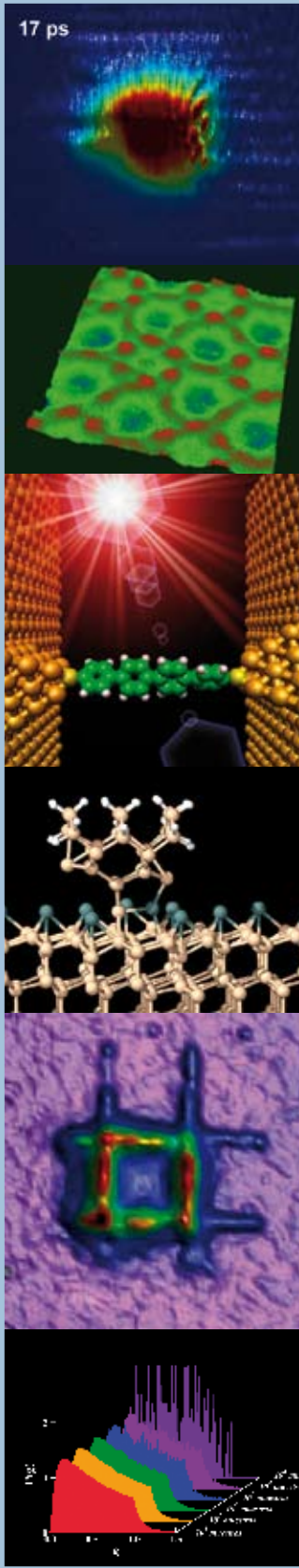




Research Report

2007 -2008



INSTITUTO NICOLÁS CABRERA

**Instituto Universitario
de Ciencia de Materiales
“Nicolás Cabrera”**



Research Report

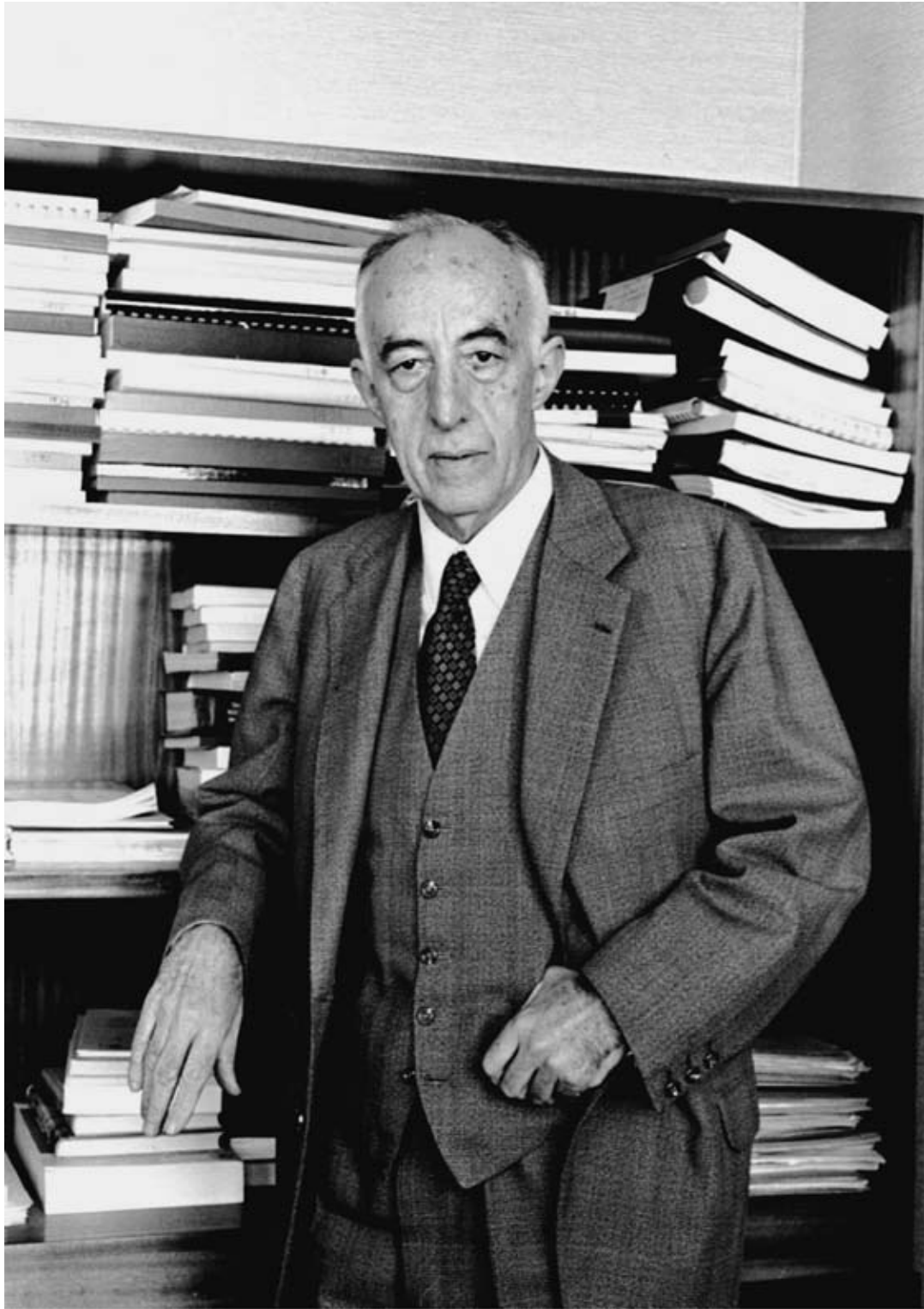
2007 -2008

Edited by: José Gabriel Rodrigo

<http://www.nicolascabrera.es/>

■ INDEX

Presentation.....	9
Members	11
Research groups & reports	13
Activities	85
List of Publications	109



Nicolás Cabrera was born in Madrid in 1913. His father, Blas Cabrera, made pioneering experiments in magnetism and was the leading Spanish physicist of the first third of the 20th century. After the Spanish Civil War, the Cabrerias went into exile to Paris and Nicolás eventually established in Bristol, where he wrote classic papers with N. F. Mott, W. K. Burton, and F. C. Frank on the theories of oxidation and crystal growth. In 1952 he joined the Physics Department at the University of Virginia where he was Head for many years and led a vigorous research program which, among other achievements, laid the foundations of the theory of atom surface scattering. In 1969 Nicolás Cabrera returned to Spain to provide leadership in the creation of the Physics Department at the newly founded Universidad Autónoma de Madrid. He passed away in 1989. Don Nicolás is remembered by his colleagues and disciples as an outstanding scientist and a true gentleman.

INC Research Report 2007-2008

Forewords and Presentation

This research report presents a summary of the experimental and theoretical research work developed at the Instituto de Ciencia de Materiales Nicolás Cabrera of the Universidad Autónoma de Madrid during the period 2007-2008. Our Institute is heir to the tradition of academic and scientific excellence pioneered by Prof. Cabrera (1913-1989) who played a decisive role in the creation of a world-class Physics Department at the Universidad Autónoma de Madrid.

Currently, our Institute comprises more than 100 professors and post-doctoral researchers in the field of Materials Science supported by approximately the same number of graduate students, thus involving more than 200 scientists. All aspects of the research on Materials Science are covered including a pioneer group in Biophysics. This research work is complemented with the participation of the members of our Institute in up to 6 postgraduate Masters related to Materials Science, Nanotechnology and Biophysics. The reports presented below are a valuable piece of evidence of the excellence of the research developed in our Institute.

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“Nicolas Cabrera” Material Science Institute Research Groups & Reports

• Transport and Superconductivity in Mesoscopic Systems	15
• Laboratory of Coatings and Nanostructures: Magnetic Coatings and Nanostructures Group	17
• Laboratory of Coatings and Nanostructures: Oxide Nanostructures Group	21
• Ab Initio Studies of Lanthanides in Solid-state Lighting and of Actinides in Advanced Nuclear Energy Systems.	25
• Biophysics of Neuronal Systems	29
• Biodynamics and Computational Biology.	30
• Electron Transport and Dynamics in Magnetic and Superconducting Nanostructures - MAGNETRANS	32
• Semiconductor Group (SEMICUAM).....	35
• Ferroelectric Materials & Phase Transitions	38
• Materials of Interest in Renewable Energy Research Group (MIRE).....	41
• Functional Nanostructures.....	43
• Group of Laser Spectroscopy	45
• Non-Linear Optics and Optical Waveguides Group	47
• MoLE (Moving Light and Electrons)	48
• Paramagnetic Resonance Spectroscopy of Solids	52
• Electronic Properties of Novel Materials (EPNM) Group	54
• Scanning Probe Microscopy in Ultra-high Vacuum and Nanoscience: NanoSPM Group	56
• Group of Surfaces and Thin Films at CMAM.....	59
• Photovoltaic Materials Group.....	62
• Liquids and Complex Systems Group.....	65
• Scanning Probe Microscopy Theory & Nanomechanics Group	67
• Surface Science Laboratory at UAM (LASUAM).....	69
• Low Temperature Laboratory (LBTUAM).....	73
• Advanced Materials for Integrated Guided Optics.....	78
• Group of “Crystal Growth Laboratory, CGL”	80
• AFM and Nanosystems Group.....	82

Transport and Superconductivity in Mesoscopic Systems

TRANSPORTE Y SUPERCONDUCTIVIDAD EN SISTEMAS MESO-NANOSCÓPICOS

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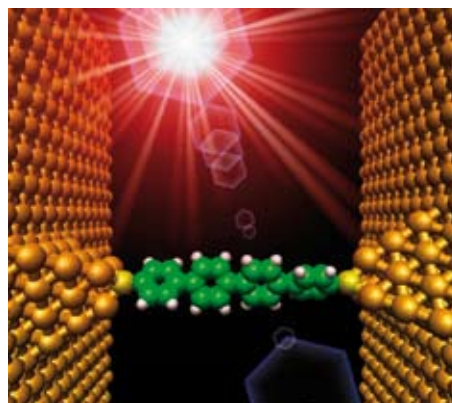
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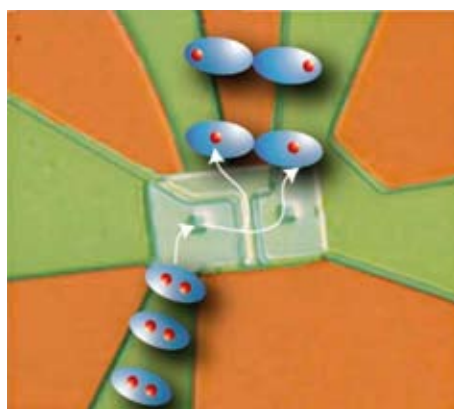


The tendency to miniaturization in micro-electronics has had a strong influence in the evolution of Condensed Matter Physics in the last 20 years. In addition to its technological interest, nanoscale devices are of great interest from the point of view of basic research. Thus, since the last 80's there has been a strong activity in the study of quantum effects in the transport properties of systems whose dimensions are comparable to the electronic phase coherence length (the so called mesoscopic systems). More recently the interest is shifting towards nanoscopic or even systems with typical dimensions in the atomic or molecular scale. The combination of these devices with superconducting elements give rise to a new and rich phenomenology which in turn is providing a more deep and detailed knowledge of well known phenomena like the Josephson effect.

OBJECTIVES

There are currently worldwide activities aiming at a better understanding of effects that could serve as a basis for future nanoelectronic devices. The theoretical analysis of systems of potential technological interest is an indispensable part of this process. A strong collaboration with experimental groups is of great importance to guide the theoretical research in the appropriate direction.

Our initial hypothesis is that it is possible to predict and analyze quantitatively the properties of nanostructures using microscopic models with different levels of approximation. Thus, in the case of systems including traditional superconductors and ferromagnets they can be described using effective models in the mean-field approximation, whereas in the case of molecules the use of ab-initio methods could be necessary. On the other hand, the transport phenomena in these systems can be adequately obtained using non-equilibrium Green functions techniques in their different formulations.



The general aim of our project is the theoretical study of different phenomena associated with electronic transport in devices which combine different materials at the nanoscale. The project is divided into three main lines of research:

1. Electronic transport in atomic and molecular size systems. Main objectives within this line are: ab-initio description of transport through single molecules and study of electron correlation effects.
2. Non-equilibrium phenomena in nanostructures with superconducting electrodes. Objectives: study of ac driven transport, noise properties and non-local transport in multiterminal structures.
3. Hybrid nanostructures including ferromagnetic and novel materials. Objectives: consequences of induced triplet superconductivity and proximity effect in graphene and other carbon based nanostructures.

SCIENTIFIC AND TECHNICAL CONTRIBUTIONS

This project is focused on fundamental electronic transport properties of nanostructures. The work is expected to be carried out in close collaboration with experimental groups and we expect to obtain quantitative predictions which could be verified in the near future as well as to produce a proper theoretical description of recent experimental results.

Although contributions of a technological character cannot be expected in the short term, our study is oriented towards the foundation of a new type of electronics based on nanostructures and functional molecules.

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Laboratory of Coatings and Nanostructures: Magnetic Coatings and Nanostructures Group

LABORATORIO DE RECUBRIMIENTOS Y NANOESTRUCTURAS:
GRUPO DE RECUBRIMIENTOS Y NANOESTRUCTURAS MAGNÉTICAS

Members of the Group: *Pilar Prieto, José María Sanz*

The magnetic group of the Laboratory of Coatings and Nanostructures (LRN) is working on the development of new nanocrystalline magnetic thin film for high frequency applications as well as magnetic nanostructures based on arrays of nanoholes, (i.e., anti dots arrays) which are promising nanostructures for the new generation of ultra-high-density magnetic storage media. In summary we try to tailor the magnetic properties of magnetic materials in two ways: 1) by incorporating nitrogen into its lattice to obtain nanocrystalline magnetic materials with an adequate combination of magnetic properties for use on high-frequency devices and 2) by introducing arrays of ordered nanoholes to obtain high density antidots nanostructures with controlled magnetic properties.



HIGH-FREQUENCY MAGNETIC MATERIALS

The requirements to the physical properties of the magnetic materials for use in gigahertz inductive devices are a high permeability, compatibility with under-/over-layers in multilayer device design, together with a natural ferromagnetic resonance frequency in the gigahertz range. This resonance occurs when the frequency of the applied ac field matches the characteristic precession frequency of the spins in the magnetic material and is mainly determined by the total anisotropy field experienced by the spins and the saturation magnetization. Good candidates for high-frequency applications are nanocrystalline phases of some magnetic nitrides. The incorporation of interstitial nitrogen in iron results in a substantial increase of the resistivity, induces the formation of a fine nanocrystalline material, and increases the anisotropy field, while retaining the high magnetic moment of the iron atoms. In this turn we have been studied the complete phase diagram of the Fe_xN system. The nitrogen-poor phases, i.e. α' -Fe_{x(x>8)}N, γ' -Fe₄N and ϵ -Fe_{x(3<x<2)}N are ferromagnetic compounds. A higher nitrogen content induces the formation of paramagnetic nitrides at room temperature, i.e. ζ -Fe₂N, and the recently discovered cubic phases, γ'' -ZnS and γ''' -NaCl type, with a stoichiometry close to FeN. We have demonstrated the capability of a technique like ion beam assisted sputtering deposition to obtain the different phases of iron nitride as a function of the deposition conditions. The iron nitride thin films have been chemically, electronically, magnetically and structurally characterized in terms of XRD, Mössbauer, RBS, AES, XPS, XAS, XMCD and MOKE techniques. The Mossbauer characterization has been performed in collaboration with J.F.Marco (CSIC) group and the MOKE characterization was performed in collaboration with J.Camarero (UAM, IMDEA-Nanociencia). Actually, our group has constructed a MOKE system that is now working. XAS and XMCD measurements were

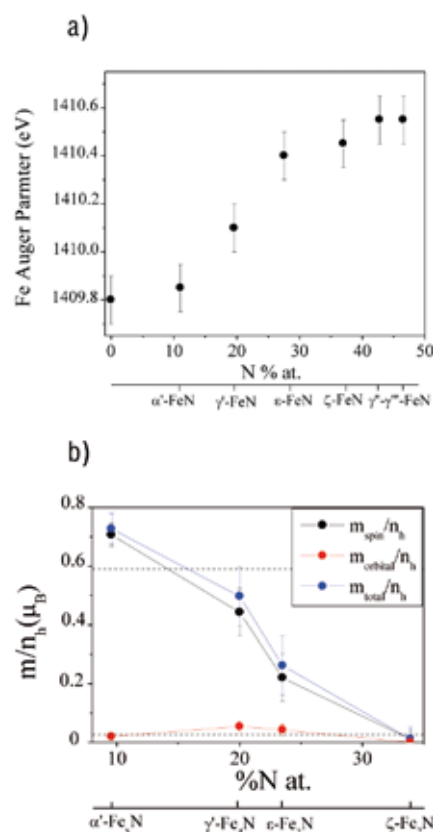


Fig1. a) Auger parameter of iron as a function of nitrogen concentration b) Spin, orbital and total magnetic moments per 3d hole as a function of nitrogen content in the film. The main phase present in the films is also included at the x axis. The values for pure iron are included (dashed lines).

performed at the advanced photoemission experiment beamline (APE) at Elettra synchrotron radiation facility (Trieste).

As a summary we have been depicted in Fig.1a the Auger parameter as a function of nitrogen content in the FeN_x film and the main nitride phase present in the film [1, 2]. Fig.1b shows the spin, orbital and total magnetic moments per 3d-hole for the different ferromagnetic nitrides. The variation of the auger parameter in the films as the nitrogen content increase is related with the 3d hole-hole interaction energy in the final state indicating changes in the localization of 3d states. The spin magnetic moments also vary considerably as the nitrogen content increase, i.e. $m_{\text{spin}}(\alpha') > m_{\text{spin}}(\gamma') > m_{\text{spin}}(\epsilon)$ and $m_{\text{spin}}=0$ for $\zeta\text{-Fe}_2\text{N}$. However, the orbital magnetic moments, i.e. m_{orb} , as well as the ratio $m_{\text{orb}}/m_{\text{spin}}$ show higher values for γ' and ϵ nitrides than those reported for pure iron. This enhancement of the orbital magnetic moments at the nitrides with respect to pure Fe is related also with the localization of the d-electrons at the Fe atoms.

Iron nitride films show thermal stability problems that can be solved by the incorporation of a third element (e.g. a transition metal) in the Fe-N system if the concentration of the third element is low. On the contrary, if the third element is Ni or Co, a higher concentration can be incorporated leading a good combination of magnetic properties. We have been explored the effect of nitrogen and nickel concentration in the Fe-Ni-N system [3,4,5]. In particular, in the case of permalloy ($\text{Fe}_{20}\text{Ni}_{80}$) it is possible to obtain nanocrystalline $\text{Fe}_{20}\text{Ni}_{80}\text{-N}$ thin films with well-defined in-plane magnetic uniaxial anisotropy and magnetically softer than the well known $\text{Fe}_{20}\text{Ni}_{80}$ films [4]. The study of magnetization reversal mechanisms in terms of the angular dependence of the coercive field indicates an evolution from domain-wall nucleation process to coherent rotation process as the nitrogen content increases in the films as it is show in Fig2b. In fact the presence of small grains of paramagnetic nitride, that we can measured by Mössbauer spectroscopy (Fig.2a) for high nitrogen concentrations, could decouple the ferromagnetic grains so that the coherent rotation reversal process, expected for single particles, is more favorable than other magnetization reversal mechanisms.

We have also been studied the low nickel content region of the Fe-Ni-N system. The more relevant result has been the fabrication of nanocrystalline $\gamma'\text{-FeNiN}$ thin ferromagnetic films with an estimated ferromagnetic resonance frequency of up to 6 GHz [5]. Fig.3a

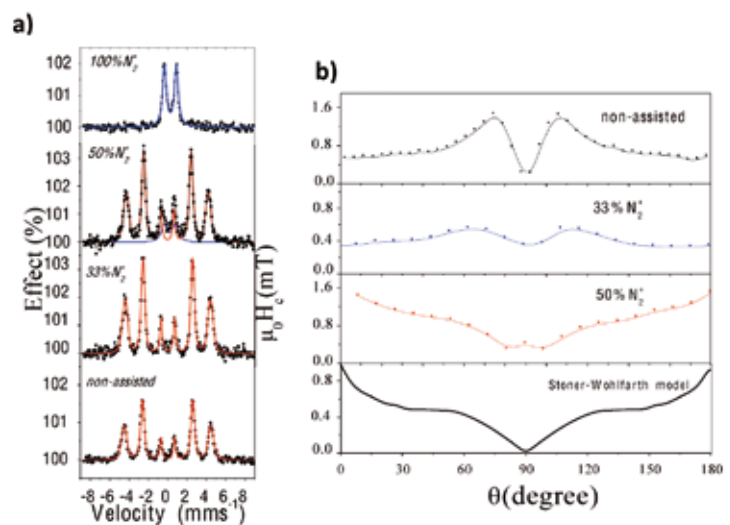


Fig.2 (a) Room temperature ICEMS spectra and (b) coercive field as a function of angle between field direction and the easy-axis for different concentration of N_2^+ in the assisted.

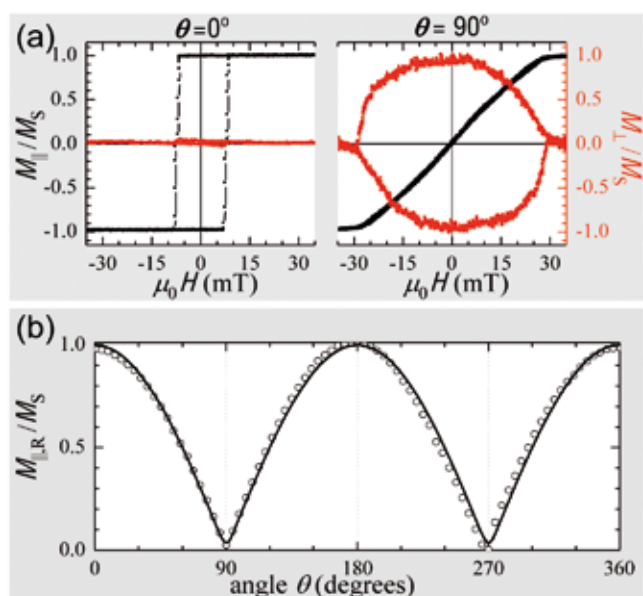


Fig.3: Magnetic properties of $\gamma'\text{-FeNiN}$ film. a) Easy-axis (0°) and hard-axes (90°) in-plane resolved hysteresis loops. b) Angular dependence of the reduced magnetization remanence (symbols) compared with the cosine behavior (line) expected for uniaxial anisotropy systems

shows the M-H loops of both perpendicular and parallel components for the easy and hard axis respectively. For the easy axis of Fig.3a ($\theta=0^\circ$), the parallel component of the magnetization does not change significantly from the saturation to remanence, i.e., $M_R/M_S=1$ and there is a sharp jump at the coercive field $H_C=7.3$ mT that reverses the magnetization state. The reversal takes place by nucleation and further propagation of magnetic domains oriented parallel to the easy-axis direction. When the field is applied perpendicular to the easy axes, i.e. $\theta=90^\circ$, the loop shows a typical uniaxial hard axis behavior with an anisotropy field $H_K=28.4$ mT. The uniaxial anisotropy of our film is also clearly observed in the angular plot of the reduced remanence (Fig.3b). The experimental data follow the typical cosine dependence expected in well defined uniaxial magnetic anisotropic systems. The high value of the ferromagnetic resonance frequency estimated in terms of saturation magnetization and anisotropy field, i.e. 6 GHz, makes this material attractive for developing of high-frequency devices.

MAGNETIC NANOSTRUCTURES: Antidot arrays

Magnetic nanostructures based on arrays of antidots have attracted extensive attention because they are promising candidates for a new generation of ultra-high-density magnetic storage media. These magnetic nanostructures are based on magnetic thin films with periodic arrays of holes usually referred as antidots. Around the antidots, a stable domain configuration is formed, which is a result of the interplay of the intrinsic uniaxial anisotropy of the magnetic thin film and the demagnetizing fields associated with the antidots. The memory bits could be trapped between consecutive holes along the intrinsic hard axis of the antidot nanostructure. The main advantage of these nanostructures is the absence of the superparamagnetic limit, once there are no isolated small magnetic entities.

We have been fabricated ordered nanoscale antidot arrays by using nanoporous alumina membranes (NAMs) as templates with different sizes and lattice geometries [6,7,8]. Two different NAMs with high order hexagonal symmetry have been used, i.e. NAMs with pore diameters ranging between 35 nm and 95 nm, but with a constant lattice parameter of 105 nm and NAMs with pores of 180 nm diameter and a lattice parameter of 500 nm. In addition we can also prepared antidot arrays where the antidot size changes by varying the thickness of the magnetic material grown on top of the NAM templates. In general, the results show a significant increase of the coercivity as well as a reduction of the remanence on the antidot arrays as compared with their parent continuous film, that depends on the size and on the density of holes introduced in the thin film. Fig.4 summarized some results for permalloy antidot arrays measured in collaboration with M.Vazquez group (ICMM-CSIC). The increase of the coercivity as the pore size increases, for a fixed antidot density, is showed in Fig.4b over a wide range of temperatures [7]. In this case we have also observed a linear dependence of the coercivity on the interantidot distance in the complete temperature range in agreement with the predictions of the coercive theories.

We have explored the magnetic domain configuration of these antidots nanostructures in the virgin state (not exposed intentionally to a magnetic film) by XMCD-PEEM at the Nanospectroscopy beamline of the Elettra Synchrotron. Ferromagnetic domains with magnetic spins parallel or antiparallel to the polarization vector

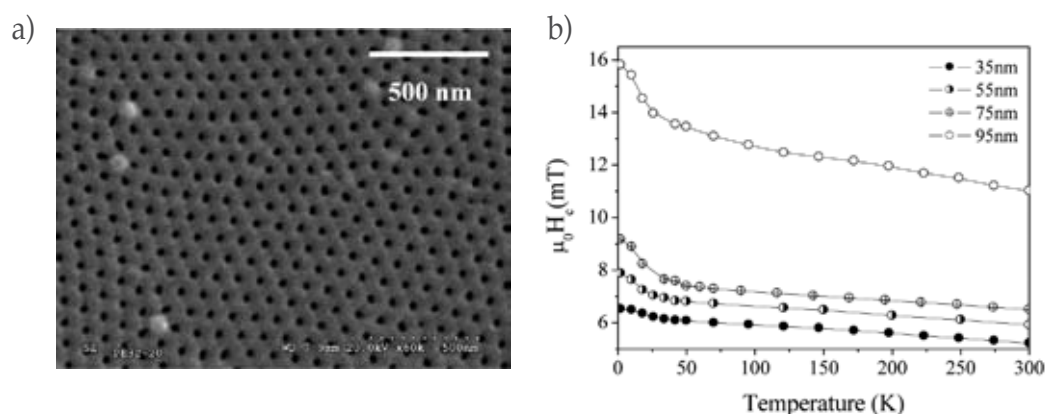


Fig4. a) SEM image of an antidot arrays b) Coercitive fields of the antidot arrays as a function of temperature. The pore diameter values indicated in the figure are those of the original NAM precursor.

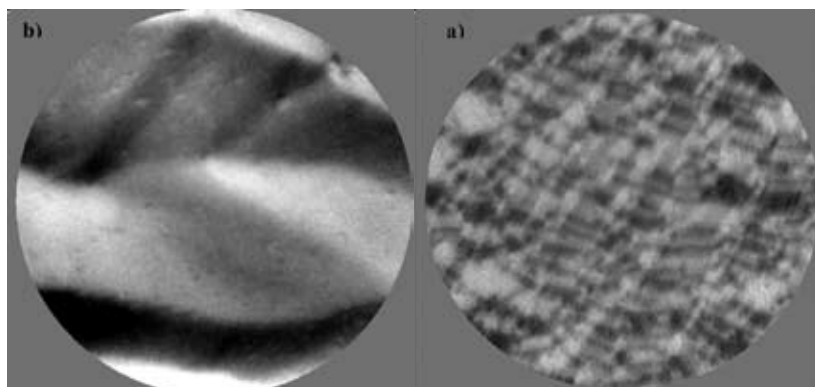


Fig. 5 a): XMCD images taken with PEEM at a field of view of 5 microns at the Nanospectroscopy beamline at Elettra of $\text{Fe}_{20}\text{Ni}_{80}$ antidot arrays with a lattice parameter $\approx 105\text{nm}$ and antidot sizes of \approx a) 45nm and b) 20nm .

appear black or white in the XMCD image, and oppositely magnetized domains with magnetic spins perpendicular to the polarization vector will both have the same grey contrast. We have been observed a larger variety of domain patterns that depend on the material as well as the characteristic sizes of the antidot nanostructure, i.e. antidot diameter and interantidot distance. Fig. 5a

and 5b show domain pattern of the magnetic antidots with a ratio between antidot diameter to interantidot distance of 0.7 and 0.2 respectively. When the ratio between antidot size and interantidot distance is 0.7, we observe the formation of domain chains with a width that correspond to the antidot nanostructure period. The length of the chains seems to be determined by self-assembled close packed domains of the NAM template. However, when the ratio decreases to 0.2 large magnetic domains, in the micrometer range, are clearly observed since the demagnetized field associated with the antidots is not strong enough to induce the formation of small domains. In this case the magnetic domain configurations as well as the magnetic properties, i.e. coercive field and saturation magnetization, are similar to the corresponding continuous $\text{Fe}_{20}\text{Ni}_{80}$ thin film.

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Laboratory of Coatings and Nanostructures: Oxide Nanostructures Group

LABORATORIO DE RECUBRIMIENTOS Y NANOESTRUCTURAS:
GRUPO DE NANOESTRUCTURAS DE ÓXIDOS

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Leonardo Soriano, Alejandro Gutiérrez, Pablo Pernas

Ph.D. Students:

Iulian Preda, Guillermo Domínguez-Cañizares, Daniel Díaz-Fernández



The group of oxide nanostructures of the Laboratory of Coatings and Nanostructures is working on the fundamental and applied research on oxide nanostructures. The fundamental research is mainly concerned on the electronic structure of oxide nanostructures, paying special attention on how surface, interface, size and other possible effects, affect the electronic properties of the nanostructures and, consequently, their physical properties. The applied research developed in our group is currently concerned on the growth of highly ordered porous oxide membranes, in particular, NiO nanoporous membranes.

SURFACE EFFECTS IN BULK NiO

The characteristic electronic structure of NiO gives rise to complex structured spectra in photoemission. In particular, for the Ni 2p 3/2 photoemission spectrum, simple theory predicts the appearance of three peaks as the results of direct photoemission (c 3d⁸), screening of oxygen neighbors (c 3d⁹L-main line) and screening of two oxygen neighbors (c 3d¹⁰L²). However, a shoulder located at 1.5 eV towards higher binding energy from the main line appears in the spectra of bulk NiO. This shoulder has already been interpreted as originated by the screening of the second oxygen neighbors and has been called as *non-local screening* peak. We have measured surface enhanced photoemission spectra of a bulk NiO sample (Fig. 1). The spectra show a clear enhancement of this shoulder, thus indicating that the shoulder has an important component from the surface. Cluster calculations performed in collaboration with Prof. M. Abbate from the Federal University of Parana, Brazil, show that part of the intensity of the shoulder comes from the contribution of the pyramidally coordinated N atoms located at the NiO surface. So that, we suggest a model in which the Ni 2p 3/2 photoemission spectra can be fitted (see fittings in Fig.1) by three peaks accounting for the main line (green), surface peak (magenta) and non-local peak (blue) respectively. This model is able to successfully explain the Ni 2p photoemission spectra in nanostructured NiO systems.

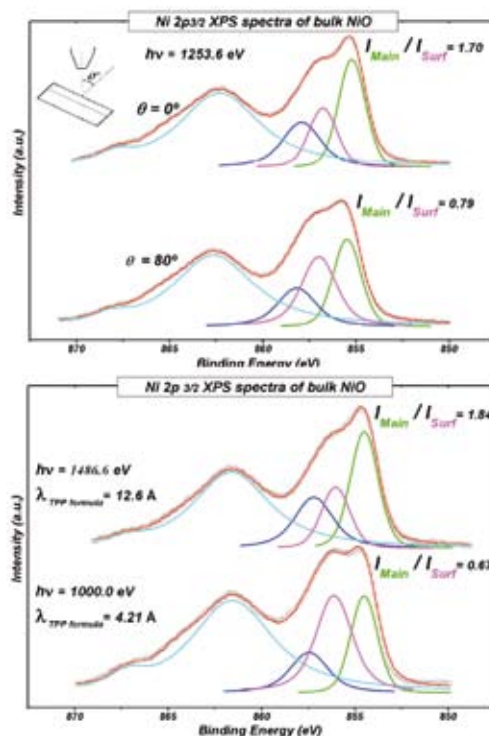


Fig1. : (upper) Ni 2p_{3/2} XPS spectra measured in take-off angle $\theta=0^\circ$ and $\theta=80^\circ$. (bottom): Ni 2p_{3/2} PES spectra measured with $h\nu=1486.6$ eV and $h\nu=1000$ eV photon energies.

SURFACE EFFECTS IN NANOSTRUCTURED NiO

It is known that, when NiO is grown on a Highly Oriented Pyrolytic Graphite (HOPG) substrate, NiO grows forming nanometric islands located at the steps and terraces of the substrate. This can be clearly seen in the AFM images shown in Fig.2. The AFM images have been measured in the non-contact mode as the contact mode produced a sweeping of the material deposited due to the low

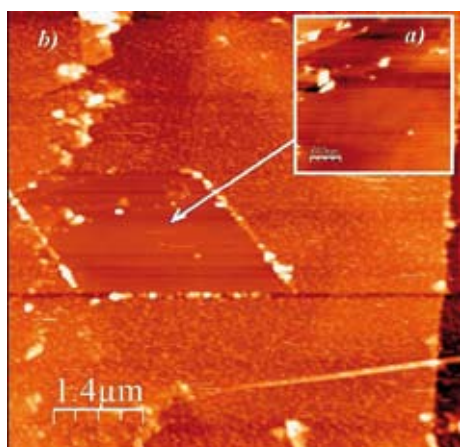


Fig.2: Tip effect of the contact AFM imaging mode of NiO on HOPG: a) 3x3 μm contact mode and b) 7x7 μm non-contact mode AFM image of 0.8 \AA NiO/HOPG.

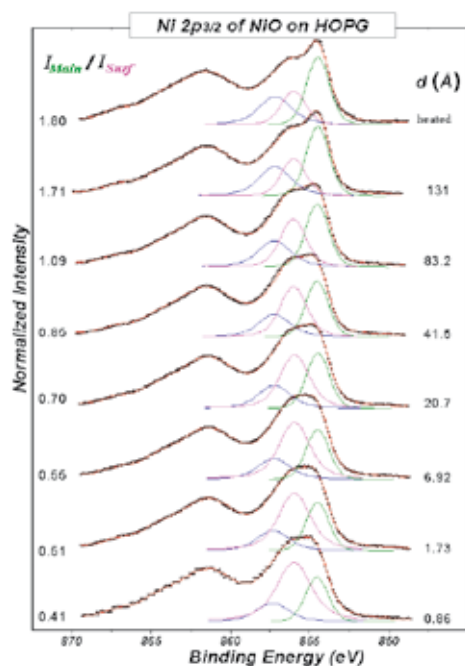


Fig.4: Fittings of the Ni 2p_{3/2} XPS spectra through the NiO growth on HOPG.

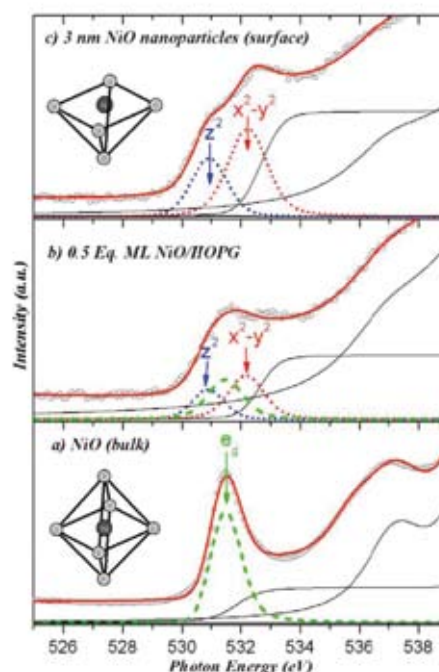


Fig.3: Experimental and calculated near edge region of the O 1s XAS spectra (dots) of: (a) large NiO coverage (bulk); (b) 0.5 ML NiO/HOPG; and (c) 3 nm NiO nanoparticles.

interaction of the deposits with the inert HOPG substrate (see inset in Fig.2). This nanostructured system, with a large surface-to-volume ratio, seems to be a suitable system to study surface effects in NiO. In fact, the O 1s X-ray absorption (XAS) and the Ni 2p photoemission spectra showed anomalous shapes with respect to those of bulk NiO.

The O 1s XAS spectrum of 0.5 equivalent monolayers of NiO deposited on HOPG is shown in Fig. 3. It is compared with similar spectra of bulk NiO (Fig. 3a) and 3 nm NiO nanoparticles (Fig. 3b). Cluster model calculations in octahedral and pyramidal symmetries indicate that the eg unoccupied electronic sub-levels of the pyramidally coordinated Ni atoms located at the surface are split into two due to the lack of the apical oxygen atoms at the surface.

On the other hand, we have also studied by photoemission the growth process of NiO on HOPG. The spectra are shown in Fig. 4. The spectra have been fitted by using the three curves according to our previous model. It can be seen that this model explain all the spectra in terms of the surface + non-local peaks. The fittings show that for low NiO coverages, where NiO forms nanometric islands, the photoemission spectra present a high intensity of the surface peak, in agreement with the AFM images. Only when coalescence is reached, the photoemission spectra agree with those of bulk NiO (upper spectrum in Fig.4).

INTERFACE EFFECTS IN NiO/OXIDE INTERFACES

As a continuation of our previous work on oxide/oxide interfaces, we have investigated the NiO/oxide systems. The oxide substrates (SiO_2 , Al_2O_3 , and MgO) have been chosen according to the nature of their chemical bonding (from a more covalent to a more ionic character). Fig.5 shows AFM images of the substrates used in these experiments. The growth process of NiO on the different substrates has been followed by photoemission. The Ni 2p 3/2 spectra have been analyzed for the three substrates throughout the growth process. In all three substrates, the final stages of growth gives similar spectra to that of bulk NiO, thus concluding

that stoichiometric NiO thin films can be grown on these substrates. However, the most interesting features of the spectra appear for low coverages. In Fig. 6 the spectra corresponding to 0.5 equivalent monolayers of NiO on the corresponding substrate are represented. It is interesting to observe that the energy shift of the two components, main line and surface line, is not constant throughout the series of spectra. In fact, the highest energy separation is obtained for the SiO₂ substrate (1.38 eV), whereas the lowest (0.90 eV) is found for the MgO substrate, and an intermediate value (1.2 eV) is observed for the Al₂O₃ substrate.

Once again, cluster model calculations show that further symmetry reduction (or further covalence reduction) from pyramidal to square planar symmetries, would produce an even larger shift. These results also help to explain our experimental results on the NiO overlayers on the different oxides. According to those calculations, the energy separation of the bulk (main line) and surface peaks decreases with the $T_{\text{apical}}/T_{\text{basal}}$ ratio. This separation is related to the changes in the covalent interaction at the NiO/oxide interface, being larger for the NiO overlayer on the more covalent SiO₂ substrate and smaller in the more ionic MgO substrate. These results are consistent with the idea of the formation of Ni-O-M cross-linking bonds (M=Si, Al, and Mg) at the interface.

In this picture, in the case of the SiO₂ substrate, the Ni 3d-O 2p overlap in the Ni-O-Si bonds is smaller than in the Ni-O-Al bonds of bulk NiO due to the strong covalent character of the Si-O bonding. On the other hand, the Ni 3d-O 2p overlap of the Ni-O-Mg bonds is larger than in the Ni-O-Ni bonds due to the more ionic character and consequently, less covalent character of the Mg-O bonds.

NANOPOROUS NiO MEMBRANES

Our applied research is focused on the growth of nanoporous NiO membranes. The membranes are grown by means of the magnetron sputtering technique. We use a nanoporous alumina membrane as substrate. Fig.7 shows SEM images of those NiO membranes. The columnar way of growth is clearly seen in the pictures, giving rise to the conservation of the porous of the alumina membrane in the NiO deposits. The possible applications of this new nanostructures are of enormous interest in different industries such as catalysis, magnetic storage, fuel cells, and Ni batteries. We are currently studying the physical and chemical properties of the membranes obtained by this method. A Spanish patent has been requested.

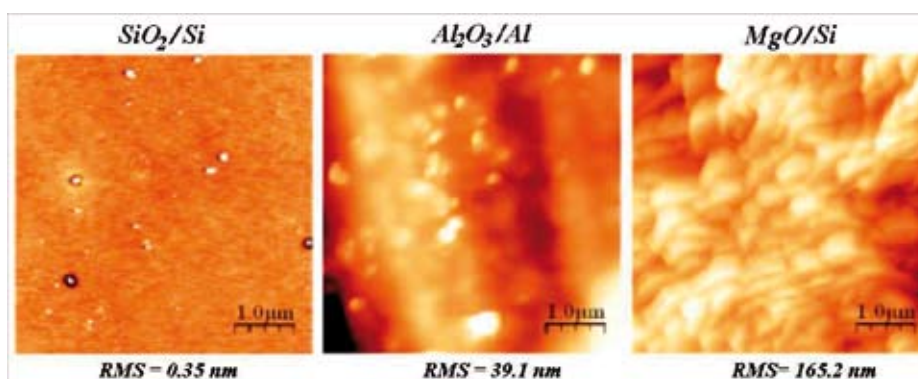


Fig.5: AFM topographic images ($5 \times 5 \mu\text{m}^2$) of the different oxide surfaces, measured in dynamic mode (tapping).

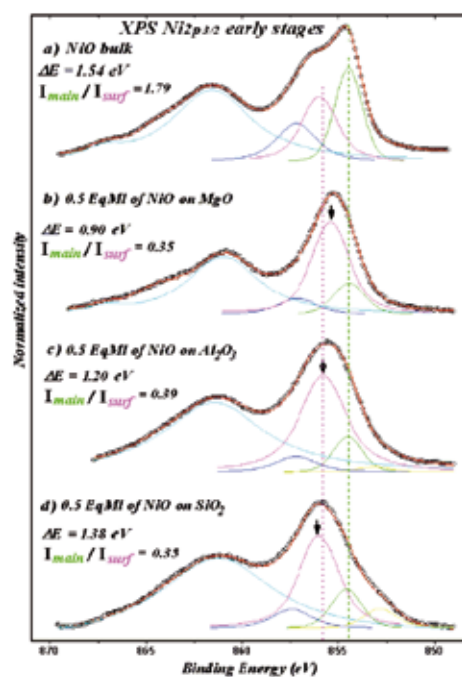


Fig.6: (a) Ni 2p_{3/2} XPS spectrum of bulk NiO, used as reference. (b-d) Ni 2p_{3/2} XPS spectra of NiO submonolayer (0.5 Eq. ML) grown on the different oxide substrates

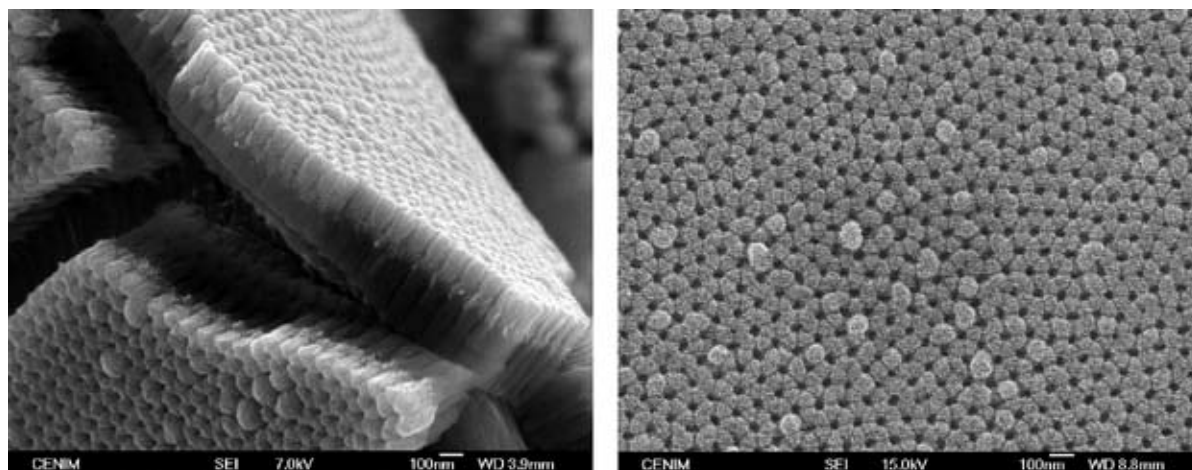


Fig.7: SEM images of nanoporous NiO membranas grown by magnetron sputtering.

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Ab Initio Studies of Lanthanides in Solid-State Lighting and of Actinides in Advanced Nuclear Energy Systems

ESTUDIOS AB INITIO DE LANTÁNIDOS EN ILUMINACIÓN DE ESTADO SÓLIDO Y ACTÍNIDOS EN SISTEMAS AVANZADOS DE ENERGÍA NUCLEAR

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SUMMARY

The research of this group is aimed at delivering high quality, first-principles, wave function based, electronic structure calculations on lanthanide-bearing materials which are phosphors useful in Solid State Lighting (SSL), like Ce³⁺-doped YAG, and on actinide-bearing materials related with Advanced Nuclear Energy Systems (ANES), like UO₂/PuO₂ mixtures. Local structures, vibrational frequencies, transition energies between the electronic states of the complex excited manifolds, light absorption and emission profiles, lifetimes and Stokes shifts of SSL-related phosphors can be calculated, using embedded-cluster wave function based methods, with a quality high enough so as to be useful in the design of colour targeted efficient phosphors and in providing basic understanding of the microscopic mechanisms involved in their luminescence. The same type of wave function based calculations performed on ANES-related actinide-bearing materials involving U⁴⁺, Pu⁴⁺, Am²⁺, Cm³⁺ and Bk⁴⁺ should help to gain basic understanding of their electronic manifolds and to develop microscopic defect models of nuclear fuels and wastes.

AIMS OF THE RESEARCH

The group has been following a line of research based on the interplay between methodological advances and systematic applications that have led to establishing practical conditions of use of wave function based ab initio methods capable to handle complex manifolds of local electronic states of heavy impurities in insulators. Along this line, the group is now in a point where it is able to calculate, on a first-principles basis and with reliability, local structures and vibrations around f-element impurity ions in insulators, in their ground state and in excited states, and energy differences between them, and, in consequence, the absorption and luminescence profiles of the corresponding materials. The group projects a step forward in the line, which basically consists of the application of the technology in their hands and of their knowledge in two fields of social interest. One of them is the prediction of the light absorption and luminescence of lanthanide-containing materials of real or potential use in Solid-State Lighting devices; this idea was promoted by Philips Lighting, Eindhoven, and substantiated in a two-year collaboration. The other one is the study of ANES-related actinide-bearing materials, aimed at developing a fundamental understanding of some of their properties, specifically the structures of local defects of fuels and wastes, and their associated absorption and emission electronic excitations.

BACKGROUND AND STATE OF THE ART

Lanthanides and SSL. SSL devices are basically made of a Light Emitting Diode (LED) which emits coloured light –e.g. blue– and a light conversion system which produces white light –e.g. by partially converting

the blue light into yellow, which mixed with the blue residue produces white light useful in lighting-. Among the phosphors used for light conversion in SSL devices, the most successful from the commercial point of view is the Yttrium and Aluminium garnet, $Y_3Al_5O_{12}$ or YAG, doped with Ce^{3+} , in its bulk form, which belongs to the family of materials made of insulators –mostly oxides- doped with lanthanide ions [1]. Other examples are Eu^{3+} -doped Y_2O_3 or Eu^{2+} -doped $BaMgAl_{10}O_{17}$ [1]. The lighting efficiencies –in lumen per watt of consumed energy– of SSL devices are now much higher than conventional lighting devices and they double each year. The same comparison and evolution rate is true for the lifetimes of the devices. On the basis of these facts, it is expected that conventional illumination will be completely substituted by SSL in the USA by 2025. Apart from the commercial impact of this, it will mean important energy savings –of 29% in general illumination and 2.5% in total energy consumption– which amount 54 Mtoe/year and 125.000 millions of US\$ from 2005 to 2025. The economic and environmental impacts of such energy savings are obvious. (These data are available in *Energy Savings Potential of Solid State Lighting in General Illumination Applications*, Office of Energy Efficiency and Renewable Energy, US DOE, November 2003, on-line version at: <http://www.netl.doe.gov/ssl>.)

The US Department of Energy does not only recognize the importance of making significant advances in SSL, but it also admits that the new technological advances will be sustained on new discoveries of basic research. In consequence with this, its *Office of Basic Energy Sciences* organized the *Basic Energy Sciences Workshop on Solid-State Lighting (SSL), held in May 2006, with the goal of: “examine the gap separating current state-of-the-art SSL technology from an energy efficient, high-quality, and economical SSL technology suitable for general illumination; and to identify the most significant fundamental scientific challenges and research directions that would enable that gap to be bridged”*. The conclusions, state as Grand Challenges “to change the very paradigm by which SSL structures are designed—moving from serendipitous discovery towards rational design” and “to understand and control the essential roadblock to SSL—the microscopic pathways through which losses occur as electrons produce light” [2].

At the same time, ab initio theoretical methods have demonstrated its power as interpretative and predictive tools in chemistry and physics of molecules and materials, including lanthanide-bearing materials. However, their use as tools that complement the experiments in lanthanide-doped solids with applications in SSL has not yet been exploited [3]. It seems to be, then, the right time to work on the prediction, via first-principles calculations, of absorption and emission profiles of solids like $YAG:Ce^{3+}$ and similar [4], which should deepen our knowledge of the details of the absorption, decay, and emission of light in these type of materials used as phosphors in SSL devices. The predictions themselves and the knowledge derived from them have a potential for leading the search for new, more efficient phosphors.

Actinides and ANES. Being able to produce enough energy steadily in a time scale of several hundred or thousand years, safely and out of risk of deriving the activity towards the production of nuclear weapons, without any negative impact on the environmental stability of the planet, and reducing and controlling the nuclear wastes, are goals of maximum social interest. This is so once it has been agreed that the energy production models that send to the atmosphere large amounts of green house effect gases, like CO_2 , are no longer sustainable, on the one hand, and having in mind that the safe storage of nuclear wastes is an important environmental issue, on the other. Developing a fundamental understanding of the properties of actinide-bearing materials is recognized as a major scientific challenge in this context.

As in the case of SSL, the *Office of Basic Energy Sciences of the US Department of Energy* organized the *Basic Energy Sciences Workshop on Advanced Nuclear Energy Systems*, which was held in July-August 2006, aimed at identifying: technology challenges; current status of research; basic research challenges, opportunities, and needs; priority research directions; and science/technology relationships. The conclusions highlight as Grand Challenges: “Resolving the f-electron challenge to master the chemistry and physics of actinides and actinide-bearing materials”, “Developing a first-principles, multiscale description of material properties in complex materials under extreme conditions”, and “Understanding and designing new molecular systems to gain unprecedented control of chemical selectivity during processing”. Specifically, (i) the development of (first-principles) quantum chemical/molecular relativistic electronic structure approaches for correlated f-electron systems and (ii) the development of innovative defect models for multicomponent actinide fuel/fission product systems, are considered crucial [5].

The need of first-principles quantum chemical/molecular studies on these problems is reinforced by the hazards inherent to the high toxicity and radioactivity of transuranium containing materials, which hinders the design and performance of experiments and, so, limit the ability to gain deeper understanding of the role of 5f electrons (also 6d and 7s) in chemical bonding in molecules, complexes in liquid solution, and solids, with respect to what happens with other parts of the Periodic Table [6]. This understanding is a fundamental issue in actinide research which remains largely unsolved, although the ability of doing reliable predictions is considered a key for separation processes, for the development of ligands to sequester actinides in the environment and to remove toxic metals from the human body, and to devise stable matrices for storage of nuclear wastes, all of which are processes of basic, technological, and societal interests.

More specifically, the study of electronic spectra of actinide-bearing materials and their correlation with molecular structure are pointed out as basic tools to reveal the role of 5f electrons in bonding. However, the hazards of the experiments (but also the strong dependence that interpretative empirical/semi-empirical theories have on them) have contributed to limit substantially experimental investigations on the relationship spectroscopy/structure/bonding. As an illustrative example, let us say that the only experimental 5f-5f spectroscopic data on free actinide ions in gas phase which are available and interpreted, are those on U^{4+} , in spite of the fact that these data are a necessary reference for understanding the manifolds of actinide ion-containing molecules and solids; all the rest of spectroscopic atomic data are extrapolations from the solid state, whose precision have been questioned [6,7]. This is also the case for spectroscopic data and reports on actinide complexes in solution and actinide ions in crystals, their numbers being surprisingly low. In these circumstances, the development and validation of quantum chemical/molecular models suitable for the calculation of the structure and spectroscopy of actinide containing molecules and their extensions to liquid solutions and to the solid state by means of quantum mechanical embedding techniques become a very promising alternative to experiments and a helpful guide to select experimental priorities, which are crucial in this field. Furthermore, their application to target actinide containing materials should lead to the necessary accumulation of knowledge on the relationship between geometry and electronic structure that should serve to shape up models for bonding and chemical thinking as powerful as those nowadays available for complexes and solids containing not so heavy elements, such as, for instance, transition metals. This research line and strategy is the backbone of the second research line in our group.

Ab initio calculations on electronic excited states of molecules and solids containing f-elements.

Although the two main lines of research seem to be very different (and they truly are from the experimental point of view), they lie in common grounds from the point of view of ab initio calculations. In effect, we face heavy element ions with unfilled shells of f-electrons (4f and 5f, respectively) doped in solids in both cases, which demand the same type of methodological requirements, namely, (i) all bonding interactions within a cluster made by the f-element and, at least, its first coordination shell, including static and dynamic correlation effects, (ii) relativistic effects of scalar (mass-velocity, Darwin) and spin-orbit coupling nature, (iii) classical and quantum mechanical embedding interactions between the solid host and the active cluster, (iv) very demanding basis sets for the active cluster, and (v) handling very large manifolds of hundreds and thousands of local electronic excited states of different configurations, e.g. those resulting from distributing all active electrons over the molecular orbitals with a main character of the actinide 5f, 6d or 7s atomic orbitals.

The quantum chemistry community has developed a variety of methods to meet the previous individual demands and several –although not many– combinations of them are possible, in principle, in order to carry out the target calculations [8]. Our group has made methodological contributions on embedding, on the inclusion of relativistic effects, via effective core potentials, and on the simultaneous inclusion of large amounts of electron correlation together with spin-orbit coupling effects [3].

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Biophysics of Neuronal Systems

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We analyze quantitatively molecular, cellular and circuit structure and function. For example, wiring and energy costs are evolutionary constraints of brains that explain features of the anatomy and function of neuronal circuits.

Our approach is quantitative, using a variety of theoretical techniques from engineering, physics and applied mathematics, as well as from systems biology and evolutionary theory. Experimentally, we use electrophysiology, imaging and behavioural measures.

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Biodynamics and Computational Biology

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BioDynamics and Computational
BIOLOGY



RESEARCH GOALS

Biological networks control an organism survival and function both at the cellular level (genetic networks) and at a global level (neural networks). As such, they do not work in isolation but are highly interconnected and embedded in a continuously fluctuating and changing environment. Despite the wealth of signals and external variations they have to deal with, they seem to have been exquisitely tuned by evolution to reliably perform specific functions. This leads to some broad questions that we try to address in the lab at different levels:

How can biological networks integrate and process information from different signals? How can they operate robustly in the presence of noise and undesirable fluctuations? What are the mechanisms underlying adaptation to environmental context? What is the relation between structure and function of simple biological networks?

APPROACHES

The advances in experimental techniques and the availability of vast amounts of data is complementing the traditional molecular approach to research in Biology with a Systems perspective, in which one tries to understand the functioning of a whole decomposing it into simpler 'modules', similar to the engineer design of complex devices. Questions can here be answered at a more quantitative level, and the combination of experiment and mathematical modeling is being proven very fruitful. While this approach has been followed by some time in Neuroscience, it is only recently becoming widely applied in Molecular and Cell Biology. It turns out that one can trace interesting parallels in the ways neural and genetic networks process information.

We use a combination of mathematical models, numerical simulation and theoretical techniques to investigate some of the above issues in relevant biological circuits. Since networks are not static entities, one of our main tools is non-linear dynamics, together with the theory of stochastic processes. Statistical physics, signal detection or information theory are also applied. We also establish collaborations with experimental groups where theoretical models can be supported by quantitative data.

RESEARCH LINES

Design principles of small genetic circuits

In collaboration with **Juan Poyatos** (Logic of Genomic Systems Laboratory, CNB) we are studying the dynamic and signal processing properties of two-component genetic circuits (two genes whose products regulate each other's expression and possibly regulate themselves). These small architectures have been shown to lie at the core of gene networks responsible for molecular clocks (for negative cross-regulation)

or cell differentiation (for positive cross-regulation). Despite its simplicity, two-component circuits are able to process signal frequency and duration in a way similar to single neurons [1] or to serve as short-term memory states allowing for flexible discrimination of transient signals, in analogy to the working memory neural circuits observed in the cortex [2]. We are currently investigating the amplitude/frequency detection of molecular signals by two-component circuits in the presence of fluctuations[3]

Chemiotherapy Resistance and Cellular Memory

One of the main shortcomings of current chemical therapies for cancer tumours is the adaptation of malignant cells to the chemical agents inducing apoptosis (cell death). In collaboration with **Cristina Murga** (Signalling Group, CBM) we are investigating the role of bistability in key apoptotic signalling components as a mechanism for cellular memory and resistance to chemiotherapeutic agents.

Variability and adaptation in neural codes

Following repeated presentations of the same stimulus, a neuron may elicit different responses. This variability is caused by intrinsic neural noise or small signal fluctuations, and may affect the way neurons transmit information or read a code. The converse is also observed in several sensory modalities: some times neurons produce similar responses to relevant stimulus features of different intensities, depending on the statistical context of the signal. Together with **Gonzalo García de Polavieja** (Instituto Cajal, CSIC, and Instituto 'Nicolás Cabrera', UAM) we have investigated the role of the intrinsic neural dynamics in response variability[4] and biophysical mechanisms of adaptation to statistics[5] taking as a model system the leech *Hirudo medicinalis*.

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Electron Transport and Dynamics in Magnetic and Superconducting Nanostructures

MAGNETRANS-UAM INC REPORT 2007-2008

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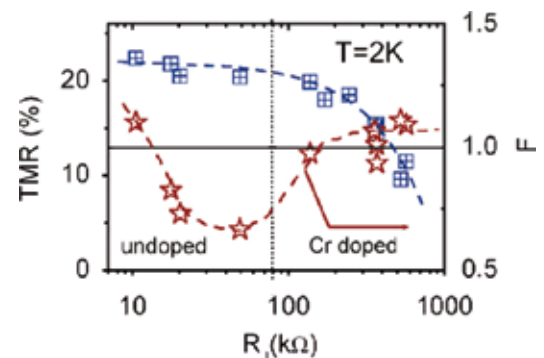
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1.1 Magnetoelectronics and spintronics – electron transport, dynamics and noise Shot noise in Co/Al₂O₃<M>/Py (M=Cr, Si) magnetic tunnel junctions

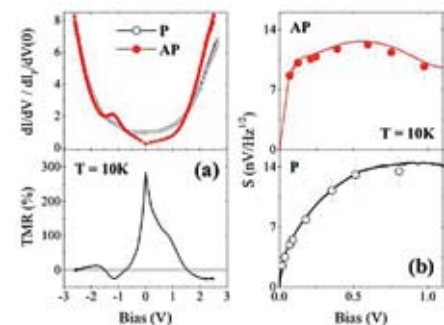
Low-frequency noise, including $1/f$ and shot noise (SN), and dynamic tunneling resistance have been studied in Co (80 Å)/Al₂O₃(14 Å)/Py (100 Å) magnetic tunnel junctions (MTJs) without doping and with Cr or Si δ -doping of the insulating barrier. The fluctuations in voltage were measured at frequencies ($200 < f < 2000$ Hz), temperatures below 10K and biases under 150 mV. For the undoped MTJs with the smallest (< 10 k Ω) and the highest (> 100 k Ω) tunneling resistances, the Fano factor shows “full” SN corresponding to uncorrelated tunneling ($F = 1$). The SN is reduced for the intermediate resistances with $F \approx 0.65$ – 0.8 indicating correlated electron tunneling, most probably through the localized states formed by the defects inside the barrier. The SN is enhanced for the antiparallel alignment of the ferromagnetic electrodes in the MTJs with tunneling weakly affected by spin-flip scattering. A model, which considers trap-assisted sequential tunneling, qualitatively explains the main experimental results.



Dependence of TMR and Fano factor on tunneling resistance for undoped and Cr-doped MTJs

1.2 High bias voltage effect on spin-dependent conductivity and shot noise in carbon-doped Fe(001)/MgO(001)/Fe(001) magnetic tunnel junctions

Low temperature (10 K) high voltage bias dynamic conductivity (up to 2.7 V) and shot noise (up to 1 V) were studied in epitaxial Fe(100)/Fe-C/MgO(100)/Fe(100) magnetic tunnel junctions as a function of the magnetic state. The junctions show large tunnel magnetoresistance (185% at 300 K and 330% at 4 K). Multiple sign inversion of the magnetoresistance is observed for bias polarity when the electrons scan the electronic structure of the bottom Fe-C interface. The shot



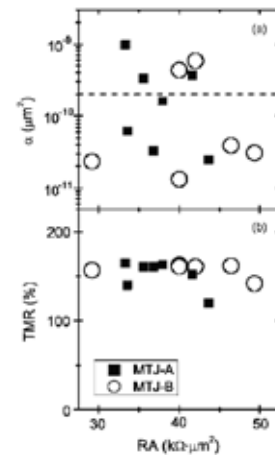
(a) Dynamic conductivities at 10 K (top panel) and related TMR (V) (bottom panel). (b) Shot noise measurements in P and AP states measured at 10 K in bias when the electrons are injected from the top toward the bottom MTJ electrode.

noise shows a Poissonian character. This demonstrates a pure spin-dependent direct tunneling mechanism and validates the high structural quality of the MgO barrier

1.3 Very low 1/f noise at room temperature in fully epitaxial Fe/MgO/ Fe magnetic tunnel junctions

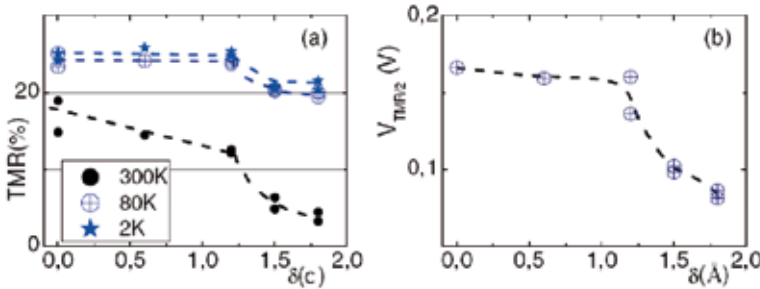
We report on room temperature 1/f noise in fully epitaxial Fe (45 nm)/ MgO (2.6 nm / Fe(10 nm) magnetic tunnel junctions (MTJs) with and without carbon doping of the Fe/MgO bottom interface. We have found that the normalized noise (Hooge factor) asymmetry between parallel and antiparallel states may strongly depend on the applied bias and its polarity. Both types of MTJs exhibit record of low Hooge factors being at least one order of magnitude smaller than previously reported.

Normalized noise measured at +200mV (a) and zero-bias TMR(b) as a function of RA product. The dashed line (part a) indicates the lowest Hooge factor value previously reported



1.4 Low frequency noise in Co/Al2O3<Si>/Py Magnetic túnel junctions

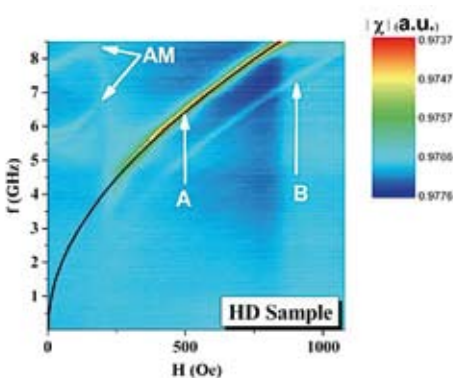
Low frequency noise and dynamic tunneling resistance have been studied in Co(80Å)/ Al2O3(12Å)/ Py(100Å) magnetic tunnel junctions (MTJs) with and without asymmetric Si doping of the insulating barrier (Si ≤ 1.8 Å).



a) Dependence of TMR on Si content at three selected temperatures. b) Bias dependence of TMR (VTMR/2) on Si content.

Variation of the dynamic resistance and tunneling resistance with Si doping and applied bias in these MTJs indicate a transition from the Si-doped regime to Si cluster formation above a δ -layer thickness of about 1.2 Å, close to 1 monolayer coverage. The measurements show anomalously strong enhancements of the low frequency noise for Si thickness above 1.2 Å, mainly due to the appearance of random telegraph noise. A simple model, which considers suppression of Coulomb blockade in the array of Si dots, opening two-step tunnel channels, qualitatively explains the variation of both conductivity and noise with Si content.

2.1 Magnetization dynamics in dots in magnetic vortex state



3-D plot for the magnitude of the susceptibility for HD sample when magnetic field is applied along Diagonal direction, with the corresponding theoretical Calculation of the uniform mode

Study of magnetization dynamics at room temperature in periodic arrays of 50 nm thick FeNi (Py) circular magnetic dots of 500 nm radius and different center to center distance (1200 and 2500 nm), had been performed using a broadband magnetometer based on Vector Network Analyzer which works between 300 kHz and 8.5 GHz. A comparison between the dynamic response, ferromagnetic resonance (FMR) and its line-width, with static magnetic characteristics such as magnetization curves had been presented and lead to more profound vision about magnetic vortex state. The FMR peak appears just above the nucleation field and is perfectly described by Kittel formula taking into account the demagnetizing factor of an individual magnetic dot. In addition to FMR we observed a spin wave resonance below the uniform mode (mode B at Figure), which could be attributed to spin waves in confined systems. The FMR line-width shows a significant broadening close to the field region corresponding to nucleation of magnetic vortex.

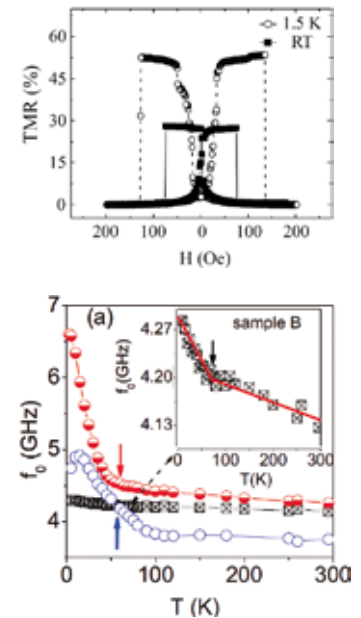
2.2 Magnetization dynamics in magnetic tunnel junctions

Fully epitaxial Fe(110)/MgO(111)/Fe(110) magnetic tunnel junctions (MTJs) have been tested with respect to symmetry-enforced spin filtering. These epitaxial but symmetry-mismatched MTJs yield tunneling magnetoresistance (TMR) values of 54% at 1.5 K and 28% at room temperature (see the figure). The TMR value and the estimated tunneling spin polarization are consistent with a partial spin filtering.

TMR at RT and LT in Fe(110) MgO(111)Fe(110)MTJs

Ferromagnetic resonance and static magnetic properties of CoFe/Al₂O₃/CoFe/Py and CoFe/Al₂O₃/CoFeB/Py magnetic tunnel junctions and of 25 nm thick single-layer Permalloy (Py) films have been studied as a function of temperature down to 2 K. The temperature dependence of the ferromagnetic resonance excited in the Py layers in magnetic tunnel junctions shows “kneelike” enhancement of the resonance frequency accompanied by an anomaly in the magnetization near 60 K (the figure shows the resonance frequency as a function of temperature for different samples). We attribute the anomalous static and dynamic magnetic response at low temperatures to interface stress induced magnetic reorientation transition at the Py interface which could be influenced by dipolar soft-hard layer coupling through the Al₂O₃ barrier.

FMR frequency vs. temperature in Py/Al₂O₃/CoMTJs



3. Phase transitions at surfaces and in thin films

Low temperature scanning microscopy measurements on (111) surface of Si with a monolayer of Pb adatoms forming $(\sqrt{3}\times\sqrt{3})R30^\circ$ structure have been made to study vertical displacements of the Pb adatoms of the monolayer by intentionally introduced additional adatoms. Also perturbations of the monolayer by pairs of the additional adatoms as well as correlations in the positions of the additional adatoms have been studied. A specific pattern of the vertical displacements produced both by single adatoms and by their pairs has been explained taking into account the $\sqrt{3}\leftrightarrow(3\times 3)$ transition taking place at a lower temperature than the temperature of the experiment. The same approach has been used to explain the interaction between the adatoms which is experimentally revealed in correlations of their positions.

Possibility of ferroelectric memory in very thin films is closely associated with stability of single domain ferroelectric state in films with real metallic electrodes. It has been argued that due to finite screening length in real metals the single domain state is at best metastable in thin ferroelectric films. Therefore, to reveal the possibilities of the ferroelectric memories one has to determine not the minimal film thickness compatible with ferroelectricity as many authors do but to determine the thickness corresponding to a sufficiently long escape time from the metastable state permitting realization of the memory of a desired duration. The problem of calculation of this escape time is very complicated but a possible path to realize the calculation has been indicated.

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Semiconductor Group (SEMICUAM)

GRUPO DE SEMICONDUCTORES-SEMICUAM

MEMBERS:

Staff:

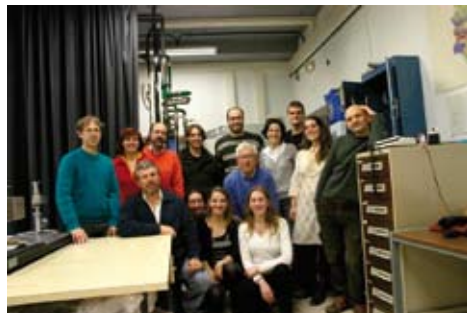
José M. Calleja
Luis Viña
Carlos Tejedor
Herko Van der Meulen
Dolores Martín
Daniele Sanvitto
Francesca Marchetti.

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Emiliano Cancellieri

Ph.D. Students:

Eva Gallardo
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Guilherme Tosi
Alejandro Gonzalez Tudela



Research at SEMICUAM has been focused both theoretically and experimentally on the light-matter interaction in semiconductors since 1983. The group contains one theory subgroup led by Prof. Carlos Tejedor and two experimental subgroups devoted to time-resolved spectroscopy (Prof. Luis Viña) and continuous wave spectroscopy (Prof. José Manuel Calleja). The main recent activities of the group are the following:

THEORY OF LIGHT-MATTER INTERACTION

Carlos Tejedor has produced seminal contributions to the theoretical understanding of light emission and absorption spectra as well as electrical transport in low-dimensional semiconductor structures. He has applied many-body theory to explain Fermi-edge singularities in quantum wires and BCS techniques to describe excitonic interactions. He has also worked in exciton condensates, spin textures in electron bi-layers and isolated or coupled QD, transport properties of QD in the Kondo-regime and light emission by coherent excitations in Qd immersed in optical microcavities. His group has performed calculations of photon correlation functions in single quantum dots, of polarization entanglement of photon pairs emitted by a quantum dot embedded in a microcavity and proposed a cavity-assisted generation of entangled photon pairs by a quantum-dot cascade decay. Recently, this theory group has started working in the quantum optics produced by more complicated and real systems as those ones formed by several unequal QD's or interacting bosonic complexes describing cavity polaritons.

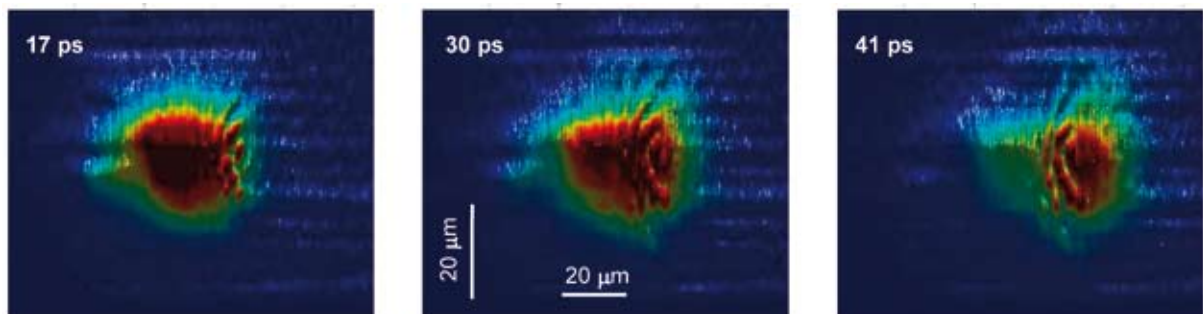
ULTRAFAST SPECTROSCOPY

The subgroup led by Luis Viña has large international recognition in ultrafast optical spectroscopy, starting with the collaboration of the group of Prof. J. Shah at the ATT- Bell-Laboratories at Holmdel (N.J., USA). This group has published the first experimental results on spin relaxation in doped quantum wells. He also discovered exciton interactions strongly dependent on spin. In the last years the group interest is focused on quantum microcavities based on semiconductor nanostructures and on the preparation of Bose-Einstein condensates in solid state systems. The group has produced pioneering work on the spin dynamics of polaritons in microcavities, which have triggered a lot of activity in the theoretical description of these processes. The group has set up the first laboratory of ultrafast optical spectroscopy (pico- and femto-seconds) in Spain.

Two of the members of the group are young “Ramón y Cajal” researchers with a significant experience in ultrafast spectroscopy and on the Physics of microcavities. M. Dolores Martín has contributed with pioneering works on the spin properties of polaritons in microcavities and has studied diverse phenomena under resonant excitation during her postdoctoral stay at Southampton University. Daniele Sanvitto held a “Marie Curie fellowship” in Paris and worked at Sheffield University until the beginning of year 2007. His main interests are in the Physics of microcavities in the strong coupling regime and in photonic crystals: from individual quantum states to collective behavior of polaritons.

In the last months the group has started a new activity on the study of hydrodynamics of polaritons, which is based on obtaining either simultaneously spatially and temporally resolved images (near-field microscopy with time resolution) or simultaneously angularly and temporally resolved images (far-field microscopy with time resolution). These studies have obtained the first experimental evidences of existence of polaritons’ superfluidity (Nature 457, 291 (2009).)

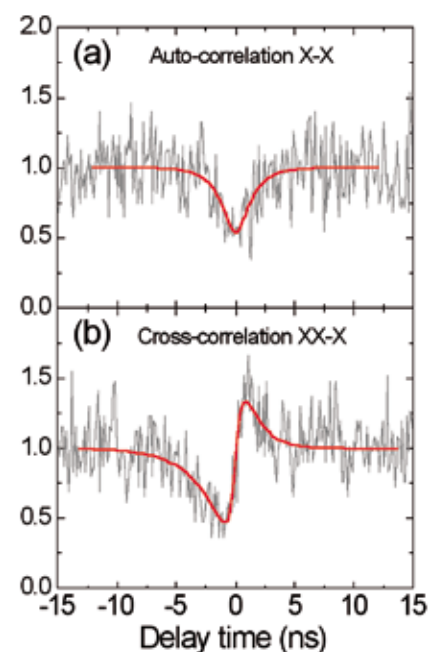
Three images of a polariton condensates flowing through a defect



CONTINUOUS WAVE SPECTROSCOPY

The CW subgroup led by J.M. Calleja is active on optical spectroscopy and light-matter coupling in semiconductor low-dimensional systems. Specific topics are:

- Single quantum dot spectroscopy** on InAs/AlAs and InP/InGaP systems, emitting in the visible region. The light emission spectra of single quantum dots reveal fine details and trends of the electronic structure (bright exciton splitting, biexciton binding energy) as a function of QD size and composition, as well as the exciton coupling mechanisms to phonons. Spatially resolved magneto-optics measurements give values of the diamagnetic shifts and Landé factors of single quantum dots.
- Exciton-photon coupling** in single InAs/GaAs quantum rings (QR) emitting in the near infrared, embedded in photonic crystal microcavities. The QR exciton emission energy is externally tuned into the cavity modes either by temperature or by thin film deposition. On resonance, changes in the light emission intensity, polarization and width reveal fundamental characteristics of the light-matter coupling mechanisms in these systems.
- Single photon emitters (SPE).** The second order photon correlation functions are measured by Hanbury-Brown and Twiss interferometry to assess emission of individual photons by quantum dots and rings. The effects of coupling to an optical microcavity, as well as excitation energy and temperature on the SPE efficiency are



Second order correlation functions of a InAs/GaAs quantum ring. The antibunching dip in (a) indicates single photon emission.

studied. Cross-correlation measurements of the biexciton-exciton (XX-X) cascade of the same or different QD allow exploring the production of entangled photon pairs for **quantum information** applications. The degree of polarization entanglement is measured by quantum tomography techniques.

c) **Nitride-based nanostructures.** Group III-nitride nanostructures emitting from the near IR (InN) to the near UV (AlGaIn) are investigated for their possible applications in high temperature-high power optoelectronic devices. The joint use of optical emission and Raman spectroscopy determine relevant parameters as crystal orientation, composition and strain. In particular the electron surface accumulation in InN nano-columns is studied by the coupled phonon-plasmon modes observed in Raman experiments.

SEMICUAM has produced the following results in the last five years:

- More than 100 papers published in international journals on the optical and electronic properties of low-dimensional semiconductor structures.
- Numerous contributions to International Conferences (> 80), of which 32 have been invited. More than 15 participations as members of the International or Programme Committees
- Participation in different European projects.
- Organization of meetings and International Conferences (Workshop INTAS in Madrid; Euro-conference on "Ultra-fast Processes in solid state nanostructures: Quantum state engineering", Toledo 2003; Optics of Excitons in Confined Systems -OECS11, Madrid September 2009).
- Direction of 11 doctoral theses finished and 7 more under elaboration.
- Participation in the "Programas de Doctorado de Calidad Física de la Materia Condensada" and "Física de Materiales" of the Universidad Autónoma de Madrid.

■ Ferroelectric Materials & Phase Transitions

Carmen Aragón López, Manuel I. Marqués Ponce

Research in ferroelectric materials and ferro-paraelectric phase transitions is being carried out in the Laboratory of Ferroelectric Materials, Department of Materials Physics, C-IV (UAM). Many applications of ferroelectric materials come from their pyroelectric and piezoelectric properties; but the more relevant are those based on its own characteristic behavior, the possibility to reverse its spontaneous polarization under the influence of an external field (switching). On this way, ferroelectric nonvolatile memories (NVFRAM) or periodically poled crystals of Lithium Niobate (PPLN) with alternating refracting index are two of the most relevant applications. Nowadays, the trend is to minimize the thickness of the ferroelectric materials in order to improve its performance in waveguides or integrated circuits.

RESEARCH PROJECT (I+D, FIS2008-00715)

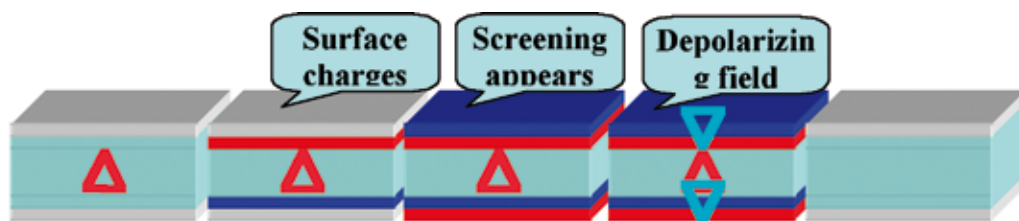
“RELAXOR FERROELECTRIC THIN FILMS: Nanometric Memories”

RESEARCH LINES

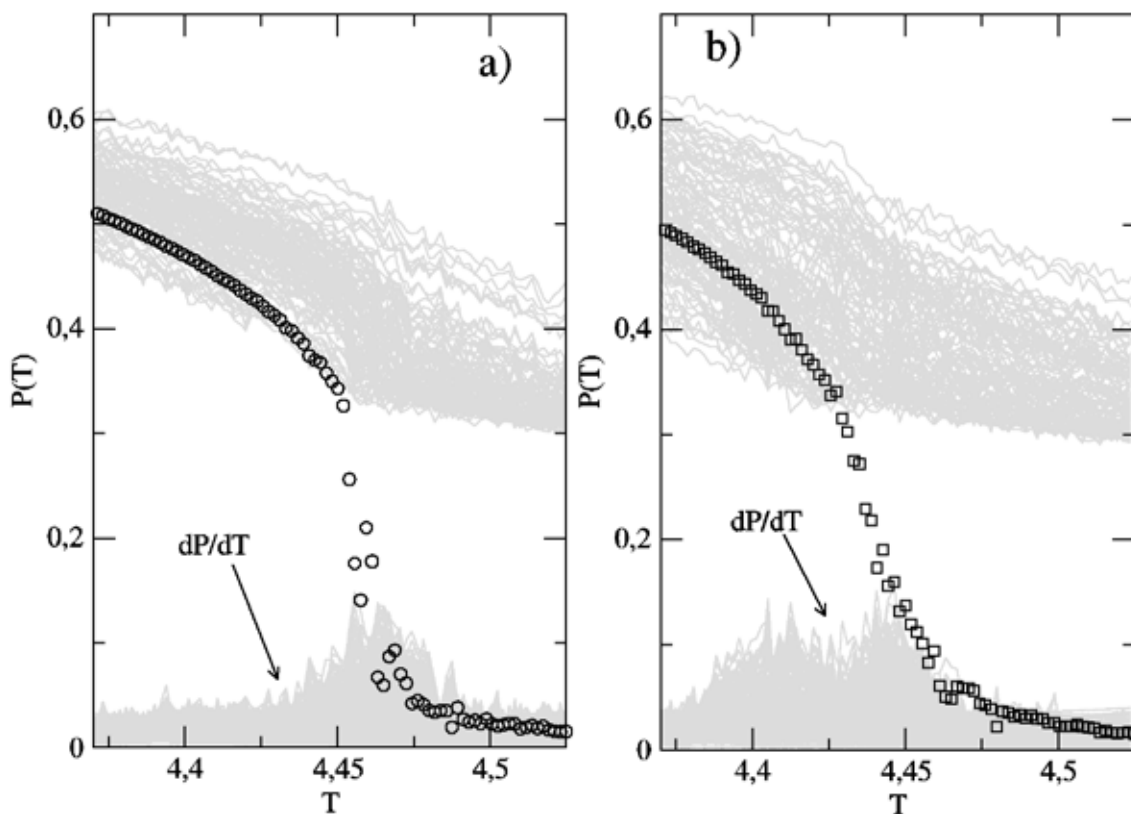
The characterization of ferroelectric materials and its corresponding ferro-paraelectric phase transition is approached from two perspectives, experimental and theoretical, both of them closely related.

A specially interesting group of ferroelectric materials, named relaxor ferroelectrics, undergoes a diffuse transition with smeared dielectric constant peak and spontaneous polarization remaining over its Curie temperature T_C that, in addition, changes with the frequency of the electric field applied. This behaviour is usually explained on terms of an intrinsic structural disorder caused by nanodomains that persist well over the transition temperature, until a higher temperature called Burns temperature T_B . All these features make them candidates as functional materials, and its behavior has been explained by a Random Field Ising Model (RFM)

Ferroelectrics are becoming outstandingly relevant in the world of technology applications at the nanoscale. In fact, recent findings of ferroelectric stability in ultra-thin films, with a thickness of just a few nanometers, have opened a complete new world of possibilities for these materials. A controllable variation of the thickness has turned out to be an effective tool for tailoring the domain structure and changing the value of ferroelectric parameters. Thin film memories based on ferroelectric materials are now a topic of main interest in the computer industry. Nanomemories consisting on a few layers of ferroelectric materials could be a promising solution to the problem of miniaturization. However, when a ferroelectric memory is written by inducing a polarization different from zero in the thin film, a depolarizing field spontaneously appears, due to the existence of uncompensated charges at the substrate. If the width of the memory is very small (down into the range of nanometres) the depolarizing field increases to a value large enough to cancel the polarization. In order to avoid this inconvenience we are planning to implement relaxor ferroelectrics thin films and to check our theoretical model, suggesting that they could be one solution to the depolarizing field problem.



Spontaneous polarization in a ferroelectric thin film memory may be unstable due to the existence of a depolarizing field created at the substrates.

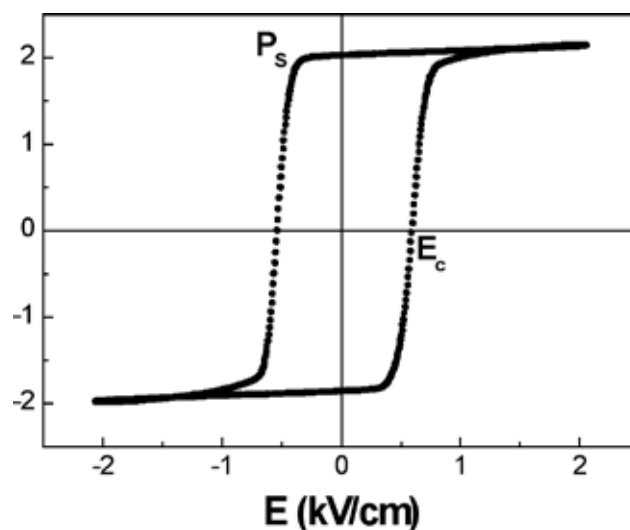


Computer simulation of spontaneous polarization of a relaxor ferroelectric in a random field Ising model for a system: a) strongly prepolarized and b) slightly prepolarized. These results show that a change of universality class may be explained by a redistribution of nanodomains caused by the prepolarization of the system.

EXPERIMENTAL TECHNIQUES

- Hysteresis Loops

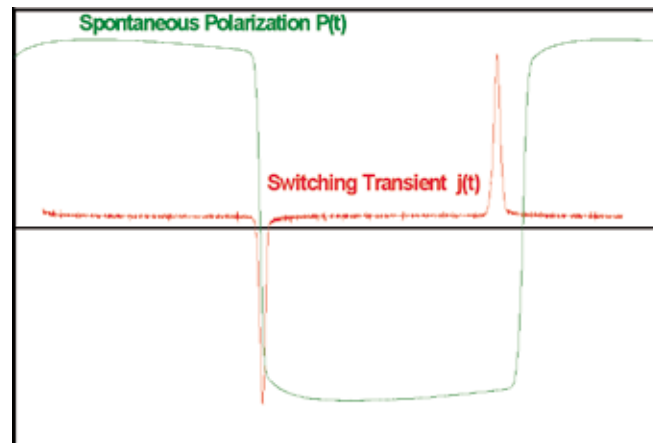
In order to observe the hysteresis loops of the ferroelectric materials, a classical DDP bridge, connected to an oscilloscope, is being used. The acquisition of the spontaneous polarization data and its analysis is fully automated. In all measurements a control of temperature (with a precision of 0.1 K) is held.



Hysteresis loop obtained for triglycine sulfate (TGS) at room temperature

- **Switching Transient**

Switching pulses on ferroelectric crystals are driven by a bipolar rectangular voltage that can be amplified until $\pm 1000\text{V}$. The length of the pulses is of $500\ \mu\text{s}$ each one and they are separated 10 ms. The maximum intensity current as well as the field amplitude at which this maximum occurs can be observed and measured simultaneously in an oscilloscope. It must be noted that we are restricted to relatively low fields and that, due to the fact that the amplification rise time is long, the rectangular voltage turns out to be almost linear with an exponential decay.



*Time dependence of the polarization $P(t)$ as obtained from hysteresis loop.
The peak of the switching transient $j(t)$ corresponds to the inversion of the slope of $P(t)$*

- **Dielectric Measurements**

The dielectric properties (dielectric constant, losses) through the transition are measured by means of a LCR bridge, with a frequency range from 20Hz to 1 MHz and a voltage range from 5 mV to 20V. The sample holder used is a liquid nitrogen cryostat that allows a temperature range from 100K to 400K.

- **Pyroelectric Measurements**

The measurement of pyroelectric current gives us decisive information about the temperature dependence of the spontaneous polarization. A special device has been constructed in order to make possible such measurements. The system possesses a charge integrator that allows the recording of the charge accumulated by means of a capacitor of $10.5\ \mu\text{F}$. Another experimental setup related with pyroelectric measurements is a thermal-electric energy converter, based in the good pyroelectric performance of ferroelectric materials.

- **Birefringence**

A high precision birefringence system is available to provide a more complete overview of the relationship between ferroelectric and optical properties.

Materials of Interest in Renewable Energy Research Group (MIRE)

MATERIALES DE INTERÉS EN ENERGÍAS RENOVABLES

MEMBERS:

Head of the Group:

Carlos Sánchez López

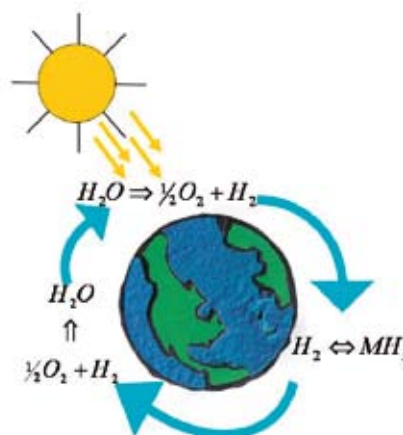
Members of the Group:

Isabel Jiménez Ferrer, José Francisco Fernández Rios,
José Ramón Ares Fernández Fabrice Leardini,
Daniel Koon (guest professor during the 2007-2008 course)

Ph.D. Students:

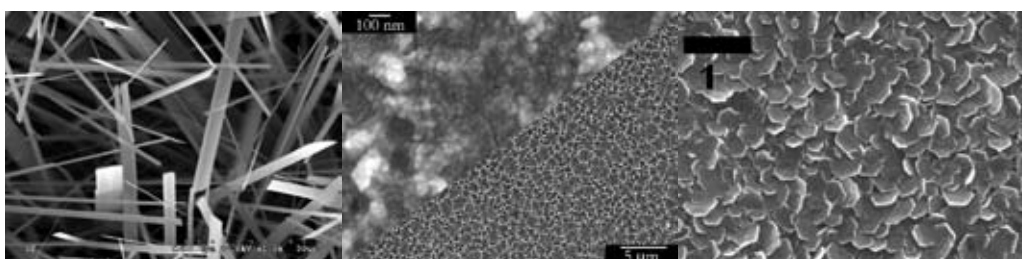
PabloDíaz Chao, Julio Bodega Magro,
José Manuel Clamagirand

Technician: Fernando Moreno de las Heras



The aims of this research group stretch from the preparation of materials useful for energetic applications to their characterisation and optimisation in experimental devices. Two fields are being investigated: metallic hydrides as hydrogen storage materials and metallic dichalcogenides thin films for hydrogen production and photovoltaic and thermoelectric applications. The group has been working in these fields for the last 20 years. Along this time, a wide experience in the preparation of materials has been developed: metal alloys (mechanical alloying, arc melting, thermal evaporation ...) and thin films of metallic dichalcogenides (flash and thermal evaporation, sulfuration, screen printing...), as well as, in characterisation techniques (structural, compositional and morphological).

We are involved in the study of storage and kinetic properties of low weight materials based on magnesium. With respect to the metallic dichalcogenides, the research is focused in transition metal sulfides (FeS₂, NiS₂, TiS₃, TiS₂, CoS₂, PdS...).



SEM micrographies of different thin films materials obtained in our lab: TiS₃, PdS and MgH₂.

EXPERIMENTAL TECHNIQUES

Experimental techniques for material synthesis available in our laboratory are the following:

- Thermal and Flash evaporation equipment, in which it is possible to prepare thin films formed by up to four different elements in vacuum and in a controlled atmosphere.
- A vacuum closed space system in a controlled temperature furnace to make sulfuration of metallic films.
- Planetary ball mill system, hydraulic press (up to 15 Ton), arc furnace machine, used for the synthesis of alloys.



SEM micrographies of MgNi alloys

- Two facilities for solid-gas reaction synthesis of metal hydrides at H₂ pressure up to 60 bar.
- Facility for electrochemical synthesis of metal hydrides with an in-situ measurement of hydrogen concentration in the metal.



Arc oven and planetary ball mill system

In relation to the characterisation of the materials developed, our lab has several experimental techniques:

- A Tian-Calvet high pressure differential scanning calorimeter suitable for “in situ” hydrogenation studies of metallic alloys.
- Thermal Desorption spectroscopy system.
- Differential Scanning calorimeter coupled to a thermal desorption spectroscopy system. Simultaneous measurements of the heat and mass evolved during the decomposition of metal hydrides can be done.
- Optic microscopy system comprising a high temperature stage for “in situ” measurements of hydride formation and decomposition.
- Profilometer system of thickness measurement for thin films.
- Experimental set up for optical, electrical (Hall effect and resistivity) and thermoelectric characterisation of the films.
- Experimental system for “in situ” measurement of electrical and thermoelectric parameters during the film formation process.

The structural characterisation is usually done by XRD, available in the SIDI service at Autónoma Univ. SEM and EDX facilities are also provided by this service. TEM is usually used in collaboration with P. Adeva (CENIM-CSIC). The group has also access to Ion Beam techniques (RBS, ERDA) and Neutron spectroscopy techniques (diffraction, INS, QNS, etc) from their collaboration with other national and foreigner groups.

FINNANCIAL PROJECTS

Financial support through the projects:

- *“Almacenamiento de hidrógeno en nanopartículas de magnesio”*. Supported by CAM. (2007).
- *“Complex metallic alloys”*. European Excellence Network. Supported by E.U. (2005-2009).
- *“Sistema Solar-hidrógeno: Materiales para la fotogeneración de hidrógeno y su acumulación en hidruros metálicos”* supported by MEyC (2005-2008).
- *“Sistema Solar-hidrógeno: desarrollo de nuevos materiales para la fotogeneración de hidrógeno y su acumulación en hidruros metálicos”* supported by MCINN (2009-2011).
- DEIMOS Project: *“Desarrollo e Innovación en pilas de combustible de membrana polimérica y óxido sólido”*, financed by CDTI through the CENIT program (2007-2011).

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Functional Nanostructures

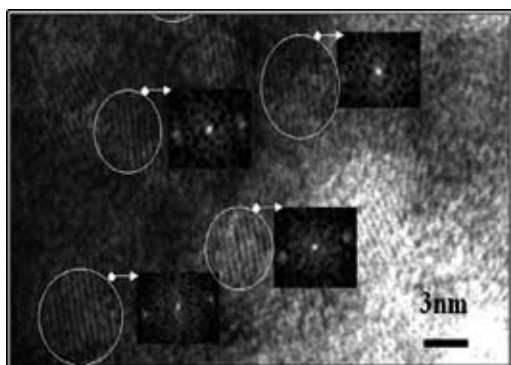
NANOESTRUCTURAS FUNCIONALES

Staff: Prof. Aurelio Climent-Font, Prof. Manuel Hernández Vélez, Prof. Miguel Manso Silván, Prof. Raul José Martín Palma, Prof. David Martín y Marero, Prof. José Manuel Martínez Duart, Prof. Vicente Torres Costa.

PhD students: Alvaro Muñoz Noval, Esther Punzón Quijorna.

Outline: The Functional Nanostructures Group is integrated by experimental scientists working in the Cantoblanco Campus (Madrid, Spain). Its members belong to the Department of Applied Physics, Universidad Autónoma de Madrid (UAM). Every member presents a characteristic skill conforming a pluridisciplinary team. The common interests are blended in the development of a diversity of research projects. The activities of the group are divided into three main research areas:

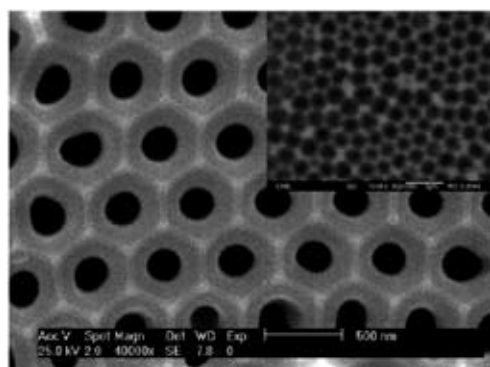
MESOPOROUS MATERIALS



X-TEM image from the PS layer grown by illumination during HF electrochemistry

The group counts with expertise in the processing, nanostructuring and optical characterization of thin films that have been applied in many scientific and industrial projects. Expertise in the preparation of nanostructured Si surfaces and their optical and electrical characterization has been acquired during the last 15 years. With these tools optoelectronic devices based in porous silicon (PS) have been prepared by electrochemical means (photovoltaic cells, Bragg reflectors, filtered emitting microcavities, gas sensors, etc.[1]) The evolution of the PS devices has even allowed proposing an optically based immuno sensor. Current activities with porous silicon include the creation of 3D refractive index contrasts for the development of

photonic crystals. These could be at the origin of new transducer mechanisms for chemical and biochemical sensors. Recently we started also the study of PS particles bearing a magnetic load or a particular surface termination. These can be used as tracers in biomedical field as fluorescent or magnetic markers.

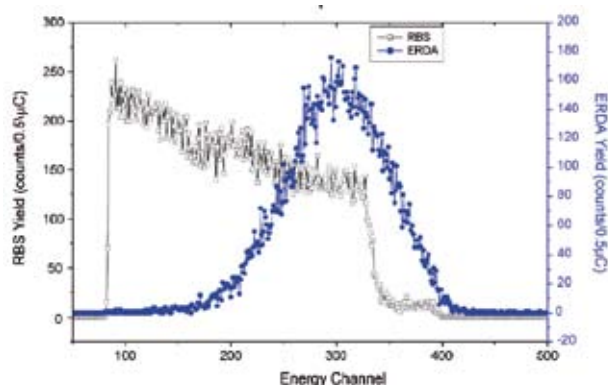


SEM image of a mesoporous alumina membrane before and after biofunctionalization (inset).

Porous alumina and titania membranes (PAI, PTi) have been also an intense subject of study for the last 10 years. Ordered structures have been obtained with different electrochemical environments and applications have been envisaged for the processing of high aspect ratio semiconductors and magnetic materials [2]. Furthermore, these materials can be biofunctionalized exhibiting biosensing properties by optical transduction. Recent applications include their use as masks for ion beam modification allowing transferring the structure of the membrane to the underlying material.

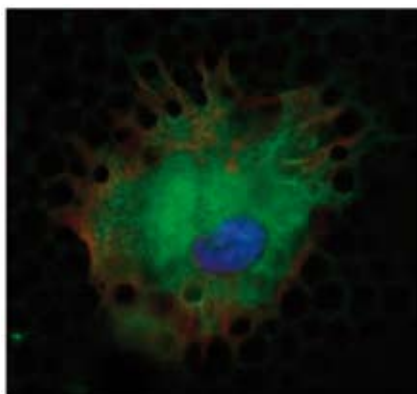
ION BEAM MODIFICATION AND CHARACTERIZATION

Most of the materials processed in the group are the subject of a deep microanalysis characterization. Techniques available at CMAM include RBS and ERDA, allowing in depth compositional distribution studies. Modification is also possible by using a wide bunch of ions in the MeV range. Currently, the effects



of Si implantation in Si wafers and its influence in formation of PS is under study. The selective transformation of TiN into TiNO is also under development. From the biomedical point of view, ERDA characterization is especially useful since it allows the detection of light elements from the surface involved in functional groups (N, C, O, S) [3] or in the degree of denaturation-condensation of biomedical polymers (H content).

BIOMEDICAL MATERIALS AND SENSORS



The preparation and characterization of biomaterials, both in the organic and inorganic world, is one of the emerging activities of the group. This line includes the chemical functionalization and colloidal nanostructuring of surfaces. To achieve so, the group relies in both plasma deposition and sol-gel chemistry equipment. In the recent past the collaborations have further grown along the biomedical field. Materials and systems designed and controlled in the group have been assayed at molecular and cellular level at the Department of Molecular Biology. Moreover, since the beginning of a research line based on the differentiation of Human Mesenchymal Stem Cells (HMSC), the group has designed both materials and systems to help determining the parameters that

control that differentiation. However, further ingredients to achieve controlled differentiation of HMSC are needed [4].

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Group of Laser Spectroscopy

GRUPO DE INVESTIGACIÓN EN ESPECTROSCOPIA LASER

Members of the Group:

Luisa E. Bausá
 José García Solé
 Daniel Jaque
 Carmen de la Heras
 Juan Antonio Sanz
 Maria de la O Ramírez

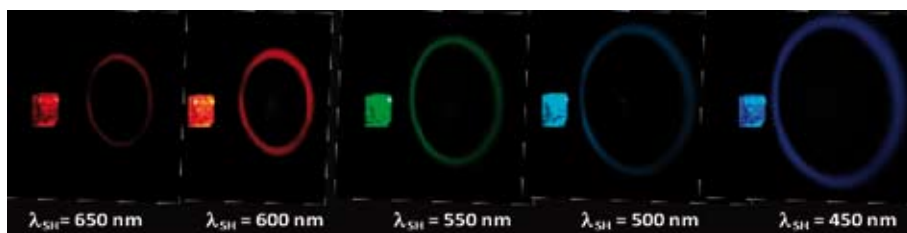
Ph.D. Students

Pablo Molina
 Airan Ródenas
 Emma Martín
 Jesús Vicente García Santizo
 Antonio Benayas



The research activity of GIEL has been centred on solid state lasers, covering basic stages such as material preparation, optical spectroscopy, and laser gain. Recently, the group has been also interested in other aspect such as frequency conversion processes, tunability or optical bistability, which constitute additional functions that can be integrated in the active laser media and which can confer a multifunctional character to solid state lasers. A way to enlarge the range of materials useful for controlling and handling light is, for instance, adjusting the composition of materials to the molecular level, which means looking for completely novel material, or by looking for novel processes. Another way is using new types of configurations or superstructures on known materials. Structuring the materials in the micro and sub-micrometer region constitutes a good method to get a spatial or spectral control of the electromagnetic radiation. In particular, when an appropriated structure is practised on a solid state laser crystal, new optical functions can be added. The aim of our work is the extension of the functionality of optically active materials to include new linear and non-linear processes provided by different configurations. We address the problem by using different approaches:

TWO DIMENSIONAL NONLINEAR PHOTONIC CRYSTALS ON SOLID STATE LASERS



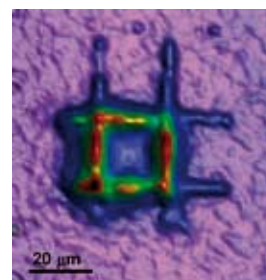
Far field pattern of ringshaped second harmonic generated from a Nd³⁺ doped SBN laser crystal in the range 430-680 nm.

The functionality of ferroelectric-based laser materials can be extended by using different types of ferroelectric domains structures practised on those solid state laser crystals. We

will show how by using two-dimensional anti-ferroelectric micro-domain structures novel frequency conversion processes can be obtained. Specifically, we will show how by means of the appropriated structure and configuration, multiple-direction second harmonic generation can be continuously tuned in an extremely broad frequency range covering the whole visible spectrum. The results are promising for novel optical multifunctional devices based on solid state lasers, which can simultaneously act as multiple harmonic generators, nonlinear prisms or all optical deflectors.

MICRO AND NANO PROCESING BY ULTRAFAST LASER INSCRIPTION

The ability of ultra-short laser pulses to modify at the micrometric and sub-micrometric scale the refractive index of transparent materials is being used for the fabrication of novel photonic devices. Among the different photonic devices that can be fabricated is worth to mention the fabrication of optically activated waveguides and three dimensional photonic crystals capable of controlling the spontaneous emission provided by trivalent Rare Earth ions. Despite the practical interest of these devices, ultra-fast laser inscription also opens a new window for the study of light matter interaction at extreme conditions such as strong spatial and temporal confinement of photons. In this sense the group is also making an effort trying to understand the nature and extension of the effects induced in the irradiated material.



Confocal fluorescence of induced stress in Nd³⁺:YAG ceramic after inscription with 150 fs laser pulses

OPTICALLY ACTIVE DIELECTRIC NANOPARTICLES

Some of our interest is now focussed in inorganic nanocrystals (sizes shorter than 100 nm) that can produce visible light under infrared (IR) illumination for high resolution optical imaging in biomedical applications. We are mostly dealing with two kinds of systems: (i) Dielectric nanocrystals (mostly fluorides) doped with pairs of trivalent rare earth optically active ions (for instance Yb³⁺/Er³⁺), which can produce visible fluorescence under two-photon IR excitation processes (up-conversion) and (ii) nanoparticles made of non-linear crystals that convert input IR radiation into visible light via second harmonic generation. For this last purpose we investigate different non-linear Niobate crystals (LiNbO₃; NaNbO₃, KNbO₃ and Sr_{0.6}Ba_{0.4}Nb₂O₆) with different particle sizes.

MULTILAYERS FOR REFLECTION AND ANTIREFLECTION COATING

The group is also working in the growth and characterization of different types of multilayers (namely, Sb₂S₃/MgF₂ and ZnS/MgF₂) useful as reflection and antireflection coatings for laser crystals. Structural and microstructural properties of grown samples are studied. The grown samples are optically analyzed by measuring the transmittance and reflectance in the VIS and IR range. Multilayers properties are studied in relation to the number of layers and also in relation to the first deposited layer material on the substrate.

In the two-year period 2007-2008 the group has carried out an intense activity, participating in different research projects and given rise to around 40 papers published in international journals, 11 invited presentations at international conferences, organization of the international meeting DPC07, presentation of 2 doctoral thesis and four more under elaboration.

Non-Linear Optics and Optical Waveguides Group

Members:

Prof. Mercedes Carrascosa Rico, *permanent member*.
Prof. José Manuel Cabrera Castillo, *permanent member*.
Dr. Ángel García Cabañes, *permanent member*.
Dr. Olga Caballero Calero, *post-doc*.
Mr. Javier Villarroel Freites, *graduate student*.
Mr. Jesús Carnicero Gómez, *graduate student*.

Research lines:

1. Nonlinear waveguide fabrication and characterization:
 - Proton exchanged waveguides
 - Novel nano-structured waveguides produced by swift-heavy ion irradiation
 - Electro-optical and nonlinear optical behaviour
2. Photorefractive effect and holographic devices
3. Photorefractive optical damage inhibition in high power devices
4. Quasi phase-matching by ferroelectric domain inversion.

Research projects

- “Dispositivos no lineales, holográficos y electroópticos en materiales ópticos nanoestructurados obtenidos por irradiación con iones de alta energía”. DGICYT, Ministerio de Educación y Ciencia (MAT2005-06359-C03-01). (Sub.: 148.750 €).
- “Dispositivos fotónicos en guía de onda mediante micro- nano- procesado por irradiación con iones pesados de alta energía”. DGCYT, Ministerio de Ciencia e Innovación (MAT2008-06794-C03-01). (Sub.: 116.160 €).

Thesis

- Jun – 2007. Olga Caballero Calero, “Nonlinear optical waveguides in LiNbO_3 and Periodically Poled LiNbO_3 ”. European Thesis.

MoLE (Moving Light and Electrons)

MOLE (MOVIENDO LUZ Y ELECTRONES)

Members:

Head of the Group:

Prof. Juan José Sáenz

Members of the Group:

Dr. Pedro García-Mochales,

Dr. Manuel Marqués

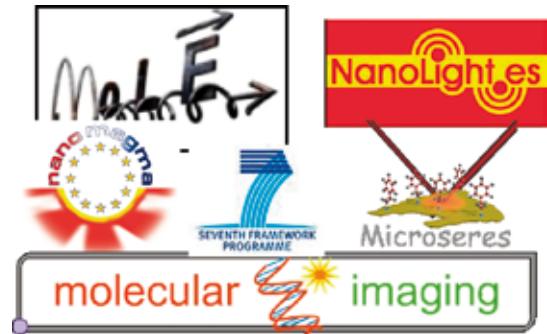
Dr. Manuel Donaire,

PhD Student:

Silvia Albaladejo,

Enrique Sahagún

Irene Suárez



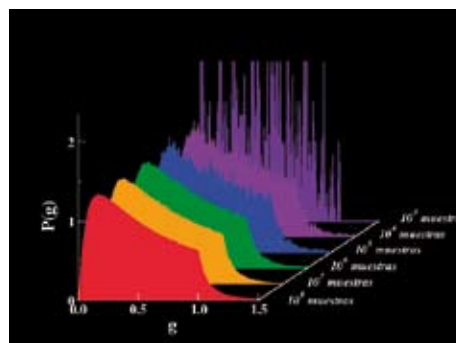
The group research is focused on different theoretical and modelling aspects related to nanoscience. At present the group research interests include theoretical modelling of scanning probe microscopies (SPM), quantum electron transport through nanocontacts, wave transport through complex media and optical phenomena at the nanoscale. MoLE group is involved in the organization of the annual meetings of the Spanish Nanotechnology Network (NANOSPAIN) and the prestigious “Trends in Nanotechnology” (TNT) conference series since 2000.

The group is partner of the Consolider Project **Nanolight**, **Microseres-CM** and of the European Projects **Molecular Imaging** (“Integrated Technologies for in-vivo Molecular Imaging”) and the **NanoMagMa** (Nanostructured active Magneto-plasmonic Materials)

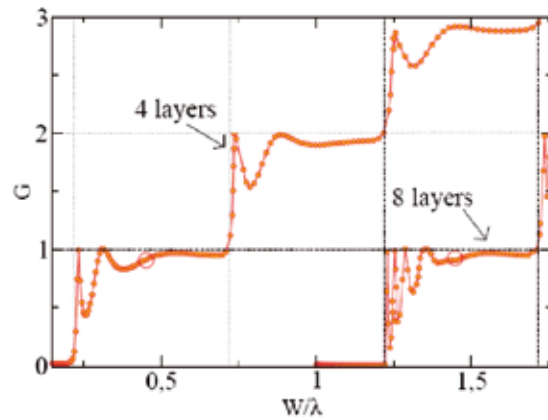
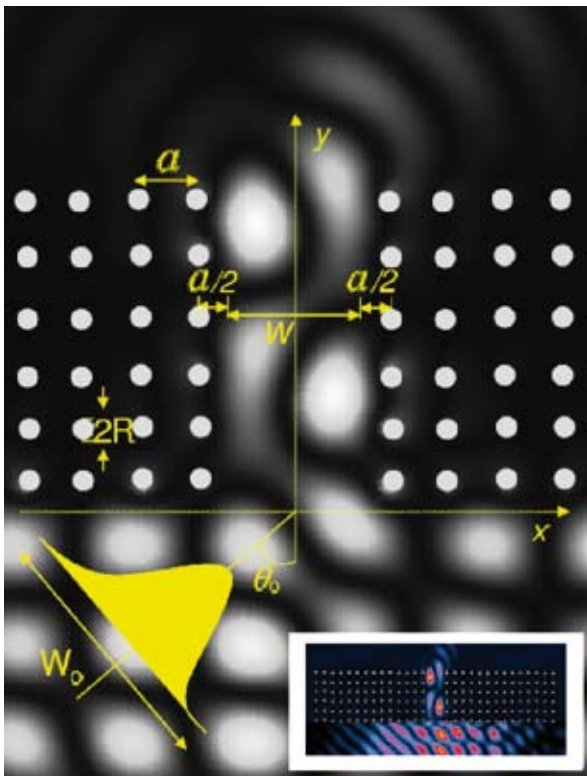
Wave Scattering in Complex Media

The research covers different aspects of interest in classical and quantum wave transport through mesoscopic systems. We focus on the properties and the calculation of the Scattering Matrix of very different systems. We have developed a very efficient numerical scheme that uses an exact mode-matching technique together with a generalized scattering matrix method. For disordered systems the statistical properties are analyzed in terms of Random Matrix Theory. Our current work along this line covers:

- Quantum Conductance in Nanometer Sized Contacts.
- Wave Transport through Surface-Corrugated Waveguides
- Conductance Distributions in Disordered Wires.
- Intensity Correlations and Fluctuations in Random Media.
- Electromagnetic Field-Particle Interactions in Waveguides.
- Electrodynamic interactions in Photonic Crystals.



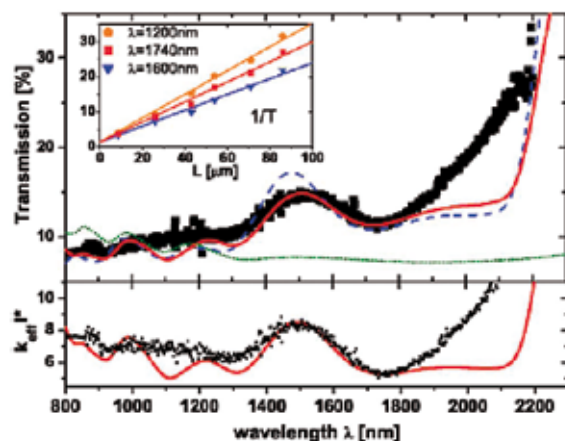
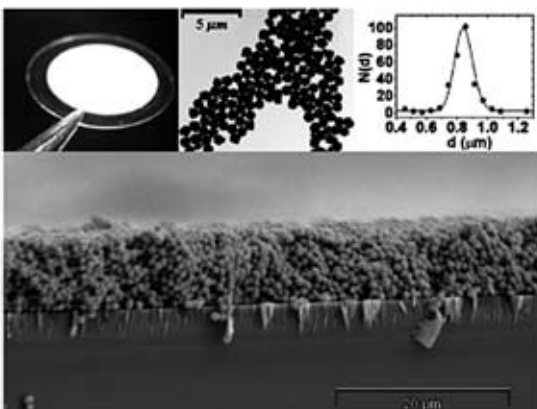
Here we discuss briefly some of the new concepts developed during the last two years (07-08).



Optical Conductance: We introduced the concept of optical conductance in order to characterize the transport properties of **waveguides built into finite photonic crystals**. The conductance is given by the integral of the transmission cross section as a function of the incoming angle. This concept is illustrated by exact calculations of the light-guiding properties of a waveguide built into a photonic crystal slab based on a square lattice of dielectric cylinders in air. In analogy with their electronic

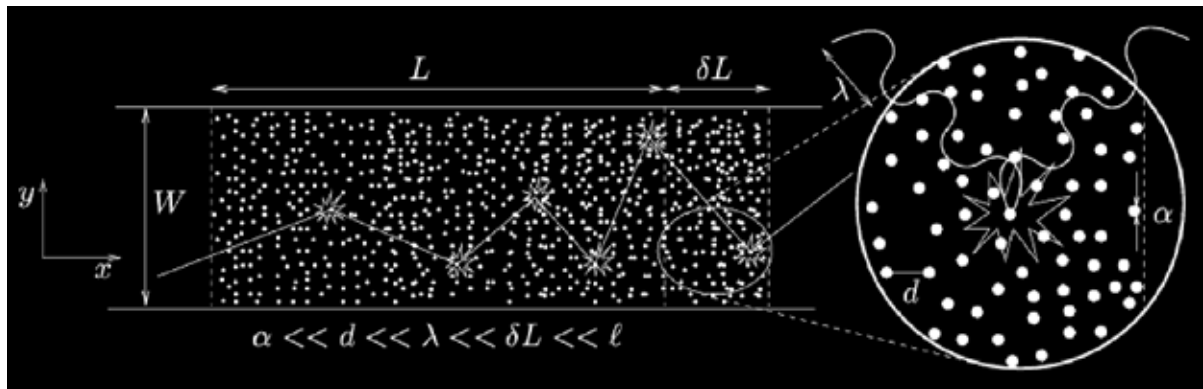
counterparts, the optical conductance of a waveguide is quantized and thus provides a direct measure of the number of guided modes supported by the system. (After Albaladejo et al. Appl. Phys. Lett. (07))

Transport of light in amorphous photonic materials (In collaboration with Prof. Scheffold's group at Fribourg): We have analyzed the optical properties of amorphous photonic materials based on dense assemblies of high refractive index spherical particles are presented. Light transmission through these photonic glasses shows nontrivial wavelength dependence. The transmission spectra can be quantitatively reproduced by modeling theoretical properties starting from their building blocks. Our results emphasize the relevance of including short range order correlations and an appropriate effective refractive index in the analysis of light transmission through amorphous photonic materials. (After Reufer et al. Appl. Phys. Lett. (07))

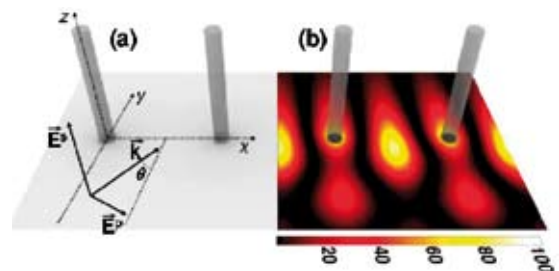


Statistical scattering of waves in disordered waveguides: In collaboration with Prof. Mello group at UNAM, we have developed a new theoretical approach to analyze the statistical properties of wave transport through a disordered sample. In this new theory, which generalizes previous Random Matrix

theory approaches, we analytically derive the statistical properties of a thin slab (“building block”) of length dL from a potential model and used to find the evolution with length of the expectation value of physical quantities. We found that the corresponding statistical properties of the full system depend only on the mean free paths and on no other property of the slice distribution. We pointed out the relevance of correlations between the spatial positions of the scatters. We founded that light transmission through disordered media with strong spatial correlations shows nontrivial wavelength dependence in the transmitted intensity.



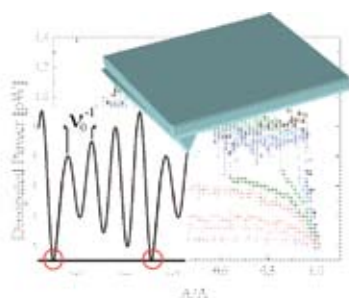
Fluorescence lifetime (In collaboration with Prof. Carminati’s group at ESPCI Paris): We have focused on single-molecule fluorescence in complex systems, where the complexity comes from the interaction with nanoscale structures or a disordered environment. We have shown how periodic nanostructured dielectric substrates or metallic systems involving coupled surface electromagnetic modes can be engineered to control spectrally and spatially the fluorescence dynamics. We have designed numerically dielectric structures (gratings of nanocylinders) which lead to spatially localized fluorescence enhancement without quenching. Such structures could improve the sensitivity of ex-vivo imaging and biosensing techniques bringing current concepts of nanophotonics to the field of fluorescence detection and imaging. (Laroche et al. Opt. Lett (07)).



We have studied fluorescence lifetime fluctuations in a disordered system with nanoscopic length scales, in both the single and the multiple scattering regimes. Numerical experiments and theoretical modelling have been performed using a 3D cluster of dipole nanoparticles as a model system. We have shown that lifetime fluctuations carry information on the local (submicron) scale around the emitter, and that the scattering properties (structural information) and the absorption (spectroscopic information) could be somehow decoupled. This might lead to novel ideas in the field of fluorescence imaging in complex media.

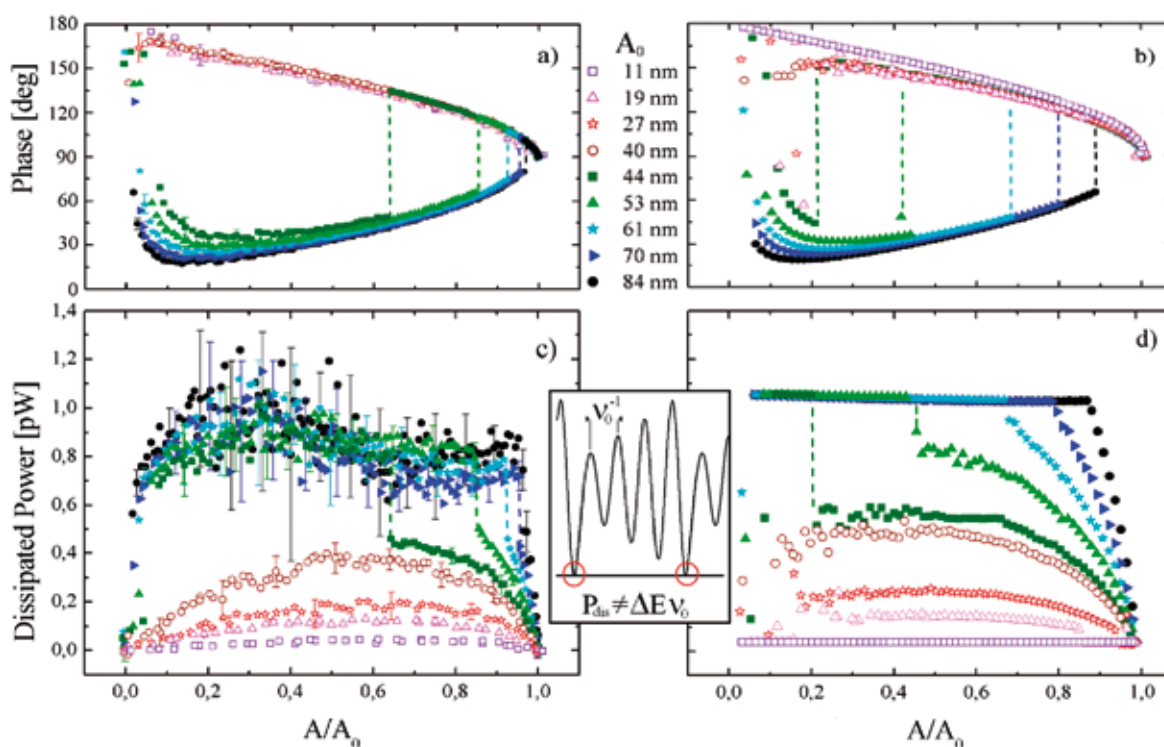
Dissipation at the nanoscale:

Adhesion hysteresis in Dynamic Atomic Force Microscopy



Recently we have developed a method for the measurement of hydrophobicity using a conventional AFM. Acquiring amplitude (A) and phase (φ) it is possible to calculate power dissipated P_{dis} . In presence of humidity capillary condensation takes place linking the tip to the substrate. The power dissipated in the neck breaking process depends directly in the size of the condensed water neck that in turn depends on the hydrophobicity of the sample (Sahagún et al. Phys. Rev. Lett. (07)).

We have also studied the effects of adhesion hysteresis in the dynamic-dissipation curves measured in amplitude-modulation atomic force microscopy. Hysteresis in the interaction forces is shown to modify the dynamics of the cantilever leading to different power dissipation curves in the repulsive and attractive regimes. Experimental results together with numerical simulations show that power dissipation, as measured in force microscopy, is not proportional to the energy dissipated in the tip-sample interaction process.



Experimental (a) and calculated (b) phase shift and experimental (2c) and theoretical (2d) dissipated power versus the oscillation amplitude obtained as the tip-sample distance is reduced. Symbols correspond to different free oscillation amplitudes A_0 . Experimental data were smoothed (average over 10 data points) and the standard deviation is shown. The time evolution of the tip-sample distance in the attractive regime is sketched in the central inset.

(After M. Köber et al, PSS-RRL 2, 138 (2008).

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Paramagnetic Resonance Spectroscopy of Solids

GRUPO DE RESONANCIA PARAMAGNÉTICA DE SÓLIDOS

Members:

Staff:

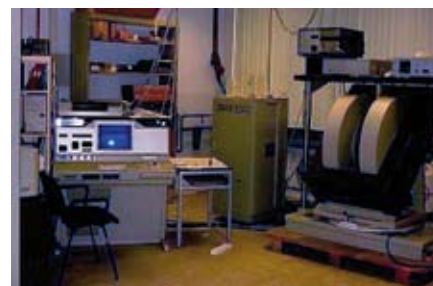
Fernando J. López
David Bravo

Other Centers members:

Agustín Martín

Ph.D. Students:

Juan C. Lagomacini



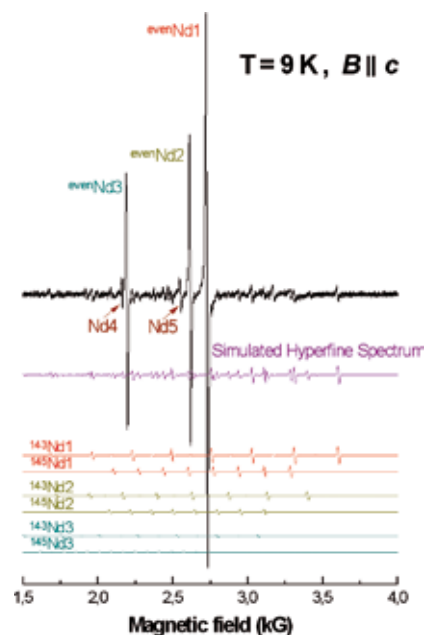
THE TECHNIQUE

In this Laboratory the Electron Paramagnetic Resonance (EPR) technique is used to investigate different solid state materials both dielectric and semiconductors. This technique gives very detailed information about the microscopic structure of point defects in crystals. In particular, it is possible to determine the symmetry of the environment of the paramagnetic entity which is detected (usually a paramagnetic impurity or intrinsic defect) so that the arrangement of the surrounding ions can be deduced. Moreover the spin of the paramagnetic ion or defect is determined. With all these information it is possible to propose a detailed model for the defect.

RESEARCH LINES

Photonic materials

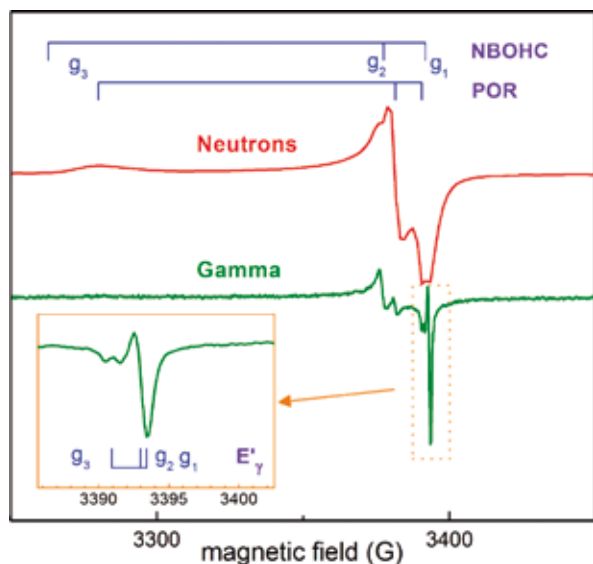
Research include the understanding of the photorefractive properties of various materials and their relationship with impurities. Also, new candidates for solid state lasers are studied. These lasers consist on a crystal host doped with one or more laser-active impurities. The EPR technique allows determine the microscopic structure of emitting centers.



EPR spectrum of Nd³⁺ impurities in β -BaB₂O₄ single crystals.

Insulating materials for fusion technology

In the future thermonuclear fusion reactors a number of insulating and transparent elements will be exposed to very strong irradiation of various types: gamma, neutrons and ions. The defects produced drastically modify their properties making them unusable. This research intends to determine the nature of defects produced by irradiation, their evolution as well as the thermal stability in order to propose the most adequate materials to be used in such environment.



EPR spectrum of vitreous silica irradiated with gamma or neutrons showing various electron or hole centers.

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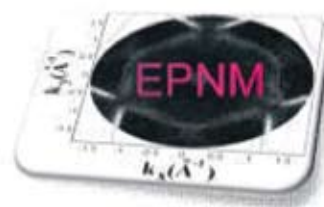
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Electronic Properties of Novel Materials (EPNM) Group

GRUPO “PROPIEDADES ELECTRONICAS DE NUEVOS MATERIALES”

Members:

Prof. Enrique García Michel
 Dr. Pilar Segovia
 Dr. Silvina Bengio
 Dr. Miguel Angel Valbuena
 Ph.D. Students: Lucas Walczak

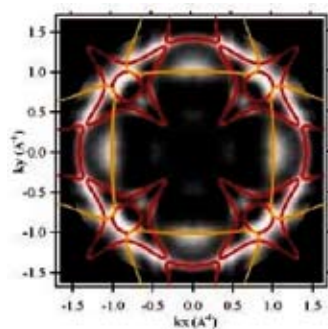


The Electronic Properties of Novel Materials (EPNM) group belongs to the Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid (UAM). Our main research interest is the study of the electronic and crystalline structure of surfaces and interfaces and of low dimensional materials.

Our primary technique is Angle-Resolved-Photoemission Spectroscopy (ARPES) that we employ to study the electronic structure of solids. Also Low Energy Electron Diffraction (LEED), Auger Electron Spectroscopy (AES) and X-ray Photoelectron Spectroscopy (XPS) are currently performed in our laboratory for complementary structural information and previous characterization of the surface. In addition to the in-house activities, some experiments are carried out in several Synchrotron Radiation Facilities, where we have regular access. For instance, Surface X Ray Diffraction measurements at the ESRF (Grenoble) or HRPES at Elettra (Trieste), MaxLab (Lund) or the SLS (Villigen). Besides this, we participate in different international collaboration programmes.

Our research topics include:

SURFACE PHASE TRANSITIONS



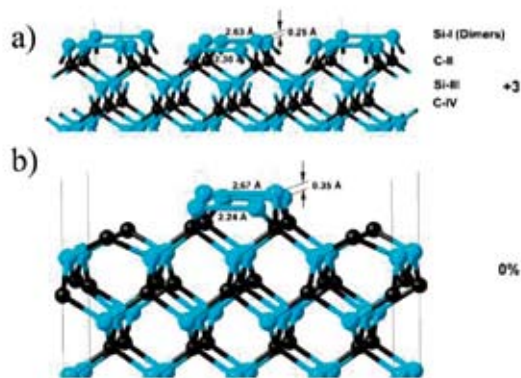
Fermi surface of 0.5 ML of Sn on Cu(100). Nesting in this Fermi surface drives a temperature induced phase transition [1].

We study the modification of the electronic structure induced by Surface Phase Transitions. Charge density waves (CDW) or Mott transitions are representative examples of two dimensional structural phase transitions associated to an electronic gap opening at the Fermi level. The stabilization of a charge density wave state by the Peierls mechanism is due to the opening of a band gap in the Fermi Surface for some reciprocal space regions that are coupled efficiently by a phonon (Fermi Surface nesting by electron-phonon interaction). The Mott transition is due to electron-electron interactions. In other cases studied the phase transition is triggered only by dynamical fluctuations. In order to visualize the electronic properties Angle Resolved Photoemission (ARPES) is the technique of choice, due to its ability for providing a direct measurement of the spectral function for each momentum and energy. Fermi Surface mapping measurements offers detailed information about the electronic structure changes during

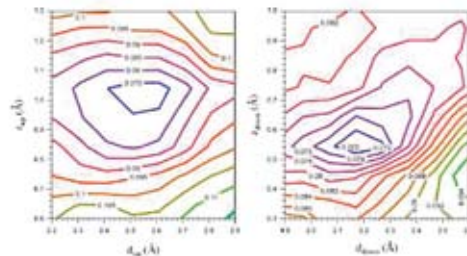
the transitions. Complementary Surface X-ray diffraction (SXRD) measurements provide information on the crystalline structure of the different phases.

SILICON CARBIDE

Silicon carbide has superior properties for several applications, compared to silicon. Besides these features, its complex surface reconstructions exhibit fascinating physical properties. We have determined the structure of several of these reconstructions of cubic SiC using photoelectron diffraction. In particular, the nature of the $c(4 \times 2)$ reconstruction of 3C-SiC(001) has been analyzed in detail [2]. The results support the alternating-up-and-down-atom model (AUDD), thus solving a long controversy on this matter.



Calculated SiC(001)-(4x2) reconstruction. For clarity, only the top layers of the 11-layer models are shown. (a) AUDD reconstruction (obtained for as 3% strain) . (b) AUDD structure for 0% lateral strain.



R-factor contour plots in the vicinity of the optimal crystalline structure.

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[2] *Atomic structure determination of the 3C-SiC(001) c(4x2) surface reconstruction: Experiment and theory* A. Tejeda, E. Wimmer, P. Soukiassian et al. *Physical Review B* 75 (19) (2007) 195315

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Scanning Probe Microscopy in Ultra-High Vacuum and Nanoscience: NanoSPM Group

MICROSCOPIA DE PROXIMIDAD EN ULTRA-ALTO VACÍO Y NANOCIENCIA:
GRUPO NanoSPM

Members:

Prof. José M. Gómez-Rodríguez

Dr. Celia Polop (*Ramón y Cajal researcher*)

Dr. Iván Brihuega (*Ramón y Cajal researcher*)

Dr. Nicoleta Nicoara (*Post-doc*)

Ph.D. students:

Antonela C. Marele

Antonio J. Martínez-Galera

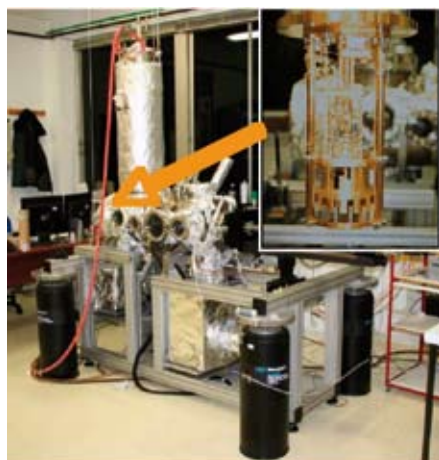
Miguel Moreno Ugeda

Bruno de la Torre



The main research lines of the NanoSPM group are summarized in the following:

SPM INSTRUMENTATION IN ULTRA-HIGH VACUUM

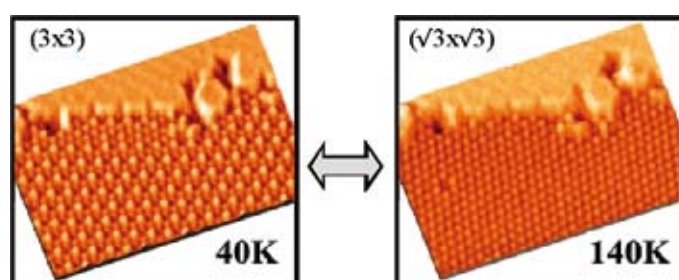


Home-made 4K UHV scanning tunneling microscope

The NanoSPM group has a long standing tradition in the development and construction of advanced instrumentation in scanning probe microscopy [1]. In particular, this group has designed and built several variable temperature scanning tunneling microscopes [2] able to operate between 40 and 400 K under ultra-high vacuum (UHV) conditions. Its most recent accomplishment has been the design and construction, for the first time in Spain, of a low temperature (4 K) UHV scanning tunneling microscope. This new system, fully developed in the course of Miguel Moreno Ugeda's PhD thesis, is completely operative since 2008 and it is being used at present for the analysis of the electronic properties of surfaces and nanostructures with high spatial and energy resolutions.

Currently, another ambitious instrumentation project is under development by Dr. Nicoleta Nicoara: a non-contact atomic force microscope (NC-AFM) that will operate under UHV conditions and low temperatures (4K). Again, this will be a unique instrument in Spain that will allow to gain access not only to metal or semiconductor surfaces and nanostructures but also to insulating materials at the nanoscale.

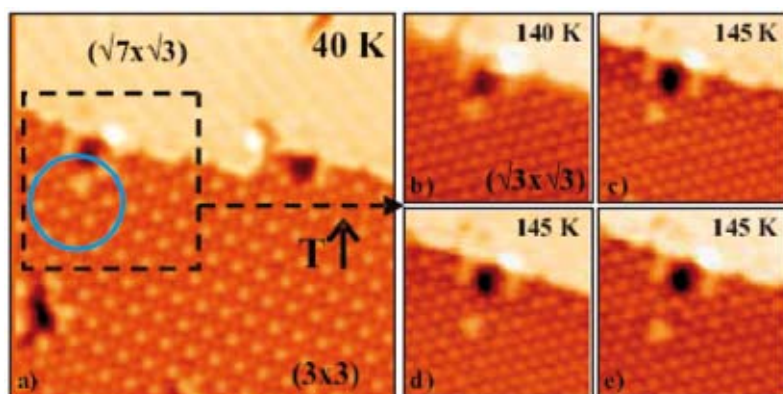
SURFACE PHASE TRANSITIONS ON METAL-SEMICONDUCTOR SYSTEMS



"True" variable temperature STM measurement of a surface phase transition on Pb/Si(111). Exactly the same region is observed with atomic resolution below (left) and above (right) the critical temperature [3]

We have carried out in the last few years several studies on surface phase transitions taking place at low temperature on metal-semiconductor systems. In particular, we have analyzed the (3×3) to $(\sqrt{3} \times \sqrt{3})$ phase transition on Pb/Si(111) and Pb/Ge(111) surfaces [3,4] by means of variable temperature STM. In a peculiar way of operating the STM that we have called "true variable temperature", we have been able to image exactly the same surface areas with atomic resolution while varying the temperature. This has allowed us to detect the intrinsic character of the phase transition regardless of the presence of atomic defects on the surface and to extract the critical exponents and critical temperature of the phase transition. Moreover, we have also reported for the first time the existence of a new kind of substrate mediated interaction between adatoms adsorbed on surfaces that present the softening of phonon modes associated with the presence of low temperature phase transitions [5]. This works have been performed in collaboration with several theory groups at UAM (Profs. A. Levanyuk, J.J. Sáenz, R. Pérez and Dr. A. Cano) and experimentalists at Osaka University (Prof. S. Morita and Dr. O. Custance).

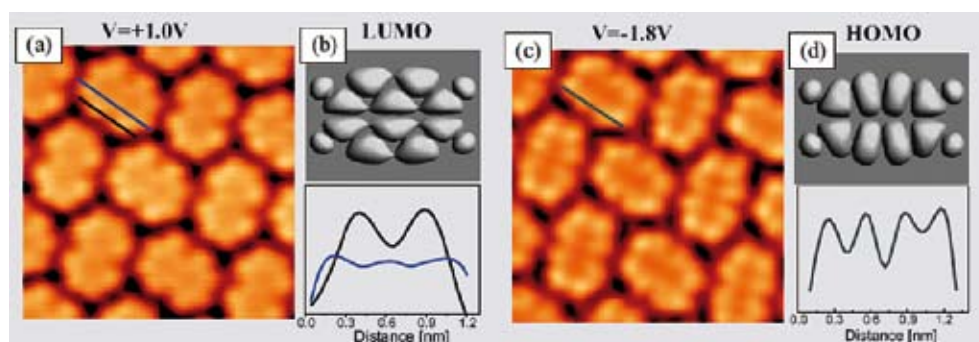
SURFACE DIFFUSION ON SEMICONDUCTORS



STM images showing exactly the same single adatom (outlined with a circle) on a Pb/Si(111) surface in a temperature range between 40 and 145 K. The latter temperature is the onset for surface migration of the adatom to neighboring sites [6].

was performed at temperatures well below room temperature but above the critical temperature for the phase transition that this surface experiences. In this way, the activation energy and the preexponential factor for the surface diffusion of single adatoms on the high temperature phase have been obtained. It was also studied the role played by the underlying low temperature (3×3) phase at these higher temperatures.

GROWTH AND ELECTRONIC STRUCTURE OF SELF-ASSEMBLED MOLECULAR LAYERS ON SURFACES



Comparison of STM images on PTCDA/Au(111) with DFT calculated molecular orbitals of the free PTCDA molecule [7].

We have carried out several studies on the adsorption, growth and electronic properties of self-assembled molecular layers on metal and semiconductor surfaces by means of scanning tunneling microscopy

and spectroscopy combined with photoemission experiments and first-principle calculations performed in collaborations with other experimental and theoretical groups (Profs. J.A. Martín-Gago, J. Méndez and E. Román in ICMM-CSIC, Prof. J.M. Soler and Dr. O. Paz at UAM, Prof. N. Lorente at ICMB-CSIC, among others). Several organic/inorganic systems have been analyzed, e.g. PTCDA (3,4,9,10-perylene-tetracarboxyl dianhydride) on Au(111), Cu(111), Si(111)-(7x7); triazine on Cu(111) and 4,4'-bipyridine on Au(111), Ag(100) and Cu(110).

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Group of Surfaces and Thin Films at CMAM

GRUPO DE SUPERFICIES Y PELÍCULAS DELGADAS DEL CMAM

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Victor Joco

The Surface and Thin Films group at the Centro de Microanálisis de Materiales (CMAM) of the Universidad Autónoma de Madrid (UAM) is devoted to the growth and characterisation of new materials in systems of reduced dimensionality. A new experimental system is currently in its final stage of construction and commissioning. It is an ultra-high vacuum (UHV) designed to carry out accurate structural studies in thin films, surfaces and nanostructures. In-situ sample growth can be performed by molecular-beam epitaxy (MBE) in an auxiliary chamber equipped with up to six evaporators, as well as with facilities for substrate cleaning, surface preparation and deposition control, such as a gas inlet system, a sputtering gun and a quartz microbalance. There is the additional possibility to install a radiofrequency atomic source for the growth of films of metal nitrides and oxides. A powerful set of characterization facilities will be available in situ, including an electron optics for the performance of low-energy electron diffraction (LEED) and Auger spectroscopy, and the equipment required for high- and low-energy ion beam analysis (IBA). The system is coupled to the 5 MV tandem accelerator of the CMAM, which can be applied for sample modification and for High-Energy Ion Scattering (HEIS) studies. A low energy (up to 10 keV) ion source for high-resolution Low-Energy Ion Scattering (LEIS) studies is also attached to the main UHV chamber. Surface studies are particularly powerful due to the combined use of MBE, LEED/Auger and LEIS/ToF. The use of low energy ions (up to about 10 keV) allows to extract precise structural information about the first few monolayers of the sample.

The system at this moment is starting to be used for the growth of magnetic materials. Information storage in magnetic media is a very important field of research, and the search for magnetic materials with the required properties is an active field of research. It is expected not only to increase the capacity of conventional magnetic devices, but also to develop spintronic elements that should allow new architectures like for example magnetic MRAM memories based on magnetoresistive elements or magnetic tunnel junctions (MTJ). We aim at the fabrication and characterisation of thin films with this type of magnetic properties. A group of materials very interesting in this respect are the oxides of transition metals and rare earths in which conduction electrons can show high degree of spin polarization. We plan to grow epitaxial iron oxides on metallic as well as insulating substrates and perform a detailed structural characterisation due to the strong dependence of the magnetic properties particularly in epitaxial systems.

We are also involved, in collaboration with the Applied Physics Department of the UAM (Prof. C Palacio and Dr. A Arranz), in the development of new alternatives to synthesize mixed-oxide thin films in order to be able to design thin films with the possibility to tune their properties between those specific of the binary oxides forming the film for their use as variable refractive index films for functional and/or structural applications. Choosing the appropriate mixed-oxides will allow to obtain not only thin films with suitable optical properties but also to improve their tribological properties. The mixed-oxide thin films will be based on transition metals (Cr, Ta and Hf) and Si or Al. The films will be synthesized by ion beam methods (ion beam mixing, IBM, and reactive co-sputtering) and in particular we will explore as a novelty the synthesis by IBM using O₂⁺ on bilayers. The mixing will be carried out at low energies (0–6 keV), for films below 100 Å, and also at high energies, 200–300 keV, for films of thicknesses above 2000 Å. AES, XPS, ARXPS, ISS, UPS, EELS will be used for analysis as well as RBS, GDOES, XRD, AFM and optical characterization techniques. This characterization should allow establishing a correlation between the physical-chemistry properties of the films and the deposition parameters in order to facilitate the synthesis of thin films with specific properties in a controlled way.

The work of the group has focussed in the last years in the construction of the above mentioned experimental systems, while it has been also active in the following fields of research:

An essential element in order to achieve a reliable structural characterization using ion beams is the possibility to perform accurate and fast simulations. We have developed a new computer code for the simulation of ion scattering in solids. This program TRIC (Transport of Ions in Crystals) combines the power of a "brute force" method, in which trajectories are simulated realistically, with a high computing efficiency, which allows its use for structural determination in a wide range of ion energies and experimental conditions. The program applies the ideas of importance and stratified sampling, well known in other applications of Monte Carlo simulations by concentrating samples in the regions of phase space which give the highest contribution to the yield in the detector and correcting with the appropriate weighing factor. This is implemented by the generation of showers of scattered and recoiled atoms in directions close to the detector at every close encounter of an ion with an occupied lattice site [5].

We have studied the stability of three-dimensional islands (quantum dots) formed under highly mismatched epitaxy by means of atomistic simulations using simple analytical interatomic potentials. We have studied their nucleation behaviour [3] and the influence of classical effects arising from the competition of step-edge energy and strain release at steps on the stability of coherent islands. The conclusion is that these need to be taken into account, in addition to the electronic contribution to the cohesion energy, in order to understand the observed height distribution of coherent islands [1].

We have studied the electronic structure and magnetic properties of systems of rare-earth metals by spectroscopic methods. We have performed an extensive study of the electronic structure of Tb(0001) by means of angle-resolved photoemission spectroscopy [2] and we have found a strong temperature dependence of the magnetic interlayer exchange coupling between magnetic rare-earth metals Gd and Tb separated by nonmagnetic Y that even leads to reversals of the sign of the coupling [4]. This has been explained in terms of magnetization-dependent reflectivity of electrons of opposite spins at the magnetic-nonmagnetic interfaces.

We have been working in the synthesis and characterization of coatings (oxides, nitride, and borides) for improved oxidation resistance [6] or mechanical properties [7-10]. In particular, we have done an extensive research in the design of new multifunctional biocompatible coatings for load-bearing applications [11-13]. Finally we have developed improvements in the depth profiling of thin films by GDOES in the nanometric range [14-15] and in terms of multilayer modeling [15], or nitrogen calibration [16-17] for accurate quantitative analysis.

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Photovoltaic Materials Group

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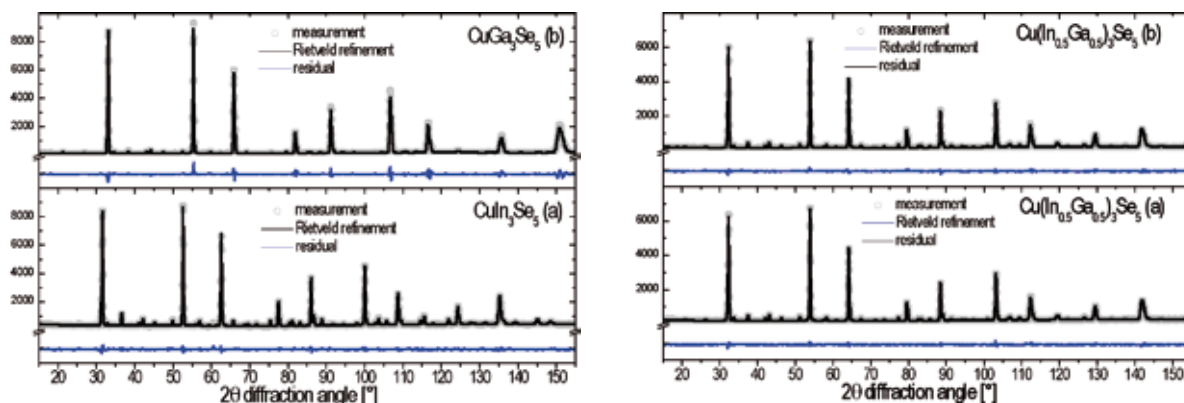
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Photovoltaic Materials Group

The Photovoltaic Materials Group has a large experience in the synthesis and characterisation of several ternary and multinary compounds, among them $\text{Cu}(\text{Ga},\text{In})(\text{Se},\text{Te})_2$ -type compounds as well as $\text{Cu}(\text{Ga},\text{In})_x\text{Se}_y$ -type, more commonly known as “ordered defect compounds” (ODC), have extensively been studied. We have dealt with a considerable number of characterisation techniques such as X-ray and electron diffraction, Rietveld refinement of powder X-ray diagrams, Laue techniques, transmission electron microscopy (TEM) and extended X-ray absorption fine structure spectroscopy (EXAFS), as well as energy dispersive X-ray analysis, optical transmission and reflectance and ellipsometric measurements. Our experience also involves thin films deposition with several evaporation techniques (thermal, “flash”, e-beam) among which the “flash” evaporation method has been extensively used to deposit and characterise $\text{Cu}(\text{Ga},\text{In})\text{Se}_2$ and $\text{Cu}(\text{Ga},\text{In})_x\text{Se}_y$ thin films for Mo/ $\text{Cu}(\text{Ga},\text{In})\text{Se}_2$ /ODC/CdS/ZnO-type solar cells.



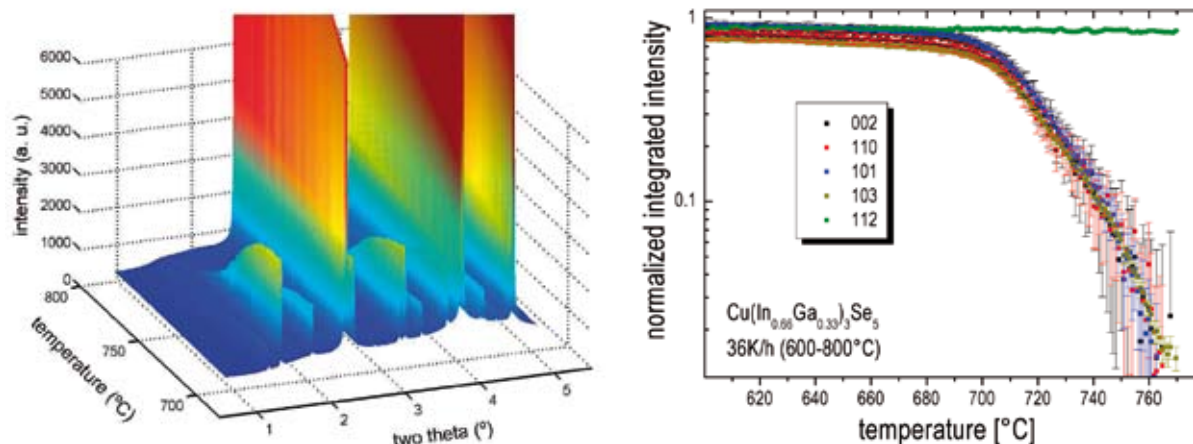
Neutron powder diffraction measurement (grey circles), Rietveld refinement (black line), and the corresponding residuals (blue line) for the boundary compounds CuIn_3Se_5 , CuGa_3Se_5 and for $\text{Cu}(\text{In}_{0.5}\text{Ga}_{0.5})_3\text{Se}_5$ synthesised in two different ways.

OPTICAL AND STRUCTURAL ANALYSIS OF SINGLE CRYSTALS AND THIN FILMS OF SEVERAL “ODC” FOR PHOTOVOLTAIC APPLICATIONS

In collaboration with several groups from different former Soviet Union countries (Department of Semiconducting Materials Science Institute of Applied Physics, Chisinau, Moldova; Department of Semiconductor Materials Technology, Tallinn Technical University, Tallinn, Estonia; and Department of Radioelectronics, Belarusian State University of Informatics and Radioelectronics, Minsk, Belarus) and coordinated by the Photovoltaic Materials Group, we have synthesised and explored the structural and mainly the optical properties, by ellipsometric measurements, of several ternary compounds belonging to the ODC family, namely CuGa_xSe_y and CuIn_xSe_y , with $x = 3, 5, 7$ and $y = 5, 8, 11$. All these works have been published in many contributions to different journals (see the publication list)

STRUCTURAL STUDIES ON THE PHASE TRANSITIONS IN THE CuIIISe_2 - $\text{CuIII}_3\text{Se}_5$ - $\text{CuIII}_5\text{Se}_8$ SOLID STATE SYSTEMS

On the other side, in collaboration with the “Helmholtz Zentrum für Materialien und Energie” (HZB), we have studied, by neutron diffraction at the Berlin Neutron Scattering Center (BENSC), and refined the crystalline structure of different compounds belonging to the $\text{Cu}(\text{Ga},\text{In})_3\text{Se}_5$ and $\text{Cu}(\text{Ga},\text{In})_5\text{Se}_8$ solid state systems, previously synthesized in our laboratories. Such work has been presented at the MRS-Spring Conference.

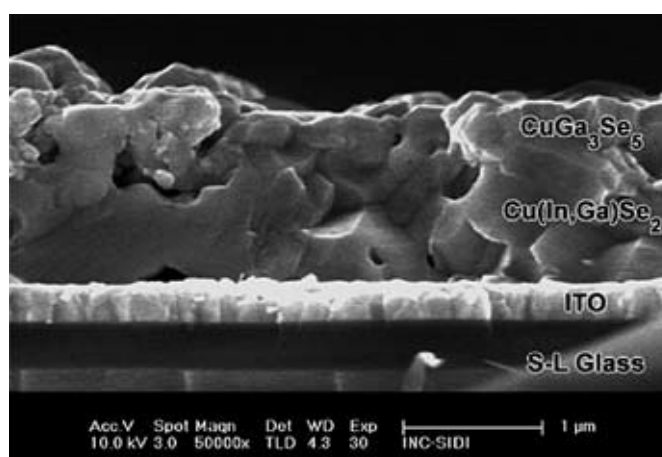


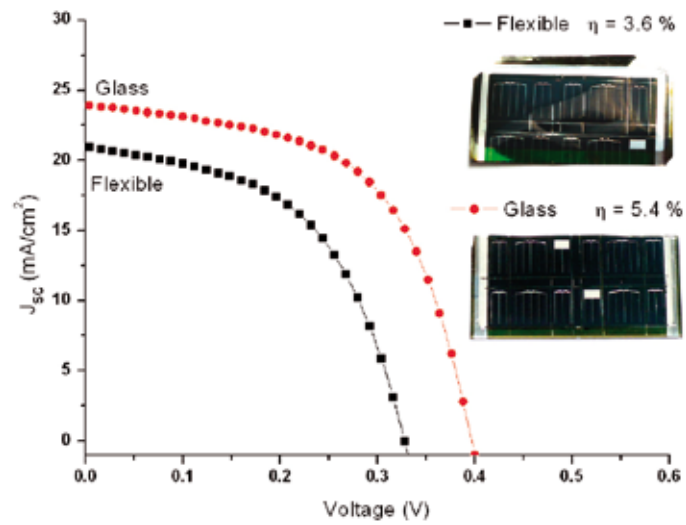
Intensity evolution with temperature of some reflection peaks (left) and integrated intensities vs. temperature (right) for the $\text{Cu}(\text{Ga}_{0.33}\text{In}_{0.66})_3\text{Se}_5$ sample.

More recently, jointly also with the HZB group and the High Energy Beamline (ID15) from the E.S.R.F., we have also studied the phase transitions in both solid state systems by X-ray diffraction at different temperatures, refining as well the diffractograms for each compound. The analysis of the diffusion mechanisms that control these phase transitions is now in progress.

FLEXIBLE SOLAR CELLS

The Photovoltaic Materials Group has also developed the deposition by the “flash” evaporation method of thin films of $\text{Cu}(\text{Ga},\text{In})\text{Se}_2$ and $\text{Cu}(\text{Ga},\text{In})_3\text{Se}_5$ for solar cells fabrication onto rigid (soda-lime glass) and flexible (polyimide) substrates, in collaboration with the Energy Department, Renewable Energies Division (CIEMAT), Institute of Polymer Science and Technology (CSIC) and Institute of Technology E-I3 (Helmholtz-Zentrum Berlin für Materialien und Energie). In such way, several photovoltaic devices on the basis of Glass or polyimide / Mo / $\text{Cu}(\text{Ga},\text{In})\text{Se}_2$ / $\text{Cu}(\text{Ga},\text{In})_3\text{Se}_5$ / CdS / ZnO have been fabricated and tested, and are currently under improvement.





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■ Liquids and Complex Systems Group

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The Liquids and Complex Fluids Group aims to advance research on the liquid state of matter and soft matter in general by applying numerous theoretical techniques based on equilibrium and non-equilibrium statistical mechanics, such as density-functional theory and computer simulations. Our scope encompasses both the microscopic and mesoscopic length scales in systems that range from 'simple' liquids to soft condensed matter and biologically-inspired systems. Topics range from the structure and dynamics of pure liquids and their interfaces, to complex fluids such as colloids, liquid crystals, biological membranes, vesicles, etc. The group has strong interest in biopolymers, and more specifically on protein filaments that play a role in cell division and structural stability of cells. Other topics covered include liquid crystal mixtures, confined liquids and fluids at interfaces, and more recently granular matter. An active and fruitful collaboration with the experimental group of Marisela Vélez (IMDEA-Nanociencia) is now under way. Likewise a strong link exists with the group of Enrique Chacón of the Madrid Materials Science Institute (CSIC) and various groups in Europe.

CAPILLARY WAVES AT INTERFACES

Our work in the field of capillary waves in the liquid-vapour interface has been modulated by the recent, increasingly accurate, experimental measurements which confirmed the existence of a layered structure in the normal direction in the liquid-vapour interface of some metals. Some workers have related this oscillatory structure to the metallic character of the fluid. However, already in our first paper, we suggested that this peculiar property was not specific to the metallic state, but actually much more general and associated with fluids with a high ratio of melting to critical temperatures. This work led us to face the problem of trying to establish a connection between the mesoscopic capillary-wave theory (CWT) and the microscopic van der Waals theory. In later work we have been successful in establishing such a connection by formulating an operational definition for the 'intrinsic surface' of microscopic configurations obtained from Monte Carlo simulations. We concluded that the use of CWT as done by the experimentalists is not entirely correct. Our intrinsic density profiles exhibit a marked structure, in agreement with experiment but, in line with our previous work and contrary to the contention of experimentalists, this structure is a general behaviour of fluids: it is the poor experimental resolution that hides this structure, except in metals where the oscillations are much more pronounced. As a result, a new picture emerges where the liquid surface resembles a solid surface, with only two parameters containing the relevant microscopic information of the surface: population of first layer, and distance between the first two layers. Both these parameters are accessible experimentally. On the other hand, the new picture may have an impact on other relevant problems, such as: reactivity in liquid surfaces, observation and manipulation of liquids using force microscopy, etc. Finally, in the last two years we have generalised this approach to molecular liquids, such as water and alkane fluids, and have studied the connection between hydrodynamics and capillary waves at the nanoscopic scale.

PROTEIN FILAMENTS AND THEIR ROLE IN CELL DIVISION

Work in this area involves the study of properties of protein filaments and their role in the mechanical forces necessary for cell division. By using coarse-grained model for the proteins, based on information extracted from Atomic Force Microscopy images of adsorption of FtsZ bacterial polymers on mica, we have provided a mechanical explanation for the formation of cytoskeletal rings and helices under the constraints imposed by the curved cell membrane and shown that the phase diagram of possible shapes depends crucially on the existence of lateral interactions. Also, these interactions suggest a mechanism by which these polymers could generate the force on the cell membrane necessary to initiate cell division. These and future studies on this problem rely very strongly on experimental information obtained from biosynthetic experiments performed by the experimental Group of M. Vélez (IMDEA – Nanociencia), with whom we have a strong and fruitful collaboration.

HYBRID COMPUTER SIMULATION TECHNIQUES

In this research line, led by Rafael Delgado-Buscalioni starting from his recent enrollment in the group as a Ramón y Cajal researcher, we develop simulation methods that combine microscopic scales (based on particles and interactions) with mesoscopic scales (in terms of effective particles or coarse-grained models) and continuum theories, with methods to correctly and consistently match the two descriptions. More specifically, we have developed a method to couple the dynamics of a liquid at the nanoscale (atomic detail) with a surrounding liquid described by fluctuating hydrodynamics by exchanging fluxes in a way that respects the conservation laws of fluid mechanics. Application of these methods to dynamical and flow problems involving shear and sound waves have been performed. This line is heavily connected with some of the previous lines. For example, the dynamics of nanoscopic capillary waves in simple liquid surfaces has been analysed using these methods, and hydrodynamics have been shown to be valid for surprisingly small wavelengths (of a few molecular diameters) provided the wavenumber dependence of the surface tension is considered.

FRUSTRATION EFFECTS IN CONFINED LIQUID CRYSTALS

Liquid crystal, characterised by an average direction of molecular alignment (director), have a large susceptibility to external fields (in the form of bulk fields, surface fields or, in the case of smectics, confinement along the direction of the director, which creates commensuration effects). Most application of liquid crystals in display-cell technologies rely on these properties and it is crucial to understand theoretically the underlying physics of confinement. When a confined nematic material is subject to antagonistic boundary conditions at two surfaces (e.g. slit pore geometry), say planar (parallel to surface) and homeotropic (perpendicular to surface), several director configurations may result. The final configuration arises from competition between elastic, surface and capillary effects. A step configuration (where the director changes abruptly in some region of the cell) has been shown to be stable under some conditions. The popular elastic theory predicts either a continuously tilted director configuration or a uniform configuration and it fails, by construction, to account for the step phase. Monte Carlo (MC) simulation studies on a lattice Lebwohl-Lasher model give support to the step phase, but the interpretation of its role in the capillary phase diagram is misleading. A more recent MC study on a (continuum) Gaussian overlap model does not provide conclusive evidence. We have predicted the complete phase diagram using density-functional theory for models of hard rods and explained the relative phase stability of the different phases. Also, an explanation for the link between these confined phases and the wetting and bulk properties of the material has been provided.

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Scanning Probe Microscopy Theory & Nanomechanics Group

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Our work is focused on ab initio modelling of different problems in Materials Science and Nanotechnology that involve forces and currents at the atomic scale. In particular, we try to understand and develop new capacities for the basic tools in Nanotechnology, the Scanning Probe Microscopes (SPMs), that enable us to use currents and forces to visualize and manipulate matter at the nanoscale.

We work, in close collaboration with experimental groups worldwide, in topics such as:

1. Scanning Tunneling (STM) and Atomic Force (AFM) Microscopes: Atomic contrast, energy dissipation mechanisms and nanomanipulation.
2. Nanomechanics: Fracture. Friction and Wear at the atomic scale. Mechanical and Transport properties of nanocontacts.
3. Adsorption, reactivity, and self-organization of fullerenes and other organic molecules on surfaces.

We use a suite of total-energy methods based in Density Functional Theory (DFT) , --from very efficient codes based on local orbitals (like FIREBALL and OPENMX) to more accurate implementations based on a plane-wave basis (CASTEP, VASP)-- in order to provide a realistic description of the mechanical and electronic properties. The transport properties are calculated with a non-equilibrium Green's function formalism, that can be naturally linked with the local orbital DFT methods.

Recent Research Highlights

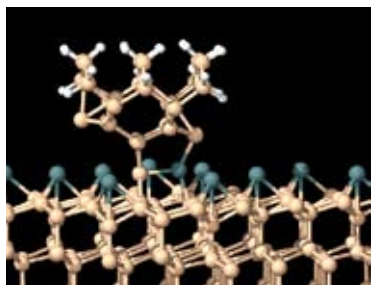
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G. Otero, G. Biddau, C. Sánchez-Sánchez, R. Caillard, M. F. López, C. Rogero, F.J. Palomares, N. Cabello, M.A. Basanta, J. Ortega, J. Mendez, A.M. Echavarren, R. Pérez, B. Gómez-Lor and J. A. Martín-Gago, Fullerenes from aromatic precursors by surface-catalysed cyclodehydrogenation, *Nature* 464, 865-869 (2008)

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Research Activities

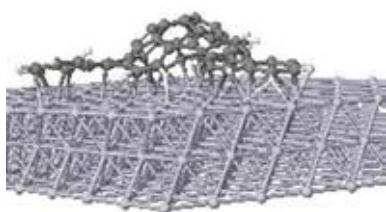
Imaging, Manipulation, Chemical Identification with Dynamic AFM



Scanning Probe Microscopes are the basic characterization tools in Nanotechnology. The Atomic Force Microscope (AFM) has recently shown its ability for atomic-scale imaging of surfaces, using the force acting between tip and sample when they are in close proximity.

Our group employs first-principles atomistic simulations to study the basic properties underlying AFM operation and to extend its outstanding capabilities to include single atom manipulation, chemical identification and nanotribology.

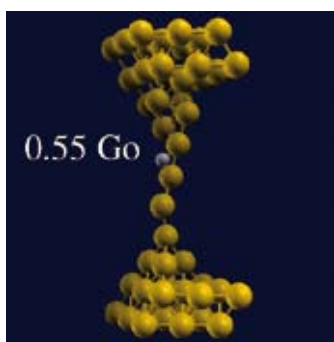
Adsorption & Reactivity of Organic Molecules on Surfaces: Towards the Synthesis of Fullerenes and Triazafulerenes



Tuning the unique electronic and mechanical properties of fullerenes by selective “doping” will pave the way for nanotechnology applications, including molecular electronics and nanomagnetism. However, heterofullerenes and endofullerenes are very difficult to synthesize.

In a collaboration with organic chemists and surface scientists, we have been exploring alternative routes for azafullerenes based on planar aromatic precursors and the catalytic role of reactive metallic surfaces in the activation of cyclodehydrogenation processes.

Nanocontacts: Conductance, Forces & Reactivity



Nanometer-scale structures differ substantially from their bulk counterparts in the transport properties --e.g. conductance quantization in metallic nanocontacts-- and in the chemical reactivity --catalytic activity of oxide-supported gold nanoparticles--.

Our group has pioneered the simulation of the whole breaking process for metallic nanocontacts, including the presence of defects and different molecular species, in order to get access to realistic structures before the final nanocontact break.

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Surface Science Laboratory at UAM (LASUAM)

LABORATORIO DE SUPERFICIES DE LA UAM-LASUAM

Members:

Head of the Group: Rodolfo Miranda

Members of the Group: Juan José de Miguel, Amadeo López Vázquez de Parga, Jesús Alvarez, José María Gallego, María José Capitán, Juan José Hinarejos, Daniel Farías, Julio Camarero

Postdocs: Bogdana Borca, David Ecija, Antonio Politano, Nikolai Mikuszeit, Julio Camarero, Miguel Ángel Niño

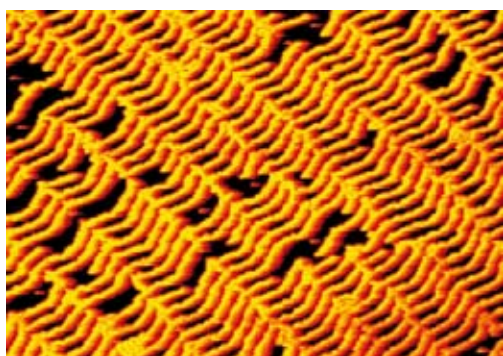
Ph.D. Students: Marta Trelka, Daniel Barredo, Pablo Nieto, Christian Urban, Erika Jimenez, Josefa María Rodríguez, Sara Barja, Manuela Garnica

The Surface Science Group (LASUAM) of the Universidad Autónoma has kept the tradition for research in surface science initiated by Prof. N. Cabrera. The research team is headed by Prof. R. Miranda, an experienced scientist in surface science for over 20 years. The group's members participate in a large number of research projects and contracts, both national and international. An important scientific output has derived from this activity, including more than 100 international publications, a similar number of communications to specialized conferences and 14 PhD's.

The main facilities of the laboratory include: High-resolution Helium Atom Scattering; LEED; photoemission electron spectroscopies (XPS, UPS); variable temperature and 4K STM and STS, AFM; facilities for molecular beam epitaxy (MBE) under UHV; in situ (UHV) magneto-optical Kerr effect (MOKE) and Kerr microscopy. The main recent research activities of the group are the following:

ORGANIC MOLECULES ON SOLID SURFACES

The ability to design, synthesize and organize organic molecules with different functionalities has increased during the last years in a spectacular way. This has led to the development of a new field, organic electronics, which has made possible a more flexible, light and cheap technology, including the fabrication of organic displays, solar cells, and field effect transistors.



Self-assembly of the organic acceptor PCBM on Au(111).

The subgroup TIREMISU (Time Resolved Microscopy of Surfaces), led by Roberto Otero and José M. Gallego, has focused its research activity during the last years on the study, by scanning tunneling microscopy, of the self-assembly of organic molecules on solid surfaces onto functional molecular nanostructures with photovoltaic functionality. In general, these studies have been complemented with other *external* techniques such as photoemission spectroscopy or theoretical calculations.

As a model system for a bulk heterojunction photovoltaic device (i.e., an all organic photovoltaic device consisting in thin films of blended electron acceptors and donors), we have investigated the lateral segregation of donor/acceptor binary mixtures on a Au(111) surface. We have shown that the nanopattern imprinted on the surface by the gold reconstruction directs the growth of a lateral superlattice of donor and acceptor areas, about 10 nm-wide, a morphology that has been described as ideal for the performance of this type of cell.

In hybrid photovoltaic devices charge separation is started by a charge transfer from the photoexcited dye molecule to a solid surface. The role of the dye molecule is just that of an antenna to capture sunlight and release electrons, the same function carried out by biological antenna complexes, which trigger

photosynthesis after photon absorption. We have studied the self-assembly of a Zn-porphyrin derivative on different metal surfaces, demonstrating that this species self-assemble into long 1D coordination polymers with a structure that closely mimics that of the antenna complexes in green photosynthetic bacteria.

Another research line is the investigation of the assembly and reactions of chiral aminoacids on dehydrogenating catalytic surfaces. The target of this research line is the development of new enantioselective heterogeneous catalysts for the chemical and pharmaceutical industries.

MOLECULAR BEAM STUDIES OF REACTIVITY OF SOLID SURFACES

Studies of elementary collision processes of H₂ with metal surfaces can provide benchmark tests of theoretical methods that are used to aid the design of new heterogeneous catalysts. Molecular beam and associative desorption experiments have been carried out to understand the main factors that govern H₂ dissociation at the surface, while vibrationally inelastic and rotationally inelastic scattering experiments have provided useful information on how certain features of the potential energy surface (PES) control the experimental observations.

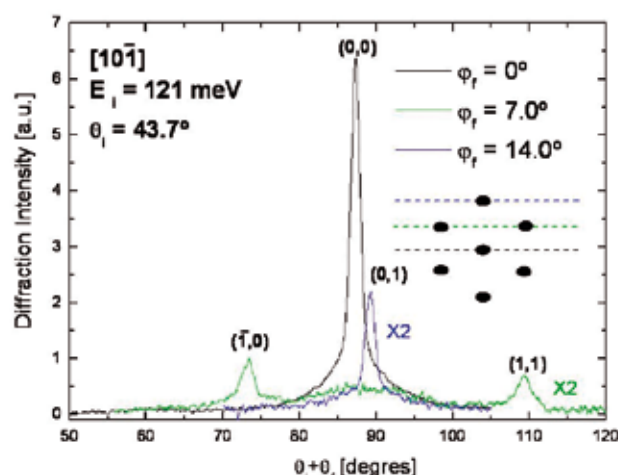
A different point of view is provided by diffraction experiments. H₂ diffraction from metal surfaces is more complex than He diffraction, since the PES is six-dimensional and the coupling with the dissociative adsorption channels comes into play. Thus, H₂ diffraction is a very promising technique to gauge the molecule-surface PES and dynamics. Using the two high-resolution molecular beam systems at LASUAM under the guidance of Daniel Farías, we have recently shown that this is possible by performing H₂ diffraction experiments on reactive Pd(111) and non reactive NiAl(110) surfaces at 60-150 meV. By comparing with six-dimensional quantum dynamics and classical trajectory calculations performed by Fernando

Martín we showed that accurate diffraction patterns can be obtained from state-of-the-art PES based on DFT calculations. Once the PESs are validated, they can be used to study in detail the different channels involved in H₂ reactivity, like direct dissociation and dynamic trapping. Finally, we address the problem of the validity of the Born-Oppenheimer approximation for molecule-metal surface reactions, which has been recently questioned due to the possibility of electron-hole pair excitations. We have performed experiments and six-dimensional quantum dynamics calculations on the scattering of molecular hydrogen from Pt(111), obtaining absolute diffraction probabilities. The comparison for in-plane and out-of-plane scattering, and results for dissociative chemisorption in the same system, shows that for hydrogen-metal systems, reaction and diffractive scattering can be accurately described using the Born-Oppenheimer approximation.

QUANTUM SIZE EFFECTS IN NANOSTRUCTURES

Quantum Size Effects (QSE) in ultrathin metal films, where electrons are confined in the perpendicular direction by suitable energy barriers (e.g. band gaps in the substrate and image potential in the vacuum side), lead to oscillations in many physical properties upon variation of the film thickness. This is produced by the systematic variation in the Density Of States (DOS) at the Fermi level due to its periodic crossing by the Quantum Well States (QWS) created by the confinement of electrons.

In the last few years, the subgroup VT-STM led by Amadeo López Vázquez de Parga has been investigating by means of Scanning Tunneling Microscopy and Spectroscopy (STM/STS) the QSE on Pb/Cu(111) and Pb/Si(111). The layer-dependent electronic energy contributed by QWS to the total energy of ultrathin metallic films with confined electrons has been shown to influence the thermal stability of ultrathin metallic

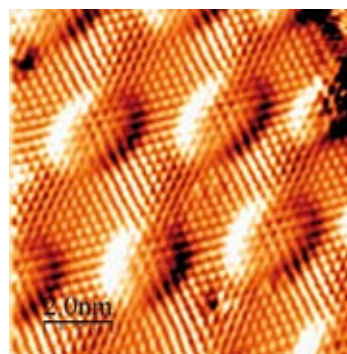


*H₂ diffraction spectra recorded from Pt(111).
The surface temperature is 463 K.*

films. STM at variable temperature have been used to follow the evolution of the morphology of the films during a quasi-static annealing with a temperature ramp of 1 K per minute. Films of different thicknesses have been grown at low temperature and their surface roughness transition has been studied as function of the Pb thickness. For Pb on Si(111) we have the same type of QSE but the film stability is better due to the low density of steps of the substrate. The resulting film with a magic thickness does not show a single step in images that are 500 nm wide. This has been used to fabricate a quantum- stabilized mirror for He atoms of unprecedented structural perfection depositing a Pb film of magic height on a 50 micron thick Si(111) wafer.

EPITAXIAL GROWTH OF GRAPHENE ON METALLIC SUBSTRATES

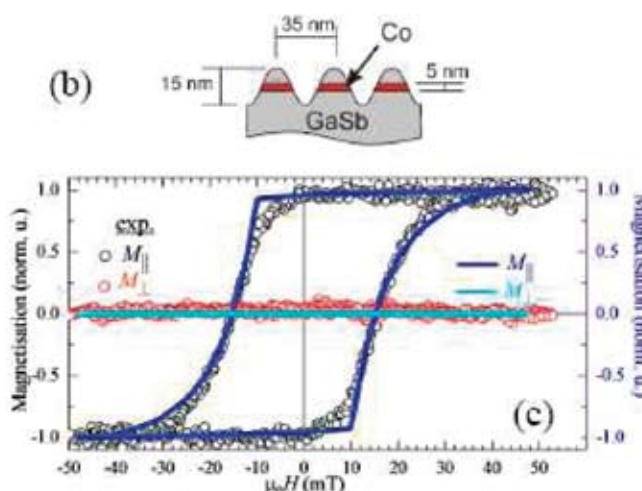
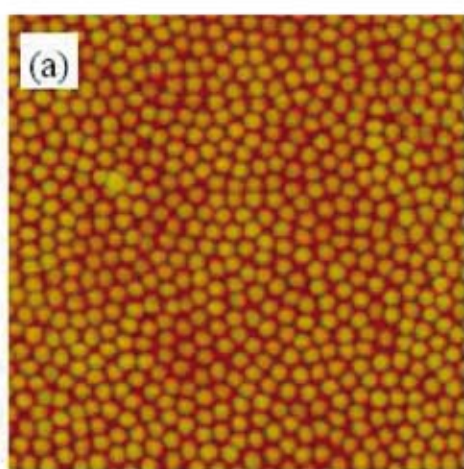
We have developed a general method to fabricate and characterize highly perfect, *periodically rippled* graphene monolayers and islands, epitaxially grown on single crystal metallic substrates under controlled UHV conditions. The periodicity of the ripples is dictated by the difference in lattice parameters of graphene and substrate, and, thus, it is adjustable. We characterize its perfection at the atomic scale by means of Scanning Tunneling Microscopy (STM) and determine its electronic structure in the real space by local tunnelling spectroscopy. Both the geometric and electronic corrugations of the rippled layers are detected, as well as the lack of reactivity of the graphene monolayers which allow us to transfer the samples prepared in UHV to external systems for studies with other experimental techniques.



STM image of graphene on Ru(0001) showing the Moire pattern and the atomic corrugation.

SELF-ORGANISED ARRAYS OF NANOMAGNETS ON SURFACES

The Nanomagnetism subgroup led by Juan José de Miguel and Julio Camarero has worked out a way to prepare self-organized arrays of nanomagnets with a density of 0.5 Tbit/in² by a variety of methods, that include ion bombardment at high fluxes of Co layers sandwiched between GaSb layers or shadow deposition of Co on nanostructured SiGe substrates. Magneto-optic (MOKE) measurements have shown that the nanomagnets have remanence at 300 K, with single-domain magnetically independent behavior. The spin reorientation transition from out-of-plane to in-plane of the nanodot arrays has been studied by x-ray magnetic circular dichroism (XMDC).



(a) AFM image of the surface topography of a Co nanodisc array obtained by ion-sputtering patterning an intercalated Co layer, as schematically depicted in (b). (c) In-plane and out-of-plane hysteresis loops (circles) measured by MOKE at 300 K, and theoretical fits (solid lines) to the data.

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Low Temperature Laboratory (LBT-UAM)

LABORATORIO DE BAJAS TEMPERATURAS

Members

Head of the Group: Sebastián Vieira

Members of the Group: Nicolás Agrait, Miguel Ángel Ramos, José Gabriel Rodrigo, Gabino Rubio-Bollinger, Hermann Suderow.

Ph.D. Students: Andrés Castellanos, Vanesa Crespo, Isabel Guillamón, Bisher Kabtoul, Merzak Hassaine, Tomás Pérez-Castañeda

An important part of the LBT-UAM research is devoted to the physics of new superconductors by studying its local density of states with STM/S techniques, the fabrication and characterization of superconducting nanostructures, including superconducting tips, and the study by a combination of STM and AFM of single molecules, atomic chains and contacts. A promising field is the combination of all this know-how with nanolithographic techniques to produce nanostructures, which can be fabricated now in the UAM. Another important research line at LBT-UAM is devoted to the study of anomalous behavior of glassy or non-crystalline solids at low temperature. With such an aim, calorimetric and specific heat measurements performed at LBT-UAM are combined with x-ray diffraction and light-scattering or neutron-scattering experiments in other laboratories.

In the recent years new original equipment has become operational at the Low Temperature Laboratory, LBT-UAM. This equipment supported our participation in different programs of excellence like Consolider Ingenio 2010 "Nanociencia Molecular", and "Ciencia y tecnología en el milikelvin" (www.uam.es/citecnomik), from Comunidad de Madrid. The abovementioned equipments and instruments allow the study of superconducting and magnetic properties of material by means of local scanning tunneling microscopy and spectroscopy (STM/STS) techniques, well below 1K, down to 100 mK, and with magnetic fields up to 13 T. The versatility of these systems, built with the support of SEGAINVEX, makes them unique in some aspects. For example, it is possible to prepare, in-situ, in cryogenic ultra high vacuum, both tip and sample, allowing to perform the experiments in contaminant free conditions.

It is noteworthy that LBT-UAM owns the only dilution cryogenic system in Spain capable of reaching 8 mK, with a remarkable cooling power of $400\mu\text{W}$ at 100 mK. This system includes devices that allow a shared use by different groups. LBT-UAM systems include also several ^3He and dilution refrigerators, as well as usual ^4He cryostats, all of them equipped with superconducting magnets. Different cryogenic instrumentation is also built and developed in collaboration with SEGAINVEX: superconducting coils for high magnetic fields with vector control, USB controlled voltmeters and sources, liquid nitrogen and helium transfer systems, helium level meters, and temperature measurement and control systems.

LBT-UAM is also involved in collaboration projects with companies like EADS-CASA and INTA. LBT-UAM is an Associated Unit to ICMC-CSIC, involved both in technical and scientific fields.

Our group has an ongoing scientific collaboration with different groups, like P.C. Canfield (Ames, USA), Thomas Frederiksen, Andrés Arnau (DIPC San Sebastian), Alfredo Levy Yeyati, Juan Carlos Cuevas, (UAM), Nazario Martín (UCM), and the low temperature groups at Grenoble (France), Leuven (Belgium), Bath (U.K.), Kosice (Slovakia), Leipzig (Germany), Messina (Italy), Kharkov (Ukraine), and INA at Zaragoza.

LOCAL TUNNELING SPECTROSCOPY ON SUPERCONDUCTORS

The development of local tunneling spectroscopy, at very low temperature, allows to perform a great variety of experiments. It opens the possibility of using completely new local probes, based on the use of superconducting tips in the STM, capable of determine at a local scale the Josephson effect, the magnetic field above the surface of the sample or the spin polarization in the tunneling current.

2H-NbSe₂ is considered a prototype material for the study of superconductivity by local probes. It is a complex material, showing two band superconductivity coexisting with a charge density wave (CDW), as confirmed, between others, by works at LBT-UAM. We found on this material atomic scale variations of the superconducting density of states. These variations exist also in the presence of vortices, as shown in figure 1, which present a clear six-fold star shape. The origin of this structure has been in discussion for the last two decades, and recently we have shown that in NbS₂, a superconductor with no charge density wave, the six-fold star is absent in the vortex structure. Therefore, the presence of the CDW strongly determines the anisotropic characteristics of NbSe₂.

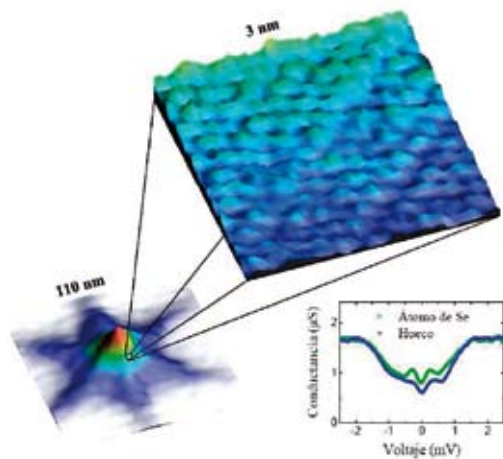


Fig.1. Six-fold star shaped vortex in NbSe₂ and atomic scale variations of the superconducting DOS.

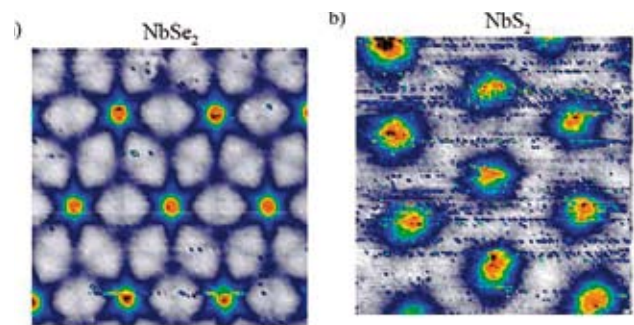


Fig.2. Vortex lattice in NbSe₂ and NbS₂. Both the star-shaped vortices and CDW are absent in NbS₂.

The multiband character of superconductivity in NbSe₂ also arises when the vortex lattice is imaged by STS at 6K, when the gap in one of the bands at Fermi surface is closed. The differences regarding the absence of six-fold symmetry at some energies, compared to the results at low temperature are shown in fig.3.

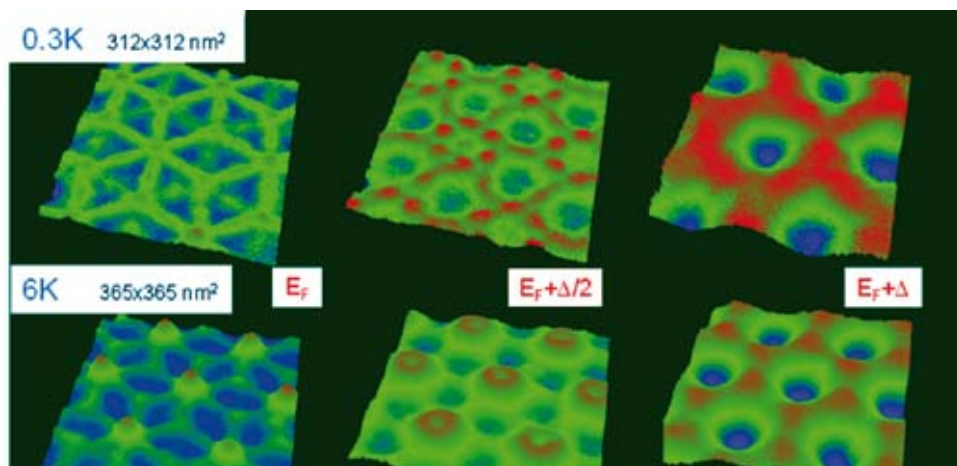


Fig.2. Evolution of vortex patterns in NbSe₂ obtained at different energies using STS with a superconducting tip. Differences are due to multiband superconductivity.

SINGLE MOLECULE ELECTRONICS

Among the possible alternatives for future miniaturized circuits, molecular electronics proposes to use single molecules as wires and active components. A first basic step in this direction is the **understanding** and **control** of the **electrical conduction** through a **single molecule**. We use proximity probe techniques based on STM to study the electrical properties of molecular junctions in dry and liquid environment at room temperature, and in vacuum at low temperature.

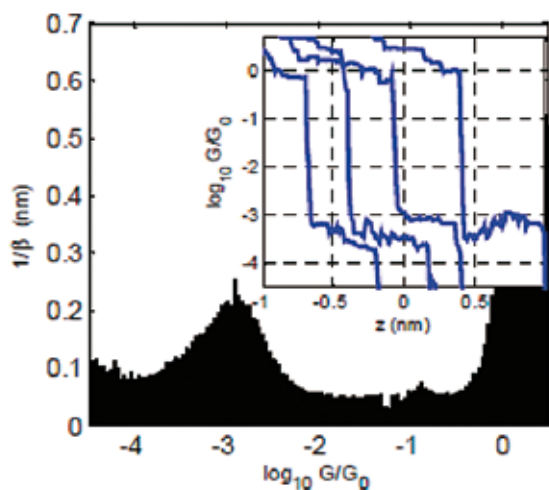


Figure 1. Conductance traces in a break-junction in the presence of pentanedithiol molecules. The plateau at $G = G_0$ corresponds to a single gold atom contact, while the plateau at $G = 10^{-3} G_0$ corresponds to a single molecule junction.

vibrations by the traversing electrons. We have performed IETS measurements in short alkanedithiol molecules, showing the effect of elastic deformations and elucidating the electron pathway through the molecule (see Fig. 2).

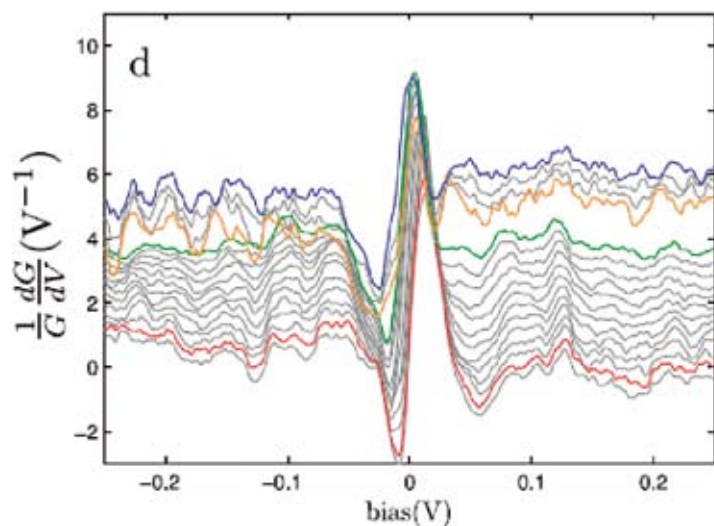
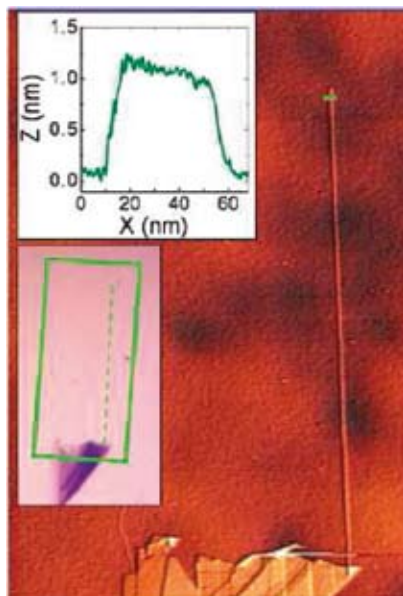


Figure 2. IETS spectra of a single pentanedithiol molecule between gold electrodes, at 4 K.

In particular we use the **break-junction approach** which consists of forming and breaking repeatedly metallic junctions by moving the STM tip down till contact with substrate and retracting it back. In the presence of molecules ending in the proper anchoring groups, the gap between the metallic electrodes can be bridged by molecules with certain probability. Studying the variation of the conductance G while retracting the STM tip, we detect the formation of stable configurations by the observation of a flat plateau. This is the case for one gold atom contact, at $G_0 = 77.5 \mu S$, and for junctions with bridged molecules, at G values several times less than G_0 (see Fig.1).

A powerful tool that has proved to be very useful for understanding electron transport in atomic wires of gold is inelastic tunneling electron spectroscopy (IETS). This technique, which requires the use of low temperatures, is based on the variations in the conductance caused by the excitation of the molecular

GRAPHENE ELECTRONICS



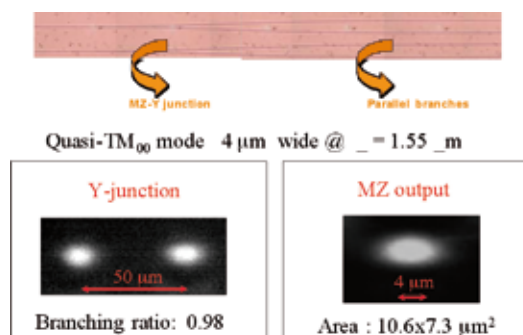
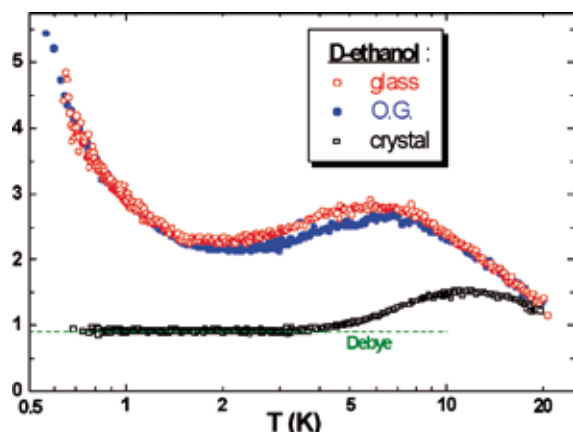
An alternative approach to silicon electronics could be based on carbon. Indeed, the two-dimensional crystalline form of carbon, graphene, has a potential for serving as an excellent electronic material and can be used to develop new kinds of transistors based on quantum physics. When a graphene flake is reduced to a long nanometers-wide ribbon, additional properties emerge in the already rich scenario of graphene. In particular, lateral confinement of the charge carriers causes the opening of an energy gap, which depends on the width of the nanoribbon. The presence of such a gap is essential for future applications. Using a new technique based on micromechanical cleavage, we have succeeded in producing long graphene nanoribbons of well-defined edges, and we are currently studying their transport properties.

Figure 3. AFM image of a 37 nm-wide and 25 micron-long graphene nanoribbon.

THERMODYNAMIC PROPERTIES OF GLASSES:

Glass is a well-known and widely used material by mankind since thousands of years ago. Nevertheless, the very nature of the glassy state and its physical properties remain an issue of vivid debate within the scientific community. Indeed, when some prominent scientists analyzed the main challenges to be addressed in the 21st century, it was stated that *“The deepest and most interesting unsolved problem in solid state theory is probably the theory of the nature of the glass and the glass transition”* [P. W. Anderson, *Science* 267, pp.1615-1616 (1995)]. The main reason for this problem to remain unsolved is that two different, contradictory aspects play an important role to understand the glass-transition phenomenon: kinetics and thermodynamics. Although many experiments on any kind of glasses have been performed all along past 20th century, the answer to many key questions is still to be found.

On the other hand, the anomalous behavior of glassy or non-crystalline solids at low temperature remains an interesting and much debated issue. It was showed clearly almost 40 years ago, that low-temperature thermal properties of non-crystalline solids exhibit a universal behaviour, that differs significantly from that observed in fully-ordered crystals obeying Debye’s theory. In particular, specific heat of glasses depends linearly on temperature below 1 K, what was soon ascribed to the existence of tunneling states, whereas, above 1 K, C_p still strongly deviates from the expected Debye-like behavior $\propto T^3$ due to lattice vibrations, exhibiting a characteristic broad maximum in a C_p/T^3 vs T plot. This maximum in C_p/T^3 is closely related to the so-called boson peak, observed by low-frequency vibrational spectroscopies such as Raman- or neutron-scattering, which arises from a broad maximum in the vibrational density of states normalized to the quadratic Debye one, i.e. $g(\nu)/\nu^2$, occurring around $\nu \sim 1$ THz. Above mentioned glassy anomalies for $T < 1$ K were soon accounted for, at least phenomenologically, by the *Tunnelling Model*, that postulates the universal existence of atoms or groups of atoms in any amorphous solid, which can tunnel between two configurations of similar energy. Nonetheless, the also rich and universal glassy behaviour for $T > 1$ K (the maximum in C_p/T^3 , a universal “plateau” in thermal conductivity within 2–20 K, the above mentioned boson peak in vibrational spectroscopies...) remained unexplained.



The main research line of our group aims to deepen in our understanding of abovementioned properties universally exhibited by non-crystalline solids at low temperatures, in conjunction with the more general problem of the very nature of the glass-transition phenomenon and the glassy state itself. In particular, we have implemented and used a low-temperature, home-made calorimetric experimental system, either in cryogenic environments at liquid helium temperatures, or at temperatures above that of liquid nitrogen, in order to study and characterize substances that are liquid at room temperature and can solidify into both glassy and crystalline phases. A special attention has been paid to pure ethanol. Our main result has been to find out that the “orientational glass” (*i.e.* a crystal with orientational disorder) possesses qualitatively, and even quantitatively, the same “excess” of specific heat as the structural glass (an amorphous solid), so demonstrating that the lack of long-range translational order is not an essential requisite for the existence of the typical “glassy properties”. Furthermore, their very similar “glass transitions” (that is, the freezing-in from an ergodic state into a non-ergodic one) show that the very phenomenon of the glass transition can be a more general process than just the kinetic arrest experienced by a supercooled liquid when its viscosity dramatically increased when cooling, and it becomes a non-crystalline solid. Also, we have recently found the big influence of several factors (water impurity in ethanol, the employed experimental cell, and even the thermal history of the liquid) in the kinetics of the different phases of ethanol. In addition to ethanol, we have used the same techniques to prepare and measure the specific heat of 1-propanol and 2-propanol, as well as of glycerol, both their stable crystal and conventional *glass states*. We are currently investigating these thermodynamic properties on 1-butanol, that has been claimed to exhibit an unusual so-called “glacial state”, as well as on ethanol-water binary mixtures and on geological glasses.

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Advanced Materials for Integrated Guided Optics

Staff:

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PhD Students

M. Quintanilla, J. Lamela and J. Barrio

The Advanced Materials for Integrated Guided Optics (AMIGO) group focuses its activity in the study of optical materials and photonic devices.



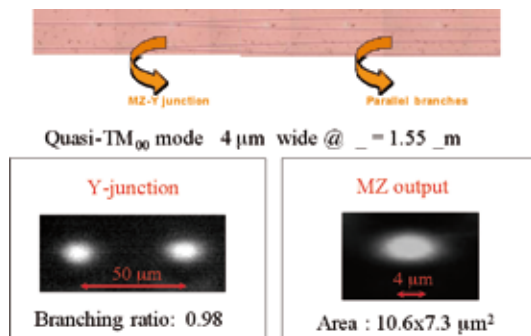
The areas of activity cover a broad range of interest, which includes: Crystal growth; Spectroscopic characterisation; Planar and channel waveguide fabrication; Waveguide characterisation; Modelling and simulation of waveguide devices; Integrated lasers and amplifiers; Non-linear devices; Integrated optical sensors; Near Field Optical Microscopy (SNOM); and Optical properties of RE-doped nanoparticles



Growth of rare earth-doped LiNbO₃ monocrystals. The laboratory has the facilities for Czochralski growth and experience in growing rare-earth doped LiNbO₃ single domain and PPLN.

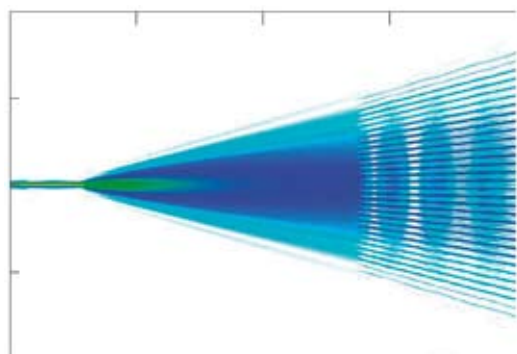
LNB:Nd³⁺ monocrystal.

Spectroscopic characterisation. The group has facilities for a variety of spectroscopic techniques, including absorption, luminescence (CW and lifetimes), and photoacoustic spectroscopy, with excitation and detection in the visible-IR range (Ti-Sapphire and MOPO sources).



Planar and channel waveguide fabrication by Zn-diffusion in LNB and waveguide evaluation (modal spectra, modal fields, attenuation and spectroscopy)

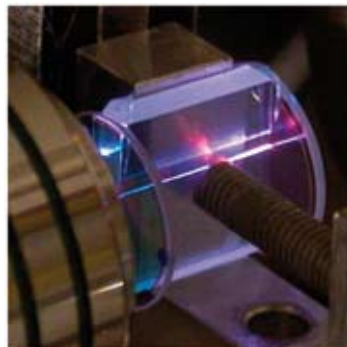
Characterization of MZ interferometer



Modelling and simulation of waveguide devices. Several software packages have been developed for the modelling and simulation of a variety of integrated photonic devices including photonic crystals.

Modelling of the input star of an Arrayed Waveguide Grating.

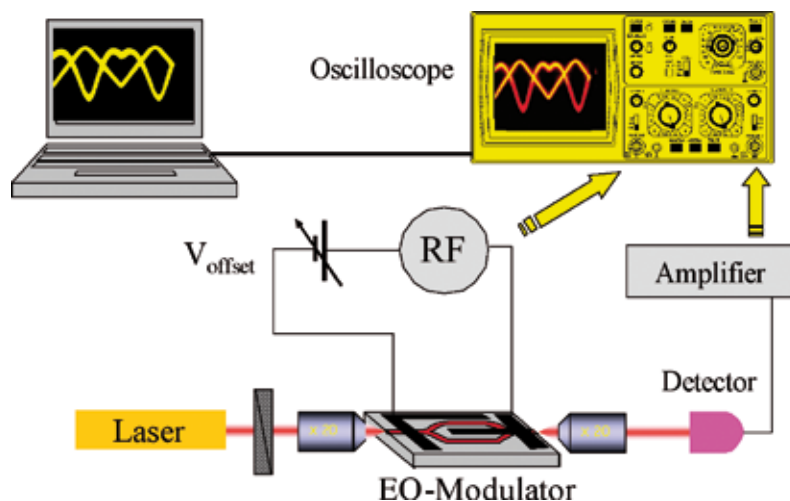
Integrated lasers and amplifiers. Rare-earth doped lithium niobate integrated lasers have been fabricated showing very low threshold and high PR damage resistance.



LNB Tm³⁺ laser

Non-linear devices. Using periodically structured LNB channel waveguides, second harmonic generation in the blue range has been demonstrated

Integrated Mach-Zehnder interferometers are under development for electro-optic & acousto-optic devices and opto-chemical-sensors.



Group Of “Crystal Growth Laboratory, CGL” of the University Autonoma of Madrid

Members:

Head of the Group:

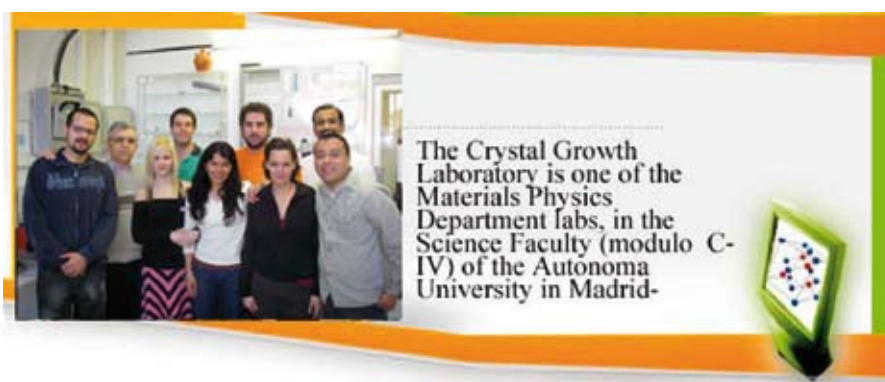
Prof. Ernesto Diéguez

Members of the Group:

Dr. José Luis Plaza, Dra. Susana de Dios. Project Manager: Iván Benito

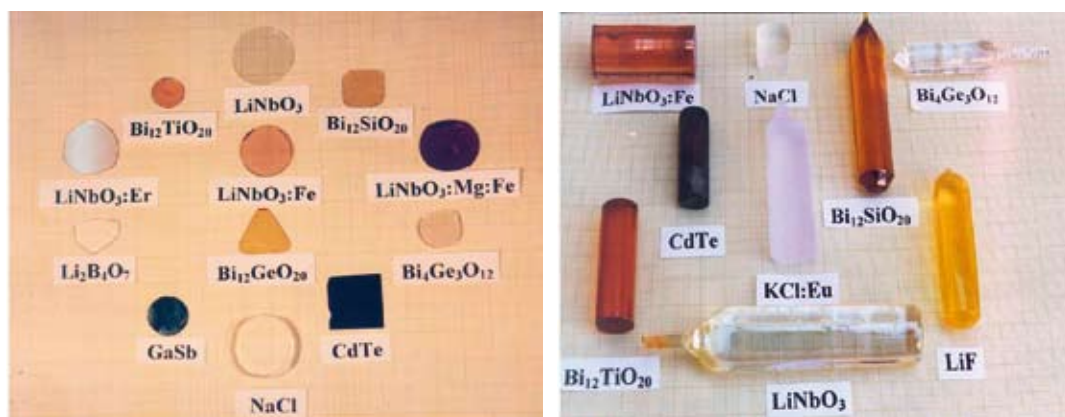
Ph.D. Students:

Javier Olvera; Verónica Carcelén; Jerome Grocco;Cristina Ramírez



The Laboratory of Grystal Growth (CGL) of the University Autónoma de Madrid essentially dedicates its investigation to the preparation and characterization of crystalline materials, semiconducting and insulating materials. In more than thirty years of its operation, has centered its investigation in crystalline materials such as: Halogenides (LiF, KCl, NaCl,) for the study of its crystalline and optical properties, Ferroelectric materials, with special mention to the LiNbO₃, Semiconducting materials such as the GaSb InSb, InGaSb, of great application in the manufacture of Termophotovoltaic Cells and optoelectronic devices and the CdTe and CdZnTe that is nowadays the fundamental base of present financing of Laboratory through projects of the Ministry of Education and Science and of the Community of Madrid. The CGL recently also dedicates an important investigating work destined to the polycrystalline lamina manufacture of ZnO on diverse substrates. Through the CGL more than fifteen PhD students have defended their PhDs. The cgl has published more than 250 international publications in the last 25 years. For more information, to visit the pages Web

For more information: <http://www.uam.es/cgl> <http://www.uam.es/sensorcdt>



Crystals Grown at CGL

Running projects based on RADIATION SENSORS ON CdZnTe/CdTe

**Scientific objective:* the development of high resolution/large volume devices based on the CdTe/CdZnTe family semiconductor compounds

**Technological objective:* to implement in our laboratories the methodology and technology required for the production of such sensors with the dimensions, spectrometric resolution and reliability required in the state-of-the-art of medical application such as SPECT or PET imaging.

**Strategic value:* Sensor technology based on semiconductor materials that can be operative at room temperature is a relevant area of interest in the field of the Europe research and industrial community considering the great number of applications where these materials can be used, namely X-ray and gamma imaging, gamma radiation detectors for nuclear medicine, biosensor materials, security and non-proliferation of hazardous materials, or environmental applications.

**Final Application:* the scientific properties of CdTe based materials are the best candidates for X-gamma-Ray detector. Recent publications in this field have concluded that CdTe family materials are the best candidates for cardio-vascular and thyroïdal imaging; the best candidate for neurology, cardiology and oncology, with applications such high energy tomography and Z-ray Computed tomography. The CdTe family can contribute to the improvement in critical aspects such as patient dose reduction and high contrast imaging.

Projects

"Radiation detectors based on CdZnTe/CdTe, SENSORCDT", financed by CAM (2006-2009). "Cooperation across Europe for Cd(Zn)Te based security instruments, COCAE" financed by FPVII (2009-2011). "Crystallization of CdTe and related compounds on microgravity conditions", contract ESA (2006-2010).

AFM and Nanosystems Group

GRUPO MICROSCOPIA DE FUERZAS ATÓMICAS Y NANOSISTEMAS

Members:

Prof. Julio Gómez

Dr. Pedro José de Pablo (Assistance professor)

Dr. Cristina Gómez-Navarro (R&C researcher)

Dr. Lorena Welte (Post-doc)

Dr. Miriam Jaafar (Post-doc)

Ph.D. students:

David Martínez-Martín

Francisco Javier Guzman

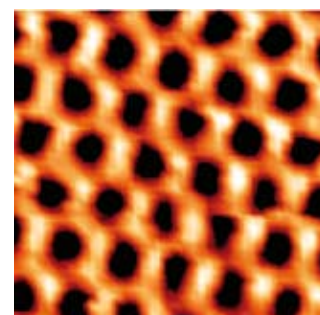
Mercedes Hernando

The main research lines of the NanoSPM group are summarized in the following:



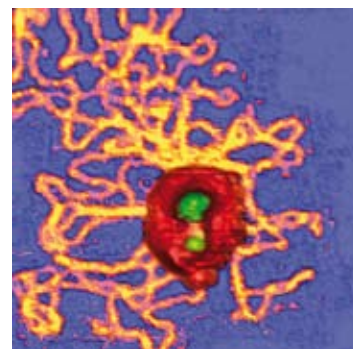
AFM INSTRUMENTATION

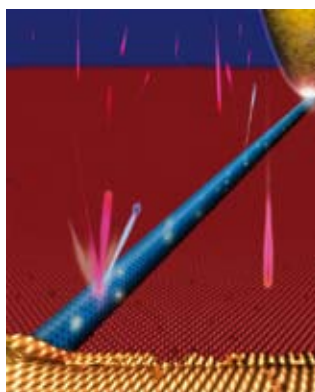
The **AFM and nanosystems group** has a long standing tradition in the development and construction of advanced instrumentation in scanning probe microscopy. WSxM software used for thousands of researchers worldwide is a perfect showcase for our instrumentation developments [1]. In particular, his group has designed and built several AFM systems that work from high vacuum up to liquids [2], including external magnetic fields [cita], variable temperature etc. David Martínez Martín has recently been able to obtain true atomic resolution on a mica (001) surface, immersed on a buffer solution, using an AFM working on frequency modulation. This achievement has been possible thanks to a new AFM design in collaboration with Nanotec Electrónica SL.



BIOPHYSICS.

Dr. de Pablo is the director of the biophysics line of the group. During the last 5 years we have carried out different studies on the physical properties of single viral particles, ranging from mechanical stiffness [2] to the use of viral cages to understand the behavior of water in closed confined geometries. Specifically we are mainly interested in the role of the nucleic acid in the stabilization of viruses by studying the influence of the viral DNA in the stiffness of the capsid shell. This may have important implications in their infectivity as well as in the design of new materials with tuned mechanical properties.





ELECTRICAL TRANSPORT

Dr. Gomez-Navarro is the director of this line of the group. Scanning probe microscope has been a powerful tool to measure electrical transport at the nanoscale. Our experience in this field started many years ago with the studies of **nanocontacts** [4] and from there we moved to problems related with electronic transport in **DNA** [5], **carbon nanotubes** [6], **metal organic** systems [7] and very recently **graphene** [8]. Graphene can be considered as a particularly simple example of a 2D polymer. We are now initiating a new line towards isolation of individual layers of more complex laminar polymers.

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Web page: [http://www.uam.es/departamentos/ciencias/fismateriac/especifica/Nuevas Microscopies_webpage/Index.html](http://www.uam.es/departamentos/ciencias/fismateriac/especifica/Nuevas_Microscopies_webpage/Index.html)



Activities:

**International Summer Schools,
Seminars, Conferences, Courses**



International Summer School “NICOLÁS CABRERA”

The International Summer School "Nicolás Cabrera", in a series with the generic title "Frontiers in Science and Technology", is the best example of the commitment of the INC with excellence in Science. This commitment is shared by the BBVA Foundation ("Fundación BBVA"), through its continuous financial support of the activities of the International Summer School "Nicolás Cabrera".

Funded by Fundación BBVA

Fundación **BBVA**

XIV International Summer School

“Nicolás Cabrera” - 2007

Frontiers in Science and Technology:
NANO-PHOTONICS AND OPTICS

17-21 September 2007

Residencia La Cristalera, Miraflores de la Sierra (Madrid, Spain)

DIRECTORS

J.J. Sáenz (INC, MOLE Group, UAM)

F.J. García-Vidal, (INC, UAM)

Secretary: Silvia Albaladejo (MOLE Group, UAM)

OBJECTIVES

The aim of this school is to introduce some relevant topics in nanophotonics to young physics and graduate students.

There are some topics included in this summer school:

1. Plasmonics
2. Photonic Crystals
3. Metamaterials
4. Biophotonics

The International Summer School is primarily addressed to young researchers in the fields of Materials Science, Condensed Matter Physics and Optics. The maximum number of participants is 55, excluding the lecturers. Full board and lodging is limited to 35 participants on the basis of double room. Some scholarships covering all but travel expenses will be provided for students, their number depending on the financial support obtained.

SPONSORED BY:

Fundación BBVA



Fundación **BBVA**

Instituto Madrileño de Estudios Avanzados



Universidad Autónoma de Madrid



LECTURERS:

- **Sajeev John** (*Univ. of Toronto, Canada*)
- **Sergey Bozhevolnyi** (*Univ. Aalborg, Denmark*) "Nanophotonics using channel plasmon polaritons"
- **Thomas Ebbesen** (*Univ. Louis Pasteur, France*) "Light in Tiny Holes: Fundamentals and Applications"
- **Luis Martin-Moreno** (*Univ. de Zaragoza, Spain*) "Scattering of light and surface plasmons by surface corrugations"
- **Javier Garcia de Abajo** (*IO-CSIC, Spain*) "Mastering optical near fields in nanostructured materials"
- **Gaspar Armelles** (*IMM-CSIC, Spain*) "Magneto-optical effects in plasmonic nanostructures"
- **Costas Soukoulis** (*Iowa State University, USA*) "Bending Back Light: The Science of Negative Index Materials"
- **Ulf Leonhardt** (*Univ. of St Andrews, UK*) General Relativity in Electrical Engineering (Metamaterials)
- **Remi Carminati** (*Ecole Centrale Paris, France*) Single molecule fluorescence in nanoscopic environments
- **Carlos Tejedor** (*Univ. Autonoma Madrid, Spain*) "Semiconductor nanostructures as components for quantum optics"
- **Javier Aizpurua** (*D.I.P.C, Spain*) "Optical antennas for field enhanced microscopy and spectroscopy"
- **Niek F. Van Hulst** (*ICFO, Spain*) "Controlling single photon emitters in space and time"
- **Frank Scheffold** (*Univ. Fribourg, Switzerland*) "Transport and fluctuations in strongly scattering colloidal assemblies "
- **Rainer Hillenbrand** (*Max-Planck Inst., Germany*) "Near Field Optical Nanoscopic"
- **Manuel Nieto Vesperinas** (*ICMM-CSIC, Spain*) "Photonic Forces in the Near Field"
- **Francisco Meseguer** (*ICMM-CSIC/UPV, Spain*) "Photonic nanostructures based on Coloids"
- **Paul Mulvaney** (*Univ. Melbourne, Australia*) "Single Quantum Dot Spectroscopy"
- **Luis Liz-Marzan** (*Univ. de Vigo, Spain*) "Surface Plasmon Resonances in Metal Nanoparticle Colloids"
- **Concha Domingo** (*IEM- CSIC, Spain*) "Molecular chemosensors based on nanostructured metal surfaces: SERS (*raman*), SEIRA (*infrared*) and SEF (*fluorescence*)"
- **Philippe Lalanne** (*CNRS, France*) "Surface waves generated by subwavelength slits"
- **Jose A. Sanchez-Gil** (*IEM- CSIC, Spain*) "Surface plasmon optics on metal nano-structures"
- **Cefe Lopez** (*ICMM-CSIC, Spain*) "Photonic crystals and glasses by self assembly"
- **Hernan Miguez** (*ICMSE , Spain*) "Solar Cells Coupled to Photonic Crystals"
- **Lluís Marsal** (*Univ. Rovira i Virgili, Spain*) "Photonic crystals: fabrication and applications of ordered micro and nanostructures by electrochemical etching"
- **Jaime Gomez Rivas** (*AMOLE, The Netherlands*) "Optical anisotropic, light scattering and birefringence of nanowires and nanorods"
- **Jordi Martorell** (*ICFO, Spain*) "Nano and micro quadratic nonlinear optics"
- **Maria Ujue** (*ICFO, Spain*) "Plasmon Nano-Optics: from the manipulation of light at the nanoscale to the manipulation with light of nanoobjects"
- **Jorge Ripoll** (*FORTH, Greece*) "Optical tools in Molecular Imaging"

XV International Summer School

“Nicolás Cabrera” - 2008

Frontiers in Science and Technology:
100 YEARS LIQUID HELIUM:
NEW PHYSICS AT THE EDGE OF ABSOLUTE ZERO

14-19 September 2008

Residencia La Cristalera, Miraflores de la Sierra (Madrid, Spain)

DIRECTORS:

Sebastián Vieira (INC, Lab. de Bajas Temperaturas, UAM)
Hermann Suderow, (INC, Lab. de Bajas Temperaturas UAM)
Secretary: Yousely Gonzalez Lemus (Física de la Materia Condensada, UAM)

Local organizing committee:

- M.A. Ramos (UAM, Spain)
- J.G. Rodrigo (UAM, Spain)
- G. Rubio Bollinger (UAM, Spain)

Scientific advisory committee:

- N. Ägrait (UAM, Spain)
- J. Bartolomé (ICMA-CSIC, Spain)
- J.C.Gómez Sal (UC, Spain)
- F. Guinea (ICMM-CSIC, Spain)
- R. Ibarra (ICMA, Spain)
- F. Sols (UCM, Spain)
- J. Tejada (UB, Spain)
- J.L. Vicent (UCM, Spain)
- F. Vidal (USC, Spain)
- R. Villar (UAM, Spain)

OBJECTIVES

The aim of this Summer School is to provide graduate students, post docs, and last year undergraduates with exceptional marks and motivation for physics, of a general introductory overview of some of the most exciting topical developments on Condensed Matter and Nanoscopic Physics. The Summer School will consist on a series of introductory lectures given by internationally recognized leading experts. The school will span a wide range of topics across low temperature physics, connected by common theoretical or experimental methods, with the main aim to give the students an overview of some of the most intriguing open questions and of the technical abilities required to be able to make successful top level research close to absolute zero.

PARTICIPANTS

The International Summer School is primarily addressed to young researchers and students with interest in Condensed Matter Physics and Nanotechnology, and a background in physics. The maximum number of participants will be around 60 including about twenty invited speakers that are internationally recognized experts. Scholarships covering full board (no travel expenses) will be provided for students, their number depending on the financial support obtained. The Summer School is organized within the framework of the excellence research program “Science and Technology at the milikelvin” (CITECNOMIK), funded by the Comunidad Autónoma de Madrid.

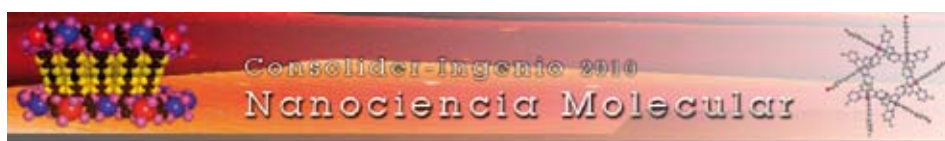
The Summer School is funded by the following institutions and research programs:

1. Fundación BBVA. <http://www.fbbva.es>
2. Universidad Autónoma de Madrid. <http://www.uam.es>
3. CITECNOMIK and CONSOLIDER-INGENIO 2010 "Molecular Nanoscience" programs. <http://www.uam.es/citecnomik> and <http://www.icmol.es/consolider/>
4. Instituto Madrileño de Estudios Avanzados en Nanociencia. <http://www.imdea.org>

Sponsored by:



CITECNOMIK
CIENCIA Y TECNOLOGÍA EN EL MILIKELVIN



LECTURERS:

- **A. Andreev** (*Kapitza Institute, Russia*) Fundamental ideas of low temperature physics.
- **S. Balibar** (*CNRS/Laboratoire de Physique Statistique de l'ENS, France*) Supersolidity and disorder. The discovery of superfluidity. .
- **A. Benoit** (*Institut NÉEL/CNRS, France*) High sensitivity measurement of Cosmic Microwave Background Anisotropies using low temperature bolometers. Balloon and satellite experiments.
- **J. P. Brison** (*CEA/Grenoble, France*) Experimental aspects of multigap superconductivity in strongly correlated systems.
- **A. Buzdin** (*CPMOH/University of Bordeaux 1, France*) Coexistence of ferromagnetism and superconductivity.
- **B. Cabrera** (*Stanford University, USA*) The Search for Dark Matter in the form of WIMPs and the CDMS experiment
- **P. Canfield** (*Iowa State University, USA*)
- **J. T. Devreese** (*University Antwerpen, Belgium*) Hot topics in cold atoms.
- **C. Enss** (*Universität Heidelberg, Germany*) Interplay between nuclear magnetic moments and atomic tunneling systems in glasses at low temperatures.
- **A. Feher** (*P.J. Safarik University, Slovakia*)
- **J. Flouquet** (*INAC/SPSMS, France*) Phase diagram of heavy fermion systems : pressure and magnetic field scan.
- **I. Fomin** (*Kapitza Institute, Russia*) Superfluid Helium-3 in aerogel.

- **H. Godfrin** (*Institut NÉEL/CNRS, France*) Liquid Helium-3: The canonical Fermi liquid.
- **F. Guinea** (*ICMM/CSIC, Spain*) Electronic and structural properties of graphene.
- **A. Levanyuk** (*UAM, Spain*) Liquid helium and theory of phase transitions.
- **V. Moshchalkov** (*Catholic University of Leuven, Belgium*) Nanostructured superconductors: new frontiers at low temperatures.
- **J. Pekola** (*Helsinki University of Technology, Finland*) Single electron tunneling: physics and devices.
- **G. Pickett** (*Lancaster University, UK*) Superfluid Helium3 in the Zero Temperature Limit: Simultaneously a Model System and Tabletop Universe.
- **F. Vidal**. Measuring the superconducting transition in inhomogeneous highTc cuprates: the superfluid ^4He in the rearview mirror.... and also forward
- **G. Volovik** (*Helsinki University of Technology, Finland*) Helium liquids and the Universe.
- **F. de Waele** (*Eindhoven University of Technology, Netherlands*) Cryocoolers: basics and applications
- **F. Yndurain** (*UAM, Spain*)
- **R. Miranda** (*UAM, Spain*)

INSTITUTO NICOLÁS CABRERA



**SEMINARS:
“SEMINARIOS-CAFÉ”
SERIES 2008**

Seminars:

“Seminarios – Café”

Series 2008

- **Problemas actuales sobre grafito y grafeno** (*Dr. Miguel Angel Ramos, Prof. Pablo Esquinazi*)
- **Problemas actuales sobre Nanomagnetismo** (*Dr. Farkhad Aliev*)
- **Catálisis Biológica y Bioenergía: pilas de combustible microbianas** (*Dr. Raul Guantes*)

Wednesday 30 January 2008

Dr. Paco Guinea (ICMM-CSIC), Dr. Amadeo López Vázquez de Parga (UAM).

Problemas actuales sobre grafito y grafeno (1)

Wednesday 13 February 2008

Prof. Julio Gómez Herrero (UAM), Dr. Pedro L. de Andrés (ICMM-CSIC), Dra. Pilar López Sancho (ICMM-CSIC).

Problemas actuales sobre grafito y grafeno (2)

Wednesday 27 February 2008

Dr. Juan José Palacios (Universidad de Alicante), Dra. M^a Ángeles H. Vozmediano (ICMM-CSIC).

Problemas actuales sobre grafito y grafeno (3)

Wednesday 26 March 2008

Dr. Javier Sabio (ICMM-CSIC), Dr. Nicolás García (FSP-CSIC).

Problemas actuales sobre grafito y grafeno (4)

Wednesday 28 May 2008

Dr. Farkhad Aliev (Universidad Autónoma de Madrid), Dra. Oxana Fesenko-Chubykalo (ICMM-CSIC), Dra. M^a Puerto Morales, (ICMM- CSIC).

Problemas actuales sobre NANOMAGNETISMO (1)

Wednesday 4 June 2008

Dr. Juan de la Figuera (Instituto de Química-Física Rocasolano-CSIC), Dr. Juan José de Miguel (Universidad Autónoma de Madrid).

Problemas actuales sobre NANOMAGNETISMO (2)

Wednesday 11 June 2008

Dr. Manuel Vázquez (ICMM- CSIC), Dr. Farkhad Aliev (Universidad Autónoma de Madrid).

Problemas actuales sobre NANOMAGNETISMO (3)

Friday 24 October 2008

Prof. Miguel Ángel García (Universidad Complutense de Madrid), Dr. Miguel A. Ramos (Centro de Microanálisis de Materiales).

Problemas actuales sobre NANOMAGNETISMO (4)

Wednesday 29 October 2008

Dr. Víctor M. Fernández (Instituto de Catálisis. CSIC.),
Dr. Abraham Esteve (Centro de Astrobiología. CSIC-INTA).

Catálisis Biológica y Bioenergía: Pilas de combustible microbianas.

INSTITUTO NICOLÁS CABRERA



SCIENTIFIC MEETINGS FOR YOUNG RESEARCHERS

SCIENTIFIC MEETING FOR YOUNG RESEARCHERS 2007

20 de Diciembre de 2007

Residencia La Cristalera de Miraflores de la Sierra

X JORNADA DE JÓVENES CIENTÍFICOS
DEL INSTITUTO DE CIENCIA DE MATERIALES NICOLÁS CABRERA

PROGRAMA

9:45 Inauguración de la X Jornada Científica del INC por el Director del INC

Moderador: Prof. Luis Viña Liste

10:00 *"Superfluidez de polaritones en microcavidades semiconductoras"* **Daniele Sanvitto** (C-IV)

10:30 *"Dinámica del potencial eléctrico superficial en grafito"* **David Martínez Martín** (C-III)

11:00 Café

Moderador: Prof. Raúl Guantes Navacerrada

11:30 *"Efectos de superficie e intercara en NiO"* **Iulian Preda** (C-XII)

12:00 *"Imágenes simuladas de STM mediante cálculos de primeros principios"* **Óscar Paz** (C-III)

12:30 *"Calculo de la repulsion Coulomb intra e inter-molecular en conductores orgánicos moleculares"* **Laura Cano-Cortés** (C-V)

13:30 Comida

Moderador: Prof. Julio Camarero de Diego

15:30 *"Optimización de sistemas nerviosos"* **Alfonso Pérez Escudero** (Grupo Biofísica)

16:00 *"Luz y materia en acoplo fuerte"* **Elena del Valle** (C-V)

16:30 Clausura de la Jornada Científica por el Excmo. Vicerrector de Investigación, **Prof. J. M. Sanz**

SCIENTIFIC MEETING FOR YOUNG RESEARCHERS 2008

17 de diciembre de 2008.

Residencia La Cristalera de Miraflores de la Sierra

XI JORNADA DE JÓVENES CIENTÍFICOS DEL INSTITUTO DE CIENCIA DE MATERIALES NICOLÁS CABRERA

PROGRAMA

9:45 Inauguración de la XI Jornada de Jóvenes Científicos del INC por el Director del Instituto
Moderador: Prof: Carlos Sánchez

10:00 *Simulación de grano grueso de procesos de agregación de moléculas anfifílicas*
Teresa Ruiz Herrero (Dpto. de Física Teórica de la Materia Condensada)

10:25 *Autoensamblaje de nanotubos de porfirina con cadenas unidimensionales de Zn-O como espina dorsal: complejos antena biomiméticos*
Marta Trelka (Dpto. de Física de la Materia Condensada).

10:50 Café

Moderador: Prof: Rodolfo Miranda Soriano

11:30 *Las bombas de Na⁺/K⁺ adaptan el disparo en ráfagas a la estadística del estímulo.*
Sara Arganda Carreras (Grupo de Biofísica del INC)

11:55 *“Observación directa de la fusión de la red de vórtices superconductores: desanclaje térmico y nuevas fases entre el líquido y el sólido”,*
Isabel Guillamón Gómez (Dpto. de Física de la Materia Condensada)

12:20 *“Efecto de proximidad y transporte no local en interfases grafeno-superconductor”,*
Pablo Buset Atienza (Dpto. de Física Teórica de la Materia Condensada)

12:45 *Estudio de interacciones magneto-eléctricas en sistemas multiferroicos mediante espectroscopia óptica no lineal*
María de la O Ramírez Herrero (Dpto. de Física de Materiales)

13:10 Comida

Moderador: Prof: Carlos Tejedor de Paz

15:30 *Fotodiodos de Avalancha de GaN: Conteo de Fotones de UV en Modo Geiger*
Jose Luis Pau Vizcaíno (Dpto. de Física Aplicada)

15:55 *Crecimiento y caracterización de nitruros de cobre.*
Nuria Gordillo García (CMAM)

16:20 Clausura de la Jornada Científica por el Excmo. Vicerrector de Investigación Prof. **José María Sanz Martínez.**

INSTITUTO NICOLÁS CABRERA



MASTER IN BIOPHYSICS

MASTER IN BIOPHYSICS

MÁSTER EN BIOFÍSICA

The Postgraduate Program in Biophysics is fundamentally an introduction to the experimental sciences area research. Its main goal is to teach the physical principles of biological processes and the used techniques and Physical methodologies for its study.

Master en Biofísica · 60 ECTS
Doctorado

Instituto Universitario de Ciencia de Materiales
«Nicolás Cabrera»

Coordinadora:
Marisela Velez Tirado

Teléfono: +34 91 497 4689
Fax: +34 91 497 8734
biofisica@uam.es
<http://www.uam.es/biofisica>

UAM
UNIVERSIDAD AUTÓNOMA
DE MADRID

biofísica

programa oficial de posgrado
2006 · 2007

Universidad Autónoma de Madrid

Centro de Estudios de Posgrado y Formación Continua

MASTER + PHD PROGRAM

The Postgraduate Program in Biophysics consists of a Master course (600 hours in a whole academic year, although part of it can be validated by subjects passed in other academic programs) and a Doctorate where the student will develop an original research project in one of the groups associated to this program. Subjects of the Master course will be imparted in spanish and english.

Organizing Entities

Universidad Autónoma de Madrid (UAM)
 Public and Private Collaborating Institutions:
 Centro Nacional de Biotecnología(CSIC)
 Others (Companies Biomol Informatics and Nanotec Electrónica)
 Instituto de Química Física Rocasolano(CSIC)
 Centro de Investigaciones Biológicas (CSIC)
 Instituto Cajal (CSIC)
 Institut Curie. Section Recherche.UMR CNRS/IC

Aim

This program is an experimental research oriented masters Degree oriented to research in biophysics. The main working perspective for those who attend the Master will be their incorporation in a research group for the accomplishment of a Doctoral Thesis. Their specific objectives are:

To provide knowledge on Biology and basic Biochemistry or on Physics and Mathematics, necessary to attend the rest of the program. For that reason several updating subjects are offered to students so that they alternatively attend them according to their background (Elements of Physics and Mathematics and Elements of Biochemistry, Molecular Cellular and Genetic Biology).

To provide a general overview of biological processes at different organization levels (molecular, cellular, histological and physiological) emphasizing the physical principles of the biological functions (Molecular Interactions, Cellular Organization, Development Biology, Systems Organization).

To provide a basic knowledge of the advanced experimental and computing techniques that provide deeper insight of the biophysics of biological systems (Technical Biophysics, Biocomputing, Noninvasive Methods of Medical Diagnosis).

To provide a practical knowledge of some of the studied techniques (laboratory guided training).

Admission Profile

The students who have a Degree in Experimental Sciences, Health Sciences or Engineering, or who prove to have surpassed at least 240 credits corresponding to a First Cycle Degree will be admitted, as long as between these credits will be included the totality of the common academic contents of some of those Graduate Degrees, in agreement with the established effective legislation.

Admission Requirements

The criteria of the students' selection will be based on the valuation of the academic record, personal reference letters, interviews and English level. The admission of students with foreign Degrees, that fulfil the general requirements to access, will be made individually by the coordination committee.

Syllabus and Organization

Crédits: 60 ECTS.

The Masters Degree consists of 70 credits, 20 corresponding to levelling courses and 50 to courses specific to this masters degree. Students accepted in the program that come from the existing Degrees or from Degrees with 240 ECTS credits will fulfill 60 credits until completing a total of 300 that allows them access to the doctorate. Of these 60 credits, 10 will correspond to leveling courses to be chosen from the ones offered in the program. The remaining 50 will be completed with the 30 credits offered as mandatory plus 20 credits obtained from practical work to be completed in any one of the laboratories available for it. Additional credits can also be obtained from courses offered in different graduate programs in other Spanish or European Universities.

Special mandatory courses offer (50 credits):

First semester

- Elements of Biochemistry and Cellular Biology(10 credits) or
- Elements of Physics and Mathematics(10 credits).
- Bioinformatics (3 credits)
- Molecular Interactions (4 credits)
- Cellular Biophysics (3 credits)
- Experimental Techniques (8 credits)

Second semester

- Neuroscience and Systems Biology(6 credits)
- Image Analysis in Biology (3 credits)
- Developmental Biology (3 credits)
- Master Thesis (20 credits)

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A.F. Andreev (left) and B. Cabrera (right) during their lectures at the XV International Summer School Nicolás Cabrera, "100 years liquid helium: new physics at the edge of absolute zero", in September 2008.

These Summer Schools, which carry the generic title "Frontiers in Science and Technology", are the best example of the commitment of the INC with excellence in Science.

The Summer Schools are financially supported by the BBVA Foundation.

Fundación **BBVA**