRAMA

	Miércoles 6 de Febrero de 2008	Jueves 7 de Febrero de 2008	Viernes 8 de Febrero de 2008
9:00	**Robert Cava** Princeton University (EEUU) **Structure, Superconductivity and Thermolectric Effects in Metal Chalcogenides**	**Brian Korgel** The University of Texas at Austin (EEUU) **Elucidating Nanostructure Properties using Colloidally-Grown Nanomaterials.**	**John Pendry** Imperial College, Londres (Inglaterra) **A Cloak of Invisibility**
10:00	Jesús Ricote (ICMM, Madrid) Size effects on the ferroelectric properties of polycrystalline ultrathin $PbTiO_3$ films	Miguel Correa, (Univ. Vigo) Carbon Nanotubes as Useful Templates for the Development of Novel Composites	Maria Ujue González (ICFO, Barcelona) Surface Plasmon photonics: development of plasmonic elements
10:25	Jofre Gutierrez (ICMB, Barcelona) Flux pinning in MOD-TFA YBCO nanostroctured films	Leonor Chico (Univ. Castilla la Mancha) Nanotubos de carbono: simetría y propiedades electrónicas	Mauricio Morais de Lima (ICM, Valencia) Surface acoustic waves as tools for building photonic functionalities
10:50	J. M. Hernández (UB, Barcelona) Two novel experiments using rotating magnets and surface acoustic waves combined with high frequency paramagnetic resonance to study the pumping spin states	Juan Carlos Sánchez-López (ICMS, Sevilla) Aplicaciones de las técnicas espectroscópicas al estudio tribológico de sistemas nanoestructurados de carbono	Daniele Sanvitto (UAM, Madrid) Efectos colectivos no-lineales de polaritones en microcavidades
11:15	Coffe break	Coffe break	Coffe break
11:45	Elena Bascones (ICMM, Madrid) Competing scenario in high-temperature superconductors	Luis Hueso (Univ. Leeds, UK) Room temperature operation and energy model of Alq3-based spintronic devices	Aitor Mugarza (ICMB, Barcelona) Single-molecule chemistry of water on Ru(0001) by scanning tunneling microscopy
12:10	Carlos Carballeira (USC, Santiago) Quantization effects in nanostructured superconductors and hybrid superconductor/ferromagnet nanostructures	Thomas Frederiksen (DIPC, San Sebastián) Elastic and inelastic tunneling of electrons through Au-alkanedithiol-Au junctions from first principles	Gerardo Goya (INA, Zaragoza) Nanopartículas Magnéticas y Radiofrecuencia: nuevos nanogeneradores de calor para destruir microestructuras celulares.
12:35	Maria José Calderón (ICMM, Madrid) Silicon based quantum computing	Susana Cardoso (INESC Microsystems & Nanotechnologies, Portugal) Magnetic tunnel junctions for spintronics and sensors: material optimization and device nanofabrication	**Mesa Redonda y Clausura**
13:00	Oscar Iglesias (UB, Barcelona) Modelling the magnetic properties of nanoparticles: finite-size, surface and exchange bias effect	David Sánchez (Univ. Illes Balears) Breaking the Onsager symmetry: rectification effects and nonequilibrium environments	
13:25	Comida	Comida	Comida

15:30	M. Guibert (ICMB, Barcelona) "Interfacial self-assembled oxide nanostructures from chemical solutions: a powerful methodology for surface nanostructuration""	P. Guardia (UB, Barcelona) "Synthesis of iron nanoparticles of controlled size, shape and magnetic properties"	
15:45	P. Alonso Gutierrez (ICMA, Zaragoza) "Efectos de desorden local en el espectro Raman de la serie Zn (1-x) Mn(x) Ga(2) Se(4)"	V. Salgueiriño-Maceira (USC, Santiago) "Ni/NoP nanowires deposited onto CNTs/Pt nanocomposites"	
16:00	A. Palau (Univ. Cambridge, UK) "Magnetic vortex pinning in superconductor/ferromagnet nanocomposites"	M. Spuch-Calvar (UV, Vigo) "Anisotropic Iron Oxide Particles coated with gold colloids"	
16:15	J. Vicente Alvarez (UAM, Madrid) "Coexistence of Superconductivity and Antiferromagnetism, Model Hamiltonian and ab-initio calculations in Ce-based compounds"	A. Rodenas (UAM, Madrid) "Estructuras fotónicas escritas con pulsos ultracortos: de guías de onda a cristales fotónicos"	
16:30	M. Kovylina (UB, Barcelona) "Magnetoresistance in positive and negative exchange bias Ni/FeF_2 bilayered 200 nm antidots"	M. D. Martín (UAM, Madrid) "Transporte de luz en un vidrio fotónico mediante resonancias de Mie"	
16:45	J. Herrero Albillos (ICMA, Zaragoza) "Parimagnetismo en ErCo2: un nuevo tipo de desorden magnético"	F. López-Teijeira (ICMA, Zaragoza) "Modulación del acoplo de luz-pasmón mediante el uso de nano-indentaciones"	
17:00	Coffe break	Coffe break	
17:30	Posters	Posters	
19:00	Posters	Posters	

SESIÓN EXTRAORDINARIA PATROCINADA POR EL CENTRO DE ESTUDIOS AVANZADOS DE LA USC

Jueves 7 de Febrero 2008, 18:00 horas

Miguel Angel Alario Franco: Universidad Complutense de Madrid, España

"A Strategy in the Search of New Materials (A non-scheptical chemist view)"

Robert Cava, University of Princeton, USA.

"Research on New Electronic and Magnetic Materials: Where are we and where should we go?"

Daniel Khomskii, University of Cologne, Germany.

"Main problems and current challenges in systems with strongly correlated electrons"

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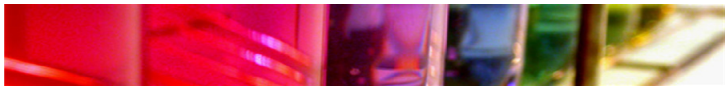

Santiago de Compostela, 6-8 Febrero 2008

CONFERENCIAS PLENARIAS:

Miércoles 6 de Febrero: Dr. Robert Cava, Princeton University, USA

Jueves 7 de Febrero: Dr. Brian Korgel, The University of Texas at Austin, USA

Viernes 8 de Febrero: Dr. John Pendry, The Imperial College, UK

Structure, Superconductivity and Thermoelectric Effect in Metal Chalcogenides

R.J. Cava

Department of Chemistry
Princeton University

The layered early transition metal dichalcogenides have been model systems for charge density wave behavior since the 1970s. In virtually all cases, the CDW has been attributed to a special nesting condition of the Fermi surface that arises in part from the two-dimensional electronic character of the compounds. For $TiSe_2$, however, nominally a “normal valence” compound, the cause of the three-dimensional CDW has been controversial for 30 years. We have recently found that $TiSe_2$ can be made superconducting through the intercalation of Cu, and have further characterized the host compound itself, providing further evidence for its unconventional nature. Similar to the layered dichalcogenides, the binary bismuth tellurides have served for years as a model system for excellent thermoelectric behavior. We have recently shown that the nine distinct bismuth-tellurium compounds ranging from pure Bi to Bi_2Te_3 can be described as members of a single homologous series. They in fact appear to represent the best case of an “infinitely adaptive” series known to date. In this talk I will describe our work in both these chalcogenide systems and place it in the context of previous studies on these and related materials.

ELUCIDATING NANOSTRUCTURE PROPERTIES USING COLLOIDALLY-GROWN NANOMATERIALS

Brian A. Korgel

Departament of Chemical Engineering, Texas Materials Institute, Center for Nano- and Molecular Science and Technology, The University of Texas at Austin, Austin, TX 78712, USA.

Colloidal synthetic approaches have proven to be very effective for making nanostructures, such as semiconductor quantum dots and nanowires. These nanomaterials exhibit unique size-dependent properties due to their nanoscale dimensions and might be exploited in a variety of applications, ranging from light-emitting diodes, displays, sensors, medical diagnostics and therapy, and computational logic and memory. There is still, however, significant uncertainty about the fundamental properties of nanostructures—in particular, semiconductor nanowires—because small variations in size, crystal structure and surface chemistry can lead to dramatic differences in the properties of the nanomaterials. This is true in the case of semiconductor nanowires, as orders-of-magnitude differences in carrier mobilities and conductivities are typically found in an ensemble of nanowires. Analytical tools with the capacity to measure the properties of individual nanostructures while providing simultaneous feedback about the crystal structure and surface chemistry are needed to provide a basic understanding of these issues. These kinds of analytical tools are becoming available. This presentation will highlight two examples of property measurements carried out on individual colloidally-grown nanostructures with simultaneous imaging: (1) mechanical property measurements of oscillating nanowires and (2) energy loss spectroscopy mapping of the electronic properties of individual semiconductor nanowires.

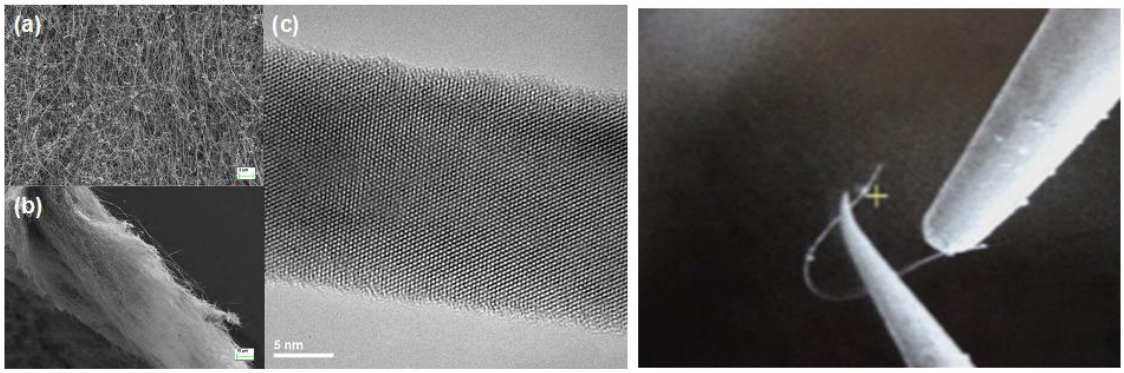

Figure 1. (Left) Germanium nanowires synthesized colloidally by the supercritical fluid-liquid-solid (SFLS) route; (Right) A single nanowire being bent by two independently moveable scanning probe tips in a scanning electron microscope.

A Cloak of Invisibility

John Pendry

The Blackett Laboratory
Imperial College London
South Kensington Campus, London SW7 2AZ

Refractive materials gives us some limited control of light: we can fashion lenses, and construct waveguides, but complete control of light is beyond simple refracting materials. Ideally we might wish to channel and direct light as we please just as we might divert the flow of a fluid. Manipulation of Maxwell's equation shows that we can achieve just that provided we have access to some highly unusual material properties. Metamaterials open the door to this new design paradigm for optics and provide the properties required to give complete control of light. One potential application would be to steer light around a hidden region, returning it to its original path on the far side. Not only would observers be unaware of the contents of the hidden region, they would not even be aware that something was hidden. The object would have no shadow.

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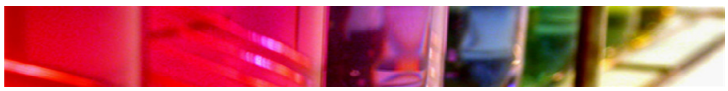

Santiago de Compostela, 6-8 Febrero 2008

COMUNICACIONES ORALES INVITADAS:

Miércoles 6 de Febrero de 2008

SIZE EFECTS ON THE FERROELECTRIC PROPERTIES OF POLYCRYSTALLINE ULTRATHIN $PbTiO_3$ FILMS

J. Ricote, R. Fernández, M.L. Calzada, R. Jiménez

Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain

The integration of ferroelectrics in nanodevices requires the preparation of high quality ultrathin films. Among the methods used, Chemical Solution Deposition (CSD) is considered as a rapid and cost-effective technique for preparing high quality oxide films, but which has traditionally been regarded as unsuitable to fabricate films with thickness below 100 nm. A careful control of the deposition parameters has lead to the successful preparation of ultrathin films down to 18 nm by CSD [1], and even structures with nanometric lateral dimensions [2]. The effects of size reduction to the nanoscale on the properties of ferroelectrics attract a lot of attention nowadays, normally studied in structures epitaxially grown, and using for their electrical characterization local approaches based on scanning probe microscope techniques. However, the fabrication of macroscopically addressable ferroelectric ultrathin capacitors with good properties to be integrated in real devices is rarely studied, regardless its technological importance. In this work we present the analysis of the dielectric, piezoelectric and ferroelectric properties of $PbTiO_3$ ultrathin films measured on extense electrodes. This study shows at the same time the quality of the CSD ultrathin films over large areas, which made them promising materials for their integration as transducer elements in Nanoelectromechanical Systems (NEMS). The polycrystalline nature of these films add complexity to the mechanisms that rule size effects in these ferroelectric materials, and the roles of interfaces, grain boundaries, ferroelectric domains and crystallographic orientations are discussed.

Referencias

[1] Ricote J., Holgado S., Ramos P., Calzada M.L. Piezoelectric ultrathin lead titanate films prepared by deposition of aquo-diol solutions IEEE *Trans. Ultrason. Ferroelectr. Freq. Control* **53[12]**, 2299 (2006).

[2] Calzada M.L., Torres M., Fuentes-Cobas L.E., Mehta A., Ricote J., Pardo L. Ferroelectric self-assembled $PbTiO_3$ perovskite nanostructures onto (100)$SrTiO_3$ substrates from a novel microemulsion aided sol-gel preparation method *Nanotechnology* **18,** 375603 (2007)

Flux pinning in MOD-TFA YBCO nanostroctured films

J. Gutiérrez, T. Puig, A. Pomar, A. Llordés, M. Gibert, C. Moreno, N. Romà, J. Gázquez, S. Ricart, F. Sandiumenge, N. Mestres, X. Obradors

Institut de Ciencia de Materials de Barcelona, CSIC, 08193 Bellaterra, Spain

A methodology of general validity to study vortex pinning in $YBa_2Cu_3O_{7-\square}$ YBCO) is described. It is based on measuring the angular dependent critical current density in a large range of temperatures and magnetic fields. It permits to identify, separate and quantify three basic vortex pinning contributions associated to anisotropic-strong, isotropic-strong and isotropic-weak pinning centers. Thereof, the corresponding vortex pinning phase diagrams for the three mentioned contributions are built up. This methodology is applied to the recently discovered solution-derived YBCO nanostructured films which present a rich variety of pinning landscapes. Our approaches have focused on generating nanostructured YBCO coated conductors using low cost and scalable chemical solution deposition methodologies. We have controlled interfacial pinning by the growth of nanostructured templates by means of self-assembled processes, which has allowed us to grow $Ce_{0.9}Gd_{0.1}O_{2-y}$, and La_2O_3 interfacial nanoislands [1]. On the other hand, nanocomposites have been prepared by modified solution precursors, i.e. Ba and Zr-salts have been added to the anhydrous YBCO-TFA solution.

The application of the vortex pinning methodology and comparison with a standard solution-derived YBCO film [2], enables us to identify the nature and quantify the effect of the additional pinning centers induced through the nanostructuration of the films. In the case of $BaZrO_3$-YBCO nanocomposites, maximum vortex pinning forces (78 GN/m^3 at 65 K) have been achieved showing so far, the highest efficiency pinning properties in high temperature superconductors [3]. We have identified the isotropic-strong defects contribution being at the origin of their unique properties. On the other hand, in the case of the nanostructured templates, an increase in the in field critical current densities at high temperatures has been achieved as a consequence of a great enhancement of the anisotropic-strong defects along the c-axis of the film.

[1] M. Gibert et al, Advanced Materials vol 19, p. 3937 (2007)

[2] Puig.T et al SuST EUCAS 2007 (to be published)

[3] J. Gutierrez et al, Nature Matertials vol. 6, p. 367 (2007)

* This work has been supported by HIPERCHEM, NANOARTIS and MAT2005-02047.

Two novel experiments using rotating magnets and surface acoustic waves combined with high frequency paramagnetic resonance to study the pumping spin states

A Hernández-Mínguez, F. Macià, J.M. Hernàndez, C. Carbonell and J. Tejada

Dep. de Física Fonamental, Universitat Barcelona Diagonal 647, Barcelona 08028

We report here two new experimental techniques to monitor spin population dynamics. One deals with huge rotating fields whereas the other combines the use of surface acoustic waves and high frequency electron paramagnetic resonance. Both techniques allows us to probe spin relaxation on reasonably fast times scales detecting either the inversion of the whole spin states or the population and relaxation rate of the different quantum spin levels in the two wells of the anisotropy Hamiltonian. These two very new techniques could help to carry out new experiments in a number of different fields broaden substantially the scope of their use until now.

References

A Hernandez-Minguez *et al. Applied Physics Letters* **91**, 203502 (2007)

F. Macià, *et al*. to appear in *Physical Review B,* **77 Issue 2** (2007)

Competing scenario in high-temperature superconductors

E. Bascones(*)

Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, 28049 Madrid

The properties of high-temperature superconductors, also called cuprates, are controlled by the doping of the Cu-O band which crosses the Fermi level. At half-filling, undoped cuprates are Mott insulators with antiferromagnetic ordering. Antiferromagnetic order is destroyed by doping with electrons or holes and superconductivity appears.
For low doping superconductivity opens in a pseudogap state with unconventional properties. The pseudogap dominates the phase diagram of hole-doped cuprates but there are claims that a pseudogap (of maybe different nature) is also present in electron doped cuprates. The origin of the pseudogap is not well understood. There are two main scenarios in one of the pseudogap is a precursor of superconductivity while in the other one superconductivity and pseudogap competes.
I will present a theoretical analysis of experimental results in the superconducting state of hole and electron doped cuprates within a scenario in which the pseudogap truncates the Fermi surface, competes with superconductivity and below a critical doping is present in the superconducting state.

(*) in collaboration with Belen Valenzuela

Quantization effects in nanostructured superconductors and hybrid superconductor/ferromagnet nanostructures

C. Carballeira

Laboratorio de Baixas Temperaturas e Superconductividade (LBTS), Departamento de Física da Materia Condensada, Universidade de Santiago de Compostela, 15782-Santiago de Compostela, Spain.

The intrinsic quantum nature of superconductivity makes superconductors with dimensions of the order of $\xi(0)$, the Ginzburg-Landau (GL) coherence length, particularly sensitive to confinement effects. In the last years, significant advances in different nanofabrication techniques have promoted the systematic study of the properties of micro- and nano-superconductors [1]. This research has demonstrated that sample's topology can be used to enhance considerably the superconducting critical parameters, thus opening new perspectives for the potential applications of superconductivity.

In this Contribution we first illustrate why the Ginzburg-Landau (GL) phenomenological theory of superconductivity is, probably, the most appropriate tool to study the quantization effects in mesoscopic superconductors. Close to normal/superconducting phase boundary it may be applied in the form of the linearized GL-equation, that preserves in its solutions the symmetry imposed by the boundary conditions. As we will see, by using a vector potential gauge transformation that accounts for the superconducting/vacuum boundary condition, this property allows to study the confinement effects on the nucleation of superconductivity in mesoscopic regular polygons [2]. These effects include, for instance, the spontaneous generation of vortex-antivortex patterns that comply with the symmetry of the sample [2,3]. The same procedure can be adapted to study the influence of a disk-shaped magnetic dot on top of the superconductor, that may induce at the boundary multiquanta vortex entries and an expansion of these vortex-antivortex patterns [4]. The outliving of these symmetry-induced properties deep inside the superconducting phase will be also considered within the GL-framework [5,6].

[1] See, e.g., V.V. Moshchalkov *et al.*, in *"Handbook of Nanostructured Materials and Nanotechnology*", edited by H.S. Naiwa (Academic, San Diego 1999) Vol.3, Cap. 9, p.451.
[2] L.F. Chibotaru, A. Ceulemans, M. Morelle, G. Teniers, Carlos Carballeira and Victor V. Moshchalkov*,* J. Math. Phys. **46**, 095108 (2005).
[3] L.F. Chibotaru, A. Ceulemans, V. Bruyndoncx and Victor V. Moshchalkov, Nature **408**, 833 (2000).
[4] C. Carballeira, L.F. Chiboraru, A.Ceulemans and V.V. Moshchalkov, Phys. Rev. Lett. **95**, 237003 (2005).
[5] C. Carballeira, G. Teniers, V.V. Moshchalkov, L.F. Chiboraru, and A.Ceulemans, Europhys. Lett. **75**, 936 (2006).
[6] Qinghua Chen, Carlos Carballeira and V.V. Moshchalkov, Phys. Rev. B **74**, 214519 (2006).

SILICON BASED QUANTUM COMPUTING

María José Calderón

Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, 28049 Madrid

Doped Si is a promising candidate for quantum computing due to its scalability properties, long spin coherence times, and the astonishing progress on Si technology and miniaturization in the last few decades (Moore's law). This proposal for a quantum computer [1] ultimately relies on the quantum control of electrons bound to donors near a Si/barrier (e.g. SiO_2) interface (see Fig. 1). I will discuss several important issues related to the manipulation of donor electrons by means of external fields in such architecture [2, 3].

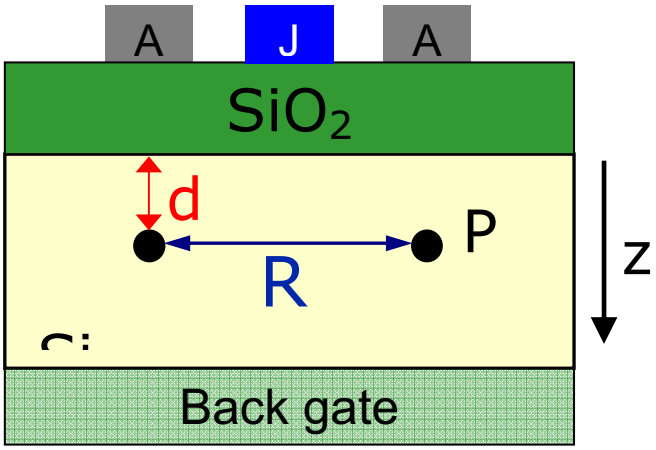

Fig. 1. Schematic view of the proposed P-doped Si quantum computer [1]. Surface A- and J-gates control one- and two-qubit operations. In the present study, we consider uniform electric and magnetic fields applied in the z-direction.

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MODELLING THE MAGNETIC PROPERTIES OF NANOPARTICLES: FINITE-SIZE, SURFACE AND EXCHANGE BIAS EFFECTS

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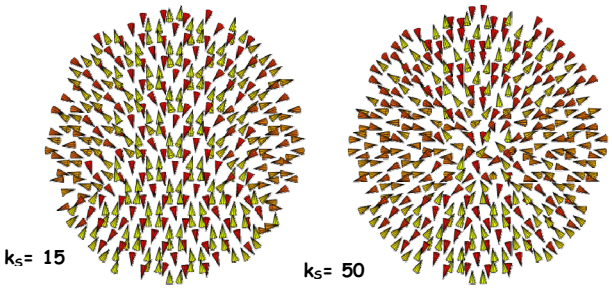
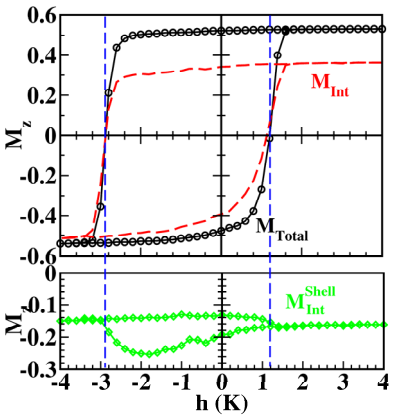
Magnetic nanomaterials present new magnetic and transport properties that arise due to a complex interplay between the intrinsic properties of the constituents (such as specifically tailored microstructure and finite size or surface effects) and the interactions among the entities forming them [1]. Among them, magnetic systems formed by nanosized particles have attracted increasing interest during the last decade because of their technological applications, ranging from magnetic data storage to biomedical applications. From the fundamental point of view, the computational approach to the modelling of such peculiar phenomenology is an attractive challenge because, usually, it involves a wide range of time and length scales. In this talk, we will review our recent work on the modelling of magnetic nanoparticles. We will focus on Monte Carlo simulation methods to study the phenomenology associated to finite-size and surface effects in models for a single nanoparticle [1], and on the study of the microscopic origin of exchange bias effects in nanoparticles with core/shell structure [2,3]. The need for new computational schemes and algorithms and plans for new investigations on different kinds of nanoparticle systems will be stressed.

Funding from the Spanish MEyC NAN2004-08805-CO4-02, CONSOLIDER CSD2006-12 and MAT2006-03999 projects, and Catalan DURSI (2005SGR00969) is acknowledged.



Magnetic configurations of maghemite particles with surface anisotropy k_S.



Shifted hysteresis loop of a core/shell nanoparticle and the interface contribution.

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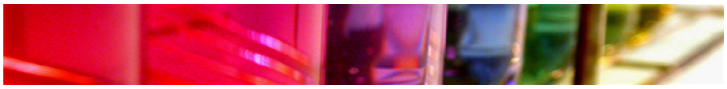
V REUNIÓN DEL GRUPO ESPECIALIZADO DE FÍSICA DEL ESTADO SÓLIDO (GEFES)



Santiago de Compostela, 6-8 Febrero 2008

COMUNICACIONES ORALES INVITADAS:

Jueves 7 de Febrero de 2008

Carbon Nanotubes as Useful Templates for the Development of Novel Composites

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CNTs can be considered as ideal templates for the formation of one dimensional nanoparticle assemblies. Despite their relative chemical inertness, several strategies have been followed for the preparation of CNT–nanoparticle composites, either through in situ nanoparticle synthesis or by the assembly of pre-formed nanoparticles. In both cases surface modification is required, sometimes implying the chemical development of defect-sites and subsequent covalent functionalization or non-covalent adsorption of macromolecules on the side walls. Herein, we report on the fabrication of one dimensional nanomaterials based on the non-covalent functionalization of CNTs by means of a combination of polymer wrapping and layer-by-layer assembly (figure 1a) through the deposition of nanoparticles of different nature (magnetic, metallic semiconductor) and the description of the properties of the resulting hybrid materials. [1-5] As a second approach it will be shown the covalent functionalization based on the acidic chemical oxidation of the CNTs surface, which can be used for the self assembly of CNTs on colloidal templates. Additionally it will be shown how these composites help for the synthesis of particles with an increased complexity and functionality through the surface modification of the adsorbed CNTs either through nanoparticles assembly or through uniform surface coating [6-7].

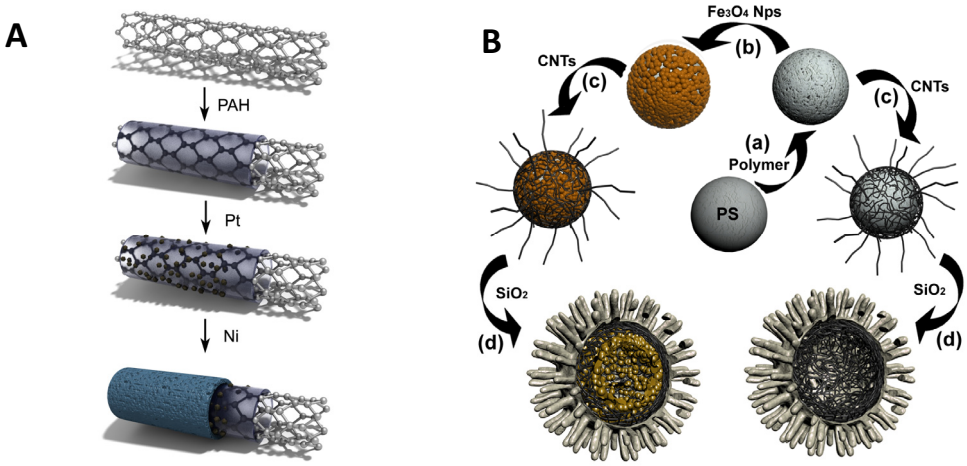

Figure 1: Schematic illustration of the synthetic procedures comprising the polymer wrapping of CNTs, the electrostatic self-assembly of pre-synthesized Pt nanoparticles and the Ni salt reduction with the consequent formation of Ni/NiO nanowires supported onto the CNTs (A); and the polyelectrolyte coating of PS spheres (a), adsorption of Fe_3O_4 nanoparticles (b), adsorption of CNTs (c, d), and SiO_2 coating of the individual CNTs (B).

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NANOTUBOS DE CARBONO: SIMETRÍA Y PROPIEDADES ELECTRÓNICAS

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Los nanotubos de carbono son un nuevo tipo de materiales cuasi-unidimensionales que pueden comportarse como metales o semiconductores según su geometría. Esta relación entre estructura y comportamiento electrónico ha llevado a proponer una nanoelectrónica basada en el carbono, en la que los componentes básicos de los circuitos sean dispositivos de nanotubos de carbono.

En esta charla describiré las propiedades electrónicas de sistemas basados en nanotubos de carbono. En particular, mostraré el papel de la simetría en el transporte en los mecanismos de confinamiento electrónico[1,2,3] y en la interacción espín-órbita[4] en estos sistemas unidimensionales.

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APLICACIONES DE LAS TÉCNICAS ESPECTROSCÓPICAS AL ESTUDIO TRIBOLÓGICO DE SISTEMAS NANOESTRUCTURADOS DE CARBONO

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La tribología estudia la fricción, el desgaste y la lubricación que tienen lugar durante el contacto entre superficies sólidas en movimiento. La aplicación de técnicas espectroscópicas y microscópicas al estudio de materiales usados con fines tribológicos resulta de vital importancia para la comprensión de su respuesta en funcionamiento y su posterior mejora tecnológica. La realización de una diagnosis adecuada implica el estudio de las dos superficies en contacto a escalas de tiempo y dimensiones adecuadas para poder conocer los fenómenos implicados y su correlación con las características iniciales. El desarrollo de nuevos materiales multifuncionales con estructuras complejas a nivel micrométrico o nanométrico dificulta su análisis dado que se requiere un mayor grado de conocimiento de sus particulares estructuras y una mayor especificidad y resolución espacial de las técnicas empleadas.

En esta charla se presentarán diversos ejemplos de caracterización a escala nanométrica de películas delgadas basadas en compuestos de carbono como recubrimientos protectores o lubricantes llevados a cabo en nuestro grupo. En concreto, se presentarán diferentes muestras representativas de formas del carbono tales como nanocomposites de carburos metálicos embutidos en carbono amorfo (MeC/a-C); nitruro de carbono amorfo (CN_x), diamond-like carbon (DLC) o nanotubos (CNTs). A través de estos sistemas se ilustrará el empleo de distintas herramientas analíticas como la espectroscopia de pérdida de energía de electrones (EELS) [1,2], espectroscopia de fotoelectrones de rayos X (XPS) y electrones Auger (AES) [2], resonancia magnética nuclear (RMN) [3] o la espectroscopia Raman [4] para la interpretación de la respuesta tribológica observada. Gracias a la información estructural y química obtenida con buena resolución lateral (<100 nm) de las superficies iniciales y con posterioridad a los tests de fricción es posible conocer los fenómenos fisico-químicos ocurridos en la región de contacto y las trasformaciones sufridas durante su uso, lo que puede servir para diseñar nuevos materiales con mejores propiedades de fricción y desgaste.

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ROOM TEMPERATURE OPERATION AND ENERGY MODEL OF Alq_3-BASED SPINTRONIC DEVICES

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Spin transport in organic semiconductors has been receiving widespread attention since the first experimental demonstration of magnetoresistive effects (change in resistance under an applied magnetic field) in hybrid ferromagnetic/organic/ferromagnetic structures [1]. Continuous effort in the field has led to the realization, for example, of vertical organic spintronic devices with different organic semiconductor layers [2,3] or organic tunnel barriers [4]. However, there is still a lack of understanding on the mechanism that governs spin injection and transport in organics, leading to general disagreement even on the expected sign of the devices output magnetoresistance.
With the aim to clarify the spin transport behaviour in organic semiconductors, I will present new results on hybrid inorganic/organic spin valves with the most successful up-to-date combination of materials [2-4]. The highly spin polarized manganite $La_{2/3}Sr_{1/3}MnO_3$ and Cobalt have been used as ferromagnetic electrodes for spin injection into thick layers (up to 200 nm) of tris(8-hydroxyquinoline)aluminum(III) (Alq_3). In a critical design improvement, we have for the first time introduced an artificial tunnel barrier (Al_2O_3 or LiF) between the organic and the Co top electrode to study its influence on spin injection into organic semiconductors and to improve the chemical stability and reproducibility of the devices.

In this talk I will: explore the importance of artificial tunnel barriers for spin injection in organics, show room temperature magnetoresistance, demonstrate that only ferromagnetic electrodes and not organic semiconductor limit device output and, finally, sketch an energy diagram able to explain negative magnetoresistance in LSMO/Alq_3/Co spin valves.
The work I will present is a step forward in the new field of organic spintronics, as we prove that organic semiconductors do not have a clear limit for spin transport performance and we introduce a reliable model that could be easily extrapolated to predict the output of different materials combinations in hybrid spin valves.

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Work in collaboration with V. Dediu, I. Bergenti and A. Riminucci (ISMN-CNR, Bologna, Italy)

Elastic and inelastic tunneling of electrons through Au-alkanedithiol-Au junctions from first principles

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The electronic conductance of alkanedithiol molecules bridging two gold electrodes is investigated using the TranSIESTA scheme for first-principles quantum transport simulations [1]. We investigate how the conductance per molecule is affected by molecular coverage, tilt angle, and carbon back-bone length.

Based on the scheme described in Ref. [2] we also calculate the effects in the current from the coupling to molecular vibrations as revealed in inelastic electron tunneling spectroscopy (IETS). We explore the interplay between the microscopic configuration and the IETS.

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MAGNETIC TUNNEL JUNCTIONS FOR SPINTRONICS AND SENSORS: MATERIAL OPTIMIZATION AND DEVICE NANOFABRICATION

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This work describes material optimization and nanofabrication of magnetoresistive devices based on magnetic tunnel junctions. Since the first demonstration of large tunnel magneto-resistance in magnetic tunnel junctions (MTJ) at room temperature [1], large progress have been made in the MTJ engineering and in its implementation as the new generation of magnetoresistive sensors with controllable resistances from few $\Omega.\mu m^2$ to several hundred $k\Omega.\mu m^2$. The research on improved materials, study of interfaces, and switching mechanisms in low dimension devices is of major importance today, motivated by the progresses achieved every year in pushing the magnetoresistance values up to 500% [2,3] Several topics are addressed in this presentation, starting with the optimization of spin valve and magnetic tunnel junction growth by magnetron sputtering and Ion Beam deposition [4]. The nanofabrication techniques for current-in-plane (spin valves) and current perpendicular-to-plane architectures (magnetic tunnel junctions) are described. Application of magnetoresistive stacks for MRAMs [5] and new switching mechanisms are shown including spin transfer [6] and thermally assisted switching [7,8].Also, examples of magnetoresistive biochips and portable/integrated platforms will be shown [9], as they have increased attention in the past years among the biotechnology community. Finally, MgO based magnetic tunnel junctions with controlled linear range, sensitivity and noise are optimized [10,11] to fabricate ultra low field (target sensitivity 1pT/sqrt(Hz)) detectors for biomedical imagiology [12].

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BREAKING THE ONSAGER SYMMETRY: RECTIFICATION EFFECTS AND NONEQUILIBRIUM ENVIRONMENTS

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The Onsager relations applied to electronic transport establish that the conductance of a two-terminal conductor is an even function of the applied magnetic field. However, breakings of this symmetry may take place in the nonlinear regime [1]. We find that magnetic-field asymmetries arise in mesoscopic systems only as a consequence of the charge response of the conductor, thus being a pure interaction effect [1,2]. Furthermore, we investigate magneto-asymmetries in the linear response regime when a mesoscopic system interacts with its environment [3]. Interestingly, we find that the interaction between the two systems causes an asymmetry when the environment is out of equilibrium. We elucidate our general result with the aid of a quantum dot capacitively coupled to a quantum Hall conductor and discuss the asymmetry dependence on the environment bias and induced dephasing.

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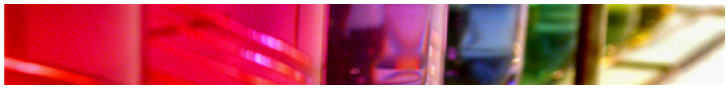

Santiago de Compostela, 6-8 Febrero 2008

COMUNICACIONES ORALES INVITADAS:

Viernes 8 de Febrero de 2008

SURFACE PLASMON PHOTONICS: DEVELOPMENT OF PLASMONIC ELEMENTS

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Surface plasmon based photonics, commonly referred as plasmonics, is a promising route towards highly integrated optics. A surface plasmon (SP) is basically an electromagnetic wave bounded to a metal/dielectric interface exhibiting a high confinement of the electric field perpendicular to the interface, which makes it very suitable for the development of optical devices in coplanar geometry, for biochemical sensing or for enhanced spectroscopy.

An important effort in the development of plasmonic devices, both passive and active, is necessarily dedicated to the design of systems allowing the two dimensional control of SP propagation. Different approaches can be considered to obtain these SP-optical elements. In this talk, we will present some of these methods, as well as the characterization of the SP elements designed through them.

First, we consider the introduction of a corrugation in the metallic layer as a way to modify the dispersion relation of the propagating SP. By this method, very efficient SP Bragg mirrors can be obtained [1]. On the other hand, the use of structured dielectric layers on top of the metallic film allows altering the SP effective refractive index, n_{eff}. In this way, SP optical elements are designed based on n_{eff} contrast, analogously to conventional optics [2]. Finally, introducing metallic nanoparticles supporting localized surface plasmon resonances also allows the SP dispersion relation engineering. By designing the appropriate configuration, this can be used to efficiently extract light through a metallic layer [3].

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Surface acoustic waves as tools for building photonic functionalities

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The acoustic excitation of semiconductor-based photonic structures is an emerging field with great potential for new types of photonic manipulation [1]. We will review recent experiments, where a surface acoustic wave (SAW) is used to modulate photons and polaritons in planar semiconductor microcavities. In addition, we will discuss novel approaches to use the phase coherence of these waves to build extremely compact optical devices for light propagating in-plane. The strong interaction between a high population of non-thermal acoustic phonons (in the form of SAWs) and photons trapped in a semiconductor microcavity gives rise to a tunable optical superlattice with a folded dispersion relation and well-defined energy-gaps, which were probed by reflectivity and diffraction experiments [2]. Placing a quantum-well with excitonic energy matched to the cavity mode allows for the investigation of the acoustic modulation of microcavity-polaritons in the strong-coupling regime. In this case, as the phonon population increases, one identifies the transition from a polariton superlattice to an array of weakly coupled polariton wires [3]. These experimental results are in very good agreement with a comprehensive model that takes into account the phonon-induced strain, the elasto-optical interaction, and the deformation potential. Finally, we will discuss a novel device concept based on the modulation of the refractive index of ridge waveguides (WGs) by SAWs. Recently, we have demonstrated an extremely compact (active region of approx. 15 microns) Mach-Zehnder modulator with 10 to 90 % peak to peak modulation and fundamental frequency above 500 MHz [4]. This concept has been extended to structures with several WGs, which are acoustically modulated with a specific phase relationship. These devices allow for the implementation of complex optical functionalities such as optical switches, harmonic generators and pulse shapers [5].

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Collective Phenomena of Polaritons in Microcavities

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Microcavity polaritons offer a new test bed for phenomena related to BEC, which up to now were only studied in atomic diluted gases. Though, due to the very short cavity lifetime, thermal equilibrium is not easily reached and polariton particles dwell in the condensed state only a few picoseconds. On one hand, this could be an advantage since in such a system the number of particles is not conserved and so a better defined phase can be obtained. However, on the other hand, the short lifetime of this system prevents the observation of collective dynamic phenomena, like superfluidity. To allow condensed polariton states to be observed over a relatively large amount of time, we have made use of a combination of a continuous-wave (CW) pump and a picosecond-pulse probe to trigger an optical parametric scattering process in the desired state along the polariton dispersion. In this way, using ultrafast detectors, it is possible to follow the dynamics of driven polariton condensates for hundreds of picoseconds. Using this technique we have been able to observe the appearance of a linear dispersion, similar to that one obtained in condensed superfluid atomic gases along which we have created a condensed phase of polariton with finite momentum. The collective state of polaritons running at ~ 1 μm/ps in the linear Bogoliubov dispersion shows a diffusion-free motion while a similar polariton state in a dispersive quadratic dispersion would double its size. At the same time, the coherent polariton signal state is peaked at a specific k vector, which is maintained throughout the travelling time [1]. Similar behaviour is obtained for signal polaritons running against obstacles as long as the size of these defects is kept smaller than the coherent polariton wavepacket. For bigger size obstacles, the polariton signal splits into two independent condensates with a defined momentum as narrow as that of the original polariton state.

It is interesting to note that the effect of a point-like defect on the pump states is quite different, due to the higher velocity of the pump polaritons, which travel at supersonic regime. In this case, as predicted by Ref. [2,3], and observed experimentally for an atomic condensate [3], the effect of a barrier- like defect in the cavity is to generate Čerenkov shock waves.

Acknowledgments

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Single-molecule chemistry of water on Ru(0001) by scanning tunneling microscopy

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The adsorption of water on Ru(0001) containing a small amount of C impurities and its stability upon dissociation has been studied by using a low temperature scanning tunnelling microscope (STM). Apart from standard imaging, the STM has been used as a tool to selectively manipulate individual molecules by using inelastic electrons tunnelling from tip to surface or viceversa. The inelastic electrons excite internal vibrational modes of the molecules which in turn decay by inducing different processes. Depending on the molecule, tip structure and the voltage pulse applied, the induced process can be molecular diffusion and dissociation, formation and breaking of intermolecular bonds, desorption, or reversible surface-tip transfer of the molecule. From the energies involved in the vibrational excitation we can identify the chemical nature of the molecule and obtain detailed information about the reaction path and energy barriers of the induced process.

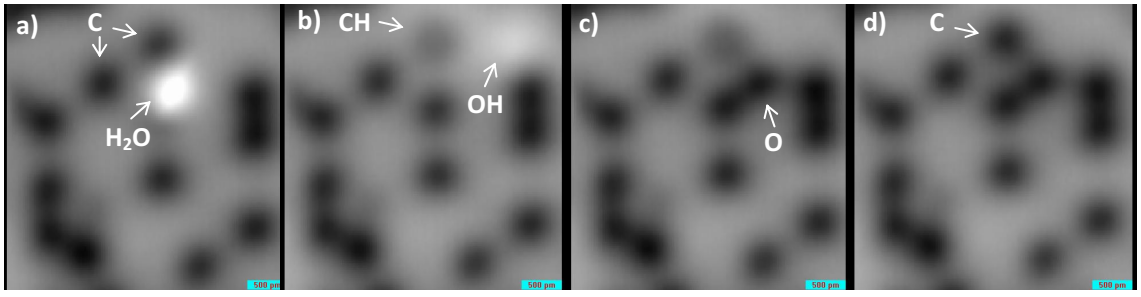

Figure 1: Series of STM images showing a manipulation sequence by using voltage pulses of difference energy when the tip is located on top of the molecule to be manipulated. From left to right: a) A water molecule (bright dot) bonded to a carbon molecule (dark dot). b) After a voltage pulse of 1.5 V, the water has dissociated forming an OH (faint bright dot), and the released H has reacted with the C to form a CH molecule (grey dot). c) After a voltage pulse of 2.45 V on the OH, it has dissociated, leaving an O atom on the surface. e) After a voltage pulse of 1.2 V on the CH, it has dissociated back leaving the C atom on the surface.

NANOPARTÍCULAS MAGNÉTICAS Y RADIOFRECUENCIA: NUEVOS NANOGENERADORES DE CALOR PARA DESTRUIR MICROESTRUCTURAS CELULARES.

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La absorción de energía en nanopartículas magnéticas sometidas a radiaciones electromagnéticas abarca una gran diversidad de mecanismos, que van desde la rotación mecánica hasta excitación de plasmones. Algunos de estos mecanismos son bien conocidos y han dado lugar nuevas y potentes tecnologías[1], mientras que otros son aun objeto de estudio y su potencial tecnológico es aún incierto. La generación de calor por sistemas nanoestructurados mediante la aplicación de ondas de radio (f < 1 MHz), conocida como Hipertermia con Fluidos Magnéticos, es un campo nuevo y creciente de gran interés por su potencial como protocolo clínico para terapias no invasivas y de alta selectividad.[2] Consiste en inducir la muerte celular través de la absorción y liberación altamente local de energía, mediante la aplicación remota de un campo magnético sobre nanopartículas magnéticas previamente ligadas a las células diana. Su aplicabilidad para el tratamiento de tumores está siendo actualmente evaluada en protocolos clínicos de Fase III. Para su aplicación en sistemas vivos, es de fundamental importancia una estrategia viable para la vectorización de las nanopartículas a las células diana, capaz de evadir la acción del sistema reticuloendothelial que actúa captando y eliminando las nanopartículas inyectadas.[3]

En este presentación se discutirán los mecanismos de absorción y liberacion de energia en sistemas nanometricos, y su efecto en la microestructuras celulares. Comentaré asimismo las estrategias seguidas en el Instituto de Nanociencias de Aragón (INA) para la construccion de aplicadores de campos para a) caracterizacion de ferrofluidos, b) experimentos en cultivos celulares y c) experimentos in vivo. En relacion a los sistemas biológicos se discutirán las estrategias de vectorización seguidas en el Servicion de Oncologia del Hospital Clinico 'Lozano Blesa', y los primeros resultados positivos para control de organismos unicelulares.

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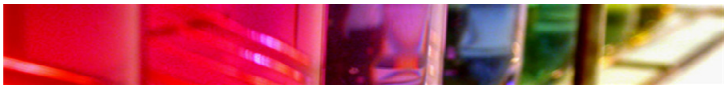
V REUNIÓN DEL GRUPO ESPECIALIZADO DE FÍSICA DEL ESTADO SÓLIDO (GEFES)



Santiago de Compostela, 6-8 Febrero 2008

COMUNICACIONES ORALES REGULARES:

Miércoles 6 de Febrero de 2008

Interfacial self-assembled oxide nanostructures from chemical solutions: a powerful methodology for surface nanostructuration

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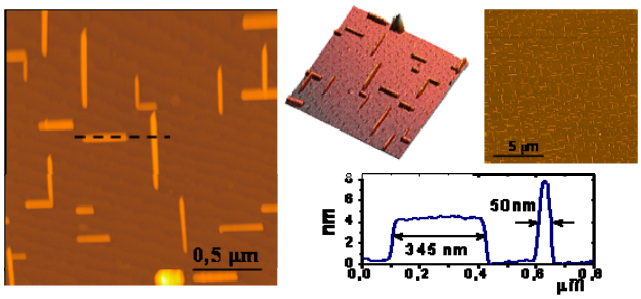
The tendency of some complex oxides to form ordered arrays of nanostructures constitutes a very attractive path for the implementation of new devices with emerging properties and applications in fields such as ferromagnetism, ferroelectricity, optics or superconductivity. Consequently, it is a real scientific challenge to understand the formation mechanisms of oxide nanometric structures. In this work, we present a very general methodology for the generation of strain-induced self-assembled oxide nanostructures prepared by means of chemical solutions, a technique of great interest for many functionalities and applications when the deposition of large areas is required. Special attention has been given to the growth of fluorite structure CeO_2 and $Ce_{1-x}Gd_xO_{2-y}$ (CGO), which has been proved to have an ultrafast kinetics that make it very suitable for the study of mechanisms leading the evolution of the interfacial nanostructures [1]. This enhanced kinetics is due to the particular crystallographic orientation of the resulting epitaxial nanostructures, (011)CGO[1-10]||(001)ABO_3[100], which is achieved through the tuning of interfacial energy by growth atmosphere. A detailed study based on atomic force microscopy has devised the formation of the first stable nucleus, isometric and of just 1-2 unit cell height. In a further evolution stage, nanodots follow a dynamic coalescence process resulting in highly anisotropic nanostructures. Even though nanoislands' height remains fairly constant (h~8 nm) through evolution, lateral aspect ratio (c=long axis/small axis) raises as island's size increases, reaching values c~35. The existence of this shape instability is being attributed to optimization of the elastic energy relaxation of the system. As a result, we have the ability to tune morphology (isometric, anisotropic), size (short and long axis), distribution (organization of nanostructures along one unit cell steps of the vicinal substrate or along its main crystallographic directions), etc. of the resulting interfacial oxide nanostructures through the control of growth conditions (time, atmosphere, temperature, etc.). The presented methodology is also being applied to the generation of other strain-induced self-assembled oxide nanostructures ($BaZrO_3$, rare earth oxides, etc.) on different substrates ($SrTiO_3$, $LaAlO_3$, $NdGaO_3$, YSZ, etc), evidencing its great validity and generality.



Highly anisotropic self-assembled $Ce_{1-x}Gd_xO_{2-y}$ nanostructures on $LaAlO_3$ prepared from chemical solutions.

[1] M. Gibert et al.; Self-organization of heteroepitaxial CeO_2 nanodots grown from chemical solutions, Advanced Materials, **19**, 3937 – 3942 (2007); *mgibert@icmab.cat*

Efectos de desorden local en el espectro Raman de la serie $Zn_{1-x}Mn_xGa_2Se_4$

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La serie $Zn_{1-x}Mn_xGa_2Se_4$ pertenece a la familia de semiconductores tetraédricos con vacantes ordenadas. En estos compuestos el orden catiónico varía con x, desde orden total en el $MnGa_2Se_4$ (grupo espacial $I\bar{4}$), hasta desorden parcial en el $ZnGa_2Se_4$ (grupo $I\bar{4}2m$). A lo largo de la serie el grupo espacial es $I\bar{4}$ para x > 0.5 y $I\bar{4}2m$ para x < 0.5 [1]. En este trabajo estudiamos el grado de orden a través del espectro Raman, centrado en los modos $A^{(1)}$ de 136 cm^{-1}, asignado al modo respiratorio Se-vacante, y $A^{(2)}$ (180 cm^{-1}), permitido en el grupo $I\bar{4}$ y prohibido en $I\bar{4}2m$. Un estudio del modo $A^{(2)}$ muestra que consta de dos bandas: una banda estrecha, que sólo aparece en los compuestos $I\bar{4}$ y aumenta con x, y una banda ancha, que crece en los compuestos $I\bar{4}$ al disminuir x y permanece constante en los compuestos de tipo $I\bar{4}2m$. La banda estrecha se asigna al orden $I\bar{4}$ de largo alcance y la banda ancha a rupturas locales de la periodicidad. En los compuestos $I\bar{4}$ la periodicidad se rompe por la mezcla catiónica, o por intercambios de sitios. En los compuestos $I\bar{4}2m$ la distribución catiónica aleatoria da lugar a dominios ordenados localmente que activan la banda ancha. De la relación de intensidades entre ambas bandas se obtiene un parámetro de orden que se correlaciona con los factores de ocupación del Mn. Por otra parte, el modo $A^{(1)}$ presenta una forma asimétrica atribuida en el $MnGa_2Se_4$ a un acoplamiento anarmónico [2]. En el resto de los compuestos el modelo de acoplamiento no reproduce la asimetría, por lo que se añaden efectos de desorden estructural utilizando el modelo de correlación espacial [3], según el cual el tamaño finito o la presencia de dominios activan modos con q≠0. Los parámetros del modelo son la forma de la relación de dispersión fonónica y el tamaño característico del dominio, *L*. Combinando los efectos de acoplamiento con el modelo de correlación espacial en el cálculo del perfil, reproducimos los espectros Raman de toda la serie. Se encuentra que *L* tiene un mínimo en x = 0.5 y aumenta hacia los extremos de la serie. El tamaño de los dominios se relaciona con la mezcla catiónica, de forma que la mezcla Ga-Zn-Mn posibilita mayor variedad estructural. El mínimo en x = 0.5 se atribuye a que en esta composición la variedad catiónica es máxima.

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Magnetic vortex pinning in superconductor / ferromagnet nanocomposites

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There has been considerable recent interest in the properties of coupled superconductor (SC) / ferromagnet (FM) systems. In addition to interactions at the electronic level the FM magnetic moment can directly influence the superconducting properties. Numerous studies have investigated the potential for strong pinning through the incorporation of FM particles within a SC matrix. However, the nature of the pinning interaction in these coupled systems is very complex and still not well-understood.

We present measurements in nanocomposite thin films consisting of a high density of small (< 10 nm) Gd particles incorporated in a Nb matrix which show enhanced vortex pinning only for decreasing fields [1]. We show that this hysteresis and enhanced pinning can be explained in terms of magnetic reversal losses in the Gd particles rather than through a direct magnetic attraction between a vortex and an isolated particle. This mechanism is therefore fundamentally different in origin to other magnetic pinning interactions previously proposed for ferromagnetic particles or other microstructural features and relies on the ferromagnetic particles having a sufficiently low coercitivity that their magnetisation can be affected by the local field changes associated with vortex motion. We demonstrate that this mechanism has wider relevance, particularly to superconductor ferromagnet bilayers and ferromagnetic superconductors and may have been observed previously.

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Coexistence of superconductivity and antiferromagnetism; Model Hamiltonian and ab-initio calculations in Ce-based compounds.

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The finite temperature phase diagram of CeRhIn5 as a function of pressure and magnetic field has three main highlights: a) the competitive coexistence of metallic antiferromagnetism and superconductivity, b) the abrupt disappearance of antiferromagnetism when the Neel and superconducting temperatures become equal at a critical pressure Pc and c) the reentrance of the antiferromagnetic phase in a range of pressures larger than Pc when a magnetic field is applied. Based on first-principles band structure calculations, we propose a quasi-two-dimensional model of interacting electrons, which reproduces, at the mean-field level, the central features of the phase diagram. We discuss the fixed-point Hamiltonian and the spectrum of excitations of such a model supporting simultaneously magnetic ordering and superconductivity. The coexistence of these two order parameters in a single phase is possible because the magnetic order is linked to the formation of a metallic spin density wave, and its order parameter is not associated to a spectral gap but to an energy shift of the paramagnetic bands. This peculiarity entails several distinct features in the phase diagram and the spectral properties of the model, which may have been observed in CeRhIn5. Apart from the coexistence, we discuss:

1.) The origin of the abrupt suppression of the spin density wave

2.) when the superconducting and magnetic ordering temperatures are equal.

3.) The divergence of the cyclotron mass extracted from de Haas van Alphen experiments as the pressure increases

4.) The structure of peaks and gaps expected in tunneling differential conductance.

5.)The size of the specific heat anomalies in the ordering transitions.

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Magnetoresistance in positive and negative exchange bias Ni/FeF_2 bilayered 200 nm antidots

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Despite the experimental and theoretical investigations, the exchange bias phenomenon (EB) in nanostructured systems remains poorly understood [1]. We used focused ion beam (FIB) lithography to prepare a series of samples of antidots of the same size and different distances in x-y directions. All of the fabrication has been performed on bilayered samples prepared by electron beam evaporation and consisted of antiferromagnetic (AF) FeF_2 (70nm), ferromagnetic (FM) Ni (50nm) and Al (4nm) as a protective layer. The square antidots with antidot size of 200 nm and x and/or y distance of 120-900 nm have been fabricated using an ion current of 30 pA. It is well known that magnetoresistance (MR) measurements can be used to determine exchange bias in thin films and nanostructures. MR was measured with the standard four terminal dc techniques in a He^4 flow cryostat equipped with a superconducting solenoid. All measurements were carried out with the field applied parallel to the easy axis of the AFM and transport data were taken with the current in plane and perpendicular to the field. The resistivity was measured at 4.2 K in various field cooling conditions. The measuring field was applied along the same axis as the cooling field.

We observed three different types of behaviour: for small cooling fields, MR displays a shift towards negative field values (negative EB), while for large cooling fields the shift is positive (positive EB). In the intermediate case, we observed two MR peaks with different height and area. In the first and second case (small and large cooling fields) the reversal is sharper in the opposite field direction to the resulting shift of MR data. It is worth stressing that the switching from positive to negative EB depends on the density and/or relative x/y distances among antidots. The positions of the MR peaks are mostly independent of the cooling field, which suggest the AF domain size is comparable to or larger than the FM domain size and that each FM domain couples only to one AF domain with a particular direction of the EB [2] . For small/large cooling fields we have only one EB direction while two appear for the intermediate cooling cases.

The funding from the Spanish MEC through a FPU grant, Spanish CICYT project MAT2006-03999 and from the Catalan DURSI (2005SGR00969) are acknowledged.

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PARIMAGNETISMO EN $ErCo_2$

UN NUEVO TIPO DE DESORDEN MAGNÉTICO

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Se presentará una serie sistemática de medidas de dicroísmo magnético circular de rayos-X (XMCD), dispersión de neutrones a bajo ángulo (SANS), y susceptibilidad magnética alterna (χ_{ac}) en función de la temperatura, el campo aplicado y la frecuencia de la fase de Laves $ErCo_2$ en zonal paramagnética. [1] Los datos de XMCD ponene de manifiesto la existencia de una amplia región del diagrama de fases en la que la imanación neta de las subredes de cobalto y erbio se encuentran orientadas en dirección opuesta, a temperaturas mucho más altas que las de la línea crítica de orden ferrimagnético, La caracterización completa del fenómeno mediante la medida de SANS y c_{ac} nos ha permitido proponer la existencia de orden ferromagnético de corto alcance en la subred de cobalto. Los resultados experimentales han sido analizados en función de las distintas interacciones magnéticas en el sistema, pudiéndose describir adecuadamente como debido a la aparición de aglomerados ferromagnéticos nanoscópicos de momentos magnéticos de cobalto. Hemos denotado *parimagnetismo* a este escenario, que comparte características con el paramagnetismo y el ferrimagnetismo y que experimentalmente podría deberse al establecimiento de una fase de Griffiths en la subred de Co de $ErCo_2$.

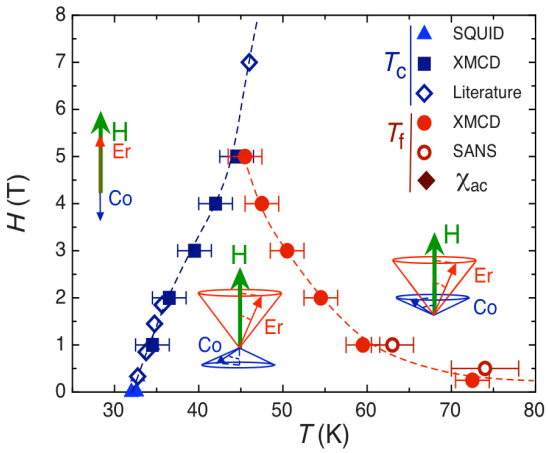

Fig.1 Diagrama de fases de $ErCo_2$ mostrando la línea de establecimiento de parimagnetismo.

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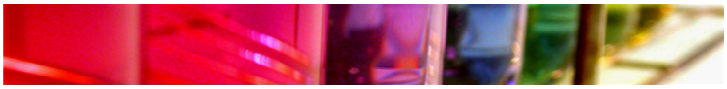
V REUNIÓN DEL GRUPO ESPECIALIZADO DE FÍSICA DEL ESTADO SÓLIDO (GEFES)



Santiago de Compostela, 6-8 Febrero 2008

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SYNTHESIS OF IRON OXIDE NANOPARTICLES OF CONTROLLED SIZE, SHAPE AND MAGNETIC PROPERTIES

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Magnetic nanoparticles (MNP) are an ideal system to study finite-size and surface effects, all these yielding new interesting phenomena and enhanced properties with respect to their bulk counterpart [1]. Besides, the potential application of MNP for biomedical purposes relies on the synthesis of high quality materials, from both the crystalline and magnetic points of view. In this work, we report on the influence of a variety of parameters in the synthesis of iron oxide nanoparticles (magnetite/maghemite Fe_3O_4/Fe_2O_3) by the thermal decomposition of an organic iron precursor in an organic media [2]. It is well known that this method allows the preparation of highly crystalline MNP with excellent magnetic parameters [3,4]. We study the role of both the reductor and surfactant on the shape, size distribution and the magnetic properties. We aim at the synthesis of MNP with an average size of a few nanometers. A narrow size distribution of spherical particles with a high saturation magnetization of 80 emu/g at low temperature, is observed when using oleic acid as a surfactant. In contrast, decanoic acid yields a wider size distribution of cubic particles with a large saturation magnetization within 90-110 emu/g at low temperature. The use of a variety reductors also monitors the magnetic behaviour. In the case of hexadecanediol, nanoparticles have a uniform oxidation and a saturation magnetization similar to the bulk counterpart. In contrast, hidracine seems to promote a non-uniform oxidation that results in the appearance of exchange bias and in a smaller saturation magnetization of about 70 emu/g. The funding from the Spanish MEC (NAN2004-08805-CO4-02, NAN2004-08805-CO4-01, CONSOLIDER CSD2006-12 and MAT2006-03999), and from the Catalan DURSI (2005SGR00969) is acknowledged.

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Ni/NiO Nanowires deposited onto CNTs/Pt Nanocomposites

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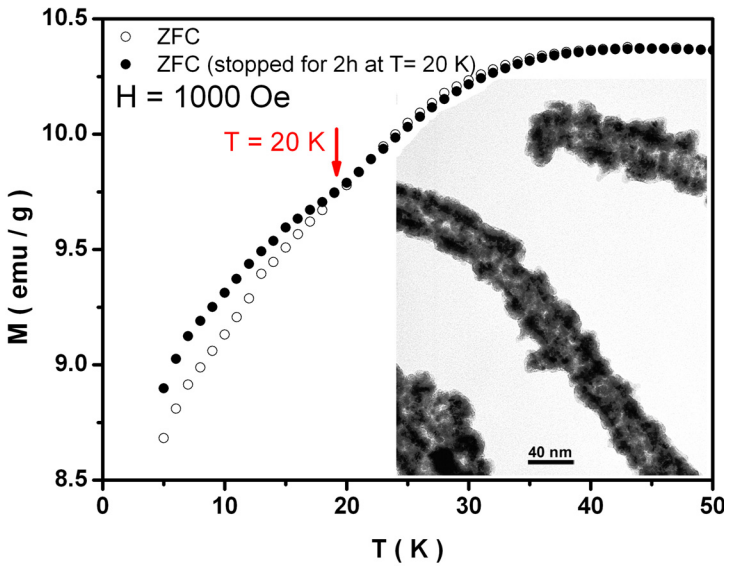
Several nanoscale-based technological applications rely on the promising scenario of highly anisotropic magnetic materials. Bearing this option in mind, we have studied the structure, magnetic properties and interfacial exchange anisotropy effects of unique wires of Ni/NiO synthesized using carbon nanotubes as substrates. Structural analyses of these nanocomposites in correlation with the magnetic measurements show that the crystalline nickel oxide outer shells cause an enhanced exchange bias, providing an extra source of anisotropy which leads to their magnetization stability.[1] These Ni/NiO nanowires with spin glass-like behaviour and magnetic moments blocked state over a wide temperature range including room temperature, should therefore inspire further study concerning anisotropic structures applicability.[2]



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ANISOTROPIC IRON OXIDE PARTICLES COATED WITH GOLD COLLOIDS

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Metal nanoparticles can display a variety of colours as a consequence of the resonance between conduction electrons on the surface of the particles with the electric field of visible electromagnetic radiation. This phenomenon is called surface plasmon resonance and the resonance frequency strongly depends on the size and the shape of the particles. In the case of gold anisotropic particles (rod-like in this case) two bands can be identified in the absorbance spectrum; one due to the transversal plasmon resonance and the second one due to the longitudinal resonance. The position of the longitudinal band is extremely sensitive to the aspect ratio of the rod.

The main aim of this work is to use anisotropic iron oxide particles (goethite rods and hematite spindles) as templates either for the assembly of Au nanoparticles or for the growth of gold continuous shells (see figure 1).

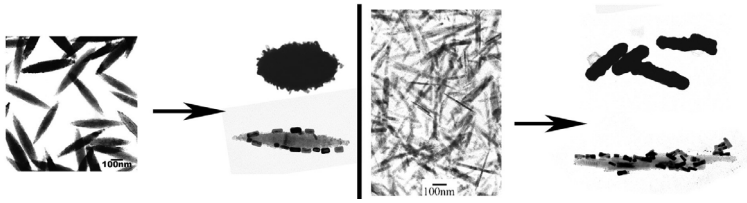

Fig. 1- Left: hematite spindles coated with gold shells (top) and with gold nanorods (bottom); Right: goethite rods coated with gold shells (top) and with gold nanorods (bottom).

The optical properties of such iron oxide@gold colloidal systems will be discussed in detail.

Acknowledgments

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Estructuras fotónicas escritas con pulsos ultracortos: desde guías de onda a cristales fotónicos

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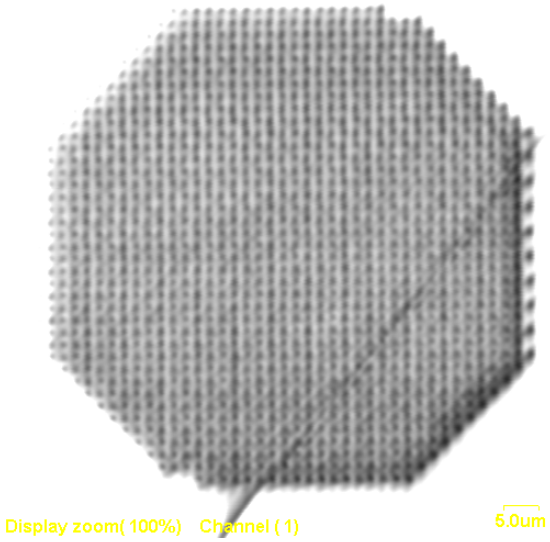
Cuando un láser de femtosegundos (pulsos de 10^{-14}-10^{-12} segundos) se focaliza en el interior de un dieléctrico se producen excitaciones multo-fotónicas en ausencia de carga térmica que, en general, dan lugar a la generación de cambios estructurales permanentes en el foco del haz láser. La extensión espacial de estos cambios estructurales permanentes depende del tamaño del haz láser en foco pudiendo llegar a ser manométricas. Los cambios estructurales producidos, suelen ira acompañados de cambios permanentes en el índice de refracción. La modificación periódica, mediante la escritura con láseres de femtosegundos, en dieléctricos puede ser utilizada para el confinamiento y control de la luz (guías de onda) así como para la creación de “Gaps” fotónicos en diferentes rangos espectrales.

En este trabajo demostramos como cuando la escritura con láseres de femtosegundos se aplica a medios de ganancia láser es posible obtener guías de onda capaces de mostrar ganancia láser. También se aporta evidencia experimental de cómo, en este tipo de materiales, es posible introducir de forma controlada bandas de baja transmitancia (“gaps” fotónicos). En la siguiente Figura mostramos un imagen de una estructura fotónica tri-dimensional creada mediante escritura con láser de femtosegundos en un cristal láser de Niobato de Litio dopado con iones Tm^{3+}.



TRANSPORTE DE LUZ EN UN VIDRIO FOTONICO MEDIANTE RESONANCIAS DE MIE

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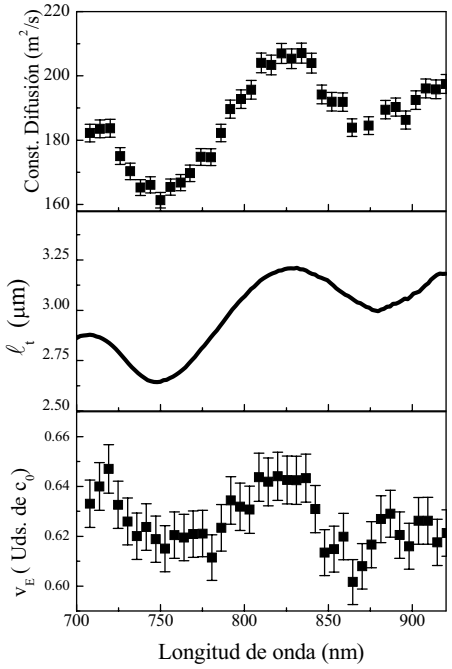
Un medio fotónico desordenado, como por ejemplo una colección de microesferas dieléctricas, es generalmente blanco y opaco, presenta únicamente una ligera dispersión y sus propiedades ópticas no dependen fuertemente de la longitud de onda.[1] Sin embargo, esas esferas pueden soportar resonancias electromagnéticas, denominadas modos de Mie,[2] los cuales pueden atrapar la luz eficientemente si la frecuencia de la luz dispersada (scattered light) es similar a la



de alguno de esos modos. La velocidad con la que la luz se propaga dentro de estos medios desordenados no esta determinada ni por la velocidad de grupo ni por la velocidad de fase, si no por la *velocidad de la energía* (v_E). Esta velocidad viene definida por el cociente entre el flujo de energía y la densidad de energía y tiene en cuenta posibles retrasos debidos al "*scattering"* resonante.Nuestro trabajo se ha centrado en el estudio de las propiedades del transporte de luz en un nuevo material fotónico, al que hemos apelado "*vidrio fotónico*", el cual consiste en una distribución totalmente desordenada de esferas dieléctricas, prácticamente idénticas, de tamaño comparable a la longitud de onda de la luz. Estas esferas presentan modos de Mie y, como resultado del efecto colectivo de todos esos modos, aparecen resonancias tanto en la *constante de difusión* (*D*) de la luz a través de este material como en el *recorrido libre medio* (ℓ_t). Hemos medido por primera vez esas resonancias macroscópicas, pudiendo determinar así la dependencia con la frecuencia de v_E, la cual se reduce por debajo de la velocidad de grupo cuando se excitan estos modos de Mie. Hemos determinado ℓ_t midiendo la transmisión total de luz a través de distintos vidrios fotónicos (tanto de distinto espesor como de distinto tamaño de esfera) utilizando una esfera integradora. Para determinar *D* hemos estudiado la transmisión (resuelta en tiempo) de un pulso ultra-corto (2 ps) de luz. Utilizando un modelo difusivo para analizar las medidas estáticas y dinámicas, podemos calcular v_E utilizando la expresión $D = \frac{1}{3} v_E \ell_t$.[3] Dentro de la ventana de frecuencias accesibles es posible observar casi dos oscilaciones completas en v_E.

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MODULACIÓN DEL ACOPLO LUZ-PLASMÓN MEDIANTE EL USO DE NANO-INDENTACIONES

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Bajo ciertas condiciones la luz puede propagarse por la frontera entre el metal y un medio dieléctrico sin alejarse de ella, adoptando la forma de una onda confinada, conocida con el nombre de "plasmón de superficie", que involucra al mismo tiempo al campo incidente y a los electrones libres presentes en el metal. Este comportamiento evanescente en la dirección perpendicular a la frontera (originado por el"exceso de momento" respecto a los fotones libres) convierte a los plasmones de superficie en candidatos ideales para el transporte de información en los dispositivos ópticos ultracompactos puestos a nuestro alcance por los últimos avances de la nanotecnología [1]. Paradójicamente, la dificultad de acoplo entre plasmones y radiación libre también constituye el principal obstáculo para el pleno desarrollo de su potencial tecnológico. En este trabajo se presenta un estudio detallado de cómo dicho acoplo puede modularse a voluntad (esto es, aumentarse o eliminarse casi por completo) incorporando una red periódica de nano-indentaciones a un esquema usual de retro-iluminación [2]. La validez de esta propuesta ha sido confirmada mediante medidas experimentales en el infrarrojo cercano y el rango de las telecomunicaciones [3].

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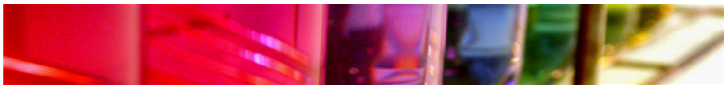
V REUNIÓN DEL GRUPO ESPECIALIZADO DE FÍSICA DEL ESTADO SÓLIDO (GEFES)



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MULTISCALE MODELLING OF THE MAGNETISATION DYNAMICS IN FEPT NANOPARTICLES

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The present paper is on the simulation of pump-probe experiments for ultra-fast magnetisation dynamics in FePt. In this experiment [1] a femtosecond laser pulse induces femtosecond magnetisation decay with subsequent picosecond recovery. We introduce a multiscale approach to model these type of dynamics. The first model is based on atomistic simulations of the stochastic Landau-Lifshitz-Gilbert (LLG) equation with Langevin dynamics, where we model bulk FePt in the ordered $L_1 0$ phase using an effective, classical spin Hamiltonian. This atomistic model [1,2] was constructed on the basis of constrained density functional theory calculations of non-collinear magnetic configurations and site-resolved magneto-crystalline anisotropy.
Our second method is a macro-spin simulation resting on the Landau-Lifshitz-Bloch (LLB) equation, which has been developed by using a mean-field approximation [4]. In the multiscale approach, the input parameters for the LLB model are gained from the atomistic model. We will show that, within certain limits, our calculation with the aid of the macro-spin are in good agreement with our atomistic model simulation. Furthermore, the macro-spin model is able to provide a suitable basis for further theoretical as well as numerical investigations of the pump-probe experiments [5].

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Structural and electrical properties of poly(3-octylthiophene) (P3OT) films: A scanning probe microscopy study.

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Poly-(3-octylthiophene) (P3OT) is one of the most promising materials for applications in organic opto-electronic devices such as field-effect transistors, light-emitting diodes or solar cells [1-3]. In the present work we use scanning force microscopy techniques to study P3OT thin films (50-500 nm) and find a very rich nanostructure. From a morphological point of view, self-assembled layered structures are formed on the surface of the films, theirs morphologies and mechanical properties are quite complex depending on the polymer films growth conditions (drop casting or spin coating).

To study the electrical properties of these films, electrostatic force microscopy (ESF), Kelvin force microscopy (KPM) and capacitance force microscopy (CFM) are applied under different working conditions; in particular under ultraviolet (UV) light illumination, while an electrical current is passing through the thin film and at different temperatures. We find that on the layered structures different surface potential domains are clearly distinguished by KPM and a very rich growth dynamic is observed under UV irradiation and at different temperatures.

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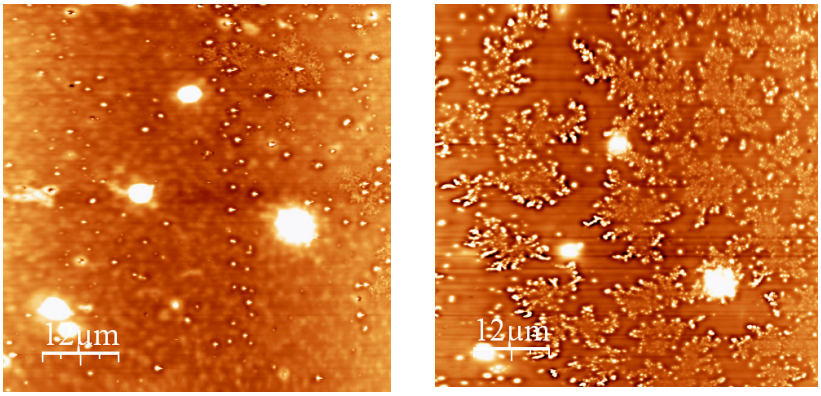

Figure: Topographic images of P3OT thin films UV irradiated. Left figure: 1 hour and 30 minutes after the irradiation. Right figure: 92 hours after the irradiation.

TEM study of a new mechanism of dots generation in MOD $La_{1-x}Sr_xMnO_3$ thin films*

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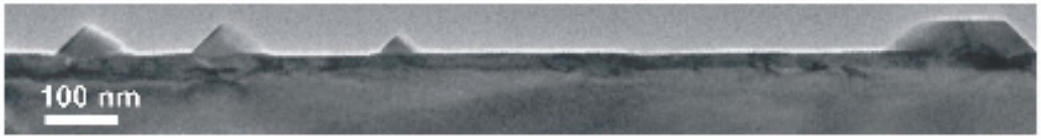
A new mechanism of dots generation segregated from $La_{1-x}Sr_xMnO_3$ (LSMO) thin films grown on $SrTiO_3$(001) substrates is studied by transmission electron microscopy (TEM). Such spontaneous phase separation mechanism leads to the formation of superficial $(Sr,La)O_x$ structures. LSMO films having a thickness around 22 nm, with self-segregated La-rich dots were synthesized by Metal Organic Decomposition (MOD). The films present high quality magnetic properties which are not affected by the formation of the self-segregated La-rich surface dots. These La-rich structures present high crystalline perfection and penetrate into the LSMO film several nanometers. The cation distribution has been investigated by energy filtered TEM and electron energy loss spectroscopy (EELS). Additional energy dispersive x-ray (EDS) measurements were performed in order to investigate the Sr distribution. The structure and microstructure of the system has been studied by HRTEM, selected area electron diffraction (SAD) and diffraction contrast imaging. The LSMO is rhombohedral, and appear partly strained at the interface. Diffraction contrast imaging of planar view foils revealed misfit dislocations spaced more than 51 nm, as required from full misfit relaxation. HRTEM and SAD characterization of the partly buried $(Sr,La)O_x$ nanodots did not allow us to identify their structure with those expected for known La_2O_3 or Sr-La oxide phases, but appear to sustain a well defined three dimensional epitaxial relationship with the LSMO film. The matching distances provided by the nanodots to the LSMO film are $d_{//}$=4.055 Å and $d_{\perp}$=4.048 Å, parallel and perpendicular to the interface, respectively, and thus the misfit strains with the LSMO films are $\varepsilon_{//}$=4.7% and $\varepsilon_{\perp}$=4.5%. As a consequence the c parameter of the LSMO film becomes tensile stretched below the nanodots by ~+0.83%, resulting in an expanded LSMO unit cell volume $\Delta V/V$~+2.5%, as compared to the bulk LSMO unit cell. The LSMO films also feature nano-inclusions of an isostructural and perfectly epitaxial phase having a larger lattice parameter than the surrounding LSMO matrix, presumably $SrMnO_3$. Strikingly, observations of a film quenched before completion of the process did not contain the above mentioned nanodots, but are characterized by a distribution of nanometric regions orthorhombic or monoclinic forms of LSMO. Our results suggests that the observed phase and structural evolution of the microstructure upon annealing constitutes a strain relief mechanism involving a complex interplay of the structural and compositional degrees of freedom exhibited by LSMO, which add to the conventional dislocation mechanism.



* This work has been supported by EU (HIPERCHEM project), Generalitat de Catalunya (2005-SGR-0029 and CeRMAE) and by Spanish MEC (MAT2005-02047, FPU program

SYNTHESIS OF GOLD-COATED IRON (Fe@Au) NANOPARTICLES

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Gold-coated iron (Fe@Au) nanoparticles have been synthesized by means of two different microemulsion methods. The samples were characterised by x-ray diffraction (XRD), ultraviolet-visible spectroscopy (UV-Vis), transmission electron microscopy (TEM) and SQUID magnetometry.

In the first system, gold-coated iron nanoparticles were prepared in a microemulsion of cetyltrimethylammonium bromide (CTAB) as surfactant, 1-butanol as co-surfactant, n-octane as the oil phase and the aqueous solution [1]. Iron(II) sulphate and tetrachloroauric acid were used as metals source and sodium borohydride was used as the reducing agent. The reduction of the iron(II) cations was performed previously to the addition of the gold(III) microemulsion and its subsequent reduction. The particle size distribution obtained form TEM shows an average size of ~6 nm.

In order to increase the particle size and to improve the particle size distribution observed, a second system was used: polyethyleneglycol (10) monoleyl ether (Brij 97) as surfactant, cyclohexane as oil phase and the aqueous solution [2]. The main size ranges between 10 and 14 nm. In order to increase the particle size, the droplet size was increased by changing the molar ratio water-to-Brij-97 ($\omega = [H_2O]/[\text{Brij-97}]$). In this case, TEM results show a main size ranging between 14 and 16 nm.

The characterization of the gold-coated iron nanoparticles was completed by measuring the temperature- and field-dependence of the magnetic properties. Superparamagnetic behaviour is observed with low blocking temperatures.

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Magneto-Optical Kerr Effect Implemented in a Time Domain Method.

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Magneto-Optical effects are important for their change in the state of polarization of incident light. One of the main applications is as an electromagnetic probe to study the magnetic structure in materials. The characteristic of this electromagnetic probe is that it does not modify the magnetic structure of the material. As an incident electromagnetic pulse is sent through an iron thin film, it produces two pulses; one with Kerr effect and the second with Faraday Effect. The incident electric field and the magnetization of the magnetic film are orthogonal. The polarization of the electromagnetic wave is rotated by the magneto-optical Kerr and Faraday Effect into the magnetic film. This phenomenon is introduced into the algorithm of Finite Difference Time Domain through the complex magneto-optical constant Q. Linear terms are retained of this magneto-optical constant which are defined by Voigt [1]; and the magneto-optical effect modifies the dielectric tensor of the magnetic film, given by

$$\varepsilon = \begin{pmatrix} \varepsilon_f & -iQ\varepsilon_f m_p & iQ\varepsilon_f m_l \\ iQ\varepsilon_f m_p & \varepsilon_f & -iQ\varepsilon_f m_t \\ -iQ\varepsilon_f m_l & iQ\varepsilon_f m_t & \varepsilon_f \end{pmatrix}$$

The magnetization only affects the electric field of the incident electromagnetic pulse. An incident pulse with linear polarization and orthogonal to the magnetization M of the magnetic film is considered. The simulation space [2] is surrounded by an absorbing boundary condition (ABC), which absorbs all the incident waves in order to reduce the effects by the finite size of the numerical space. The Perfect Matched Layer (PML) was chosen as an ABC with twelve layers, enough to reduce the reflected wave. The conductivity of these layers change from the conductivity of the medium of the wave propagation to a perfect electric conductor. The size of the cells in the space of simulation and the time step were selected in agreement to reduce the numerical dispersion and to avoid numerical instability. The size of cells was reduced 15 times in the magnetic film and the space surrounding it. In this zone, the conductivity and the cell size of the PML were modified to obtain perfect coupling. An algorithm was obtained in time domain that simulates the correct rotation of the electric field of an electromagnetic pulse as was predicted by the magneto-optical Faraday and Kerr effect. The numerical results of the Finite Difference Time Domain method were compared with the analytic solution in order to verify the algorithm and validate the numerical results.

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Micro-Raman scattering by optical and folded acoustic modes in GaAs/InGaAs nanorolls

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In this work, we investigated semiconductors nanorolls fabricated by the self rolling mechanism of epitaxially grown strained bilayers [1]. Starting point for the fabrication is a MBE-grown sample consisting of a GaAs substrate, an AlAs sacrificial layer, a strained InGaAs and a GaAs layer. The thickness d_{Ga} of the GaAs layer was varied in the different samples, whereas the thickness d_{In} and the In content x = 0.215 of the $In_xGa_{1-x}As$ layer were kept constant. The samples were scratched along the [100] direction and selectively etched. The rolled-up bilayers form multiwalled tubes with 5-6 rotations and tube radios of 0.5, 0.7 and 1.2 μm. As shown in Fig. 1 (a), through micro-Raman spectroscopy we were able to detect the residual strain of the nanoroll, which presents differences with respect to the unrolled sample and varies with the diameter of the tube.

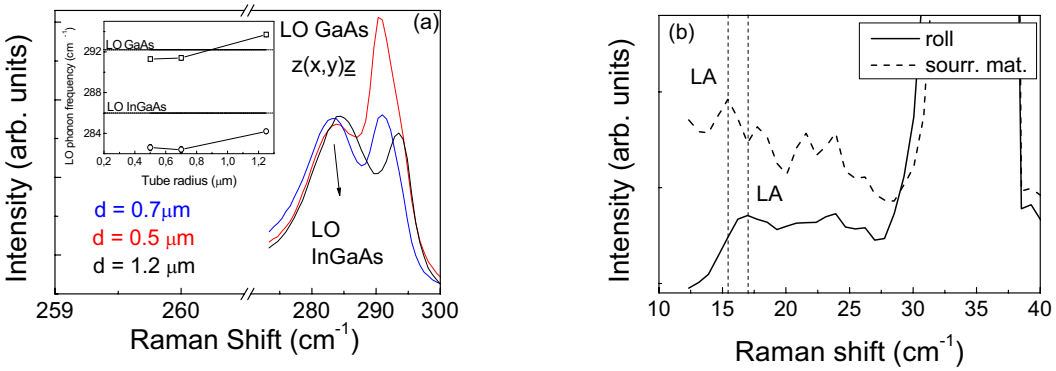

Fig. 1. (a) Raman spectra of single nanorolls. The inset shows the peak frequency of the LO modes attributed to the microtubes as a function of its radius of curvature. (b) Raman spectra of acoustic phonons collected on the nanoroll and the surrounding material.

The spectral features corresponding to the acoustic phonons of the nanoroll are different than those observed in the surrounding material, as shown in Fig. 1 (b). The wavenumber of the folded modes agree well with the theoretical calculations[2] and are consistent with the superlattice periodocity of the layers that form the heterostructure.

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Thermal decomposition of nanocrystalline magnesium hydride (MgH_2) thin films

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At present, one of the bottlenecks of the hydrogen economy and, particularly for transportation applications, is finding light materials to storage hydrogen in a reversible way at moderate pressures and temperatures. Among the different materials proposed [1], magnesium hydride (MgH_2) is one of the most promising due to its low cost, abundance and high hydrogen gravimetric density (7.6 wt%). However, the high stability of hydride (-76 kJ/molH_2), as well as its sluggish absorption-desorption hydrogen kinetics, are the main drawbacks which prevent its implementation on different applications. In order to improve the H-kinetics, a detailed knowledge of the different steps occurring during absorption/desorption mechanism is necessary. Despite numerous earlier investigations (see for instance [2]), it remains unclear which step (dissociation of H_2 molecule, H-diffusion etc) controls the hydrogen absorption/desorption in bulk magnesium, mainly because of the difficulties to achieve identical initial conditions (particle size, previous oxidation, impurities..)[3]. In that context Mg films offer an easier way to prepare well controlled material (purity, crystallite size, thickness, etc)[4] to research. Therefore, in this work, we present an investigation of the hydrogen desorption of Mg nanoscrystalline thin films prepared by e-beam deposition. Films characterization was carried out by different techniques (XRD, SEM, etc) .The influence of several parameters such as thickness, crystallite size, etc, on the desorption kinetics was investigated by DSC-MS, transport and optical measurements, etc. A tentative hydrogen desorption mechanism is proposed and compared to previous results.

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Acknowledgments

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Why "$PbCrO_3$" is not ferroelectric?

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$PbCrO_3$, a high pressure phase, is unusual among the lead perovskites, since according to early work it was reported as cubic (*S.G. Pm-3m,* a≈4.0Å) [1] while its formal analogues with Ti and V are tetragonal due to the presence of the so called inert pair on Pb(II) [2,3]. Not surprisingly, $PbCrO_3$ being cubic, this material is not ferroelectric. In the course of this work we have observed by means of x-ray powder diffraction data a "simple" perovskite cell, but with the lead ion occupying a multi-split position on the A-site. From electron diffraction we observe that the diffraction pattern along any {001} zone axis shows diffuse scattering around all the diffraction maxima, FIG. 1. By means of HRTEM and image simulations we were able to resolve its complex modulated structure, FIG. 2, that takes care of some lead understoichiometry and is distributed in microdomains [4]. We believe that this unusually complex structural and microstructural situation makes that *on average* "$PbCrO_3$" is not ferroelectric.

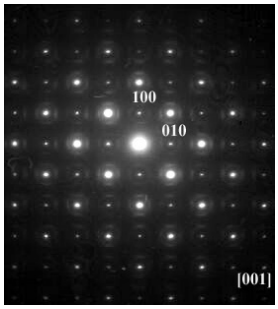

FIG. 1. SAED pattern of the $PbCrO_3$ that shows the diffuse scattering along the zone axis [001].

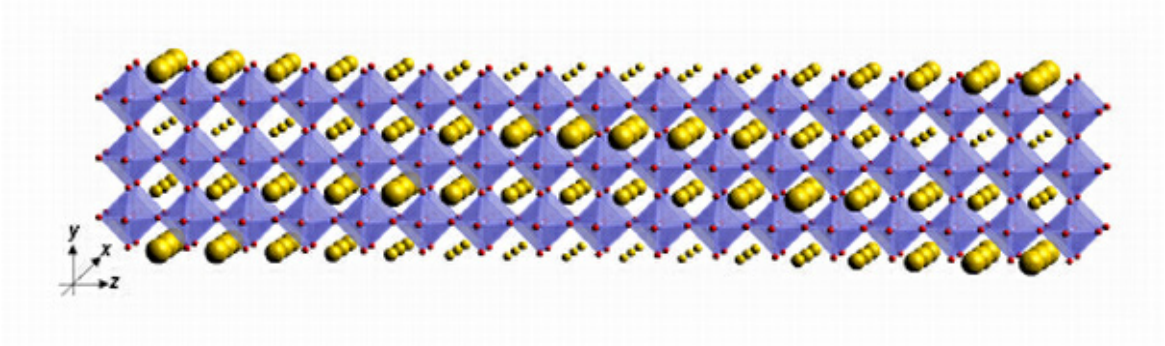

FIG. 2. Microstructural model of the "$PbCrO_3$"showingthe compositional modulation of the Lead.

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Transporte inelástico a través de moléculas individuales

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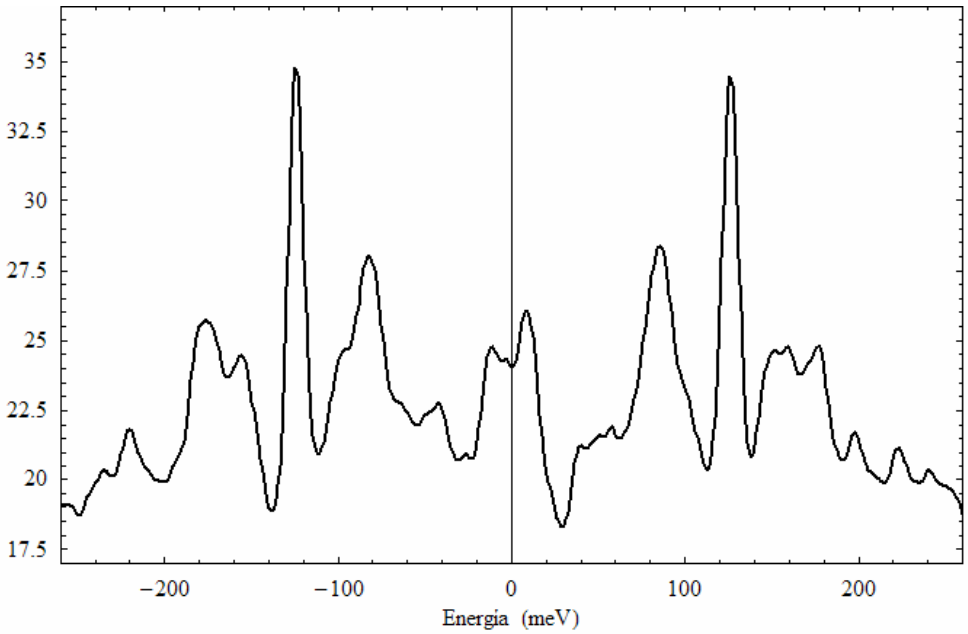
La caracterización de contactos formados por una molécula individual, conectada químicamente a electrodos metálicos, es un paso fundamental para una electrónica basada en moléculas funcionales (electrónica molecular). En este trabajo, presentamos resultados en los que se observan las vibraciones de una molécula individual suspendida entre electrodos de oro cuando se aplica una diferencia de potencial. Las medidas han sido realizadas con un microscopio de efecto túnel (STM) a bajas temperaturas (helio líquido). La técnica utilizada "Inelastic Electron Spectroscopy" (IES) permite detectar los modos vibracionales de la molécula que son excitados por electrones que la atraviesan. Los resultados obtenidos presentan un buen acuerdo con cálculos teóricos de primeros principios (DFT)[1] y con otras medidas experimentales en monocapas de moléculas autoensambladas (SAMS) [2,3].

Densidad de modos vibracionales en una molécula de pentanoditiol



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High ordered Co nanoestructures arrays

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Different techniques have been used to obtain ordered magnetic nanostructures some of them based on self-organization process. In particular, our group has long experience in the fabrication of arrays of magnetic nanowires embedded in AAM (Anodic Alumina Membrane) [1] In addition, the AAM have been used to translate the ordering degree into different material following replica-antireplica process [2]. In this work, PMMA (poly (methyl methacrylate)) patterned surfaces has been prepared. The nanostructured samples present hexagonal symmetry following the geometry of the Aluminium substrate used as a precursor. Notice that many works have been reported using the PMMA (poly (methyl methacrylate)) as a base material to perform replications for submicrometric and nanometric structures for a variety of applications [3] [4]. The aim of this work has been to use the PMMA polymer as a substrate for the deposition of magnetic materials creating a nanostructured array of magnetic nanoparticles. The morphology of the PMMA surface is controlled by the geometry of the Al precursor. In particular, hexagonal arrays of PMMA nanostructures with a lattice parameter of 105nm and 180nm have been fabricated. Magnetic thin films have been deposited by sputtering onto the polymer at different angles. We have studied the magnetic properties of these samples by using Vibrating Sample Magnetometer (VSM) and Magnetic Force Microscope (MFM). Figure 1 shows the topography and the domain structure of two samples with different lattice parameter. Figure 1 (a) and (b) corresponds to the sample with a lattice parameter of 105nm. In this case, the bright and dark magnetic contrast corresponds to the out-of-plane component of every nanoparticle. The dependence of the domain configuration with the previous magnetic history has also been observed by MFM. The samples with higher lattice parameter (180nm) present weak out-of-plane magnetization component which oscillates in up and down direction as shown in Fig 1(d).

In this work we have reported a technique to fabricate magnetic nanostructures on polymeric substrates with controllable magnetic behaviour.

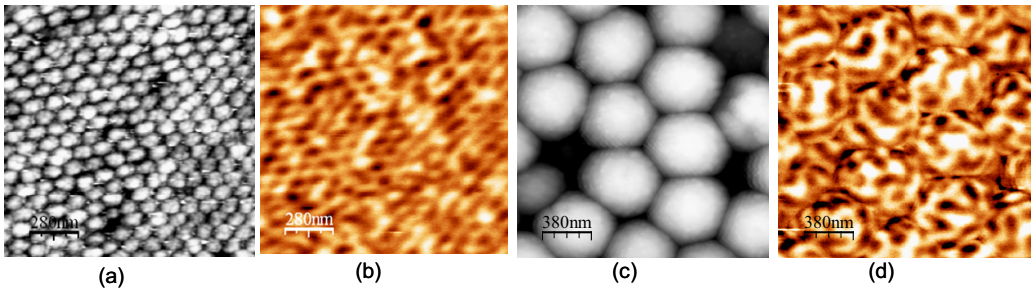

Figure 1: (a) AFM and (b) MFM image of the sample with a lattice parameter of 105nm. The Co thin film thickness is Co 30 nm. (c) AFM and (d) MFM image of the sample with a lattice parameter of 180nm. The Co thin film thickness is Co 30 nm..

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Three-dimensional elastic field of a buried inclusion in a wurtzite type half-space

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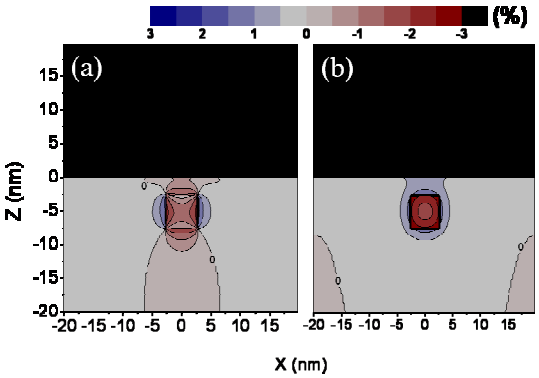
In this work (based in the previous work of Pan et al [1] on anisotropic bimaterials), we have studied the state of elastic deformation of a system formed by an arbitrarily shaped inclusion buried in a semi-infinite matrix with free surface boundary conditions, both of wurtzite crystal structure. We make use of the Stroh formalism [2] and the Mindlin's superposition method [3] in order to derive the elastic Green's function of the system as a sum of the full-space Green's function and a complementary part due to the free surface [1]. The results are expressed in terms of a two-dimensional Fourier transform in the coordinates parallel to free-surface. We give numerical examples in a system formed by a GaN inclusion buried in an AlN semi-infinite matrix. Two cases are analized: the [0001] and [11-20] axes normal to free surface, relevant for the study of polar and non-polar surfaces in III-N nanostructures. The results are useful to study the elastic field in semiconductor heterostructures as a function of the layer thickness and the effect of buried structures on adatom dynamics in epitaxial growth.



The ε_{33} strain component for a cuboidal inclusion, of size 5 nm and with the center of cuboid at 5.1 nm from the surface, for two cases: (a) free-surface normal to [0001] and (b) normal to [11-20].

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MONTE CARLO SIMULATIONS OF INTERACTING NANOPARTICLE SYSTEM

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Recently nanosized magnetic single domain particles and their mutual interactions have attracted interest both in fundamental research and applications. An ensemble of single domain particles forms a superparamagnetic state at high temperature. On lowering the temperature, the particles become blocked at a specific temperature that depends on the size and magnetic anisotropy of particles, the time scale of the experiment , the external applied field and the interactions between the nanoparticles.

The fundamental role of these interactions in the magnetic behaviour of these systems has been reported in different theoretical and experimental works [1-2]. However, there is no clear picture of how dipole-dipole interactions would affect the macroscopic magnetic response of the system.

In this work we study the influence of the dipolar interactions between magnetic nanoparticles on the blocking temperature of the system using Monte Carlo simulations [3-5]. Results show that the behaviour of the system is strongly affected by the applied magnetic field and the size of the nanoparticles.

For very small nanoparticles an increase of the concentration of particles gives always an increase of the blocking temperature of the system. However, for bigger particles and small values of external magnetic field a small decrease of the blocking temperature with increasing concentration of particles is obtained.

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Anisotropy of the Raman polarizabilities in GaN, AlN and their heterostructures

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The nitride semiconductors of the group III (GaN, AlN and InN) crystallize usually in the wurtzite structure, and present piezoelectric and pyroelectric properties. Most of the optoelectronic devices based on these materials are grown along the wurtzite c-axis. In this orientation, due to the polarization discontinuities between the active layer and the barrier, large electric fields are present in the heterostructures. Since the piezoelectric constants of the nitride semiconductors are very large, the intensity of this electric field is very sensitive to the strain state of the materials constituting the heterostructure. To reduce or even suppress this electric field, the growth of heterostructures along non-polar directions (a and m-plane of the wurtzite structure) has attracted much attention [1,2].

Raman spectroscopy is an effective technique for the optical characterization of crystal properties. It is nondestructive and contactless, and may provide information on material orientation, strain and electron concentration. Applied to semiconductor nanostructures, this technique allows the simultaneous characterization of the active layer and the matrix in which the nanostructures are embedded, the morphology of the interfaces and their relative orientation [3]. In this work we present a study of the relative values of the Raman polarizabilities of GaN, AlN and GaN/AlN heterostructures (quantum wells and quantum dots) grown along the a-plane. The relative strength of the E_2, A_1(TO) and E_1(TO) phonon modes is studied for different polarization configurations. The angle of the incident and scattered polarizations with respect to the wurtzite c axis is changed from 0 to 90º. The angular dependence of the intensity of the phonon modes allows the determination of the complex phase of the polarizations and its variation with material parameters.

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STRUCTURAL, MAGNETIC AND THERMOELECTRIC PROPERTIES OF M_xCoO_2

(M = Li, Na, K, Ca, Sr).

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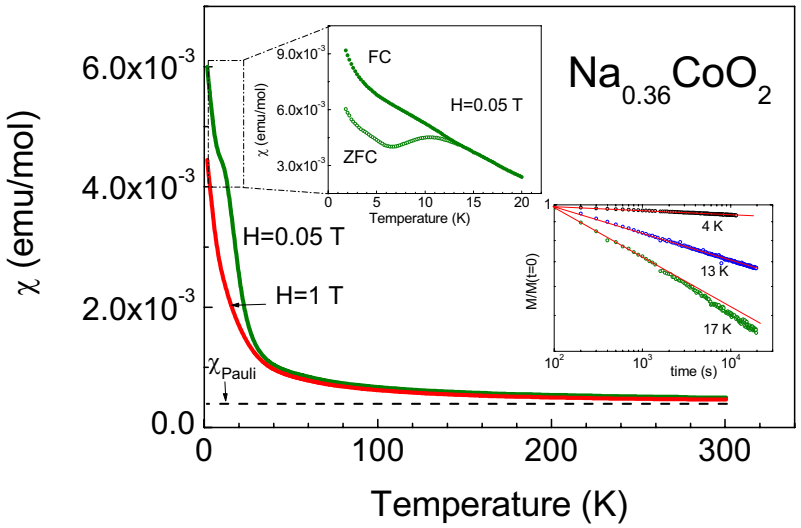
In this work we report a sistematic study of the structural, magnetic and thermoelectric properties in the layered system Na_xCoO_2. Na-deintercaleted and subsequently Na-intercaleted samples were obtained by different treatments with Br_2 and NaI in acetonitrile, respectively. The effect of annealing temperature and time was analysed in order to propose a complete magnetic/structural phase diagram. Other layered oxides M_xCoO_2 (M= Li, K, Ca, Sr) have been also synthesized by the low temperature ion exchange of layered Na_xCoO_2. Their physical properties will be shown and compared with those ones from analogous Na_xCoO_2.



ZFC magnetic susceptibility at two different fields in metallic x=0.36. The dotted line is the Pauli susceptibility determined from high temperature M(H) isotherms. Upper inset: Detail of the ZFC-FC irreversibility visible at low fields below ≈12 K. Lower inset: Relaxation rate of the normalized magnetization. Above the T_{irr} relaxation departs from the slower logarithmic behavior observed at low temperatures.

Efectos de los estados de interfase en las propiedades de transporte de heterouniones $La_{0.8}Sr_{0.2}CoO_3$/ $SrTi_{0.99}Nb_{0.01}O_3$

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En los últimos años el estudio de uniones tipo pn y Schottky fabricadas de óxidos de metales de transición (OMTs) ha recibido mucha atención.[1] Este tipo de heteroestructuras permiten cambiar la cantidad de portadores cerca de la interfase sin introducir el desorden estructural asociado al dopado por sustitución química. Asimismo estos dispositivos son muy sensibles a la aplicaciones de estímulos externos presentando diferentes fenómenos como: magnetoresistencia[2], magnetocapacitancia[3], electroresistencia[4], etc. En este contexto el estudio de las propiedades electrónicas de la interfase en dispositivos fabricados con estos materiales es relevante para entender los diferentes efectos encontrados en ellos.

Para estudiar las propiedades electrónicas de la interfase hemos realizado uniones entre el semiconductor tipo p $La_{0.8}Sr_{0.2}CoO_3$ (LSCO) y el semiconductor tipo n $SrTi_{0.99}Nb_{0.01}O_3$ (STNO). Las uniones presentan características corriente (J) – tensión (V) con buenas propiedades rectificantes en el rango de temperaturas estudiado (20K - 300K). A partir de las curvas J-V determinamos la existencia de dos mecanismos para el transporte: tunel asistido por estados de interfase para T<130K y difusión recombinación para temperaturas mayores. A partir de medidas de la capacidad de la unión (C) en función de la tensión aplicada hemos obtenido el potencial de contacto de la unión (V_{bi}) a diferentes frecuencias (F). Encontramos una relajación en la capacidad que se desplaza hacia menores frecuencias cuando la temperatura decrece y que es debida al atrapamiento/desatrapamiento de portadores en los estados de interfase.

En el trabajo discutimos la posible relación entre los estados de interfase que afectan a las propiedades de transporte J-V, a la relajación de la capacidad caracteristicas C-V-F y su posible conexión con la transferencia de carga debida al desacoplo de polaridad de la interfase LSCO-STO[5].

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FUNCIÓN RESPUESTA TERMOELÉCTRICA EN PELÍCULAS DELGADAS DE SULFUROS METÁLICOS

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Recientemente los materiales termoeléctricos se están considerando como una buena alternativa de ahorro energético [1]. Esta idea esta basada en el principio de calentamiento y enfriamiento termoeléctrico, un fenómeno que fue descubierto en el siglo XIX y que alcanzó sus primeras aplicaciones prácticas en la década de los 60 del siglo XX.

Los materiales termoeléctricos generan un voltaje eléctrico cuando se calientan de forma que exista una diferencia de temperatura entre sus extremos. Del mismo modo, cuando se aplica un voltaje eléctrico entre sus extremos uno de ellos se calienta y el otro se enfría. Sin embargo, este proceso en la mayoría de los materiales es muy ineficiente. Un buen material termoeléctrico debería tener, un alto valor del coeficiente termoeléctrico, una alta conductividad eléctrica y una baja conductividad térmica. Con este propósito muchos investigadores tratan de modificar la estructura de los materiales de alto coeficiente termoeléctrico para disminuir su conductividad térmica y aumentar su conductividad eléctrica [2-3].

En nuestro laboratorio, sin embargo, modificamos la composición del material mediante dopado para conseguir optimizar su respuesta termoeléctrica. En concreto, en este trabajo presentamos los resultados de modificar la respuesta termoeléctrica de películas delgadas de disulfuro de hierro mediante el dopado con Ti. Este proceso da lugar a respuestas termoeléctricas lineales dependientes del tiempo (ciclos de histéresis) variables en función de la cantidad de Ti introducida.

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AUSENCIA DE FERROMAGNETISMO EN NANOPARTICULAS DE TiO_2 DOPADAS CON METALES MAGNETICOS

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En los últimos años ha habido un gran interés por el estudio de los llamados DMS (semiconductores magnéticos diluidos) inducido por su posible carácter magnético y semiconductor simultáneamente. Esta posibilidad ha sido especialmente importante para el caso de los semiconductores de banda ancha tipo *p*, como el TiO_2, ya que presentarían una temperatura de Curie superior al ambiente. Desafortunadamente los resultados que hay en la literatura son totalmente contradictorios. En esta dirección, en un trabajo anterior mostrábamos que el TiO_2 no era ferromagnético en su fase rutilo cuando se dopaba con Fe [1]. En este trabajo hemos intentado generalizar el trabajo anterior con un estudio realizado sobre la estructura y las propiedades magnéticas de nanopartículas de TiO_2 dopado con metales de transición ferromagnéticos (Mn, Fe y Co) para las dos fases más comunes, anatasa y rutilo. Para sintetizar estas nanopartículas se han utilizado dos métodos. Por un lado por via química, sol-gel, para obtener la fase anatasa, y por el otro lado por condensación en fase vapor, donde la fase mayoritaria es la rutilo. La difracción de rayos X no indica la presencia de impurezas en ninguno de los casos. Los análisis realizados por XPS nos indican que la valencia del ión Ti es 4+ en todos los casos, pero el dopante presenta una valencia diferente según el ión ferromagnético que intervenga. El Mn y el Co presentan valencia 2+, lo que indica la presencia de una vacante de oxígeno por catión y el Fe presenta una valencia 3+ lo que supone una vacante de oxígeno por dos iones de Fe. En este último caso, la espectroscopia Mössbauer nos indica, por un lado, la ausencia de ferromagnetismo tanto para la estructura anatasa como rutilo. Por otro lado la presencia de dos dobletes diferentes de Fe^{3+} nos ha permitido determinar las posiciones que ocupa este ión substituyendo el Ti. Por último, las medidas magnéticas realizadas para todas las composiciones estudiadas, muestran claramente que el sistema TiO_2 dopado no presenta ferromagnetismo hasta los 5 K y el ión magnético que substituye el Ti es paramagnético.

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Progressive Breakdown of superexchange theory in magnetic insulators approaching the itinerant limit.

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The study of the metal insulator transitions that occur at T=0 K, and the new phases that emerge close to this point is one the most active areas of research in condensed matter physics. Far away from the quantum phase transition, in the insulating side, the magnetic properties of the system are well described by Superexchange theory[1]. According to this theory, the strength of the magnetic interaction can be calculated from the ratio between the hopping integral t and the Coulomb Energy U:

$$J=t/U$$

This equation is the result of a perturbative calculation (U>>t) and hence applicable only at the strongly localized limit. So, on approaching the metallic phase from the insulating side, a breakdown of this theory is expected.

In this work we studied the evolution of the Neel temperature with the volume (pressure) in a series of vanadium spinels $A^{2+}V_2^{2+}O_4$ (A= Cd,Mn,Zn,Mg), where the V-V distance is tuned by modifying the atom at the tetrahedral position. As the V-V distance decreases a systematic enhancement of the pressure dependence of T_N with volume is observed, indicating a progressive collapse of U due to partial electronic delocalization. Below a critical separation (A=Zn and Mg) charge carriers form large polarons and T_N decreases with pressure. This result shows that the insulator to metal transition occurs through an intermediate phase in which cation-clusters form into the ionic matrix.[2]

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NUEVA FASE METAESTABLE EN EL SISTEMA BINARIO Zr-Cr

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El $ZrCr_2$ pertenece a un grupo de compuestos intermetálicos denominados AB_2 que, a su vez, forman parte de un grupo más amplio conocido como las Fases de Laves. Estos compuestos intermetálicos están tomando cada vez mayor relevancia a nivel científico y tecnológico debido a sus buenas propiedades eléctricas(magnetoestricción, superconductividad), mecánicas (resistencia mecánica a altas temperaturas, resistencia a la oxidación, etc), y, especialmente, termodinámicas y cinéticas para su uso en la acumulación de hidrógeno.

El $ZrCr_2$, así como otros compuestos intermetálicos semejantes, presentan polimorfismo por lo que pueden presentarse según las distintas estructuras de Laves: C14, C15 y C36. La comprensión de las transformaciones entre estas estructuras puede ayudar a entender mejor sus propiedades y, por consiguiente, resulta muy útil un pormenorizado estudio de su diagrama de fases. Dentro de un estudio sistemático realizado en el compuesto Zr-Cr, se ha descubierto una nueva fase de naturaleza metaestable en muestras con composición nominal 36% at. Zr y 64% at. Cr, tras ser aleada en horno de arco. En este trabajo, se presenta una caracterización completa del material con el fin de identificar la composición, estructura y medir el parámetro de red de esta nueva fase. Tras análisis de microscopía óptica (MO), microscopía electrónica de barrido (SEM) y transmisión (TEM), energía dispersiva de rayos X (EDX) y difracción en polvo de rayos X (DRX), ha podido concluirse que la nueva fase posee una composición del 50% at. Zr y 50% at. Cr, estructura cúbica centrada en las caras (FCC), y un parámetro de red de ~8.17 Å. Al mismo tiempo, se ha relacionado la aparición de esta fase con la transformación metatéctica que tiene lugar para el valor de composición nominal de la muestra indicado.

Agradecimientos:

A Fernando Moreno por su apoyo técnico. Esta investigación ha sido financiada por el MEC (MAT 2005-06738-C02-01).

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Diamagnetismo alrededor de la transición Meissner en un cuprato superconductor de gran homogeneidad química y estructural

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Se presentan medidas del diamagnetismo alrededor de la transición Meissner en un monocristal de $Tl_2Ba_2Ca_2Cu_3O_{10}$ de alta calidad química y estructural.[1] Los datos experimentales son explicados cuantitativa y consistentemente en las diferentes regiones del diagrama de fases H-T, en base a la teoría de Ginzburg-Landau (GL) para el efecto de fluctuaciones de pares de Cooper y de vórtices. Este resultado confirma que la transición Meissner en estos materiales es *convencional*,[2] y cuestiona la validez del *modelo de vórtices* para explicar la falta de coherencia superconductora observada entre Tc y la temperatura del pseudogap T* en estos materiales.[3]

Este trabajo ha sido financiado por el Ministerio de Educación y Ciencia-FEDER (FIS2007-63709), y por la Xunta de Galicia-FEDER (07TMT007304PR).

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KONDO-LIKE FEATURES IN CHEMICALLY PURE MAGNETIC ATOMIC-SIZE CONTACTS

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The influence of magnetism in the electronic transport in atomic sized contacts is not yet clear [1]. However, certain features systematically appear in the conductance measurements of magnetic atomic contacts. Specifically, the spectroscopy of atomic size contacts of Ni, Fe or Co reveals the existence of a characteristic significant peak or dip at zero bias (Fig. 1) that is not present in the case of non-magnetic materials. We have measured the differential conductance as a function of bias at 4K on two houndred monoatomic contacts of Ni, Fe and Co fabricated by STM. The zero bias anomaly has been fitted with the Kondo-Fano lineshape typical of magnetic adatoms in non-magnetic surfaces [2,3]. The statistical analysis of the data results in Kondo temperatures around 250 K, 120 K and 80 K for Ni, Co and Fe respectively. A Kondo-like behaviour could arise in chemically pure magnetic contacts if tip atoms behave different due to their smaller coordination.

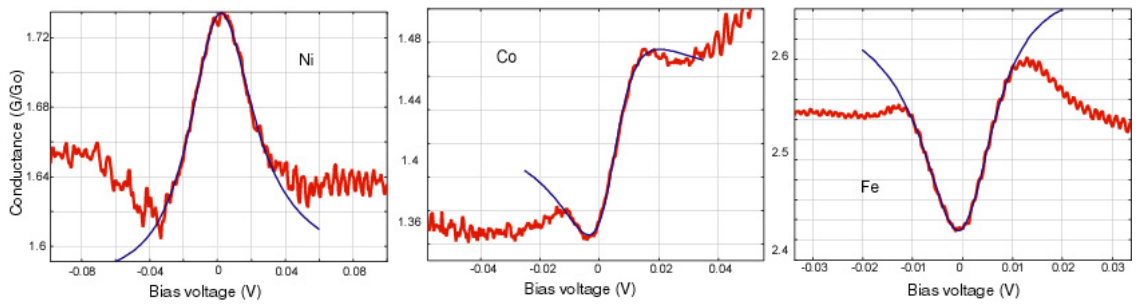

Figure 1. Spectroscopic curves for Ni, Co and Fe showing pronounced zero bias anomalies and their corresponding Fano lineshape fittings.

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Ni nanocontacts: preferential structures before failure

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The deformation of Ni nanowires is studied both experimentally and throught simulations. On one hand, molecular dynamics (MD) simulations have been performed to study the deformation of nanowires and the preferential configurations occuring before failure. The dependence of deformation on the stretching direction has been studied for [100], [111], [110] and [112] directions. For all cases two preferential structures have been observed before failure: a monomer, where a single atom acts as a bridge between the two contacts, and a dimer, where two atoms align to form a bridge between the two sides of the wire. From all cases computed (400) a total of 82% form a dimer before failure while only 18% break from a monomer. The results presented will be compared with previous calculations by other groups [1, 2]. These preferential configurations obtained from MD simulations have been used to compute the transport properties throught the first-principles implementation of Landauer's formalism included in our transport package ALACANT [3].

On the other hand, the conductance of Ni nanowires at low temperature (4.2K) was measured using a high-stability scanning tunneling microscope (STM). Traces of conductance were recorded as a function of the relative tip-sample distance as the two electrodes were brought together and separated. The experimental conductance histograms measured will be discussed considering the results obtained from the atomistic simulations described above.

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La iniciativa ESS-Bilbao: la candidatura española para albergar la Fuente de Espalación Europea (ESS)

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Bilbao está compitiendo por albergar la Fuente de Espalación de Neutrones Europea (ESS), una de las grandes instalaciones científicas mundiales que la OCDE recomendó construir en su informe de 1999 y que será utilizado cada año por más de 5.000 investigadores y dando empleo a unas 800 personas.

Son tres las candidaturas europeas que rivalizan por esta infraestructura científica europea, cuyo presupuesto rondaría entre 1.100 y 1.200 millones de euros, financiado por el país escogido y por los socios que éste consiga captar. Probablemente hasta finales del 2008 no se decidirá qué lugar, Lund (Suecia), Budapest (Hungría) o Bilbao, albergará este gran laboratorio europeo, enmarcado en la "hoja de ruta" del Foro Estratégico Europeo sobre Grandes Infraestructuras Científicas (ESFRI) presentado a finales de 2006, y cuya construcción se prevé finalice en el 2018. La candidatura de Bilbao cuenta con el apoyo de las administraciones central y Vasca, quienes por medio de la firma de un convenio han constituido un Consorcio público (ESS-Bilbao), dotado inicialmente con 10 M€, con el único objetivo de hacer que la ESS se construya en Vizcaya. Asimismo, existe una financiación comprometida, por ambas administraciones, de más de 330M€ si se elige Bilbao como sede de la ESS.

La ESS es una fuente pulsada de neutrones, producidos por espalación, de 5MW con un parque inicial de 20 instrumentos, mejorable con más instrumentos, más potencia y más blancos. Un haz de protones, producidos por una fuente de iones, acelerados a 1.3 GeV en un LINAC de unos 600 metros, colisionarán con un blanco de metal pesado, previsiblemente de mercurio, para producir pulsos largos de neutrones, en el rango de los milisegundos, a una frecuencia de 16'6666 Hz. Con estas características esta fuente de Pulso Largo proporcionará hasta dos órdenes de magnitud más flujo de neutrones en pico que las actuales fuentes.

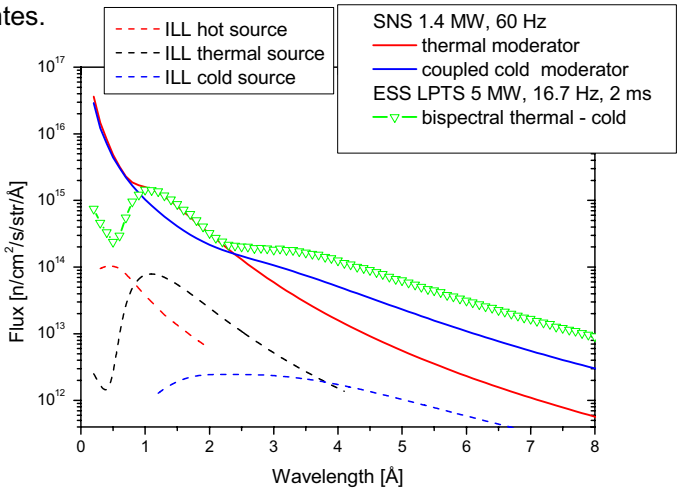

Figura 1: Espectro de neutrones producidos por el ILL, la SNS y la futura LP5MW-ESS.

ION CHANNELING STUDY IN SINGLE CRYSTALS OF CdZnTe

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CdZnTe is a very important material due to its applications such us X-rays and Gamma-rays detector [1]. For this purpose, bulk crystals of very high resistivity (>10^{10} Ω·cm) must be obtained [2]. The knowledge of the crystalline structure is an important data in order to determine the relationship among the physical and chemical properties and the crystal resistivity. In this way, lattice positions occupied by defects, impurities and dopants is a fundamental point to explain the optical and electrical properties of this material. Previous studies has been carried out using Rutherford backscattering spectrometry in channelling mode (RBS/C) [3] with 2 MeV H^+ ions. The specific lattice location occupied by Zn atoms and the composition of the CdTe:Zn [4] crystal were determined. In this work we show that pure $Cd_{0.94}Zn_{0.06}Te$ [1 1 0] oriented single crystals were successfully grown by the Vertical Bridgman method. The good crystal quality was confirmed by RBS/C experiments performed at the Standard Beamline of CMAM/UAM (Madrid), and also with Laue X-ray diffraction. The analysis of the channelling dip along [1 1 0] direction, was used to verify the existence of defects and impurities. It has been demonstrated that CdZnTe crystals of high quality were grown with the absence of defects and impurities along the [1 1 0] direction within the experimental error. The axial [1 1 0] angular scan in CdZnTe is shown in the figure 1.

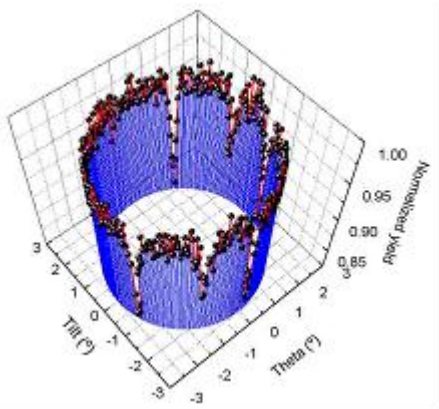

Figure 1. Angular scan around [1 1 0] axis in CdZnTe

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MODELOS DE ELASTICIDAD PERIÓDICA DISCRETA PARA DEFECTOS EN GRAFENO

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Después de la reciente observación experimental del grafeno y otros cristales bidimensionales, cobra gran importancia el estudio de la estabilidad mecánica de su red y la presencia y evolución de defectos cristalinos en ella. Hemos diseñado modelos periódicos de elasticidad discreta en redes cristalinas exagonales planas para estudiar los defectos correspondientes a dislocaciones y dipolos de dislocaciones en arista. Estos modelos se basan en discretizaciones asimétricas de la elasticidad isótropa. A temperatura cero, los defectos dinámicamente estables correspondientes a dislocaciones en arista pueden ser pares pentágono-heptágono (5-7) u octógonos dependiendo de la configuración inicial elegida. Entre los posibles núcleos para dipolos de dislocaciones están las vacantes, divacantes 5-8-5 y defectos Stone-Wales. Tanto las vacantes simétricas como las divacantes son dinámicamente estables mientras que los defectos Stone-Wales son inestables.

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Peparation of graphene layers and nanoribbons using PMDS stamps

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Graphene is an atomically thin film of graphite that presents extraordinary electronic properties. In fact graphene's electrons follow Dirac equation instead of Scroedinger equation that is followed by electrons in most of the materials producing new physical effects as anomalus quantum Hall effect, ambipolar field effect, etc. While a reproducible mass-production process is not available nowadays to get graphene sheets, micromechanical cleavage technique is the only way of producing high quality samples.

As graphene electronic properties seem to be very sensitive to the

fabrication process we have developed an 'all dry' process in which graphene sheets are not exposed to any chemical during the fabrication and the later electrode evaporation. Poly (DiMetiol) Siloxane stamps are used the cleave the high oriented pyrolitic graphite, in this way the use of scotch tape to cleave the graphite (that can leave traces of glue over the surface) is avoided. By using a shadow mask process to evaporate the electrodes, electron beam litography is not needed (that means avoiding exposition of the graphene sheets to resins and solvents).

In this work we also demostrate how with this variaton of the micromechanical cleavage technique it is possible to obtain graphene nanoribbons even thinner than the ones obtainable using electron beam litography. This ribbons can be easyly characterized by a combination of optical microscope and atomic force microscope as it is usually done with graphene flakes.

The $Sr_{1-x}Ca_xCrO_3$ solid solution.

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In 1968 Goodenough *et al*. first synthesised a polycrystalline sample of $CaCrO_3$ (S.G. *Pbnm*). Magnetic measurements suggested an AFM ordering at low temperature, ≤ 90K, along with a semiconducting behaviour explained as spontaneous collective magnetism within the electronic phase diagram. [1]. Later on, in 1971, Chamberland obtained single crystals of $CaCrO_3$ and reported metallic conductivity. The clearly metallic resistivity presents a discontinuity around 90K, which accompanies a magnetic and a structural transition. Curie Weiss law from 300-600 K is fitted with a paramagnetic moment of 3.6 MB" [2] The different properties between the two studies are attributed to the formation of insulating phases within the grain boundaries in the polycrystalline sample, and to the existence of a slightly different stoichiometry. In a recent report on $SrCrO_3$ and $CaCrO_3$, a large splitting of the ZFC and FC susceptibility curves of $CaCrO_3$ along with a small magnetization are indicative of a canted spin structure. [3] On the other hand, $SrCrO_3$, a cubic perovskite, was first synthesised by Chamberland at 65 kbars [4]. The transport properties showed a Pauli paramagnetism and metallic behaviour which have recently been matters of discussion [3, 5]. In 2006, Zhou *et al* have found itinerant paramagnetic behaviour, but metallic conduction is only observed under high pressure [3]. On the other hand, Williams *et al* have reported a low temperature phase transition to a tetragonal phase and some magnetic interactions in this compound [5]. In our recent High Pressure work we have obtained cubic $SrCrO_3$ following Curie Weiss law, with a magnetic moment slightly larger than that of Cr^{4+}, d^2 electrons and semiconducting behaviour. [6] It seems that similarly to $CaCrO_3$, small deviations in stoichiometry may occur. In view of these interesting and sometimes contradictory results, we have prepared at high pressure and high temperature the solid solution $Sr_{1-x}Ca_xCrO_3$. [7] Samples with x=0, 0.2, 0.4, 0.5, 0.6, 0.8 and 1.0, have been Rietveld refined and studied by electron microscopy. On introducing 20% calcium on the A site of the perovskite, the cubic $SrCrO_3$ transforms to tetragonal I4/mcm, $Sr_{1-x}Ca_xCrO_3$. (x≥0.2), and then to orthorhombic Pbnm (x≥0.6). Magnetic properties were also studied in all the range of solid solution. The end members show paramagnetism and an antiferromagnetic transition for, respectively, SrCrO3 and CaCrO3.

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MAGENTIC PROPERTIES OF $Eu_2Ru_2O_{7-x}$

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A sample of $Eu_2Ru_2O_7$ with pyrochlore structure has been synthesized by solid-state method and investigated with respect to their magnetic properties. The dc magnetic susceptibility under zero-field-cooled condition (ZFC) shows a cusp at 118 K characteristic of an antiferromagnetic transition. The high magnetic transition temperature and the large differences between the ZFC susceptibility and field-cooled (FC) susceptibility indicate the existence of a very strong interaction between ruthenium ions, however no magnetic hysteresis was observed. These results show that below the transition temperature local antiferromagnetic order can be coexist with a spin-glass state. When the temperature is decreased up to 5 K, magnetic hysteresis measurements indicate that exist a weak ferromagnetic contribution.

FORMACIÓN DE CRISTALES DE ÁCIDO SULFÚRICO ADSORBIDOS SOBRE GRAFENO

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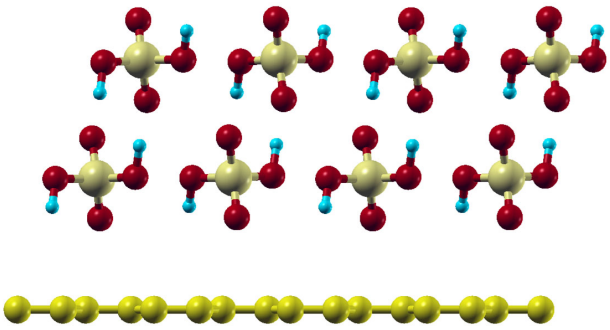
Se ha simulado la interacción entre ácido sulfúrico y grafeno (una lámina de espesor monoatómico de grafito) haciendo uso de la teoría del funcional de la densidad (DFT) con la aproximación de la densidad local (LDA). Se han analizado cuatro recubrimientos diferentes comprendidos entre una molécula de H_2SO_4 prácticamente aislada (una molécula de ácido por cada 32 átomos de carbono) y una bicapa (una molécula de ácido por cada 4 átomos de carbono, mostrada en la figura) [1]. Se han calculado geometrías de equilibrio, energías de enlace, transferencias de carga y diagramas de bandas electrónicas. A medida que el recubrimiento aumenta, las moléculas de ácido rotan, aproximándose a su orientación en el cristal, mostrando que el grafeno puede hacer de molde para el crecimiento de cristales de ácido sulfúrico de forma análoga a como parecen hacer los nanotubos de carbono [2]. Los resultados indican que hay transferencia de carga del grafeno al ácido, lo que concuerda con resultados experimentales para H_2SO_4 adsorbido en grafito pirolítico altamente orientado (HOPG) [3] y para nanotubos de carbono monocapa en ácido sulfúrico concentrado [4]. Sin embargo la estructuras de bandas del grafeno no se ve seriamente afectada por la presencia del ácido y su carácter de semimetal (semiconductor de gap nulo) se mantiene.



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Vórtices y superconductividad multibanda en NbSe2

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Se ha investigado la estructura electrónica asociada a los vórtices en el superconductor multibanda NbSe2 mediante espectroscopía túnel de barrido (STS) con punta superconductora de plomo. Este estudio permite obtener información detallada sobre la distribución espacial de las densidades de pares de Cooper y de cuasipartículas, así como de la corriente Josephson entre la muestra y la punta superconductora, en presencia de la red de vórtices de Abrikosov. La variación de estas distribuciones en función de la energía y de los parámetros experimentales temperatura y campo magnético permiten correlacionar características asociadas a los vórtices (que ocurren en una escala de cientos de nanómetros) con las propiedades electrónicas en la nanoescala (orientación de la red cristalina, estructura de la superficie de Fermi) y con el carácter multibanda de la superconductividad en este material.

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BIFUNCTIONALIZED SILICA-COATED COBALT NANOPARTICLES

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Herein we present colloidal chemistry methods for the synthesis of environmentally stable silica-coated cobalt nanoparticles, prepared combining the sodium borohydride reduction in aqueous solution and the silica precipitation in basic medium. We highlight the further functionalization of the silica-coated cobalt nanoparticles using (3-aminopropyl) tris(trimethylsiloxy) silane. These attached amino groups are used as bridges (coupling chemistry) between the magnetic nanoparticles and gold seeds, in such a way that we render the nanoparticles bifunctionalized (magnetic and optically active). Figure 1 shows a TEM image of the gold-decorated silica-coated cobalt nanoparticles and their UV-vis spectrum (red), maintaining the surface plasmon band of individual gold nanoparticles (black) but red-shifted to 560 nm.

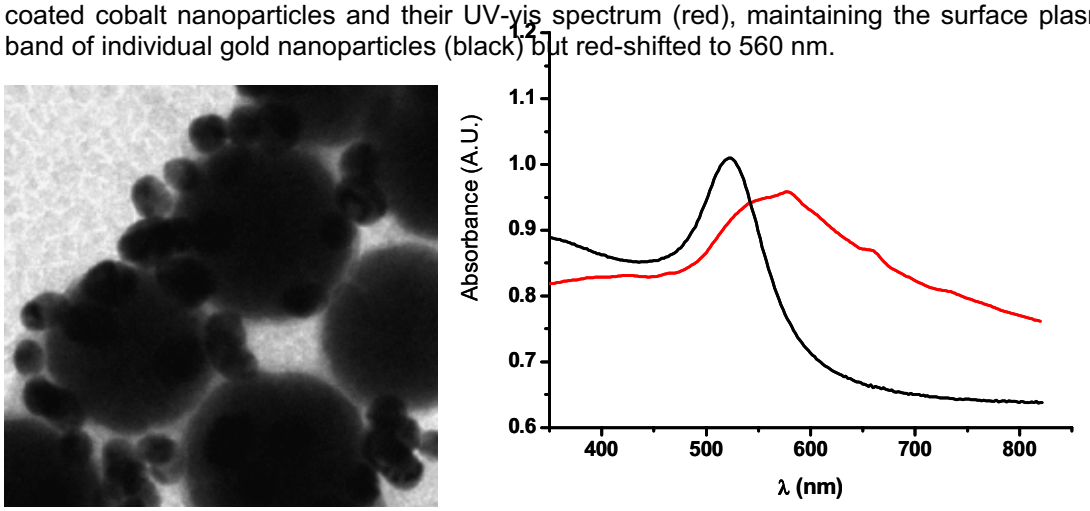

Figure 1. TEM image of gold-decorated silica-coated cobalt nanoparticles and UV-vis spectra of gold (black) and the bifunctionalized nanoparticles (red).

Acknowledgments

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Electronic Correlations and Disorder in Transport through nanoparticle arrays

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We analyze and clarify the transport properties of a one-dimensional metallic nanoparticle array with interaction between charges restricted to charges placed in the same conductor. We study the I-V curves and the potential drop through the array and their dependence on the array parameters including the effect of charge and resistance disorder. We show that very close to threshold the current depends linearly on voltage with a slope independent on the array size. At intermediate bias voltages, for which a Coulomb staircase is observed we find that the average potential drop through the array oscillates with position. At higher voltages I-V curves are linear but have a finite offset voltage. We show that the slope is given by the inverse of the resistances added in series and estimate the voltage at which this linear regime is reached. We also calculate the offset voltage and relate it to the potential drop through the array.

EFFECT OF OXYGEN DISORDER ON MAGNETIC PROPERTIES OF $RBaCo_2O_{5+\delta}$ LAYERED COBALTITES

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Remarkable research efforts are nowadays aimed to explore and understand the challenging properties of layered cobaltites of the type $R\mathrm{BaCo_2O_{5+\delta}}$ (R=rare earth and 0□δ□1). These compounds present a highly ordered structure, remarkable physical properties and a great magnetic complexity. The facility shown by Co ions (especially in perovskite-like structures) to adopt different spin states contributes to this complexity: different spins states imply different occupancies of the outermost e_g orbital and thus different magnetic interaction according to Goodenough-Kanamory-Anderson rules. Of special interest are the cobaltites with δ=0.5, with Co ions having the single Co^{3+} valence. In this case, different magnetic transitions have been reported in this series for several rare-earths ranging from the small ones (Ho, Er) to the large ones (Pr, Nd) [1]. In all cases, a spin state transition accompanied by a metal-insulator transition, and two or even three transitions involving the long-range ordering of Co ions are present [1-5]. Related with their remarkable magnetotransport properties and structural transitions, a great controversy has appeared about these magnetic structures and the spin state of Co at different sites [2-5]. Different groups report different magnetic structures and even different magnetic lattices. In particular, the comparison between the neutron studies done on single crystals, with those on powders, are especially discouraging [4,5]. Although the macroscopic behaviour does not display a clear dependence on the rare earth, apparently the ordered arrangement of magnetic moment does. In addition, this arrangement will be influenced by the ordering of oxygen vacancies and the eventual presence of misplaced oxygen vacancy-oxygen ions (disorder). Disorder is more easily present for large rare earths [5]. To elucidate any possible dependence of the magnetic structures on rare-earth size, it is mandatory to first elucidate the possible dependence on disorder to discard this origin. In this communication we compare the results obtained for two different samples of $PrBaCo_2O_{5.50}$ prepared using different routes. One of them is almost perfectly ordered while the second contains a certain amount (10%) of misplaced oxygen ions. From their comparison, we have elucidated the effect of this disorder on the magnetic properties and the magnetic order in this family.

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d^0 substitution and phase competition in $Pr_{0.50}Ca_{0.50}Mn_{1-x}Ti_xO_3$: role of short-range orbital order on thermal hysteresis

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We have studied the phase coexistence/competition and the effect of the substitution of Mn [1-2] by d^0 non-magnetic ions in $Pr_{0.50}Ca_{0.50}Mn_{1-x}Ti_xO_3$ (x=0.01, 0.03 and 0.05) manganites. Synchrotron and neutron powder diffraction has allowed us to characterize the dependence of the coexisting phases, the evolution of their relative fractions, and magnetic structures with the Ti substitution level. We have found the coexistence of two different structural phases below 240 K ($\approx T_{CO}$) with different cell distortion. The fraction of the phase with larger (smaller) distortions shrinks (enlarges) when increasing x. NPD evidences the coexisting of CE and pseudo-CE magnetic order. Ti(d^0) ions do not favor the stabilization of FM-metallic islands/regions in the AFM-insulating orbital ordered matrix. The absence of ferromagnetism was confirmed in zero-field. In consistence with the Ti^{4+} valence state (d^0), the proportion of microdomains exhibiting pseudo-CE type magnetic order increases with the Ti content at expenses of the CE type regions in the material. At low temperatures, isothermal magnetization measurements (M[H]) evidence the occurrence of avalanches in the three compounds. The melting of CE regions during the magnetization avalanche was the most apparent in NPD studies under field for the intermediate Ti-3% composition. Using the ultra high resolution of ID31 diffractometer, we have studied the microstructure of the coexisting phases. The shape of the diffraction peaks is dominated by lattice strains. These strains are considerably larger in the less distorted phase, thus presenting wider diffraction peaks. In addition, the analysis of the correlation between cell fluctuations demonstrates that strain trapped in the less distorted (short-range CO/OO) phase mimics the lattice distortions characterizing the most distorted (long-range CO/OO) phase. A characteristic feature in the low doping limit is the occurrence of a macroscopic hysteretic behavior (in the magnetization and resistivity) under heating/cooling cycle. This behavior was explained by the presence of short-range orbital ordered regions below $T_{CO}\approx$240K with a coherence length of only 200 Å [3]. On further cooling below 100 K they suddenly transform into long-ranged CO/OO domains larger than ≈1000 Å.

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STRUCTURAL INVESTIGATION AND VACANCY ORDERING IN $PrBaCo_2O_{5+\delta}$ COBALTITES VARYING THE OXYGEN CONTENT

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Due to their remarkable properties, cobalt oxides represent one of the most promising research topics in the field of strongly correlated electronic materials. Of special interest is the facility shown by Co ions (especially in perovskite-like structures) to adopt different spin states. This additional degree of freedom, quenched in other transition metal oxides, is strongly coupled with lattice, magnetic and transport properties. In this context, remarkable research efforts are aimed to explore and understand the challenging properties of layered cobaltites of the type $LnBaCo_2O_{5+\delta}$ (Ln=rare earth), with $0 \leq \delta \leq 1$ and a highly ordered structure. These compounds present remarkable physical properties: giant magnetoresistance, large thermoelectric power, metal-insulator transitions, charge-order, high oxygen mobility, mixed conduction, etc [1-10]. The magnetic and transport properties of these oxides are greatly governed by the oxygen content δ, which can be tailored by means of heat treatments under different atmospheres and different temperatures [1,7,8]. In this communication we present the results of a systematic neutron (and synchrotron) study of the location of oxygen vacancies as a function of δ and their tendency to give ordered configurations in $PrBaCo_2O_{5+\delta}$, with $0 \leq \delta \leq 1$. Detailed structural information was obtained for a series of samples with different values of δ ranging between 0.17 and 0.86. The fine knowledge of the structural details has helped us to get a more realistic picture and a better understanding of the magnetic and transport properties in this family. Both long-range and short range ordered configurations of the oxygen vacancies are described varying $\delta$and the preparation conditions. One of our main goals was to determine how the spin state transition of Co^{3+} species in octahedral environment described for $RBaCo_2O_{5.50}$, is altered by the partial presence of Co^{2+} ($\delta<0.50$) or Co^{4+} ($\delta>0.50$).

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Substrate limited electron dynamics in organic transistors (and graphene)

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In organic Field Effet Transistors (FETs), charge carriers accumulate in a two-dimensional layer at the interface between an organic crystal and a gate dielectric. The possibility of tuning several microscopic parameters such as the carrier density, the electron-electron and electron-phonon interactions makes these devices an interesting playground for fundamental physics.

Recent experiments have demonstrated that depending on the gate insulator used, the electric mobility in organic FETs can be tuned from metallic-like to insulating-like. This phenomenon can be explained in terms of the formation of small polarons, due to the remote interaction of the charge carriers with the phonons of the gate material [1]. In the devices with the highest polarizabilities, experiments performed at large gate voltages (corresponding to ~0.1 carriers/molecule) have revealed a further reduction of the mobility, suggesting the onset of electron-electron interactions [2]. The physics of this novel regime involving both strong electron-phonon and long-range electron-electron interactions will be discussed. The implications of this scenario for the transport properties of graphene will also be analyzed [3].

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TRANSICIÓN AL ESTADO NORMAL INDUCIDA POR ALTAS DENSIDADES DE CORRIENTE ELÉCTRICA EN MICROPUENTES DE PELÍCULAS DELGADAS DE CUPRATOS SUPERCONDUCTORES: INFLUENCIA DE LA DURACIÓN DEL PULSO.

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La transición al estado normal inducida en micropuentes superconductores mediante pulsos de densidad de corriente eléctrica, con amplitudes muy superiores a la corriente crítica, es un fenómeno clásico, pero todavía abierto y con un amplio interés para diversas aplicaciones [1-3]. Un aspecto importante es la influencia de la duración del pulso, en particular cuando dicha duración compite con el tiempo de relajación térmica del micropuente (alrededor de decenas de nanosegundos). En esta comunicación se presentan los resultados del estudio de las curvas de campo eléctrico frente a densidad de corriente (E-J) medidas en micropuentes de películas delgadas de $YBa_2Cu_3O_{7-\delta}$ (YBCO). Las medidas se realizaron entre Jc (la corriente a la que aparece disipación) y J* (la corriente que induce el salto al estado normal), aplicando pulsos de diferente duración temporal (desde milisegundos hasta centenas de nanosegundos). Estas medidas ponen en evidencia una apreciable disminución de J* cuando aumenta la duración del pulso Actualmente estamos analizando estas medidas utilizando un método de elementos finitos (FEM), con el fin de comprobar: i) si podemos reproducir la curva E-J incluido el salto abrupto al estado normal usando un modelo de flux-creep convencional en el que se han tenido en cuenta los efectos de auto-calentamiento, ii) si la dependencia de J* con la duración del pulso es explicada en términos de efectos térmicos.

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SILICON COLLOIDS: FROM MICROCAVITIES TO PHOTONIC SPONGES

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We report on a method for obtaining silicon colloids[1] with diameters from 0.5 μm to 5 μm. Because of their spherical shape and smooth surface, they work as optical microcavities with well-defined resonating modes in the near-infrared range. Silicon colloids may facilitate development of high quality factor optical microcavities with strong light confinement effects, allowing integration of fundamental electronic devices such as a p-n junction into a single system.

Silicon colloids have also been used as the building blocks of a new microstructured material formed by tree-like arrangements of polydisperse microspheres. We call this material 'photonic sponge' because it can scatter light strongly over a wide range of wavelengths. We expect inmediate applications of these materials in the fields of photovoltaic cells, chemical sensors, and light detectors and emitters.

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Modelización de la estructura electrónica de grafeno con defectos

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Uno de los problemas más interesantes aún inexplorados del grafeno es el de la estabilidad termodinámica y mecánica del cristal bidimensional y de los posibles defectos que se puedan nuclear. La estructura final de las muestras depende de estas propiedades que influyen de manera importante sobre las propiedades electrónicas y de transporte. La mayor parte de los trabajos existentes sobre formación y estabilidad de defectos se han realizado en nanotubos, fullerenos y grafito irradiado donde aparecen como más estables ciertos defectos topológicos, divacantes y ad-atoms. Estudios numéricos muy recientes de elasticidad realizados en la red hexagonal plana apuntan hacia la posibilidad de estabilizar otros tipos de defectos [1] que inducen curvatura negativa en la red. En este trabajo se analizan las propiedades electrónicas del grafeno con estos defectos.

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The role of nanostructure on ac response in Co-ZrO_2 granular films

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Thin films consisting of Co nanoparticles embedded in amorphous ZrO_2 matrix were grown by pulsed laser deposition in a wide range of metal volume concentrations, from dielectric regime to percolation. Transmission electron microscopy (TEM) showed spherical Co nanoparticles having very sharp interfaces with the amorphous matrix. The evolution of ac response with volume metal content x was systematically studied. A complex absorption phenomenon that mimics the universal response of disordered dielectric materials is observed but at much lower frequencies, in a narrow range of metal content ($0.20 \leq x < 0.34$) near percolation threshold. Analysis in terms of the competition between thermally assisted tunneling trhough the small and close particles (R) and capacitive conductance through further separated large particles (C) is supported by their nanostructure, directly visualized by TEM. The experimental behavior in the whole range of frequencies and temperature is successfully reproduced by a model of a simple cubic random RC-network, and the deduced parameters agree with the observed nanostrucutre.

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FUNCIONALES DE LA ENERGÍA CINÉTICA CON BAJO COSTE COMPUTACIONAL QUE TRABAJAN SOBRE LA DENSIDAD ELECTRÓNICA DE LOS SÓLIDOS.

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La obtención de las propiedades físicas de un sistema a partir de su densidad electrónica es un viejo problema de la física teórica. Este problema tiene una importancia adicional en el caso de los sólidos, ya que la propia densidad electrónica es la que en gran medida nos permite determinar la estructura de los cristales a partir de diversas técnicas como puede ser la difracción de rayos X.

La determinación de muchas propiedades físicas requiere la evaluación de la energía total del sistema electrónico. La obtención de la energía cinética es con mucho la parte más difícil de todo el proceso. Actualmente existen funcionales cinéticos de la densidad electrónica que son capaces de ofrecer valores bastante precisos de la energía cinética total. En los últimos años se han desarrollado nuevos funcionales completamente no locales, cuya no localidad se apoya en las ideas básicas de los conocidos funcionales "clásicos" de Thomas-Fermi y von Weizsäcker, y que cumplen una serie de condiciones físicas impuestas como son la reproducción de la energía y la función respuesta correspondientes al gas de electrones libres. Esto los hace especialmente adecuados para el estudio de metales simples en los que la situación de los electrones en la banda de valencia puede considerarse como cuasilibre.

Estos nuevos funcionales [1-3] gozan de la ventaja de presentar un coste computacional mucho más bajo que las técnicas tradicionales de cálculo de estructura electrónica y se han mostrado exitosos en diferentes situaciones. En este trabajo se expondrán resultados para átomos, para sistemas modelo unidimensionales (electrones en una caja de potencial infinito y en un potencial armónico) y para sistemas reales de mayor interés, como los ya mencionados metales simples.

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ATOMIC RECONSTRUCTION AT THE INTERFACE OF EPITAXIAL (ZrO_2:Y_2O_3 (8% mol) / $SrTiO_3$) HETEROSTRUCTURES.

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Complex oxides heterostructures are currently receiving much attention due to the possibility of stabilizing new phases with properties not exhibited by either of the individual constituents. The presence of a coherent interface between the two oxides impose a symmetry breakdown in the lattice periodicity and discontinuities in the chemical potential of the crystalline structure which gives rise to electronic and atomic interfacial reconstructions. Recent reports have shown an electronic reconstruction at the interface inducing a conducting state between two insulators [1] or interface ferromagnetism between two paramagnets [2]. In this communication we present an atomic reconstruction between two highly dissimilar oxide structures that increases the positional disorder at the interface and produces a fast ionic diffusion plane.

We have grown epitaxial heterostructures combining ultrathin ZrO_2:Y_2O_3 (8% mol) (YSZ / fluorite structure) and $SrTiO_3$ (STO / perovskite structure) in a high pressure (3 mbar) pure oxygen RF sputtering apparatus at high temperature (900 ºC). The electrical characterization of the samples by means of conductance spectroscopy, shows an extraordinarily high lateral ionic conductivity of the heterostructures (up to 8 orders of magnitude higher than the bulk YSZ near room temperature), and a decrease in the activation energy of the diffusion process. Electrical measurements results of trilayers and superlattices indicate that this is an interface process. In fact EELS measurement indicates that an increase of the oxygen vacancies density takes place at the interface. We propose that the atomic reconstruction at the interface and the high tensile strain (~ 7 %) in the ultrathin YSZ layer provide the large number of oxygen vacancies and a high mobility plane for oxygen ions yielding colossal values of the ionic conductivity.

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ELECTRONIC RECONSTRUTION AT $LaMnO_3$ / $SrTiO_3$ INTERFACES

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Interfaces between complex oxides are the focus of increasing research interest. Recent reports have shown novel charge transfer effects originating at polarity mismatch [1] or strain at the interface [2] which allow to modify the electronic structure [3] and to tailor novel properties and behaviours [4].

In this work we focus on the interface $LaMnO_3$ (LMO) / $SrTiO_3$ (STO), between an antiferromagnetic Mott insulator (LMO) and a band insulator (STO). The combination of these materials allow us to explore the effects of the polarity mismatch as well as the epitaxial strain at the interface induced by the different lattice parameters. We have grown ($LMO_{\ m\ u.c.}$ / $STO_{\ n\ u.c.}$) superlattices, with m and n ranging from 2 to 17, and 2 to 12 respectively, on STO (100) substrates at high temperature (800 ºC) in a high pressure (3 mbar) pure oxygen RF sputtering. EELS analysis shows that the interfaces are defined between $(LaO)^+$ planes of the LMO and $(TiO_2)^0$ planes of the STO, and that the Mn presents the nominal oxidation state (Mn^{n+}: $n=3 \pm 0.05$) in the LMO layer. X ray reflectivity patterns analysed using SUPREX 9.0 software consistently show very limited interface disorder over larger lateral distances than microscopy and also negligible chemical interdiffusion.

Our results indicate the existence of two different LMO phases depending on the relative thickness of the LMO and STO layers. The first one is a ferromagnetic-metallic phase that nucleates over highly distorted STO ultrathin films, and the second one is non ferromagnetic-insulator phase that nucleates over relaxed STO films. Ti $L_{2,3}$ edge EELS measurement reveals a “leakage current” from the $(LaO)^+$ to the $(TiO_2)^0$ interface planes in superlattices with ultrathin (2 unit cells) STO layers without changes in the Mn oxidation state. This results agrees with a hole doping in the thinnest STO layers via “polarity mismatch mechanism” at the interface [1].

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PROPIEDADES MAGNÉTICAS DE SISTEMAS $3d^6$ Y $3d^7$ CON GEOMETRÍA PLANO CUADRADA

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Se ha realizado un estudio de las propiedades magnéticas (susceptibilidad en función de la temperatura y espectroscopia de resonancia paramagnética electrónica, EPR) de diversas sales de los complejos homolépticos paramagnéticos $[M^q(C_6X_5)_4]^{-(4-q)}$, con X = Cl, F y M^q = Ni^{III}, Co^{II} y Co^{III}. En todos ellos el metal se encuentra en un entorno plano cuadrado (*SP*-4).

Los espectros de EPR de los complejos de Ni^{III} y Co^{II} se describen con espín S = ½ y un tensor giromagnético prácticamente axial. La susceptibilidad magnética en función de la temperatura (entre 2 y 275 K), se ajusta a una ley de Curie en la que el momento magnético por molécula, independiente de la temperatura, está de acuerdo con los valores principales del tensor giromagnético determinados mediante espectroscopia EPR. En el caso de las sales de Co^{III} no se observa señal de EPR. Sin embargo, las medidas de la susceptibilidad magnética revelan su carácter paramagnético. El momento magnético por molécula toma un valor constante a temperaturas superiores a 200 K ($3.7\mu_B$ para X = Cl y $4.2\mu_B$ para X = F), decreciendo fuertemente cuando la temperatura disminuye. Este comportamiento se describe con un espín efectivo S = 1 incluyendo un desdoblamiento a campo nulo (Δ = 100 $\pm$ 10 cm^{-1} para X = Cl y Δ = 135 $\pm$ 8 cm^{-1} para X = F). El comportamiento magnético de todos estos compuestos se ha sistematizado considerando los niveles monoelectrónicos, $e(xz, yz)$, $b_2(xy)$ y $a_1(z^2)$ en simetría *SP*-4. En el caso de los sistemas d^7, sales de Co^{II} y Ni^{III}, el estado fundamentel resulta ser $^2A_1$ proveniente mayoritariamente de la configuración $(e)^4(b_1)^2(a_1)^1$. En las sales de Co^{III} (d^6) el comportamiento magnético se explica considerando un estado fundamental $^3B_2$ proveniente mayoritariamente de la configuración $(e)^4(b_1)^1(a_1)^1$. Las diferencias observadas de los valores del momento magnético respecto al debido únicamente a la contribución del espín son atribuídas a la interacción espín – órbita.

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MAGNETIC AND ELECTRONIC PROPERTIES OF $Bi_{0.75}Ca_{0.25}MnO_3$

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$BiMnO_3$ is a prototypical magnetic ferroelectric, with a ferromagnetic transition at 105K. Although it is one of the very few monophasic materials exhibiting biferroicity, the origin of ferromagnetism is not yet well understood. Moreover, the dependence of the properties of $Bi_{1-x}A_xMnO_3$ compounds on the A^{2+} content is still an open issue. From magnetization data Chiba *et al.* reported that doping with Sr systematically decreases the ferromagnetic moment from the saturation value of $3.6\mu_B$, vanishing at doping levels $x \geq 0.4$ [1]. However, we have recently determined that the ground state of $Bi_{0.75}Sr_{0.25}MnO_3$ (x=0.25) is antiferromagnetic [2].

We present a study of the magnetic and electronic properties of $Bi_{3/4}Ca_{1/4}MnO_3$, investigated by means of magnetometry, neutron and synchrotron diffraction, and muon (μSR) techniques. In contrast with the Sr compound, $Bi_{0.75}Ca_{0.25}MnO_3$ presents a structural transition at 275 K. The lattice changes observed on cooling through this transition are qualitative different to the anomalies reported in $Bi_{1-x}Ca_xMnO_3$ (x>0.30), $Bi_{0.75}Sr_{0.25}MnO_3$ or $Ln_{0.67}Ca_{0.33}MnO_3$ manganites.

We have confirmed the absence of a ferromagnetic component under zero field, ruling out spontaneous ferromagnetism in $Bi_{0.75}Ca_{0.25}MnO_3$. However, the application of magnetic fields (even of a few gauss) produces a continuous progressive polarization of the Mn moments as H is increased (≈2 μ_B/Mn under 5 T at 5K). Without applied field, the low temperature state presents a high degree of spin disorder.

A remarkable result is the nonexistence of a well-developed long-range magnetic order in the ground state of $Bi_{0.75}Ca_{0.25}MnO_3$. An inhomogeneous magnetic state progressively develops below ≈150 K. In addition, a cluster-glass like transition was found below T≈70 K, and coexist with a extremely small, residual signature from minority regions with very weak pseudo-CE magnetic order. A very large majority fraction of Mn atoms in the system (≈70%) does not present local magnetic order at 5K. The unexpected magnetic behavior of $Bi_{0.75}Ca_{0.25}MnO_3$ indicates a ground state distinct to $Bi_{0.75}Sr_{0.25}MnO_3$.

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CURRENT POLARIZATION INDUCED BY THE RASHBA INTERACTION IN QUANTUM WIRES

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The manipulation of electronic spin in nanostructures is presently attracting a lot of interest in the context of the so-called spintronics technologies. Much hope is placed in devices where the spin degree of freedom is the basis for operation. In this contribution we discuss the physical mechanisms underlying one of such devices; namely the case of a spin polarizer made with a parabolic quantum wire having a region with spin-orbit interaction of Rashba type. The spin-orbit interaction acts as a spin-selective scattering center able to yield polarized transmitted currents even if incidence is fully unpolarized. Since no external magnetic field is required and the Rashba interaction can be tuned with electrical gates the system operates in practice as an all-electrical spin current polarizer [1-5].

We present numerical calculations obtained by solving the scattering problem in a grid. To gain insight in the physical mechanisms, the limit of weak Rashba coupling is analyzed using a coupled-channels model. Minimal conditions for the device operation are the presence of two propagating subbands and a phase-sensitive intersubband coupling. Analytical expressions for the transmission have been obtained using a tight-binding modelling of the equations and, also, in lowest order Born approximation. The abruptness of the space transition to the spin-orbit region is a relevant parameter. Indeed, as shown by the simplified models, in the adiabatic limit of a very smooth switching on of the spin-orbit coupling the polarization of the transmitted current completely disappears. In the strong coupling limit the systematics with Rashba coupling intensity, incident energy and Rashba region length are given numerically.

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MAGNETIC PROPERTIES OF SIZE-CONTROLLED IRON OXIDE NANOPARTICLES STABLE IN AQUEOUS SOLUTIONS.

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Iron oxide nanoparticles have lately become of great interest in biomedical applications due to their excellent magnetic properties [1], suitable for *in vitro* (separation and selection), and *in vivo* (drug delivery and NMR imaging) applications [2,3]. For that reason, the stability of the nanoparticles in an aqueous solution becomes essential. In this work, we report on a direct size-controlled synthesis of water soluble iron oxide nanoparticles (magnetite/maghemite Fe_3O_4/Fe_2O_3), with good magnetic properties, departing from iron acetylacetonate and pyrrolidone [4]. The particle size can be controlled through the concentration of the acetylacetonate, as shown by TEM micrographs and ZFC-FC measurements. The magnetic properties of both powder samples and liquid suspensions have been performed. In particular, ZFC-FC curves show significant diferences in the bloking temperature, because of the fact that dipolar interactions tend to surpressed in the aqueous solutions. The funding from the Spanish MEC (NAN2004-08805-CO4-02, NAN2004-08805-CO4-01, CONSOLIDER CSD2006-12 and MAT2006-03999), and from the Catalan DURSI (2005SGR00969) is acknowledged.

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STM/S in 2H-$NbSe_2$ at very low temperatures

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We present scanning tunneling microscopy and spectroscopy measurements at 100mK in the superconducting material 2H-$NbSe_2$. At zero field, the atomic lattice and charge density wave (CDW) are observed. STS images at atomic scale show well defined features in the superconducting density of states changing in a pattern closely following atomic periodicity. Our experiment demonstrates that the intrinsic superconducting density of states can show atomic size modulations, which reflect the reciprocal space structure of the superconducting gap. In particular we obtain that the superconducting gap of 2H-$NbSe_2$ has six fold modulated components at 0.75 mV and 1.2 mV. The tip substrate interaction in an anisotropic superconductor has been calculated, giving position dependent changes related to the observed gap anisotropy [1].

We compare these results with recent measurements in 2H-NbS_2. This superconducting material is a member of the transition metal dichalcogenides, as 2H-$NbSe_2$, and it is the only member that does not show CDW transition. We present the first spectroscopic measurements and images with atomic resolution in this material.

We will also discuss STS measurements in 2H-$NbSe_2$ at 0.1 K using superconducting tips of Al. Under magnetic fields, the peculiar electronic surface properties of vortices are precisely resolved. The tip density of states is influenced by the local magnetic field of the vortex, providing for a new probe of the magnetic field at nanometric sizes [2].

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C-axis critical current transport measurements on 3D nano-patterned YBCO TFA thin films

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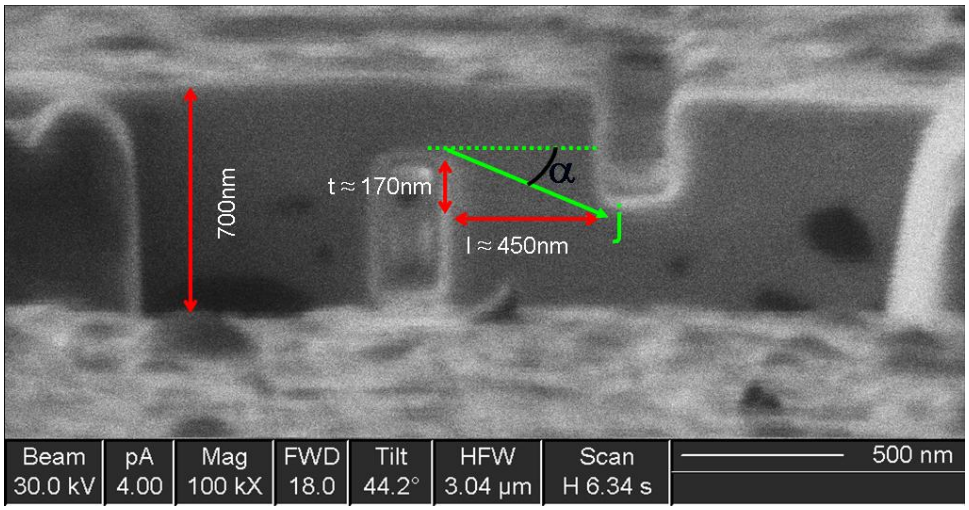
One key issue for the comprehension of vortex matter in high Tc superconductors (HTS) has been the proper understanding of vortex-vortex and vortex-defect interactions on these materials. Studies on pinning mechanisms and on methods to enhance their effectiveness in HTS is still a topic of great interest, especially in real materials like YBa2Cu3O7-x (YBCO) thin films where different sort of defects are present and their contribution to the pinning energy is difficult to isolate. Many studies already exist where the effect coming from different pinning centres has been elucidated by means of rotating the magnetic field and applying current through the ab planes. In this work we present a novel technique which allows us to apply current perpendicular to the ab plains and thus study the effect of some defects acting as pinning centres which remain masked in conventional ab current experiments. Using a focused ion beam (FIB), we have produced nano-devices on YBCO thin films in order to create vertical transport structures in which the current is constrained to flow along the c-axis. The fabrication of these devices is a challenge by itself, since it's very important to avoid gallium contamination during the FIB processing and achieve a good control of the nanostructure geometry in the thin film. With this configuration and using an 8 Tesla variable temperature two axis rotating stage cryostat we have been able to study c-axis transport critical currents at any magnetic field orientation. As far as we know this is the first time that such experiments have been performed on YBCO thin films. The analysis of the results has allowed us to identify pinning and channelling processes which remind hided in more conventional experiments where the transport current is applied along the ab-planes and the magnetic field is rotated from the c-axis to the ab-planes. With this new experiment we have been able to observe direct pinning by twin boundaries and vortex channelling in between the CuO2 planes. Moreover, we have been able to compare this results with similar measurements carried on isotropic low-Tc superconductors, which has enabled us to isolated effects coming from the intrinsic anisotropy of the YBCO material and its response in minimum Lorentz force configurations.



MICROSCOPIC ORIGIN OF EXCHANGE BIAS IN CORE/SHELL NANOPARTICLES:

VERTICAL SHIFTS AND LOOP ASYMMETRY

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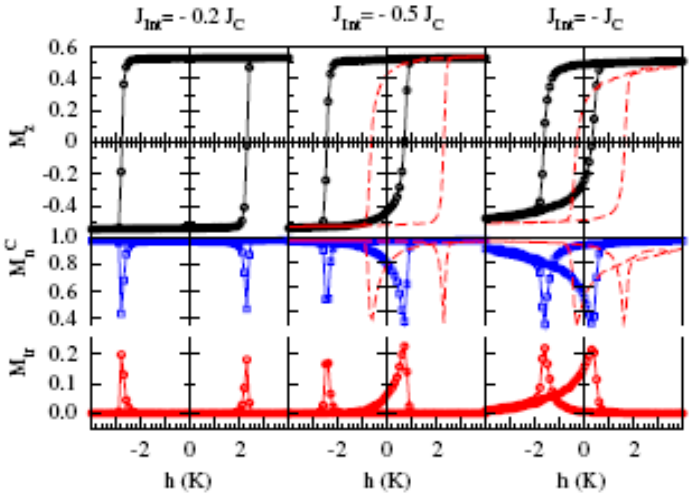
We report the results of Monte Carlo simulations for a simple microscopic model of individual nanoparticle with (ferromagnetic) core/(antiferromagnetic) shell structure which aim to clarify the microscopic origin of exchange bias in the magnetization hysteresis loops [1]. The model takes into account the different values of the anisotropy and exchange constants at the core and the shell. We have found that the increase of the exchange coupling across the core/shell interface leads to loop shifts in the field direction as well as displacements along the magnetization axis that increase in magnitude, related also to the increasing loop asymmetry between the two branches of the loops. A detailed analysis of the snapshots of the particle configurations along the hysteresis loops evidences the existence of a net magnetization due to uncompensated spins at the shell interface that is responsible for both phenomena and allows quantifying the loop shifts directly in terms of microscopic parameters, with striking agreement with the macroscopic observed value. Overlap functions computed from the spin configurations along the loops have been computed to explain the origin and magnitude of these features microscopically, giving insight into recent experimental observations. Funding from the Spanish MEyC NAN2004-08805-CO4-02, CONSOLIDER CSD2006-12 and MAT2006-03999 projects, and Catalan DURSI (2005SGR00969) is acknowledged.



Hysteresis loops obtained after FC in a field h_{FC}= +4K (circles) and h_{FC}= -4K (dashed lines) for three values of the exchange coupling constant J_{Int} at the core/shell interface. Lower panels show the average magnetization projection of the core spins along the field axis M^C_n (blue squares) and the

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SYNTHESIS OF GOLD OR SILVER-COATED MAGNETITE NANOPARTICLES

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Nanometer-size materials represent an “intermediate” dimension between bulk materials and atoms/molecules, so metallic and semiconducting particles of nanometer scale have been the subject of substantial research in recent years. Among these materials, bimetallic nanocomposites having core-shell structure have received special attention because of their electronic, magnetic and optical properties.

In this poster we describe the preparation of Fe_3O_4 nanoparticles by the coprecipitación method [1,2] and their coating with gold and silver metals, to impress optical properties to the magnetic core particles. This reaction was followed in situ by UV-visible spectroscopy confirming the presence of the Au or Ag shells because of the appearance of their plasmon absorption band. The coating was confirmed by X-ray diffraction comparing the uncoated magnetite and the gold or silver patterns with the difractograms observed of the coated particles. Transmission Electron Microscopy showed the changes in size when the Fe_3O_4 particles are covered with the gold or silver shell. The characterization of these nanoparticles was completed by temperature dependent magnetic studies, showing the effect of the shell size in the coated particles on the basic magnetic parameters.

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ESTUDIOS CALORIMÉTRICOS DEL ETANOL PURO A BAJAS TEMPERATURAS

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El etanol puro es un líquido molecular muy interesante, puesto que es posible obtenerlo en cuatro fases sólidas diferentes [1-3] dependiendo de su historia térmica: como cristal (monoclínico) completamente ordenado; como vidrio convencional (sólido amorfo) por debajo de $T_g \approx 97$ K sobrenfriando el líquido más rápido que, digamos, –20 K/min; como cristal plástico (bcc) sobrenfriando el líquido a una velocidad intermedia (del orden de –1 K/min); y como *cristal vítreo* enfriando dicho cristal plástico por debajo de la misma temperatura $T_g \approx 97$ K. Así pues esta sencilla y conocida sustancia constituye un excelente banco de pruebas para discriminar los papeles desempeñados por el desorden traslacional, rotacional y orientacional en los sólidos [2-4]. Por ejemplo, la fase de cristal con desorden orientacional o *cristal vítreo* del etanol presenta [3,4] el mismo comportamiento universal en las propiedades de bajas temperaturas y en la dinámica de bajas energías que los verdaderos vidrios (de ahí la denominación de *cristales vítreos*).

En este trabajo, presentamos nuevos experimentos de calorimetría, incluyendo resultados nuevos que arrojan más luz en el rico e interesante diagrama de fases del etanol. Combinando esta técnica con experimentos de difracción de rayos X y espectroscopía Brillouin, hemos identificado [5] la existencia de hasta cuatro variedades diferentes de la fase cristalina monoclínica dependiendo de la historia térmica. Además, mostramos ahora la influencia del entorno de la muestra (empleando distintos tipos de celda calorimétrica) en la cinética de cristalización y presentamos nuevas medidas del calor específico a bajas temperaturas para las fases de vidrio, cristal vítreo y cristal plenamente ordenado del etanol puro.

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Manganite structure: from flat surface to self-organized holes

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Oxides are one of the largest families of new materials which attract great attention due to their rich physics. Among them, the manganese perovskites showing colossal magnetoresistance and half metallic characteristics have emerged as good candidates for miniature spintronic devices. Well defined structures at nanometric scale present an increasing interest due to their unique physical properties and potential applications. However, the fabrication of artificial nanostructures of complex oxide materials appears to be a very difficult task requiring sophisticated technologies. Most of the applications require high-quality epitaxial films and heterostructures in which both the structure and the morphology play a very active role in their final performances.

In this work we report on highly epitaxial $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) thin films grown on $SrTiO_3$ (001) oriented substrates by rf magnetron sputtering. It is shown that structural strain caused by lattice mismatch between film and substrate may offer unique opportunities to control the films morphology. By choosing appropriate growth conditions a film morphology of self-organized holes can be fabricated. This morphology can be used as a nanostencil for the fabrication of self-organized nano-objects, to investigate their physical properties and to explore new device. We also have studied the evolution of the structural and magnetic properties in the same sample after different annealing treatments.

Focused ion beam fabrication of exchange bias ferromagnetic/antiferromagnetic bilayered nanostructures: sub-200 nm dots and antidots

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The exchange bias (EB) phenomenon in nanostructured systems shows many challenges with respect to their fabrication and posterior characterization [1]. Focused Ion Beam (FIB) technology, based on the nanopatterning by a highly focused ion beam, has attracted a high level of interest in the last decade as one of the potentional candidate for well-controlled and reproducible fabrication of nanostructured materials compatible with mass-production requirements or as alternative tool capable to realize fast prototyping of individual devices [2]. In this work, we report on the fabrication of two types of EB ferromagnetic/antiferromagnetic systems (FM/AFM).

The first system represents FIB fabricated FM/AFM nanodots departing from thin film samples prepared by electron beam evaporation. In this case, the samples consist of three layers: AFM FeF_2 (70nm), FM Py (70nm) and Al (4nm) as a protective layer. We fabricated nanodots from 120 to 250 nm of diameter and with the double centre-to-centre distance. Posterior atomic force microscopy characterization proved the high quality of the nanodots and the optimal choose of the FIB parameters. The second system is a series of samples of antidots of the same size and different distances in x-y direction. We prepared square antidots with the size of 200 nm and x/y distance of 120-900 nm between them.

In both of the cases the initial calibration sequence and corresponding programme elaboration were required in order to obtain the desirable nanodots/antidotes quality, removal depth and patterned area. The optimal current for FIB system [4] used in our work is 30 pA, higher currents bring to partial or complete destruction of the nanostructures.

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Exchange bias in core/shell ferromagnetic/antiferromagentic Co/Co-O nanoparticles of controlled size embedded in an insulating matrix

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Starting from the first report of exchange bias (EB) in fine particles, a huge amount of different EB system has been investigated [1]. Here we present the results of fabrication and characterization of core/shell Co/Co-O ferromagnetic/antiferromagnetic (FM/AFM) nanoparticles in an insulating zirconia matrix. These systems were prepared by pulsed laser ablation [2] at the room temperature in vacuum chamber in O_2 presence. Depending on the target component ratio, it is possible to obtain metallic particles of different sizes, above or below the percolation threshold. The samples of this study have been grown well below percolation threshold in order to exclude as much as possible the interactions between particles. We have prepared a variety of samples at different O_2 chamber pressures (p_{O2}) which resulted in different core-shell ratios. It is significant that the oxide shell forms while the Co particles fly from the target to the substrate. The investigated thin films were about 200-300 nm thick and were deposited onto different substrates according to the characterization technique to be used. The magnetic properties were measured by SQUID magnetometer. As p_{O2} increases, three interesting effects in zero field cooling/field cooling (ZFC/FC) and M(H) data can be observed: (i) the magnetization of the samples decreases due to decrease in the volume fraction of FM Co in the core of nanoparticles; (ii) the ZFC peak position moves from 6.5 K for $p_{O2} = 0$ to 12.5 K for $p_{O2} = 10 \cdot 10^{-7}$ bar, since the higher p_{O2}, the larger the mean particle size, while it broadens since the size distribution also broadens; (iii) the EB field first increases with increasing p_{O2} (increase in the AFM shell thickness at the expense of the FM core), while it decreases at large p_{O2} when the whole particle becomes AFM. Comparing the behaviour between pure AFM and core-shell particles, it is evident that the AFM nanoparticles do not present hysteresis behaviour.

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PREPARATION OF POLYMER COATED GOLD NANOPARTICLES

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The fabrication of metallic nanoparticles of controlled size, shape and functionality is the goal for the development of novel materials. In this context, the unique properties of thiolate-protected gold nanoparticles (NPs) make them excellent candidates for use in a variety of advanced technologies[1]. Among several established routes of preparation, our interest is focused on the synthesis of NPs in the presence of functionalized polymers. This strategy firstly requires the synthesis of suitable tailor made polymers with mercapto functionality, followed by the design of an effective technique for the particle synthesis which allows to directly obtaining polymer-capped gold NPs. The formation of NPs was studied in the presence of diverse polymers as capping agents, with different main chain functionalities and lengths. In this paper we reports preliminary results on the important role played by these polymeric ligands on the stabilization and control of nanoparticle formation as well as on their arrangement into ordered layers.

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ANALYSIS OF SPINOR-ELECTRON WAVEGUIDED OPTICS IN 2D AND 1D NANOSTRUCTURES BASED ON THE DIRAC EQUATION

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In this work is presented a quantum analysis, based on the Dirac equation, of the propagation of spinor-electron guided waves in 2D and 1D nanostructures. These guiding nanostructures can be regarded as the building elements of a new kind of electron wave devices based on electron wave optics such as integrated electron optical devices [1]. Likewise, it is well known that in low-dimensional structures, a pronounced wave nature of the electron is obtained and therefore interference and spinor effects must be taken into account in an enough accurate way, accordingly, the electron optics of these devices would must be formulated by a complete quantum spinor wave theory, that is, by the Dirac equation. To our knowledge, theoretical and applied studies of electron waveguides based on the Schrödinger equation have been reported [2], however, only recently the fully relativistic spinor nature of the guided electron waves has been taken into account [3], that is, it has been used a spinor-electron guided-wave optics fully based on the Dirac equation. First of all, the wave equations for Spin-Up (SU) and Spin-Down (SD) electron modes in 2D nanostructures are presented, which have been recently derived from the Dirac equation and exactly solved for electron modes in a quantum well [3]; in this work we extend these results to 1D structures; for that, we apply both the Marcatili's method and the Knox-Toulios's method, both methods being well known in integrated optics, in order to obtain, starting from fictitious 2D structures, approximate solutions of the Dirac equation for 1D nanostructures. The main consequences related to the spinor modal solutions are analysed: modal cut-off conditions; selective phase retardations, that is, retardations depending on the SU or SD spin polarization; non-relativistic limit (Schrödinger equation), and so on.

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TRANSICIÓN A UN ESTADO FUERTEMENTE DISIPATIVO INDUCIDA POR PULSOS DE VOLTAJE EN MICROPUENTES DE $YBa_2Cu_3O_{7-\square}$

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La transición a estados fuertemente disipativos inducida en un superconductor por una corriente eléctrica de amplitud superior a la crítica (a la cual se origina la disipación) es un fenómeno de gran interés tanto desde el punto de vista básico como aplicado [1, 2]. En general, esta transición ha sido estudiada imponiendo la densidad de corriente [2, 3]. Sin embargo en la mayoría de la situaciones prácticas la variable impuesta es el voltaje. En presencia, como es habitual, de efectos no lineales y térmicos, ambas situaciones conducen a un comportamiento muy diferente. En esta comunicación se resumirán algunos de nuestros resultados sobre la transición a estados altamente disipativos inducidos en micropuentes de $YBa_2Cu_3O_{7-\square}$ imponiéndoles una corriente o un voltaje *supercríticos*. Estos resultados experimentales ponen en evidencia las diferencias de comportamiento entre ambos casos, las cuales se pueden explicar asumiendo la presencia de efectos térmicos. Estos últimos se analizan a nivel cuantitativo con la ayuda de un método de elementos finitos.

Agradecimientos

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Interacción de la red de vórtices con defectos en muestras de $YBa_2Cu_3O_{7-\delta}$

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La técnica de Decoración Magnética de Bitter (DMB) es una técnica de visualización de dominios magnéticos que permite resolver imágenes a escala inferior a un micrón para superficies del orden de centímetros. El estudio de la red de vórtices en materiales superconductores mediante esta técnica permite analizar el comportamiento de la red ante la presencia de defectos en la muestra. De esta manera es posible estudiar la simetría, el grado de orden/desorden e incluso la periodicidad de la red de vórtices a partir de las posiciones de los vórtices observadas mediante experimentos de DMB.

En este trabajo se presentan resultados de DMB en muestras superconductoras monocristalinas de $YBa_2Cu_3O_{7-\delta}$ crecidas por el método de flujo.[1] Se muestran resultados del análisis del grado de orden/desorden de las muestras realizando una comparativa en función de la densidad de defectos presentes en las muestras y con películas delgadas del mismo material. Finalmente se plantea un método para el estudio por medio de DMB de la competencia entre defectos naturales y artificiales presentes en este tipo de muestras.

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Quantum magnetic deflagration in nanomagnets and manganites

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We report new experiments on magnetic deflagration on two different magnetic systems. In the case of the molecular clusters we have discovered what we have called “quantum magnetic deflagration” whereas with phase separated manganites, we have observed that the controlled ignition of the deflagration is accompanied by the colossal variations of the magnetoresistance of the material.

The experiments combine the use of microwaves to generate surface acoustic waves on piezoelectric devices and slightly perturb the samples with measurements of magnetization and resistivity.

Our observations on magnetic deflagration and their control turn out to have universal validity and consequently a new physics topic may thus lay open ahead of us both for basic science and applications.

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APLICACIÓN DE FUNCIONALES CINÉTICOS SOBRE LA DENSIDAD ELECTRÓNICA DE METALES SIMPLES: CÁLCULO DEL *BULK MODULUS* DEL ALUMINIO.

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El análisis de la densidad electrónica en sólidos es un campo de investigación de importancia creciente en la actualidad. El perfeccionamiento de las técnicas experimentales permite un estudio cada vez más preciso de la distribución de la densidad electrónica de los sólidos. Sin embargo, el conocimiento de determinadas propiedades físicas a partir de la densidad electrónica está lejos de constituir un problema trivial. En particular, el cálculo de la energía total debe salvar el escollo del desconocimiento del funcional exacto que da la energía cinética mediante el uso exclusivo de la densidad electrónica. El desarrollo de funcionales cinéticos es una línea de trabajo activa dentro del campo del cálculo de la estructura electrónica. Los nuevos funcionales desarrollados por García-Aldea y Alvarellos [1-3] satisfacen un conjunto importante de límites físicos y pueden evaluarse con un coste computacional bajo. Con la idea de poner a prueba dichos funcionales se ha estudiado el aluminio sólido en empaquetamiento cúbico compacto como un modelo real de un metal simple. Como primer paso, se evalúa la energía total del sistema de manera no autoconsistente, restando a la energía total la energía cinética Kohn-Sham y sumándole la que se obtiene mediante los funcionales cinéticos. En todos los casos se ha hecho uso del código Abinit [4], y el cálculo Kohn-Sham se ha llevado a cabo con varios pseudopotenciales. Una vez que se han obtenido las energías totales aproximadas para un barrido de distintos parámetros de red, se han ajustado mediante la ecuación de estado de Murnaghan [5]. De este modo se han obtenido los valores de las constantes de red y del "*bulk modulus*", que se han comparado con los valores experimentales y los resultados Kohn-Sham.

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FABRICACIÓN DE NANOPARTÍCULAS DE COBALTO DE TAMAÑO CONTROLADO EN CONDICIONES DE ULTRA ALTO VACÍO

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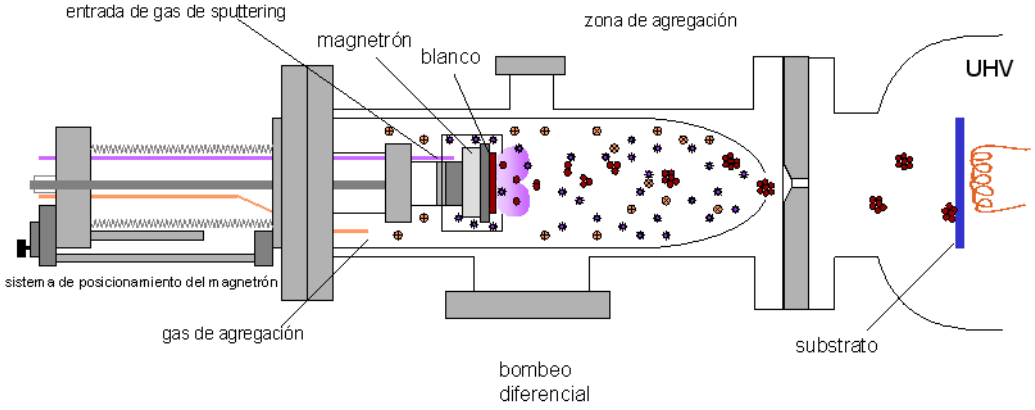
La fabricación y el estudio de nanopartículas presentan un gran interés tanto desde un punto aplicado como básico. En la última década una nueva técnica de fabricación de nanopartículas basada en fuentes de agregados o Ion Cluster Source (ICS) ha ido entrando progresivamente en los laboratorios. Esta técnica presenta algunas ventajas frente a otros métodos de fabricación de nanopartículas como son:

- control preciso del tamaño y dispersión de las nanopartículas (de 1 a 30 nm con una desviación del 5 %),

- crecimiento en condiciones de ultra alto vacío, lo que asegura la elevada pureza de los agregados depositados,

- control independiente del proceso de fabricación de las nanopartículas y del estado del substrato lo que permite emplear cualquier tipo de substrato: dieléctrico, conductor, metálico, orgánico, etc., a cualquier temperatura y con cualquier acabado superficial. En este póster se presentarán los primeros resultados obtenidos con una ICS recientemente instalada en el ICMM. La ICS está provista de un blanco de cobalto de un 99.97 % de pureza y su esquema se presenta en la figura de abajo. Mostraremos como, en función de los parámetros de fabricación, se pueden controlar los tamaños de los agregados y la densidad de recubrimiento (desde pequeñas fracciones de monocapa a multicapas). Para el análisis de los depósitos obtenidos, se ha realizado una caracterización morfológica mediante microscopía de fuerza atómica, AFM. También se presentarán resultados de caracterización estructural y magnética utilizando, TEM, VSM, Kerr, SQUID y XMCD.



EXAFS STIDUES ON THE ANOMALOUS MAGNETIC BEHAVIOR OF FeCuZr BALL-MILLED ALLOYS

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The origin of the complex magnetic properties of iron rich metallic glasses containing low concentrations of early transition metals (Zr,Sc,Hf,Y) have attracted considerable interest during more than two decades, giving rise to several controversial microscopic interpretations [1,2]. In this work we present the magnetic properties of amorphous $(Fe_{50}Cu_{50})_{100-x}$ Zr_x (x = 13, 17 at.%) alloys obtained by high energy ball-milling. It should be noticed that although iron and copper are an immiscible system, by means of this technique it is possible to obtain FeCu-rich based alloys. As can be seen in Figure 1 for x =13, the alloys show an anomalous increase of the spontaneous magnetization at temperatures above Curie´s temperature (Tc), as evidenced by thermoremanence measurements. This behaviour seems to related by an anomalous changes in the interatomic distances with temperature, as occurs in invar alloys. Such effect has been previously observed on $Iron_{rich}Zr$ based alloys [2, 3] at temperatures below Tc. At higher temperatures the normal thermal expasion takes places an a local ferromagnetic order is induced. In order to explain this effect we have performed EXAFS measurements at the Sp-line at ESRF in Grenoble, as a function of temperature. The figure 1 also shows the nearest-neighbour (D_{nn}) distances of iron atoms. It should be remarked that the D_{nn} distances are nearly temperature invariant for temperatures below Tc, as corresponding to the proposed invar effect. On the other hand, at temperatures over Tc the normal thermal expansion is evident. This thermal expansion is accompained by an increase of the magnetic signal on the thermoremanence meassurements. The increase of first near-neighbour´s distances with temperature produced by thermal expansion, can yield to and enhancement of the density of the states at Fermi level that could promote the appearance of a new magnetic order above Tc [2]

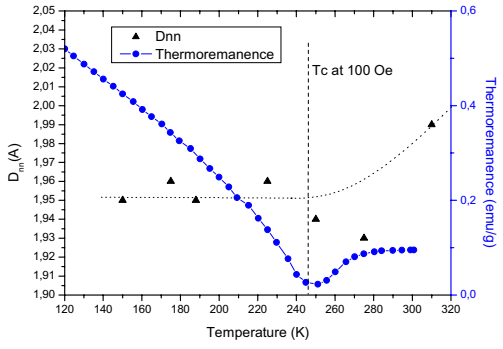

Figure 1. Dnn and Thermoremanence for x=13at%

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Fabrication and characterization of $Fe_{1-x}Co_x$ and MgO based core-shell structured nanoparticles

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Nanophase materials are a subject of very active research because of the appearance of unconventional physical and chemical properties as the size of their integrating particles is reduced down to the nanometer scale. Among others, biological applications of nanoparticles have experienced a very intensive research due to the possibility of using them as drug delivery vectors. Among the multiple hurdles that must be overcome for this purpose are the provision of a sufficiently high magnetic response and an adequate degree of biocompatibility. In this respect, the purpose of the present work was twofold. On one hand, to increase the magnetization of nanoparticles by using a $Fe_{1-x}Co_x$, since alloying with cobalt substantially increases the magnetic characteristics of iron, and on the other hand, to provide a protective biocompatible shell for the particles. In this sense, it is known that magnesia shells might provide exceptional advantages such as environment stability, controlled interparticle interactions, enhanced magnetic moments and non-toxic hydroxyl surface groups that provides intrinsic hydrophilicity and allows surface attachment by covalent linkages of drugs or biomolecules. In this work we present some preliminary results in the $Fe_{1-x}Co_x$/MgO core/shell structured nanoparticles. $Fe_{1-x}Co_x$/MgO core/shell nanophase particles have been prepared by the vaporization-condensation method in a solar reactor in the High Flux Solar Facilities in Odeillo. X-Ray diffraction and high resolution transmission electron microscopy indicate the presence of some remainders of metallic Fe and Co in addition to the $Fe_{1-x}Co_x$ alloy as well as a core/shell structure of high crystalline degree. Magnetic properties have been studied by using SQUID magnetometry and Mössbauer spectroscopy. Both techniques make evident ferromagnetic features at room temperature with values of the saturation magnetization similar to that of the bulk material.

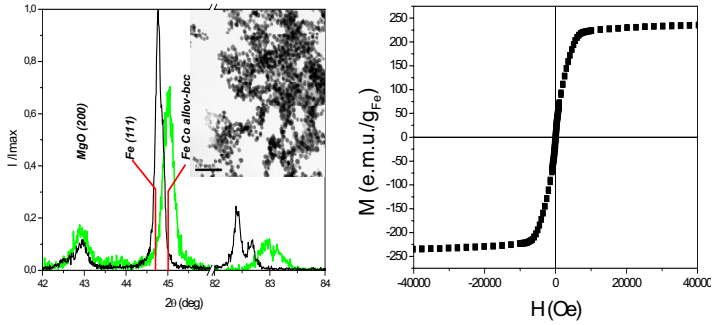

Fig. a) X-ray diffractogram of one of the $Fe_{1-x}Co_x$/MgO samples. Inset: TEM image of the $Fe_{1-x}Co_x$/MgO nanoparticles. b) Room temperature M(H) curve of one of the samples.

Optical emission in GaN/AlN non-polar heterostructures

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Heterostructures based on nitride semiconductors of the group III (GaN, AlN and InN) are usually grown in the (0001) orientation. Due to the wurtzite structure characteristic of this material system, in this orientation a strong electric field is induced along the heterostructure growth direction, which can reach values as high as 7 MV/cm in GaN/AlN QDs. As a consequence, the optical emission is red-shifted due to the large quantum-Stark effect and the radiative efficiency of the optoelectronic devices is severely reduced. It has been demonstrated that the growth of heterostructures along non-polar (m- or a-plane) directions is an effective way to eliminate or considerably reduce this internal electric field [1]. Besides the improvement in their optical properties, the heterostructures grown along these crystallographic directions present a polarized emission that depends on the dimensionality of the heterostructure (it is different for quantum wells (QWs), quantum dots (QDs) and quantum wires (QWrs)), and on its strain state.

In this work we present a comparative study, by means of micro-Raman spectroscopy and photoluminescence, of the polarized emission of stacks of GaN/AlN QWs, QDs and QWrs grown along the a- and m- planes of the wurtzite structure. The shift of the phonon modes with respect to their relaxed values allows us to determine the strain in the heterostructures and the barrier. The photoluminescence characteristics will be related with the dimensionality of the heterostructures, their orientation, shape and strain state.

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SYNTHESIS AND CHARACTERISATION OF $LA_{1-X}K_XMnO_3$ (x<0.20) NANOPARTICLES PREPARED BY THE SOL-GEL METHOD

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The Curie temperature of doped lanthanum manganites can be tuned by varying the doping agent and content. Conveniently choosing these parameters, the magnetic phase transition can occur in the neighbourhood of room temperature and show enough entropy change to be considered as suitable candidates for magnetic refrigeration at room temperature. These conditions can be met for the $La_{1-x}A_xMnO_3$ (A= Na, K) system, for x < 0.20 [1].

We have prepared $La_{1-x}K_xMnO_{3\pm\delta}$ nanoparticles (with x= 0.10 and 0.15) by the sol-gel method using urea as gelling agent [2]. Samples were characterized by x-ray diffraction (XRD), transmission electron microscopy (TEM), thermogravimetry (TGA) and SQUID magnetometry.

In the gel, ions remain randomly distributed into the structure of the gel and the crystallization of the perovskite structure occurs around 500-600 ºC. Calcination at different temperatures produces different particle sizes. Particle size ranges from 20 to 200 nm as a function of the calcination temperature.

The magnetic properties show the ferromagnetic-paramagnetic transition close to room temperature. The entropy change was studied from the initial magnetisation curves.

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PERFORMANCE OF ALACANT ON MULTIPLE COMPUTING PLATFORMS

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First-principles quantum transport packages are nowadays a fundamental tool in nanoelectronics modeling. Their main application is to compute the current through nanoscopic systems implementing, in its most generic form, the non-equilibirum Green's functions formalism in combination with first principles techniques. The software package ALACANT (Alicante Ab initio Computation Applied to NanoTransport) has been developed at the University of Alicante [1] and is available free for non-comercial institutions [2].

Here we present an analysis of some technical aspects that are usually missing in scientific publications. ALACANT has been tested on clusters that use AMD and Intel processors, such as AMD Opteron 280, Intel P4, etc. These tests have been performed by **GuiriSystems** [3], a high-performance cluster integrator devoted to help researchers in the promotion and improvement of their software. In this paper we will present the performance results of ALACANT as well as various other technical issues.

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Guiri Systems

POLYMER TEMPLATE DIRECTED CHEMICAL SOLUTION SYNTHESIS OF SINGLE-CRYSTALLINE $La_{0.7}Sr_{0.3}MnO_3$ NANOWIRES*

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One dimensional (1D) nanostructures offer a means of tuning the strong interactions that exist between magnetic, electronic and crystal structures of manganites. The development of facile, mild an effective approaches for generating size controllable 1D manganite structures remains a significant challenge. In this report, we demonstrate that self standing single crystalline $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) nanowires several microns long with controllable morphology can be successfully synthesized by template assisted chemical solution deposition (CSD) using track-etched polymer membranes of varying pore size. Nanowires were synthesized using a sol-gel based polymer precursor route allowing a good control of the viscosity and stability of the precursor solution, which are crucial parameters for template aided synthesis. The pores of the membrane were filled with the precursor solution by capillarity and subsequently heated at high temperature for polymer elimination and phase formation. Extensive characterization has been performed using XRD, SEM and TEM microscopy and SQUID magnetometry. We prove that these nanowires exhibit a monoclinic crystallographic structure not known up to now for manganite that seems to modify its electronic and magnetic properties.

Moreover, we have nanostructured single crystalline substrates with vertically aligned magnetic LSMO nanopillars and nanopyramids combining CSD with supported track-etched polymer templates, which opens the possibility to study new phenomena and interactions in nanomagnet systems embedded into magnetic/non magnetic matrices.

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El cristal Niobato de Estroncio y Bario: Un "vidrio fotónico" no lineal

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El progreso actual en el campo de la fotónica está fuertemente determinado por la fabricación y caracterización de nano y micro-estructuras en materiales avanzados útiles para la generación y el manejo de la luz. En este trabajo se ha estudiado el sistema ferroeléctrico $Sr_{0.6}Ba_{0.4}(NbO_3)_2$ (SBN) en el que existe una micro-estructuración basada en la presencia de dominios ferroeléctricos con polarización alterna con carácter bidimensional y alto grado de dispersión en tamaños. Esta distribución de dominios da lugar a una modulación de la susceptibilidad no-lineal de segundo orden útil para generación de procesos no lineales de conversión en frecuencia. Se muestran fenómenos no lineales novedosos asociados a la particular estructura de dominios en el material, tales como la obtención de procesos de conversión múltiple, tanto en frecuencia como en dirección. En particular se destaca la posibilidad de generación simultánea de segundo y tercer armónico (SHG y THG, respectivamente) ambos sintonizables en un rango continuo excepcionalmente ancho (430-680 nm para el SHG y 400-460 nm para el THG) sin necesidad alguna de sintonización angular o térmica. El carácter bidimensional de la distribución de dominios ferroeléctricos, junto con el alto grado de dispersión en el tamaño de los mismos, permiten considerar al SBN como el primer ejemplo experimental de un "vidrio fotónico" no lineal bidimensional, abriendo vías para el diseño de nuevos dispositivos fotónicos tales como generadores de armónicos múltiples, prismas no lineales o superprismas.

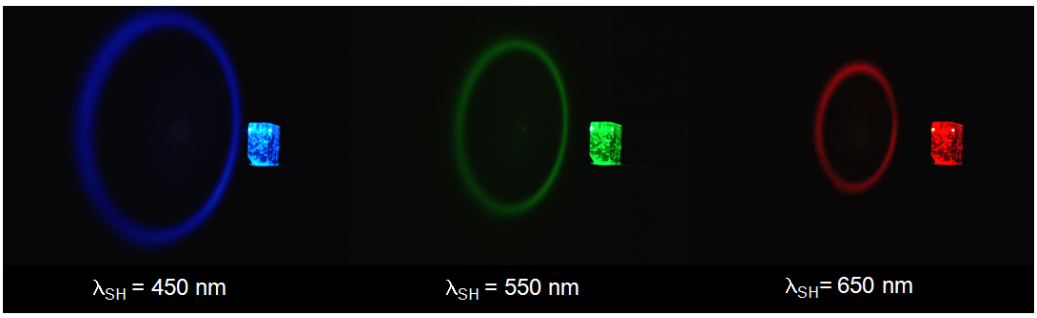

Figura 1. Generación de segundo armónico cónica para diferentes longitudes de onda incidentes (900, 1100 y 1300 nm)

P.Molina et al. Strontium Barium Niobate as a multifunctional two-dimensional nonlinear "photonic glass. *Advanced Functional Material* (in press)

Lithography by local electrochemistry on $La_{1-x}Sr_xMnO_{3-\delta}$ thin films by C-AFM

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Colossal magnetoresistance (CMR) materials have been suggested to be excellent candidates for advanced non-volatile memory devices based on its ability to switch its resistance into two different states. The origin of this phenomenon is still controversial and further investigation of the relationship of the nanostructure and electrical properties at the nanoscale is worthwhile.

We report here AFM and local current (LC-AFM) measurements of $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) thin films grown on a $SrTiO_3$ substrate by chemical solution deposition (CSD) process. These films have developed through a new process leading to epitaxial La_2O_3 nanodots at the surface. AFM topography images has allowed to identify the interfacial nanodot shape and distribution and LC-AFM has shown the insulating character of the nanodots while the LSMO films display an homogeneous metallicity.

LSMO film can be switched between a conductive ON state and a non-conductive OFF state by the application of an appropriate bias voltage.

Local *I-V* curves of the LSMO films were performed and a nonlinear and hysteretic behaviour of the transport properties is observed confirming that a resistance switching occurs. The relevance of the local nanostructure and current injection process on the resistive switching phenomenon will be discussed.

Graphene ribbons for spintronics applications

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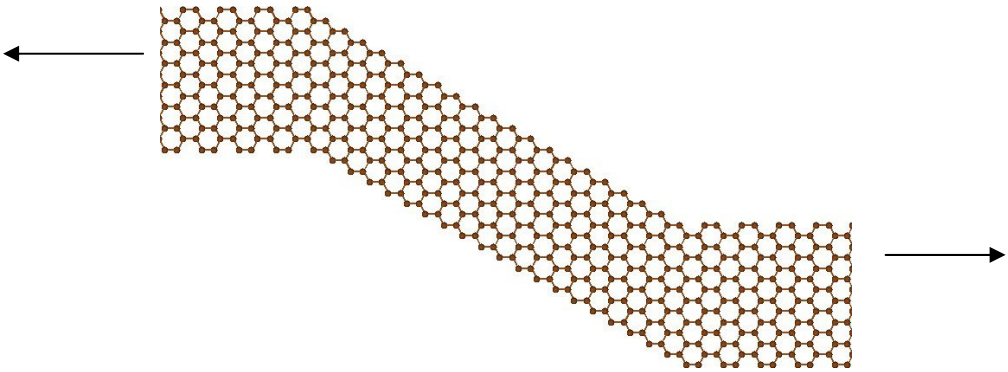
Graphene is a carbon allotrope that has recently gained popularity in nanoelectronics[1]. It is a single layer of carbon atoms ordered in a honeycomb lattice. Two-dimensional graphene presents a number of interesting properties such as a finite conductance at the Fermi energy despite presenting zero density of states at this point. Also, it presents electron-hole symmetry since its atoms are in a bipartite lattice[2]. Graphene can be cut in ribbons with two different edge shapes: zigzag and armchair. The former is an insulator with antiferromagnetically coupled magnetic edges. The latter can be metal or insulator dependig on the width of the ribbon[3].

In this work we study the electronic transport through an armchair Z-shaped ribbon as shown in the figure. A zig-zag channel is conected to a two semiinfinite graphene armchair ribbons with the same width. As expected, for low energies close to the Fermi energy, this system does not conduct. When a magnetic field is applied, it is possible to convert the insulating ribbon into a metallic ribbon. This behavior is desirable in spintronics as a on/off switch tunable with a magnetic field.



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Chemical dynamics simulations of gases scattering off a self-assembled monolayer surface

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We performed chemical dynamics simulations to study energy transfer in collisions of carbon dioxide and Ar with a perfluorinated octanethiol self-assembled monolayer (F-SAM) surface. Two different models for the F-SAM surface were used: an explicit-atom (EA) and a united-atom (UA) model along with accurate CO_2 + F-SAM and Ar + F-SAM intermolecular potentials, developed from previous *ab initio* calculations extrapolated to the complete basis set limit. The results for both models of the F-SAM surface give different results for the energy transfer efficiencies and percentages of trajectories according to the types of collisions with the surface. A new model for the F-SAM surface is suggested that reduces the CPU time with respect to the EA model with negligible loss of accuracy.

The results obtained in our simulations were compared with available experimental data. The scattered CO_2 rotational energy distributions and scattered Ar translational distributions are in excellent agreement with experiment.

KBR SURFACE MORPHOLOGY CHANGES INDUCED BY LOW ENERGY ION BOMBARDMENT: RIPPLES FORMATION

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The sputtering of insulating materials induced by ions with energies of 0.1-10keV is dominated by collision cascades due to elastic encounters between the incident ions and component atoms [1]. When an ion hits the surface, it deliver locally a certain amount of energy generating cascades of collisions in the bulk. This process induces an effective instantaneous melting of the material underneath. Due to geometrical considerations, the effect of the ion bombardment depends on the surface curvature: the energy concentrates on regions of positive curvature and this favours the excavation of valleys and the growth of hills. The excavation effect must depend on the number and velocity of the spputered ions. The local shape and orientation of the surface might play also an important role. Due to the energy transmitted by the impinging ions it concentrates more in regions with positive curvature and elements of the material have not enought energy to scape from the surface, giving, as result, ripples formation on the surface [2]. Here we examine these processes on KBr surfaces exposed to low energy ion bombardment. Non-contact Atomic Force Microscopy has been used in order to analyse the surface morphology after different times of ion bombardment. Some features in the form of ripples have been found (Fig. 1).

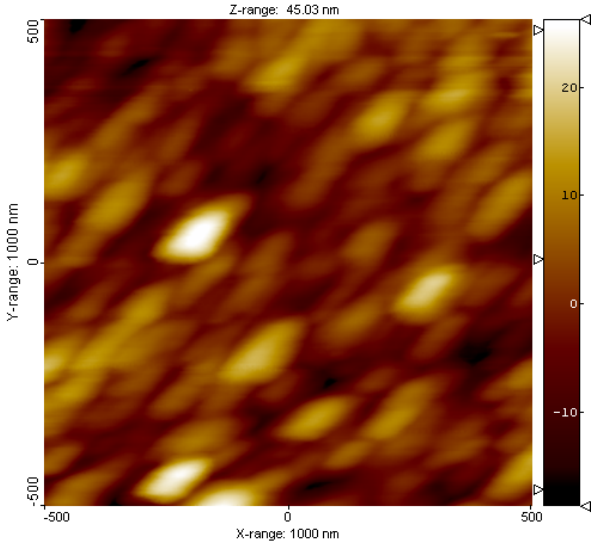

Figure 1. Ripples shape on the KBr surface by NC-AFM.

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Heteroestructuras epitaxiales Fe_3O_4/MgO/Fe para espintrónica

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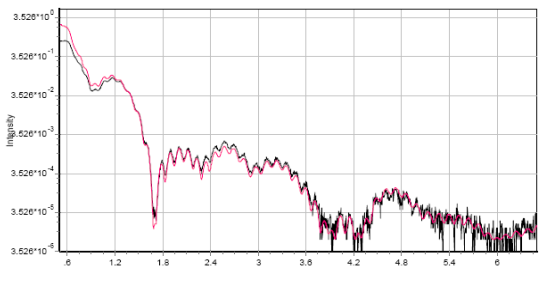
Los materiales ferromagnéticos medio – metálicos (con una polarización de espín del 100% en el nivel de Fermi) con alta temperatura de Curie son aptos para su implementación como electrodos activos en dispositivos magnetoelectrónicos[1,2] potencialmente útiles a temperatura ambiente. Un buen ejemplo de estos materiales es la magnetita (Fe_3O_4) que presenta una Tc ≈ 850 K[3]. Por ello hemos producido heteroestructuras epitaxiales tipo unión túnel con electrodos de Fe_3O_4 tipo MgO (100) // Fe_3O_4 / MgO / Fe mediante un Sistema de Deposición por Láser Pulsado (PLD). Hemos estudiado la influencia de distintos parámetros de crecimiento (presión base, temperatura del substrato, ritmo de depósito) en las propiedades estructurales y magnéticas de láminas de Fe_3O_4 depositadas sobre substratos de MgO (100), realizándose un completo estudio de las propiedades magnéticas, estructurales y de transporte eléctrico en función del espesor (t_{Fe3O4}) de dichas películas epitaxiales, entre 3nm < t_{Fe3O4} < 300 nm. Hemos obtenido las condiciones óptimas de crecimiento de la barrera de MgO y del electrodo de Fe y mediante medidas de reflectividad de Rayos X (XRR) se ha observado una baja rugosidad en las distintas intercaras (Fig.1). Mediante medidas de imanación a temperatura ambiente se observaron las contribuciones a la imanación total de cada lámina desacopladas (Fig.2), indicando la alta calidad de la barrera de MgO, sin "pinholes" que puedan producir un acoplo magnético entre ambos electrodos.



N	R	Material	Thickness	Roughness
1	1	MgO	7.85	0.398
2	1	Fe	4.49	0.198
3	1	MgO	4.82	0.231
4	1	Fe3O4	59.34	0.207
SUB	1	MgO	0.00	0.254

Fig.1: Ajuste de XRR mediante el software especializado LEPTOS

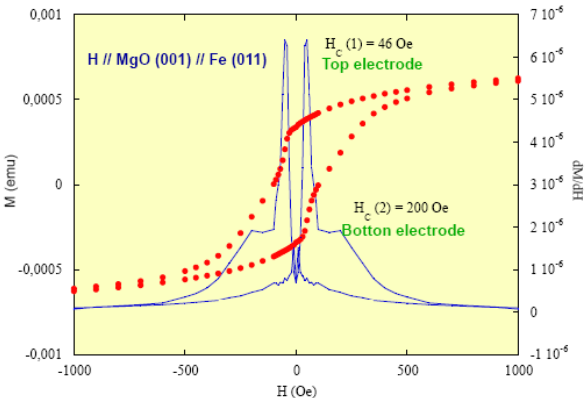


Fig. 2: Curvas de imanación en función del campo magnético a temperatura ambiente y en distintas direcciones del campo.

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EVOLUCIÓN TÉRMICA DE ZONAS DÉBILES EN UN CUPRATO SUPERCONDUCTOR

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El comportamiento térmico de zonas débiles (con menor corriente crítica) en superconductores es un aspecto todavía abierto de las propiedades de transporte de estos materiales y con amplio interés práctico [1, 2]. En esta comunicación presentamos un estudio, realizado mediante simulación numérica con elementos finitos, de la evolución térmica de un conjunto de zonas débiles artificialmente creadas en muestras superconductoras de Bi-2212. Cada zona débil se modeliza como una reducción de la sección transversal de las muestra, de modo que la corriente crítica sea localmente menor. De esta forma, se puede provocar la transición al estado disipativo de estas zonas débiles mientras el resto de la muestra permanece en estado superconductor. Cuando la corriente se hace cero, el calor generado en las regiones rebajadas fluye por conducción hacia las zonas frías adyacentes. De este modo, el proceso de refrigeración se acelera notablemente en comparación con el que tendría lugar en una muestra calentada uniformemente e inmersa en un líquido o gas refrigerante con intercambio de calor exclusivamente por convección. Estos análisis numéricos confirman nuestros trabajos previos [3-5], que ya señalaban las ventajas que supone la utilización de zonas débiles como procedimiento de refrigeración. Este método es particularmente interesante en el caso de los limitadores de corriente, para los cuales la recuperación térmica en tiempos no superiores a 1 s es de crucial importancia.

Agradecimientos

Este trabajo ha sido financiado por los Proyectos 2006/XA049 y 07TMT007304PR (XUGA-FEDER), por el Proyecto FIS2007-63709 (MEC-FEDER), y por una beca FPI del Departamento de Educación, Universidades e Investigación del Gobierno Vasco.

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Spin lattice coupling and the nature of the magnetic phase transitions

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A first-order ferromagnetic to paramagnetic (FM-PM) phase transition is an atypical phenomenon normally associated with strong coupling among different degrees of freedom. This behavior is observed in manganites, $A_{1-x}A'_xMnO_3$, with an associated CMR around a first order Tc. We will discuss a thermodynamic model in which the magnetic order parameter is coupled to the lattice, and this coupling is sensitive to chemical disorder. We will show how electron-lattice coupling promotes or suppresses first-order phase transitions, depending on whether cooperative or quenched random distortions couple to the magnetization. We will also discuss the microscopic implications of these competing effects in the properties of ferromagnetic manganites.[1][2] The applicability of this model to itinerant magnetic systems is being tested in $CoS_{2-x}Se_x$. We will show M(T,P,H) experimental results to monitor the change in the magnetic phase transition.

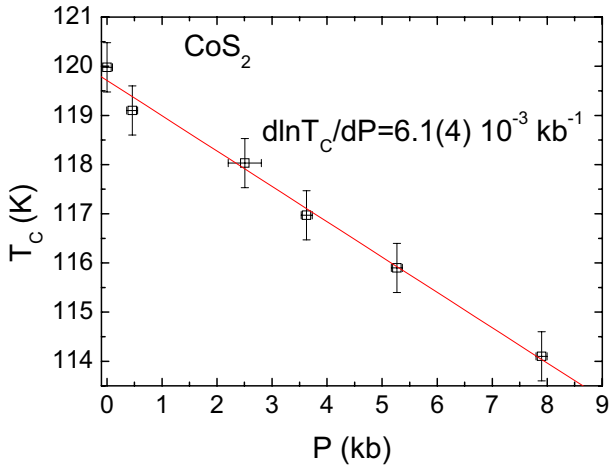

Figure: Pressure dependence of T_C in the itinerant ferromagnet CoS_2

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Preparación de Nanografenos por Aproximación Ascendente

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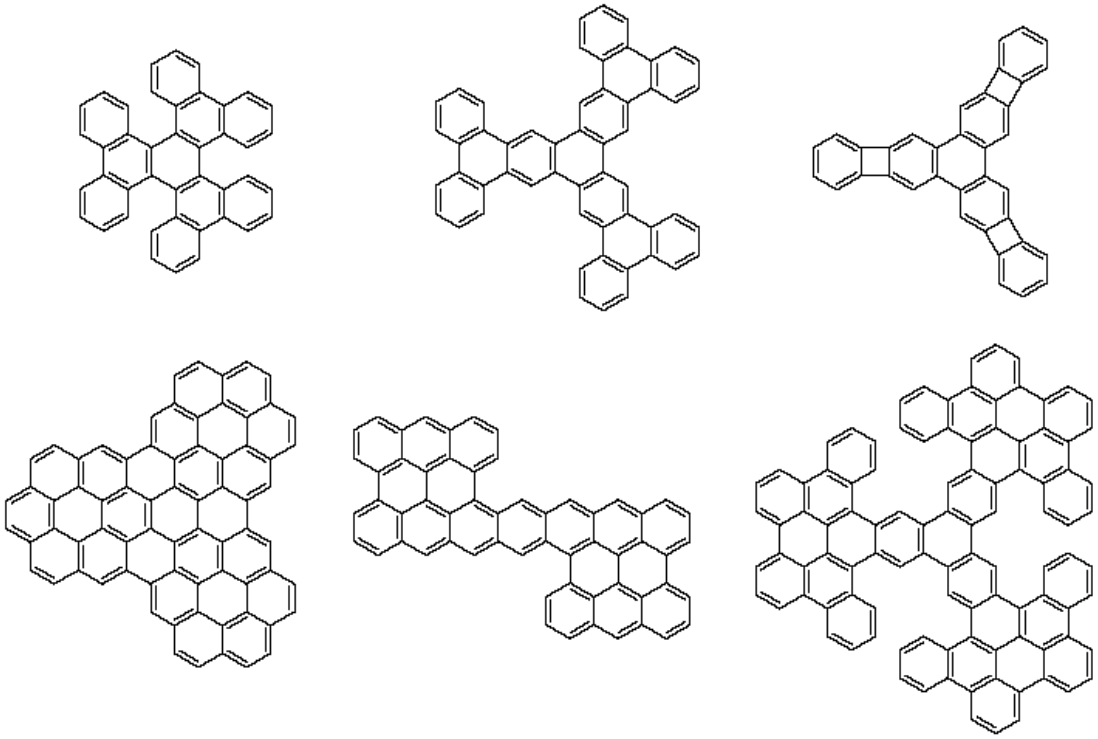
En los últimos años los grafenos han centrado gran atención de la comunidad científica por sus estructuras y propiedades únicas.[1] Uno de los retos más importantes en la ciencia de estos materiales consiste en evitar la heterogeneidad implícita en sus métodos de síntesis actuales. Los grafenos se suelen preparar siguiendo aproximaciones descendentes *(up-down)*, por exfoliación de grafito o empleando condiciones drásticas de reacción. El resultado es la obtención de nanoestructuras con diferentes tamaños y/o defectos estructurales.



En esta comunicación presentamos nuestros esfuerzos hacia la preparación de nanografenos estructuralmente definidos, empleando aproximaciones ascendentes *(bottom-up)* basadas en reacciones de cicloadición en condiciones suaves de reacción. A continuación se muestran algunas de las estructuras que se pueden preparar empleando esta metodología.[2]
Será especialmente interesante la comparación de las propiedades electrónicas, ópticas y mecánicas de estos nanografenos obtenidos por *aproximaciones ascendentes* con las encontradas para grafenos preparados por *aproximaciones descendentes*.

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SALTO ENTRÓPICO Y ORDEN DE LAS TRANSICIONES DE LA SERIE RCo_2

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Los compuestos de la serie de fases de Laves RCo_2 (R = ión de tierra rara) son candidatos como materiales con uso en refrigeración magnética [1], ya que presentan un efecto magnetocalórico elevado, aunque casi todos ellos a temperaturas relativamente bajas. Dado que los materiales más interesantes para esta aplicación son aquellos que presentan una transición de fase de primer orden, tiene interés determinar la naturaleza de las transiciones magnéticas de estos compuestos.

Nuestro objetivo ha sido realizar un estudio sistemático de la naturaleza de las transiciones de fase magnéticas en cinco compuestos puros RCo_2 (R = Er, Dy, Ho, Nd, y Pr) [2] y en la dilución sólida pseudobinaria $Er_xPr_{1-x}Co_2$ (x = 0.9, 0.8 y 0.7) empleando para ello el criterio de Banerjee [3], analizando al tiempo sus límites de aplicabilidad. Según este criterio, desarrollado para transiciones de orden magnético en el marco de la teoría de Landau-Lifshitz, el análisis del signo de los parámetros que ligan la imanación y el campo mediante la ecuación de estado de Landau en la temperatura crítica permite distinguir entre transiciones de primer y segundo orden [3].

En esta comunicación presentaremos nuestro estudio sistemático de M(H, T) de la serie de fases de Laves y se describirán:

- la aplicación del criterio de Banerjee a toda la serie, que ratifica la naturaleza de segundo orden de los compuestos $NdCo_2$ y $PrCo_2$.
- nuestro estudio del "*debilitamiento*" del carácter de primer orden en $DyCo_2$ y las diluciones $Er_xPr_{1\ x}Co_2$ al disminuir x, así como una relación fenomenológica entre el salto entrópico en la transición y un parámetro que definimos en este trabajo y que cuantifica la "*fortaleza*" del carácter de 1er orden de la transición.
- los parámetros magnetocalóricos obtenidos en esta familia de ompuestos mediante la aplicación de las relaciones de Maxwell

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Magnetization reversal mechanism of single crystalline Fe nanowires: spring like behaviour at high angles

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Magnetic nanostructures have drawn a lot of attention in recent years due to the new phenomenology they exhibit and also due to their interest for technological applications. Their magnetization processes are controlled by their intrinsic properties, which are mainly determined by the crystal-chemical structure, and by their extrinsic characteristics such as the system morphology and dimensions. The progress in the understanding of these processes has been impelled, among other factors, by high degree of improvement of lithographic tecniques [1]. In this work we present an experimental and simulational study of the magnetization processes of a set of Fe nanowires arrays lithographed on 30 nm thick Fe (001) films epitaxially grown on MgO (001) substrates by Pulsed Laser Deposition. Focused ion beam (FIB) and Electron Beam Lithography (EBL) techniques were employed to prepare the nanowires with widths of 100 and 500 nm and separations beteween 100 nm and 1 μm. The coercivity of the wires, one order of magnitude above that of the continuous films, is mainly dependent on the wires width and increases with the angle θ between the applied field and the wires axis. However, for θ>75º the loops present a fully reversible spring like behaviour with two different slopes (Fig. 1), independent of the width, separation and litography technique employed. Micromagnetic simulations have shown that this is due to the formation of two domains along the wires lateral surfaces with magnetization parallel to their axis and a perpendicular domain in the central region.

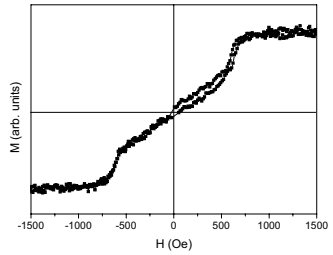

Fig. 1: Hysteresis loop of the array of wires 500 nm wide and 100 nm separation, for θ=90º.

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Fe_3O_4 nanoparticles with bulk magnetic properties

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In the search for better contrast agents suitable for magnetic resonance imaging, iron oxide magnetic nanoparticles (NP) [1] are front line candidates for substituting the widely used gadolinium chelates. One of the main goals in the design of improved Fe-O NP-based contrast agents is to obtain the highest possible saturation magnetization, M_S. Magnetite Fe_3O_4 NP synthesized by the high-temperature decomposition of an organic Fe precursor in the presence of a surfactant (oleic acid molecules covalently bonded to the NP surface) [2] show unusually high M_S values, close to the expected for bulk Fe_3O_4 [3]. Furthermore, these M_S values are much larger than those in NP prepared by the usual co-precipitation method, for which there is no chemical bond between the coating (dextrane, TMAOH, PVA, …) and the NP surface [3]. In order to understand this behavior, we have studied the surface contribution to the magnetic anisotropy and the orbital contribution to the magnetic moment of Fe_3O_4 NP particles with mean diameter of a few nanometers, as a function of the coating (oleic acid versus PVA). By means of ac susceptibility and time-dependent thermoremanence [4], we may account analytically for the surface contribution to magnetic anisotropy. The orbital contribution to the magnetic moment has been determined by XMCD, and the spin and orbital contributions are successfully correlated to the surface coating. The comparison of both techniques is presented.

The funding from the Spanish MEC (NAN2004-08805-CO4-02, NAN2004-08805-CO4-01, CONSOLIDER CSD2006-12 and MAT2006-03999), and from the Catalan DURSI (2005SGR00969) is acknowledged.

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Lattice Monte Carlo Simulation of Polymeric Reversible Gel

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Gelatine gelation has been modelled by means of a Dynamic Lattice Monte Carlo simulation of an associative polymeric solution**,** incorporating a reversible interaction on random places of interacting self-avoiding chains and an algorithm based in local movements. The simulation allows the configurational relaxation of the junction slabs without destroying it, biased by the Metropolis criterion, enabling in this way, a more realistic dynamics. The aggregation interaction is reversible so the network can follow both enthalpic and entropic relaxation during thermal equilibrium.

Static and dynamic properties of the thermally driven sol-gel transition can be obtained for a variety of gelling conditions controlled by a few parameters (helix seeds fraction, polymer volume fraction and reversibility parameter).

By imposing different gelling abilities to the system, variable network structures, gelation points and transitions have been simulated. Results are in good agreement with experimental data of gelatine gels.

Keywords: dynamic MC simulation model, polymer network, sol-gel transition.

ESTUDIO DEL COMPUESTO SEMICONDUCTOR GaSb MEDIANTE RESONANCIA MAGNÉTICA NUCLEAR CON ROTACIÓN EN ÁNGULO MÁGICO

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El GaSb es un material semiconductor con grandes aplicaciones en el campo de la optoelectrónica, las comunicaciones y la conversión de energía termofotovoltaica [1]. En este trabajo se presentan los resultados encontrados, a partir de los espectros obtenidos mediante Resonancia Magnética Nuclear con Rotación en Angulo Mágico (MAS: NMR, en Inglés), en cristales de GaSb puros y dopados con Te. Hasta donde llega nuestro conocimiento, los resultados más recientes obtenidos mediante esta técnica han sido obtenidos hace dos décadas [2] y tan solo para el GaSb puro. Existen también experimentos de NMR anteriores que se remontan a 1955 [3] pero en ningún caso se han obtenido datos en GaSb de tipo *n* (tradicionalmente GaSb dopado con Te). En este trabajo nosotros hemos estudiado los espectros de NMR-MAS en cristales de GaSb puro y dopado con Te. El primero es siempre de naturaleza tipo *p* debido a los defectos nativos, mientras que el segundo es un material de tipo *n* [1]. Así mismo, se han estudiado cristales obtenidos mediante dos técnicas de crecimiento distintas; Bridgman y Czochralski. Los resultados que se obtienen (ver Fig. 1) indican una clara diferencia entre material de tipo *p* y material de tipo *n* siendo independientes de la técnica de crecimiento empleada. Se profundizará en el análisis de las diferencias de desplazamiento químico debidas a las diferencias de carga electrónica en los diferentes materiales.

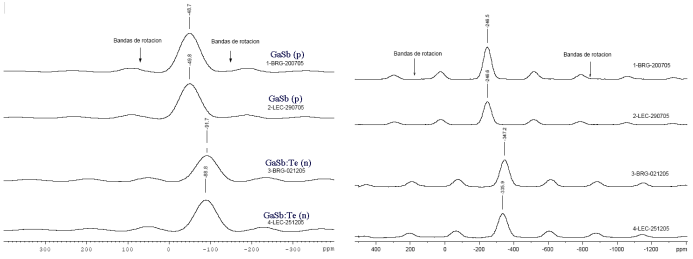

Fig. 1 Espectros obtenidos por MAS-NMR para el desplazamiento químico del (a) ^{69}Ga y el (b) ^{123}Sb**.**

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Atomically flat MOD $La_{0.7}Sr_{0.3}MnO_3$ buffer layers for high critical current $YBa_2Cu_3O_7$ TFA films

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Superconducting $YBa_2Cu_3O_7$ (YBCO) thin films have been grown by the trifluoroacetates (TFA) route onto metalorganic deposited (MOD) ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) buffer layers. Growth conditions of the LSMO films have been studied in detail and fully strained epitaxial layers with atomically flat surfaces and self-assembled nanometric islands were obtained. We will prove that the development of this surface morphology is a key parameter for achieving high critical currents in the all-chemical YBCO/LSMO multilayers, $J_c^{sf}(77K)=1.8MA/cm^2$. Angular pinning studies evidence that defect structure is modified with respect to standard TFA-YBCO films as a pronounced peak in J_c is observed for H//c at high temperatures. This indicates the presence of anisotropic defects playing an important role in vortex pinning even at the irreversibility line. The influence of the nanostructured LSMO surface on this vortex pinning behaviour will be discussed. Our results stress the suitability of these all chemical TFA-YBCO/LSMO multilayers as conductive coated conductor architecture.

This work has been supported by European Union and Spanish national funds (Hiperchem project, Consolider NANOSELECT, NAN 2004-09133-C03-01 and MAT2005-02047).

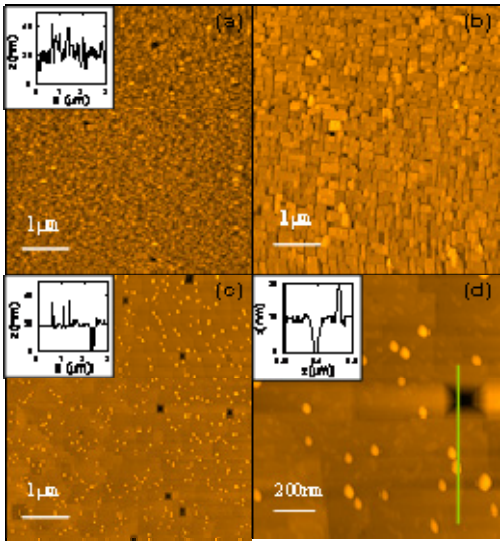

Figure 1. AFM images of LSMO films grown under different conditions showing the surface morphology evolution.

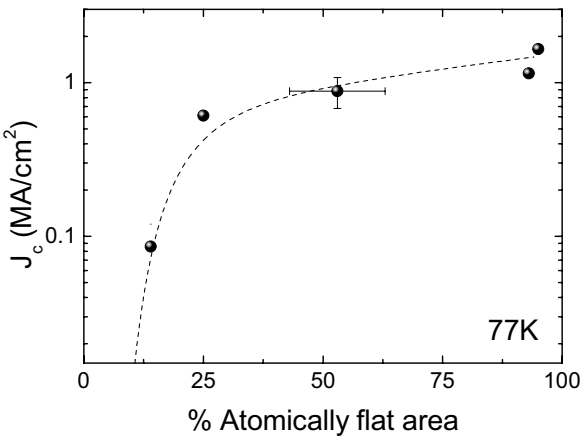

Figure 2. Critical current density of YBCO films as a function of the planarity of the underlying LSMO layer.

PROCEDIMIENTO HÍBRIDO ENTRE *FIELD COOLING* Y *ZERO FIELD COOLING* PARA INDUCCIÓN DE CORRIENTE EN ANILLOS SUPERCONDUCTORES

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Para generar una corriente persistente en anillos superconductores de tipo II se utiliza un método de tipo inductivo. Dicho procedimiento puede ser un *field cooling* (enfriamiento a campo constante) o un *zero field cooling* (enfriamiento a campo cero) [1-2]. La corriente inducida en los anillos superconductores decae de forma logarítmica con el tiempo, acorde al modelo de Anderson [3-4]. La causa del decaimiento de dicha corriente se debe al movimiento irreversible de vórtices debido a la fuerza de Lorentz [5]. Se presenta un método híbrido para la inducción de corriente en anillos superconductores de YBCO que combina las características del enfriamiento a campo cero y el enfriamiento con campo. Se pretende conseguir con este procedimiento de inducción generar vórtices atrapados opuestos para investigar el efecto sobre la pendiente de decaimiento. Primero, el anillo superconductor se enfría, a campo magnético cero, hasta una temperatura inferior a su temperatura crítica y se aplica un campo paralelo al eje del anillo. La corriente superconductora generará un campo magnético del mismo módulo y sentido opuesto al inductor. A continuación, una zona muy localizada del superconductor se calienta hasta una temperatura superior a la crítica, por lo tanto se disipa la corriente total que circula por el superconductor. Se deja de calentar el superconductor y vuelve a enfriarse hasta una temperatura inferior a la crítica en presencia del campo magnético externo. En este instante, el superconductor se encuentra en una situación similar a la que se encontraría si se hubiese enfriado en presencia de campo magnético (*field cooling*). Finalmente, se retira el campo externo y se induce una corriente en el superconductor que genera un campo magnético de la misma dirección y sentido que el campo aplicado. Para el calentamiento local del anillo superconductor, en contacto con éste y enrollado sobre él, se realiza un bobinado de hilo metálico resistente y buen conductor del calor. Esta resistencia se calienta haciendo circular por ella una corriente y a través de la misma se transmite calor al superconductor. De esta forma, aumenta la temperatura local de la muestra en la superficie en contacto con la resistencia y diminuye la corriente que puede pasar por esa zona, disminuyendo a su vez la corriente que pasa en el conjunto del anillo.

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Supercooling an ionic liquid with pressure

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Ionic liquids consist only of anions and cations like conventional salts but they can be liquid down to unusually low temperatures, even below room temperature [1]. We investigate ion dynamics under pressure in the ionic liquid 1-butyl-1-methylpyrrolidinium bis[oxalate]borate (BMP-BOB) by conductivity relaxation measurements in the temperature range 123 – 300 K and varying pressures from 0.1 MPa up to 0.5 GPa. The BMP-BOB can be supercooled near room temperature by applying pressure, and here we analyse its influence on the relaxation times and on the spectral shape of the conductivity relaxation process, which show similarities with conventional glass formers like the existence of secondary processes [2-4]. The relaxation time of the primary relaxation τ_α strongly increases with applied pressure while that of a secondary relaxation is almost insensitive to pressure [3,5]. Thus, elevated pressure separates the secondary relaxation and makes possible the appearance of an excess wing on the high frequency flank of the primary relaxation. The spectral shape of the main relaxation broadens with increasing pressure or decreasing temperature, but is found to be the same when the relaxation time is fixed, independently of the particular pressure and temperature conditions, showing temperature-pressure superposition. The pressure dependence of the glass transition temperature and the isobaric fragility show also similarities with non-ionic glass-formers.

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NUEVOS DESARROLLOS EN EL CAMPO DE LOS MATERIALES CELULARES AVANZADOS

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Los materiales celulares, constituidos por una fase gaseosa dispersada en una o varias fases sólidas, han formado siempre parte del mundo que nos rodea. Estos materiales debido a razones técnicas, comerciales y medio ambientales están incrementando su presencia en muchos sectores industriales. Así por ejemplo, los materiales celulares metálicos (Fig.1a), considerados materiales prioritarios en el VII programa marco de investigación, constituyen una nueva vía para aligerar estructuras en el sector del transporte [1], los materiales microcelulares (Fig. 1b), desarrollados inicialmente en el MIT [2], y ahora en estudio en todo el mundo permiten ahorrar materias primas en prácticamente todos los sectores industriales, los materiales celulares nanoreforzados [3] (Fig.1c), parte del esfuerzo internacional en nanotecnología, constituyen un nuevo tipo de materiales con propiedades mejoradas, útiles en múltiples campos. En este trabajo resumimos brevemente las principales contribuciones de nuestro grupo de investigación en el desarrollo de los materiales previos. En el campo de los materiales celulares metálicos se describen las mejoras de las propiedades mediante la incorporación de refuerzos internos [4]. En el campo de las espumas microcelulares se describe el proceso de fabricación desarrollado en nuestro grupo de investigación [5], y se evalúa la reducción de peso de piezas estructurales, finalmente se analizan las extraordinarias mejoras que se pueden lograr mediante la introducción de nanoaditivos [6].

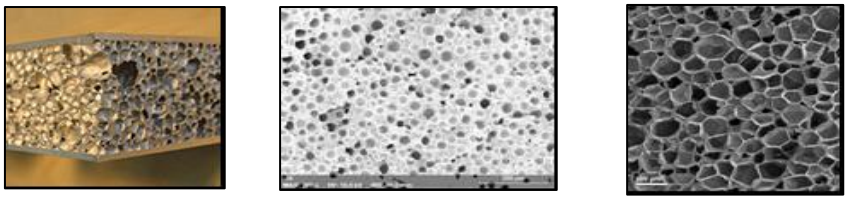

Figura 1. Ejemplo de fotografías de materiales celulares desarrollados en los últimos años. a) Material celular en base aluminio, b) material microcelular, c) material celular reforzado con nanoarcillas.

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Low-Temperature Nanotribology of Au and Pb using a Quartz Tunning-Fork

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Quartz Tunning-Fork (TF) has been in recent years successfully implemented in force detection schemes for scanning probe microscopy (SPM) applications. Here we report its use as a nanotribometer for measuring friction in atomic size areas. The idea behind such a friction detector, is to take advantage of the large Q-factor of a TF (Q_{air}~6000, Q_{vac}~20000 at room temperature) which in our set-up depends of the SPM tip-sample dissipative forces.
We have measured the Q-factor and the resonance frequency for various TFs. As a first step in the use of a TF as a nanotribometer, we studied the reactive forces that are associated with the combined local elastic properties of the sample and tip and calculated the damping rate associate with changes of the tip-sample distance.
Finally, we show the variation of the measured damping rate and local spring constants with tip-sample distances for Au and Pb. For the measurement we have used our TF-nanotribometer at different temperatures ranging from 1.5K to room temperature in high vacuum.

MAGNETIC AND TRANSPORT PROPERTIES OF MANGANITE HETEROSTRUCTURES

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Manganites present a great variety of phases as a function of composition and doping.

Those in the ferromagnetic phase are good candidates for building heterostructures with large tunneling magnetoresistance due to their high degree of spin polarization (manganites are half metals). We concentrate here in investigating theoretically an all-manganite trilayer with a thin antiferromagnetic and insulating film sandwiched between two ferromagnetic and metallic layers[1]. We study the nanoscale magnetic structure produced at the interfaces, and the conductance through the system. An example of such a heterostructure is $La_{2/3}Sr_{1/3}MnO_3$ / $Pr_{2/3}Ca_{1/3}MnO_3$ / $La_{2/3}Sr_{1/3}MnO_3$. The LSMO layers are in the ferromagnetic, metallic double exchange phase while PCMO is antiferromagnetic of the CE type and insulating in the bulk (see Fig. 1). The Hamiltonian involves double exchange, a Hubbard term to avoid double occupancy, electron-electron interaction, and an antiferromagnetic superexchange term that effectively includes the lattice contribution to the energy[2]. The model is solved self-consistently for different possible spin configurations at the interfaces. We find that the spin configuration of the intermediate layer depends on the relative magnetic orientation of the ferromagnetic electrodes and, consequently, the system presents magnetoresistance.

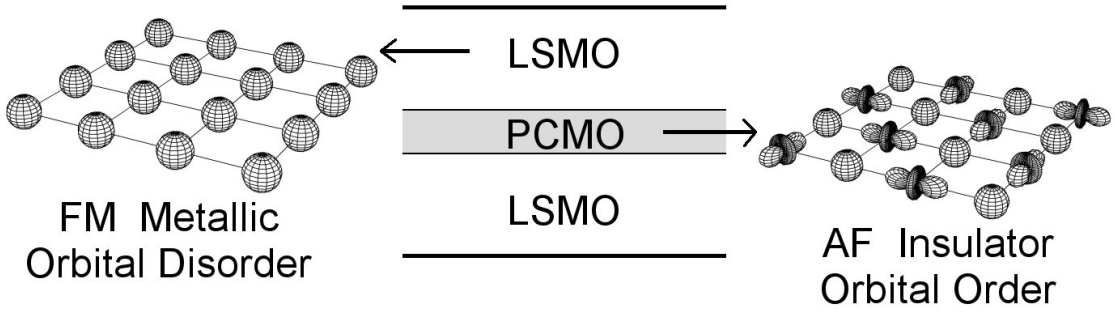

Figure 1: Heterostructure considered in this work. The PCMO intermediate level is CE antiferromagnetic and insulator, and presents orbital ordering which is absent in the metallic and ferromagnetic LSMO electrodes.

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ESTUDIO AB-INITIO AVANZADO DE PROPIEDADES ELECTRÓNICAS DE MATERIALES FOTOVOLTAICOS DE BANDA INTERMEDIA

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Los materiales de banda intermedia poseen una estructura electrónica que se caracteriza por la presencia de una estrecha banda de energía parcialmente ocupada situada en el seno de la banda prohibida de un semiconductor típico, separada totalmente de las bandas de valencia y de conducción de éste. Se ha calculado que la eficiencia termodinámica límite de una célula solar fotovoltaica construida con un material de banda intermedia es superior a la de las células convencionales de semiconductor [1]. Un método propuesto para obtener dichos materiales consiste en sustituir ciertos átomos de un semiconductor por metales de transición. Hasta la fecha se han propuestos diversos candidatos de este tipo a través de estudios de primeros principios basados en la Teoría del Funcional de la Densidad (DFT) [2]. Esta técnica se ha utilizado con éxito para el cálculo de diversas propiedades de compuestos. Sin embargo la aproximación llevada a cabo por el método DFT para la correlación electrónica es mejorable para sistemas que contienen electrones altamente localizados, como es el caso de las capas 3d de los metales de transición presentes en los materiales de banda intermedia. La inclusión de un término de correlación local de Hubbard U es una de las técnicas más utilizadas para corregir la descripción de la correlación electrónica. Sin embargo, con frecuencia el parámetro efectivo U es ajustado a posteriori para obtener una estructura electrónica lo más acorde con los resultados experimentales disponibles. En el caso de la predicción de materiales de banda intermedia no se dispone de datos experimentales, por lo que el valor de U se calcula desde primeros principios siguiendo un método de respuesta lineal [3]. Partiendo de cálculos DFT convencionales en los que se aplica un pequeño potencial adicional sobre los niveles electrónicos altamente correlacionados y viendo como varía su ocupación al relajarse la estructura electrónica se obtienen las derivadas correspondientes de las que se calcula el parámetro efectivo U. Siguiendo el método descrito se presentará la estructura electrónica obtenida para diversos candidatos a materiales de banda intermedia, señalando los compuestos más interesantes para tal fin y analizando el efecto de la correlación electrónica sobre estos novedosos materiales.

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INFLUENCE OF THE CATIONIC ORDERING IN THE DIELECTRIC PROPERTIES OF THE La_2MnCoO_6 PEROVSKITE

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Cation ordering in complex perovskite oxides with two or more cations mixed in the octahedrally coordinated B-site, is an interesting and extensively studied topic, that is known to strongly affect the structural and physical properties (magnetic, electric, dielectric) of these materials.[1]

For example, in the $La_2(CoMn)O_6$ perovskite, the transition metal ions can also be ordered to different extents using different thermal treatments (particularly annealing temperatures and cooling rates), resulting in very different magnetic behaviours, as extensively documented in the literature.[2,3]

In this work, we focus in the study of the relationship between the Mn/Co degree of ordering and the dielectric properties of the $La_2(CoMn)O_6$ perovskite. For this purpose, using different thermal treatments, we have prepared two samples of La_2MnCoO_6 differing in the degree of cation ordering and we have carried out their structural characterization by synchrotron X-ray powder diffraction (SXRPD).

According to the SXRPD and magnetic results, we have obtained a more ordered sample with a long-range cationic and valency ordered Co^{2+}:Mn^{4+} 1:1 and another more disordered sample consists in cation/valency disordered regions that coexist with cation/valency ordered Co^{2+}:Mn^{4+} regions. Very interestingly, from the dielectric point of view, the properties of these two samples are remarkably different. For example, at 300 K and $\nu = 10^4$ Hz, the dielectric constant, ε'_r, of the ordered sample is ~15 while it is much higher in the case of the less ordered material, $\varepsilon'_r \sim 10^5$.

We attribute this different behavior to the different electric and electronic characteristics arising from the different Co/Mn arrangements and valencies. The long-range ordering sample is electronic homogenous and show an intrinsic response in the whole range studied. Meanwhile, the more disordered sample is electronic inhomogenous, which gives rise to an "intrinsic" Maxwell-Wagner effect responsible for the very high ε'_r values exhibited at room temperature.

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Magnificent Sea Anemone-like Magnetic Silica Capsules reinforced with Carbon Nanotubes

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This work reports a suitable strategy for the production of hollow capsules composed of silica-coated carbon nanotubes (CNTs). This approach is based on the combination of the layer-by-layer self-assembly technique which drives CNTs onto the surface of polystyrene spheres (PS)[1] and a modified Stöber protocol for the CNTs silica coating.[2, 3] The silica coating of the individual CNTs renders CNTs-based capsules (after removing the polymeric core) very rigid and acquiring natural anemone-like morphology. (figure 1a, b). In a further improvement, previously synthesized Fe_3O_4 nanoparticles were first assembled onto the PS spheres, followed by the CNTs deposition and the silica coating, rendering the anemone-like hollow capsules magnetic. The magnetic response of these structures was evidenced by their electrophoretic deposition on a silicon substrate in the presence of an external magnetic field (Figure 1c). Such hollow structures with this unique morphology present a high surface area together with a magnetic response and the presence of CNTs which reinforces them, inspiring potential applications in various different fields.

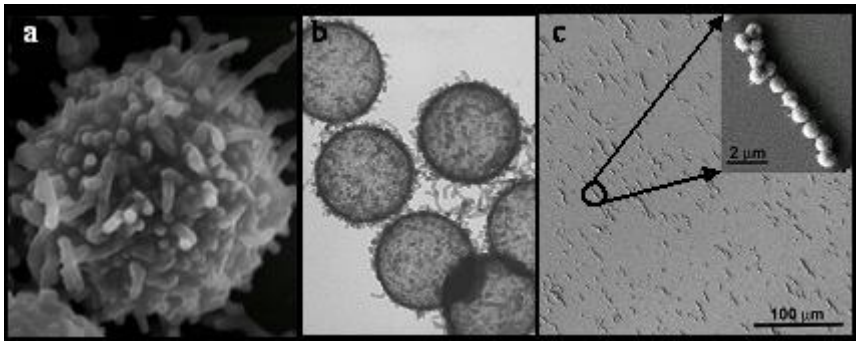

Figure 1. SEM (a,c) and TEM (b) images of the hollow capsules obtained. Alignment of magnetic hollow capsules under the presence of an external magnetic field (c).

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Nanopatterning by ion irradiation through ordered masks: structure modifications and magnetic properties

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Fabricating regular nano- and micro-patterns is of great interest due to their potential application in data storage, displays, biological sensors or photonic crystals. One way of patterning regular nano-structures is by irradiation-based lithography. Ion implantation and swift heavy ion irradiation induces very localized material transformation in matter, so-called ion tracks. Compared to e.g. e-beam or photo-lithography, ion tracks have the highest contrast between irradiated and non-irradiated regions. In addition swift heavy ions can directly transform matter in materials otherwise insensitive to electron or photon irradiation, they can induce high aspect ratio structures, and the inelastic interaction gives minute scattering.
Using these techniques with high resolution absorbing masks may thus have potential as a lithography technology for nanofabrication.
In this work on ion lithography we have used masks of commercial TEM grids and porous anodic alumina membranes (PAM) to harness the ions and transfer exact nano-patterns. Results on fabricating regular nano- and micro-structures on different materials (ZnO, TiO_2[1,2], FePt[3] and amorphous magnetic ribbons[4]) after ion irradiation through either TEM grids or PAM are presented.
ZnO and TiO_2 are oxide semiconductors with both suitable characteristics in electronic and optical applications. Ion implantation of magnetic ions confers ferromagnetic behavior to these non magnetic materials. In addition, the surface of crystalline TiO_2 has interesting properties as a photo-catalyst for some chemical reactions. Furthermore, large surface areas with highly active sites useful in photo-catalytic work can be fabricated.

FePt thin films and amorphous magnetic ribbons are different magnetic materials with direct applications in magnetic recording and sensing. The irradiation with heavy ions gives as a result the tuning of their magnetic properties.

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ENHANCED TUNNELING MAGNETORESISTANCE AT HIGH BIAS IN OXIDE MAGNETIC TUNNEL JUNCTIONS.

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Recently, large efforts have been put in using manganites as new electrodes to integrate in conventional magnetic tunnel junctions (MTJs), i.e., two ferromagnetic (FM) electrodes separated by a thin insulating barrier. Large tunneling magnetoresistance (TMR) has been observed at low temperatures in MTJs based on $La_{0.7}Sr_{0..3}MnO_3$ electrodes separated by a thin $SrTiO_3$ (STO) barrier [1]. However, all reported manganite based tunnel junctions show a rapid decrease of TMR with increasing both temperature and applied bias voltage, vanishing at temperatures well below the Curie temperature of the bulk electrodes [2-3]. Thus, the optimum value of TMR for each temperature is always restricted to low applied bias. We show the first experimental evidence of enhanced TMR with applied bias using $La_{0.3}Ca_{0.7}MnO_3$ (LC7MO) as an antiferromagnetic tunnel barrier sandwiched between two ferromagnetic $La_{0.7}Ca_{0.3}MnO_3$ (LC3MO) electrodes. This result outlines the importance of phase separation effects in modifying the ground state of tunneling barriers in MTJs [4].

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THE CHECKERBOARD PATTERN OF $Bi_{0.67}Sr_{0.33}MnO_3$ and $Bi_{0.5}Sr_{0.50}MnO_3$ DETERMINED BY RESONANT X-RAY SCATTERING AT THE Mn K EDGE

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Resonant X-ray scattering (RXS) at the Mn K-edge has been used to investigate the so-called charge-ordered (CO) phases in, respectively, $Bi_{0.67}Sr_{0.33}MnO_3$ and $Bi_{0.5}Sr_{0.50}MnO_3$ single-crystals [1,2]. A different ordered ground state and several ordering patterns have been previously proposed in $Bi_{0.67}Sr_{0.33}MnO_3$. Strong resonances were observed as the energy is tuned through the Mn K-edge for several weak superstructures of the CO phase. The energy, azimuthal and polarization dependencies of the resonant intensity have been measured for several weak superstructure (h00), (0k0) and forbidden (h/200), (0k/20) reflections with h, k odd. Additional (hk0) and (hk/20) with k odd have also been studied. The experimental results point out to a structural transition at the charge-ordering temperature (T_{CO}) that stabilizes an ordering of two non-equivalent Mn atoms in a checkerboard pattern for both x=0.33 and x=0.50 compounds. One of the atoms is anisotropic, a tetragonal distorted oxygen octahedron and the other one is isotropic, a nearly regular oxygen octahedron. The distinction of these two Mn sites is accompanied by displacements of both, isotropic and anisotropic Mn atoms. These results indicates that the checkerboard pattern is strongly stable and extends into doping concentrations x <0.5. Intermediate valence states lower than 3.5 according to fractional charge segregation were deduced for the two non-equivalent Mn atoms, i.e. $Mn^{3.30+}$ and $Mn^{3.44+}$. Consequently, the observed ordering in $Bi_{0.67}Sr_{0.33}MnO_3$ does not match with a Mn^{3+}/Mn^{4+} order, and we have established that the charge on the Mn atom is always lower than 3.5 [2]. We conclude that the checkerboard ordering of two distinct types of Mn octahedra with charge disproportionation markedly smaller than one electron (so-called CO) is a rather common feature in Bi manganites, even for compositions x far from 0.5.

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Magnetite Nanoparticles as Nanogenerators: the Influence of Particle Size and Domain Structure on Electromagnetic Absorption.

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Every one of the existing diagnostic/therapeutic techniques based on nanoparticles (NPs) requires the optimization of a specific chemical or physical property of the materials, depending on the specific function played by the NPs in that therapy (e.g., vector, porous receptacle, heating agent, magnetic moment carrier, etc…). Sometimes the particle function is activated using an external agent (magnetic fields, light, radiation, etc…) that interacts with the NPs. Magnetic hyperthermia (MH) can be defined as the rise of temperature that can be accomplished remotely by means of external alternating magnetic field acting on magnetic NPs at the targeted location. This electromagnetic radiation used by MH belongs to a frequency region where the heating effects on living tissues are negligible. The underlying physical mechanisms of MH are related to the energy dissipation when a ferromagnetic material is placed on an external alternating magnetic field. Different effects must be considered for power losses: a) magnetic losses through domain wall displacements (in multi-domain particles), Néel relaxation (in single domain particles); and b) energy loss from mechanical rotation of the particles, acting against viscous forces of the liquid medium (Brownian losses). The dominant process will depend on the specific particles used and the applied frequency range. The heating power of magnetic nanoparticles is given by the Specific Absorption Rate

$$SAR = \frac{C_S}{m_{Fe}}\left(m_{FF} \frac{\Delta T}{\Delta t} \right)$$

in W/kg, as obtained from the heating curves of the material. In this work we analyze the effect of particle size on SAR values in a series of Fe_3O_4 NPs with increasing mean particle size from 3 to 30 nm, and good control of size dispersion, especially in the small ones.

Experiments of power absorption as a function of particle size revealed the existence of a sharp increase in SAR values near the single- to multi-domain structure, irrespective of magnetization values. The largest value obtained was 130 W/g, corresponding to a mixture of 17 and 25 nm particle populations. We discuss the correlation of this behavior with magnetic parameters such as saturation magnetization, magnetic anisotropy and coercivity values.

THE SELF-ASSEMBLY PROCESS OF COBALT NANOPARTICLES CRYSTAL SUPERLATTICES

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Colloidal dispersed nanoparticles (NP) self assemble into complex structures when segregated from the solvent either by evaporation or precipitation. Thus, different micro and macroscopic structures like opals, fractals, anisotropic structures and others formed by nanoparticles are observed as a result of the balance between electrostatic forces, surface tension, entropy, topography, substrate affinity, among others, and evidently, the size, shape and concentration of the particles. In addition, in ferromagnetic materials, the dipolar magnetic interactions, add a new term in the interactions balance. In this complex context, the study of the self-assembly processes of cobalt nanoparticles onto HOPG (high oriented pyrolytic graphite) substrates gives the opportunity to study down to the minutest detail the balance between NP-NP and NP-substrate interactions in the particular case where both particles and substrate are highly hydrophobic. The micro and macro self-assembly structures resulted from the evaporation of a solution of cobalt nanoparticles onto a HOPG substrate give a conceptual framework to study the magnetic properties of both the material at the nanometric level and at the macroscopic level on the obtained structures. This is relevant, not only to built up super-structures for specific applications, like compact monolayers for magnetic recording media, but also to elucidate the behaviour of nanoparticles in liquid media, often out of equilibrium, aiming to disperse them in biological media.

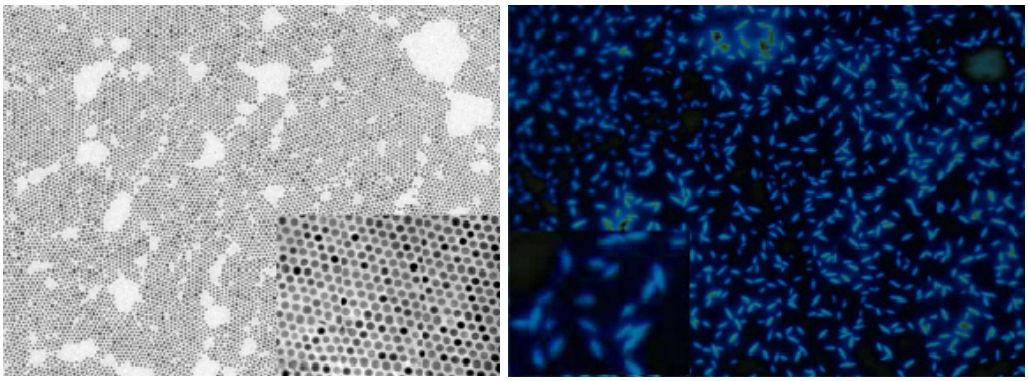

Figure 1. Left) TEM image of 10 nm cobalt nanoparticles. Rigth) Optical Image of self-assembly structures (5-9μm) of cobalt nanoparticles after its deposition onto HOPG substrate.

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Synthesis of Copper clusters in aqueous solution

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Copper nanoparticles have found applications in a variety of areas, including catalysis, electronics, photonics and thermal conducting. Although they had been obtained by different procedures, it has been found very difficult to keep Cu nanoparticles at zero oxidation state, because of the easy and fast surface oxidation. Taking into account that in small nanoparticles most of atoms are at the surface, the whole of nanosized copper aggregate will be oxidized as soon as it is in contact with oxygen, unless it has an efficient protecting layer. Therefore, the goal of our group is to achieve stables Cu^{o} nanosized aggregates, because it is of great interest for fundamental knowledge and practical applications. In this work we have used an electrochemical procedure, previously developed by our group, to produce small copper clusters (aggregates of a few number of atoms) in aqueous solution. Characterization of copper clusters and their main properties were studied by several techniques, like UV-visible absorption spectroscopy, high-resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM) and fluorescence spectroscopy.

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Propiedades magnéticas del ternario $AgCrSe_2$.

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Se realizaron medidas de susceptibilidad magnética DC y resonancia paramagnética electrónica en el rango de temperatura 2.2 K < T < 281 K para el $AgCrSe_2$ estas nos permitieron precisar las diferentes fases magnéticas y las transiciones magnéticas. De estas se obtuvo que, el $AgCrSe_2$ presenta un comportamiento paramagnético para $T \geq 105$ K, de igual forma presenta una fase ferromagnética en el rango de 67 K < T <94 K, una fase antiferromagnética entre 37 K < T <67 K y cabe destacar un tercer cambio de fase aproximadamente a 94 K atribuible a una transición ferromagnética-vidrio de espin. De igual forma con la técnica de EPR se realizo el estudio de cambio del campo de resonancia en función del ángulo de incidencia del campo magnético a temperatura constante, lo que evidenció una anisotrópia de tipo C1 consistente con una fase ferromagnética a una temperatura de 77 K.

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Magnetic depth profile of $La_{0.7}Ca_{0.3}MnO_3/YBa_2Cu_3O_7/La_{0.7}Ca_{0.3}MnO_3$ trilayers

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In recent years there has been a great interest in heterostructures of highly spin-polarized ferromagnetic $La_{0.7}Ca_{0.3}MnO_3$ (LCMO) and high-T_C superconducting $YBa_2Cu_3O_7$ (YBCO). New physical phenomena due to the complex atomic arrangement like long range proximity effect [1], induced ferromagnetism in the YBCO [2], etc., have been observed. In our experiment polarized neutron reflectometry (PNR), X ray magnetic circular dichroism (XMCD) and X-ray magnetic reflectivity (XRMS) measurements were used to investigate the origin of these phenomena through the analysis of the magnetization profile in LCMO/YBCO/LCMO trilayers epitaxially grown on (100) $SrTiO_3$. Covalent bond formation between Cu and Mn ions is suggested to be the origin of a magnetic moment rearrangement in the interface ions [3]. We performed XMCD and XRMS measurements at the Cu L_3-edge showing a surprisingly strong ferromagnetic signal probably originated at the F/S interface where the CuO_2 layers are subjected to epitaxial strain and can be strongly affected by orbital reconstruction. PNR experiments show the different magnetization of the two LCMO layers due to different strain effect from the YBCO and the STO substrate. In addition a spin-flip scattering signal indicates that the magnetization reverses by coherent rotation which means that the easy-axis is tilted away from the usual (100) direction. This signal appears at fields where preliminary transport measurements showed an unconventional large magnetoresistance peak related to the antiparallel alignment of the ferromagnetic layers [4].

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CARACTERIZACIÓN DE PROPIEDADES ELECTRONICAS Y OPTICAS DE MATERIALES TIPO CALCOGENURO PARA SU USO COMO CÉLULAS SOLARES DE ALTA EFICIENCIA

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En este trabajo se realiza una predicción y caracterización teórica de nuevos materiales fotovoltaicos de alta eficiencia. Estos materiales serían capaces de absorber de forma más eficiente la luz solar que los semiconductores utilizados habitualmente en las células solares[1]. En publicaciones previas del grupo se propusieron materiales derivados de semiconductores III-V donde uno de los átomos del semiconductor se sustituye por un metal de transición [2]. En este trabajo, mediante el uso de la teoría del funcional de la densidad (DFT), se estudiarán aleaciones de materiales conocidos tipo calcogenuro derivados de estructuras calcopiritas [3] o espinelas y sustituidos con metales de transición. Algunos integrantes de estas familias de compuestos se utilizan hoy en día ampliamente en energía solar, crecidas como células solares de capas delgadas o capas ventana para éstas. Sus estructuras junto con las sustituciones de átomos realizadas a unas diluciones concretas, dotan a estos sistemas de una estructura electrónica que presenta una banda intermedia dentro de la banda prohibida del semiconductor base. Un material con estas características se podría usar como célula solar de alta eficiencia gracias a la absorción de fotones de baja energía (menor que la banda prohibida), que permitirían un aprovechamiento mayor del espectro solar que el que realizan las células solares con una sola región prohibida de energía [1]. Existirán así tres tipos de transiciones, la usual entre la banda de valencia y la de conducción y dos excitaciones más ambas de baja energía, una de la banda de valencia a la intermedia y otra de la intermedia a la banda de conducción.

Este trabajo mediante el uso de la DFT en estos sistemas, muestra su estructura electrónica, su estabilidad termodinámica y estudios opto-electrónicos (coeficientes de absorción, transmitancias y coeficientes de refracción). De estos cálculos optoelectrónicos se deduce claramente que los fotones de baja energía debidos a las transiciones que implican la banda intermedia favorecen el incremento de la absorción total en el sistema. Se mostrará además como estos cálculos optoelectrónicos han sido refrendados por resultados experimentales.

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CHARGE ORDERING AND DIELECTRIC PROPERTIES IN THE NEAR HALF-DOPED Pr-Na-Mn PEROVSKITE

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The electronic phenomenon of charge ordering (CO) in transition metal oxides has gained renewed attention in the last years in connection with the interesting new properties and phenomenologies displayed by compounds belonging to this group, such as colossal magnetoresistance (CMR) in CO manganese perovskites [1]. More recently, theoretical studies by Efremov et al.[2] have predicted a new state near CO half-doped manganites that can lead to a non-centrosymmetric charge distribution and to a net polarization, giving thus rise to a new electronic ferroelectric (FE) state. With the aim of exploring further this possibility we have focused in the half-doped manganite $Pr_{0.75}Na_{0.25}MnO_3$, a CO compound with T_{CO} ~ 220 K, that is a Mott insulator close to an edge between a localized-delocalized state [3]. We have prepared the $Pr_{0.75}Na_{0.25}MnO_3$ compound by a solid state process, and carried out its structural characterization by synchrotron X-ray powder diffraction (SXRPD) at room temperature and at 150 K ($T< T_{CO}$). In the CO state, the SXRPD data can be refined both on the basis of the site-centred model and the bond-centred model proposed for half-doped manganites, without a clear advantage of one model over the other. Evermore, it is very plausible that the real situation is intermediate between these two extremes, as the obtained results seem to indicate. From the dielectric point of view, at the CO temperature shows a maximum in the dielectric constant whose origin is intrinsic, and can not be attributed to the presence of extrinsic factors. We relate this dielectric behaviour to the formation of polar entities at the temperature of charge condensation, due to an asymmetric charge distribution –intermediate between site-centred and bond-centred– of the type described by Efremov et al. for near half-doped manganites [**¡Error! Marcador no definido.**].

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MICROMAGNETIC MODELLING AND MFM IMAGES OF MAGNETIC STRUCTURES IN NI DOTS.

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Variable Field Magnetic Force Microscopy (VF-MFM) is a powerful tool which allows to study *in situ* magnetization processes, following the evolution of magnetic structures as a function of applied field. This is specially relevant in the magnetization studies in artificial magnetic nanostructures such as magnetic dots. The geometry of these structures offers an additional possibility to control their properties through the magnetostatic field determined by the shape of nanoelements. In the present paper we study magnetization processes in array of spherical and triangular magnetic dots of, approximately, 500nm lateral sizes and 50 nm thickness. Several sets of nanodots were prepared by means of electron lithography in Ni(111) thin films[1]. The MFM image (see. Fig1lft) shows the magnetic domains in each dot, mainly determined by minimization of magnetostatic energy for particular geometry. The magnetic structures suggest the presence of magnetic vortex at the center of each nanoelement. The VF-MFM images show that the external field produces the vortex motion in the direction perpendicular to the applied field. At the same field could also be responsible for the vortex motion, specially in the conditions of small distances between the tip and the sample. To fully understand the MFM images, we have performed micromagnetic simulations using the finite-element package Magpar [2]. We have considered isolated dots and square arrays of 2x2 and 3x3 dots. Fig1(right) shows that the simulated image at the remanence is very similar to that of the observed by MFM. We have modeled the field-dependent magnetic structures for both in-plane and out-plane applied field directions. Fig2 represents a typical simulated hysteresis cycle for a triangular Ni dot with in-plane applied field. We have observed that the demagnetization process involves the formation of the vortex at the center of the dots and a pair of the domain walls. The first reversible part of the hysteresis cycle correspond to the formation of two domains in the dot, and the consequent vortex formation which coincides with the irreversible jump. During the second reversible part the vortex moves in the direction, perpendicular to the applied field towards one of the triangle corners and the domain walls disappear at two opposite corners. Finally, the last small irreversible jump coincides with that of the disappearance of the vortex at the triangle corner. The perpendicular field hysteresis cycle is characterized by the presence of the Bloch-type domain wall across the thickness. The calculation of the hysteresis cycles confirms that small magnetic field produced by the magnetic tip is sufficient to move the magnetic vortex

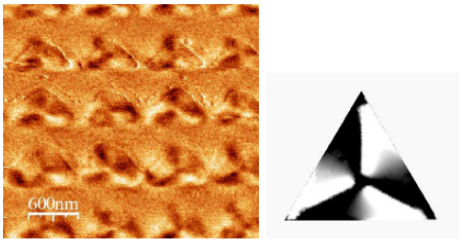

Fig. 1. MFM images (left figure) and the results of the micromagnetic modelling (right figure) of magnetic structures in triangular Ni dots.

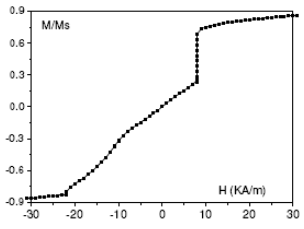

Fig. 2. Simulated hysteresis cycle in triangular Ni dots with in-plane applied field.

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NUCLEATION AND GROWTH OF TFA-YBCO FILMS FOR ALL CHEMICAL YBCO/CeO_2/$La_2Zr_2O_7$/Ni RABiTS COATED CONDUCTORS

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The development of simple architectures is of crucial importance for the achievement of low-cost $YBa_2Cu_3O_7$-based coated conductors. Fluorite CeO_2 is usually proposed as cap layer for $YBa_2Cu_3O_7$ (YBCO) deposition in most of these architectures and $La_2Zr_2O_7$ (LZO) as intermediate layer for protecting the metallic NiW RABiT substrate from oxidation. LZO is a stable pyrochlore structure with an excellent lattice matching with CeO_2 and it can be successfully grown by chemical solution deposition (CSD), opening then the possibility of a simple all-chemical architecture. However, there is a lack of knowledge on the mechanisms involving nucleation and growth of YBCO on CeO_2 top. In particular, it is known that one of the main concerns involves the high reactivity of CeO_2 with YBCO leading to the undesired formation of $BaCeO_3$. This should require a low temperature process for YBCO but the, uncontrolled non c-axis nucleation and low epitaxiality of YBCO are promoted. On the other hand, oxidation of the underlying metallic substrate should be also minimized by lowering the processing temperature. The competition between these different phenomena has been studied in the present work for YBCO films grown by the trifluoroacetates route (TFA) onto CSD-$Ce_{1-x}Gd_xO_2$ /CSD-$La_2Zr_2O_7$ on NiW RABiT substrates. Results onto CeO_2 buffered YSZ single crystals have been also used for comparison. The kinetics of YBCO nucleation has been analyzed by following the evolution of the different intermediate phases by XRD analysis. The influence of several thermal profiles has been investigated. In particular, a double step process is proposed. First, a low temperature initial stage is performed to nucleate YBCO while minimizing reactivity with CeO_2 and NiW oxidation. Second, a high temperature treatment is used to promote high YBCO crystallinity, reducing its porosity and enhancing their superconducting properties.

A successful combination of the two step process lead to an enhanced control of nucleation and growth characteristic and hence to improved superconducting properties.

This work has been supported by European Union and Spanish national funds (Hiperchem project, CONSOLIDER Nanoscaled, NESPA, MAT2005-02047 and CSIC-PIE).

GUIDED SELF-ORGANIZATION OF OXIDE NANOISLAND THROUGH SUBSTRATE MODIFICATION

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New multifunctional materials are presently being developed through bottom-up cost-efficient approaches such as self-assembly and self-organization of nanostructures. The generation of oxide nanostructured templates sets a promising path towards their applications in magnetic, ferroelectric or superconducting devices. Besides, the need of low cost and scalable methodologies has induced the development of innovative routes based on chemical solution deposition (CSD) techniques. On the other hand, complex tuning of the self-assembled processes promotes the use of new ways of intentionally directing and assisting the growth of these nanostructures.

In this work we present and confirm that the mechanical modification of the substrate by means of Nanoindentation and Focused Ion Beam are two differentiated tools for assisted self-organization of $Ce_{0.9}Gd_{0.1}O_{2-y}$ nanoislands. The application of ultra low loads (concerning Nanoindentation) and low current dosages (as regards FIB) on our single crystal perovskite substrate has derived on the localized and controlled alteration of the substrates´ elastic strain fields. CSD of the oxide precursor solution and subsequent thermal treatment at high temperatures has followed giving rise to assisted self-organization. Indeed, nucleation of nanoislands is undoubtedly affected by the presence of indented sites. In the case of $SrTiO_3$ substrate irregular-shaped nanodots preferably locate at the indented sites while in the indented $LaAlO_3$ substrate regular elongated nanoislands´ population and localization is greatly determined by the presence of indentations. We believe that the compressive or tensile nature of the strain between substrate and islands lie at the origin of the different nanostructures.

We acknowledge the financial support from MEC (MAT2005-02047, NAN2004-09133-C03-01, MAT2006-26543-E;FPU), Generalitat de Catalunya (Pla de Recerca SGR-0029 and CeRMAE), CSIC(PIF-CANNAMUS) and EU (HIPERCHEM, NESPA)

TRIGGERED OPTICAL-PARAMETRIC-OSCILLATOR PROCESSES IN SEMICONDUCTOR MICROCAVITIES

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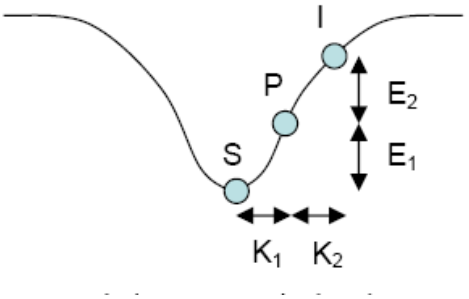
Coupled modes of semiconductor microcavities, known as polaritons, are expected to behave as bosons in the limit of low carrier densities. When this bosonic character is dominant, polariton-polariton scattering may become stimulated by final-state occupation effects and give rise to condensation, for occupancies in excess of unity. Under cw conditions, the scattering processes become self stimulated for powersproviding carrier densities sufficient to build up a final state population close to unity, and can be described as an optical parametric oscillator (OPO). As shown in Fig. 1, for pumping above a threshold, at a finite angle, a coherent signal (S) appears at the bottom of the polariton dispersion while an idler emission (I) appears at higher energies than that of the pump (P), satisfying the momentum and energy conservation rules. In this work we show that it is possible to initialize the OPO process with a pulsed probe (2 ps long) set at resonance in the polariton dispersion at the idler energy; we name this new process as a TOPO (triggered-OPO). The probe pulse provides a sufficient number of idler polaritons to activate polariton-polariton scattering from the pump to the I and S states. The OPO conditions, only initialized by the probe pulse, are granted by the reservoir of polaritons in the P state, and the final state stimulation of the pair scattering process is provided by the self sustained occupancy of the S and I states. The studied microcavity (Rabi splitting ≈ 4.4 meV), is composed by a AlAs λ/2 cavity with Bragg mirrors of Al0.1Ga0.9As/AlAs. Three GaAs quantum wells are embedded at the antinode position in the cavity, providing the excitons to form the polaritons modes. Energy and time evolutions of the photoluminescence are analyzed by a streak camera coupled to a spectrograph. The lifetime of the signal emission is orders of magnitude longer than that of the probe pulse, demonstrating that the pulse is only necessary to trigger the process (see Fig.2). The dependence of the signal emission on the probe and the pump powers shows the crucial role of the renormalization of the polariton dispersion and helps to understand the non-linear optical properties of semiconductor microcavities.



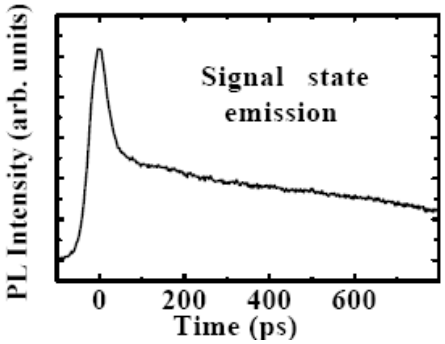


Figure 1. Polaritons are excited at the pump state with energy EP and planar momentum KP. Pair
scattering process will scatter polaritons at the signal (S) and idler (I) states, provided that the energy and momentum conservation rules can be satisfied (2EP = ES + EI; 2KP = KS + KI).
Figure 2. Signal emission from the bottom of the polariton dispersion curve. When the probe pulse
(2 ps long) excites the I state, polaritons are scattered from the P to the S and I states. Once activated, the OPO process is self sustained and lasts for hundreds of picoseconds.

S-CAPPED Au NANOPARTICLES: INFLUENCE OF THE S-Au BOND STRENGTH ON THE MAGNETIC BEHAVIOUR

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The magnetic behaviour observed in nanoparticles and capped thin films with metals like Pt1, Au2,... is one open question to be resolved. In this work we will show that thioethers can induce the damping of the surface plasmon resonance and the appearance of a ferromagnetic-like behaviour. We have synthesized two different thioether ligands, so the influence of the Au-S bond strength on both phenomena had been studied. It will be shown that, although both ligands can induce a completely damping of the Plasmon band, only with one ligand corresponding to the stronger S-Au bond is observed the appearance of a ferromagnetic-like order. This is an indication of the extreme sensitivity of the magnetism on the strength of the charge transfer at the S-Au bond.

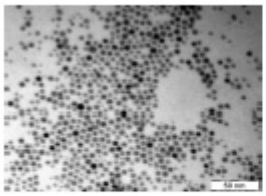

Figure 1. TEM images of thioether-capped Au nanoparticles

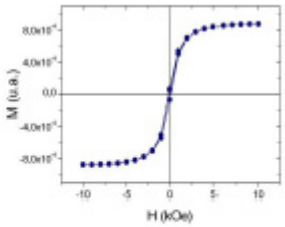

Figure 2. Magnetization curve of thioether-capped Au nanoparticles

Acknowledgements: We want to acknowledge the financial support of the MEC, Spain (projects No. MAT2005-07554-C02-01, NAN2004-09133-C03-02, NAN2004-09195-C04-01 and NanoBioMed CONSOLIDER-INGENIO 2010) and the European Union (Contract No.037465-FLUOROMAG, EU-FP6 Framework Programme LIFESCIHEALTH-6), as well as, theXunta de Galicia, Spain (Grant No. PGDIT03PXIC20907PN). RL thanks the MEC FPU grant.

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Influence of Poly (N-vinylpyrrolidone) in the electrochemical synthesis of gold clusters.

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Gold and other noble metal clusters have attracted much attention due to their completely amazing properties, and their promising applications in different branches of science [1]. We will report the synthesis and characterization of small gold clusters by a simple electrochemical technique previously described by Reetz for other metal particles [2] and then studied in our group [3,4]. Gold clusters were synthesized in aprotic solvent by the dissolution of a metallic anode. Poly (N-vinylpyrrolidone) (PVP) was chosen as the stabilizer for these clusters. The use of the PVP is due to two factors. On the one hand, this compound is used as a conductive substance that is necessary for the synthesis. And, secondly, PVP is biocompatible. Furthermore, the clusters protected with PVP are easily transferred to aqueous solutions for biological applications [5]. Several techniques are employed to characterize the clusters, like UV-vis spectroscopy, TEM and mass spectrometry, among other techniques.

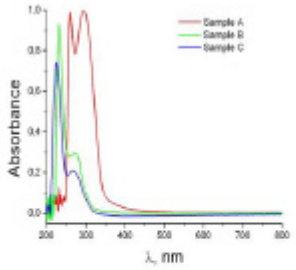

Figure 1. UV – vis Au cluster characterization: absorption spectra at different concentrations of PVP in several electrochemical synthesis of Au clusters.

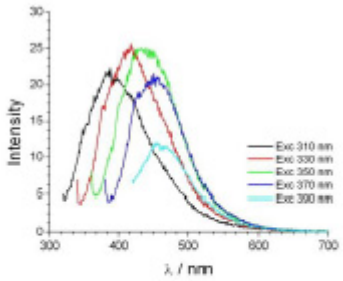

Figure 2. Fluorescent properties of the electrochemically synthesized Au clusters

Acknowledgements: We want to acknowledge the financial support of the MEC, Spain (projects No. MAT2005-07554-C02-01, NAN2004-09133-C03-02, NAN2004-09195-C04-01 and NanoBioMed CONSOLIDER-INGENIO 2010) and the European Union (Contract No. 037465-FLUOROMAG, EU-FP6 Framework Programme LIFESCIHEALTH-6). Thanks the MEC FPU grant.

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Simultaneous Two-Dimensional Mapping of Structural and Chemical Information at Atomic Resolution in $Bi_{0.5}Sr_{0.50}MnO_3$

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The simultaneous measurement of structural and chemical information at the atomic scale provides fundamental insights into the connection between form and function in materials science and nanotechnology [1,2].

We demonstrate structural and chemical mapping in $Bi_{0.5}Sr_{0.5}MnO_3$ [1] using an aberration corrected scanning transmission electron microscope. We consider the use of a high resolution scanning transmission electron microscope (STEM) which, rather than illuminating a specimen with a plane wave, scans a small Ångström-sized probe across the sample. At each probe position, electrons which have been scattered through large angles, usually by interaction with a phonon (Z-contrast imaging), can be recorded to obtain a projection of the atomic structure. Electron energy-loss (EEL) spectra can be simultaneously recorded to provide chemical identification and explore local bonding and other electronic properties. Two-dimensional mapping is thus made possible by an adapted method for fast acquisition of electron energy-loss spectra. The experimental data are supported by simulations. The specimen used in the present study, $Bi_{0.5}Sr_{0.5}MnO_3$, is one of the few materials that shows ‘‘charge ordering’’ at room temperature.

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Study of the electronic structure of $Sr_2Co_2O_5$

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Ab initio calculations and magnetic measurements were performed in $Sr_2Co_2O_5$, a strontium cobaltite that crystallizes in a brownmillerite-type structure.

The electronic structure calculations were carried out by means of a full-potential augmented plane wave plus local orbital (FP-APW+lo) method with the software WIEN2k. The magnetic measurements were performed on polycrystalline samples using a SQUID magnetometer (Quantum Design).

The electronic structure of the material and their magnetic properties were analyzed at high and low temperatures. Calculations were carried out with the structural data obtained by neutron powder diffraction at various temperatures. These measurements cannot state which space group the material crystallizes in, two space groups are possible according to the measurements. However, total energy calculations conclude that the space group Ima2 is most stable than the other possible one (Pnma).

$Sr_2Co_2O_5$ is a G-type antiferromagnet with a very high Neel temperature, the strong AF coupling between the high-spin Co^{3+} ions accounting for it. The possibility of spin state transitions in this Co^{3+} compound was explored by studying different spin state configurations in various magnetic orderings, being always the high-spin state favored and the G-type antiferromagnetic ordering being always most stable.

The magnetic measurements find a peak in the zero-field-cooling magnetization curves at about 170 K. This is not related to a spin-state transition, as our calculations predict and also the neutron diffraction data can confirm. It could be due to a weak ferromagnetism with some component of the moment along a hard axis. However, the Ima2 space group does not allow for such a component of the magnetic moment to occur. Hence, the only possible explanation for the peak is the segregation of ferromagnetic clusters that would give rise to a cluster-glass behavior (leading to a freezing temperature peak in the zero-field-cooling curves) formed by a ferromagnetic cubic perovskite phase segregated in the antiferromagnetic matrix of brownmillerite- $Sr_2Co_2O_5$. $SrCoO_{3-\delta}$ is found to be ferromagnetic for large values of δ and this would be consistent with our findings.

Monte Carlo study of the role played by the magnetic field on the magnetocaloric properties of a fine magnetic particle system

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We present in this work a Monte Carlo study of the influence of the applied magnetic field on the magnetocaloric properties of a magnetic nanoparticle system. The variation of the entropy change was obtained by means of the zero field cooling curves under different values of the applied magnetic field. It is observed that the entropy curves behave in a different fashion at low and high values of the magnetic field. At low field values, the peak of the entropy curves only slightly shifts to higher temperatures with increasing field. For larger fields, the peak rapidly shifts to higher temperatures, while the overall shape of the curve broadens over a wide temperature range. The change between both behaviors corresponds to a particular magnetic field, h*, at which the $\partial M/\partial T$ value shows a maximum. We observe too that the blocking temperature as a function of the magnetic field changes from a bell-like shape to a monotonically de-creasing function, resembling what is found experimentally for intermediate values of the sample concentration.

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Magnetic applications of small silver clusters in biomedicine.

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The ground-state properties of small silver clusters, Ag_n ($2 \leq n \leq 24$), have been studied using a linear combination of atomic Gaussian-type orbitals within the density functional theory. The results show that the Ag_{13} clusters, due to their noticeable magnetic moment and their considerable highest occupied-lowest unoccupied molecular orbital gap, are a promising candidate for the magnetic applications of nanoparticles. In particular, our study suggests that the silver nanoclusters made out of Ag_{13} clusters, as building blocks, are suitable for possible future applications in biomedicine, since they could improve some present-day difficulties of magnetic nanoparticles like toxicity and opsonization.

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Magnetostrictive-like behaviour in eight-atom gold clusters

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We have performed ab initio calculations on the lowest energy structure of eight-atom gold clusters, a tetracapped square with D_{4h} symmetry, locking it to several total magnetic moments. We have found that for nonzero values of the total magnetic moment, the D_{4h} symmetry is not stable. We have also found that for a fixed nonzero total magnetic moment, the stable structure is a distortion of the tetracapped square, along the square's diagonals. This structure has a D_{2h} symmetry. The rest of possible structures for this cluster have been calculated as well, and no magnetism-dependent deformation was found, except for the tetracapped tetrahedron with symmetry T_d , which is unstable for nonzero total magnetic moment. In this case, the favored structure is a bicapped octahedron with symmetry D_{2d} . The structural change due to magnetic constraints is relevant since the surface of gold clusters has shown a catalytic behavior highly dependent on the structure.