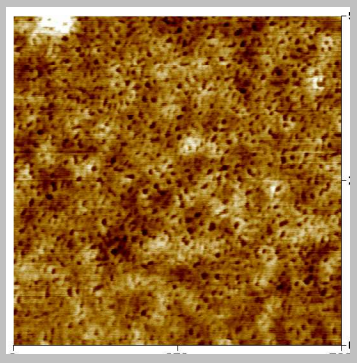
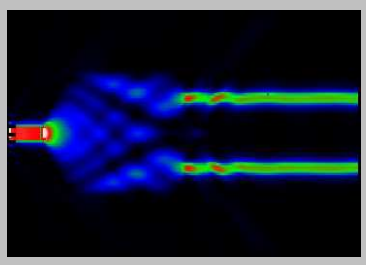
Instituto NICOLAS CABRERA

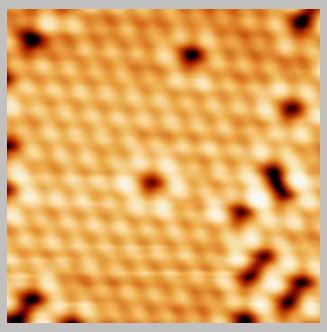
UAM UNIVERSIDAD AUTONOMA DE MADRID

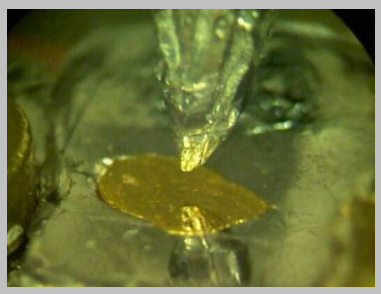
INSTITUTO UNIVERSITARIO DE CIENCIA DE MATERIALES "NICOLÁS CABRERA"

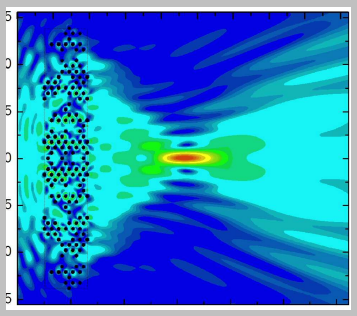
RESEARCH REPORT 2000-2001

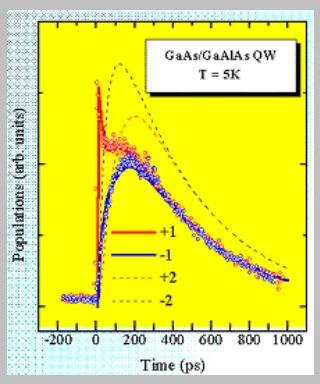


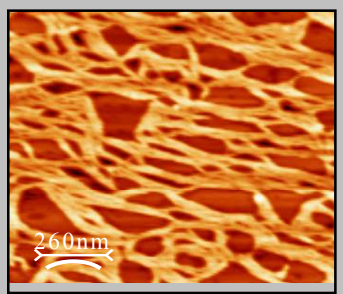


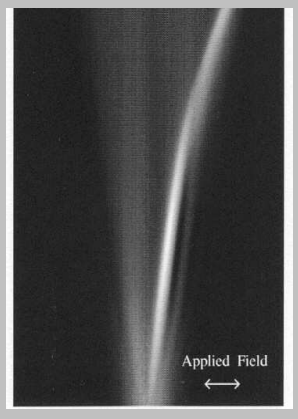


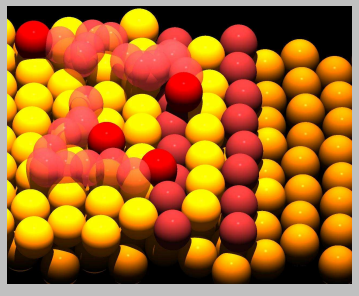


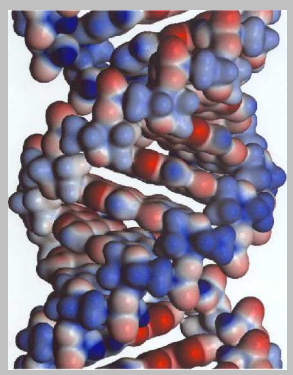












Instituto Universitario de Ciencia de Materiales "Nicolás Cabrera"

RESEARCH REPORT 2000-2001

Edited by:
Carmen de las Heras
José G. Rodrigo

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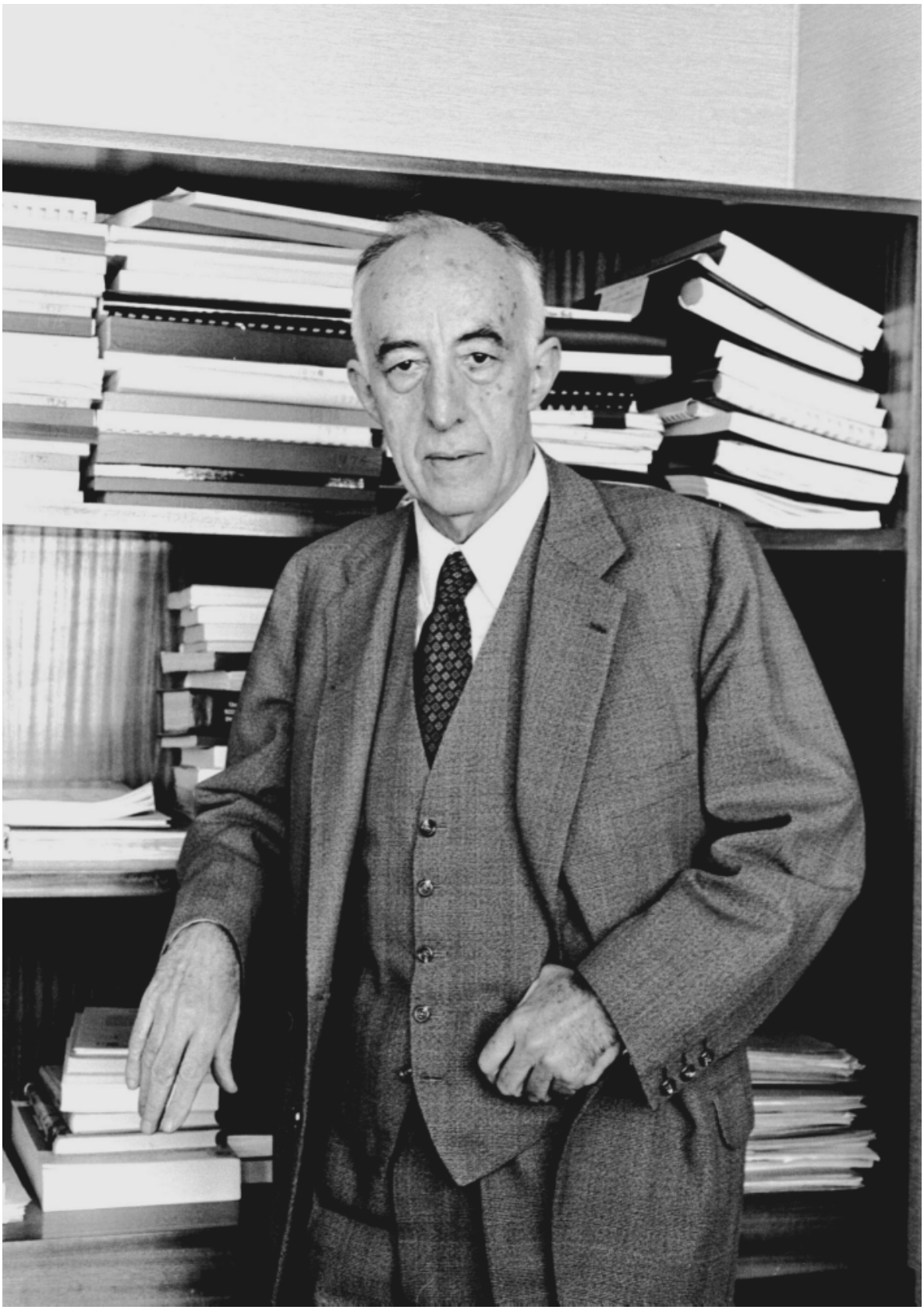
INDEX



The present publication contains a description of the experimental and theoretical research being conducted at the Instituto de Ciencia de Materiales "Nicolás Cabrera" of the Universidad Autónoma de Madrid, with specific attention to the activity performed during the period 2000-2001. Our institute comprises more than 90 professors and postdoctoral researchers at our university interested in Materials Science. Their activity is supported by an even higher number of graduate students, so that research at the Nicolás Cabrera Institute involves the work of about 200 scientists. Founded in 1989, the Nicolás Cabrera Institute has provided a valuable framework for the development of joint scientific and academic enterprises within the large community of condensed matter physicists and materials scientists of our university. Its first two directors, Fernando Flores and Sebastián Vieira, played a leading role in the creation and development of this institution as we know it today. Our institute is heir to the tradition of academic and scientific excellence pioneered by Nicolás Cabrera (1913 - 1989), who played a decisive role in the shaping of a world-class Physics Department at the Autonomous University of Madrid. This book is a fitting tribute to his memory, for it introduces the scientific research of a community of physicists that to a large extent is the legacy of Don Nicolás Cabrera.

I would like to thank our colleagues Carmen de las Heras and José Gabriel Rodrigo for their patience and competence in the process of compiling and editing the material presented in this report.

Fernando Sols
INC Director

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 Cabreras 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 an 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.

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INSTITUTE OF MATERIALS SCIENCE "NICOLAS CABRERA"

RESEARCH GROUPS

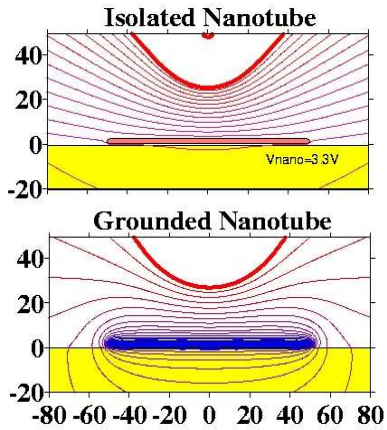
MOVING LIGHT AND ELECTRONS ("MOLE GROUP")

Prof. Juan José Sáenz.
Dr. David Jiménez. Ph. D. Students: Luis Froufe-Pérez, Raquel Gómez-Medina, Sacha Gómez-Moñivas.

The current research of the group is done along two main lines: *Scanning Probe Microscopy (SPM)* and *Wave Scattering in Complex Media*.

Scanning Probe Microscopy (SPM)

- STM: Early group's work on SPM was focused on the current-voltage-distance characteristics of the STM from tunnelling to near field emission regimes. This involved the calculation of the effective tunnelling barrier (i.e. the electric field between a nanometer sized STM-tip and the sample together with the image potential corrections).
- SNOM: We have developed a new theoretical approach to near field microscopy. It is based on the generalization of the Bardeen´s formalism (originally introduced for electron tunnelling) to electromagnetic vector waves.
- EFM: Most of the group´s current efforts in SPM are focused on Electrostatic Force Microscopy (EFM). Our goal is to develop a method to extract quantitative (topographic and electrical) information from real EFM images of inhomogeneous dielectric and conducting samples.

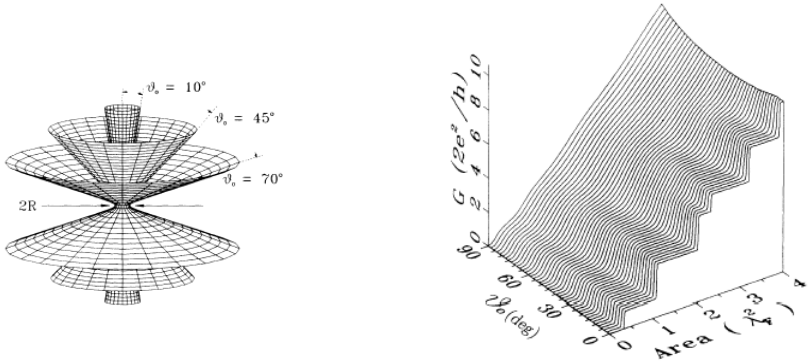


Equipotential surfaces between an EFM tip and a nanotube on a dielectric sample. [S. Gómez Moñivas et al., in preparation, 2002]

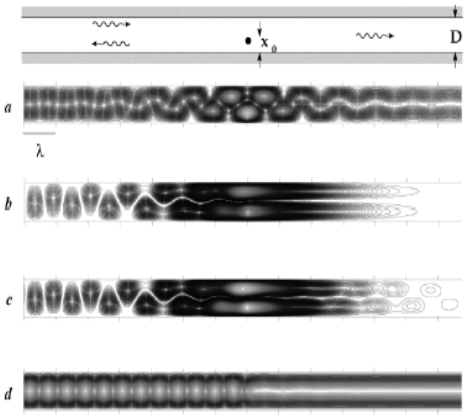
Wave Scattering in Complex Media

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:

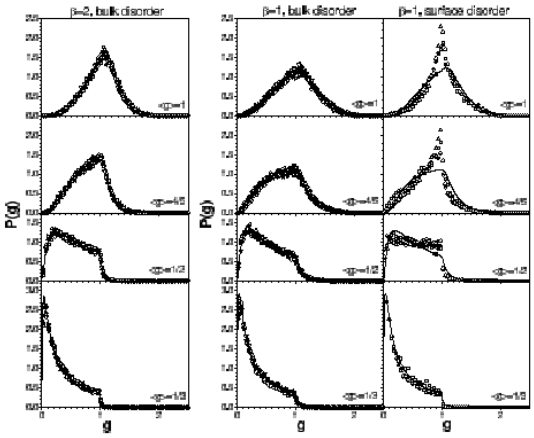
- Quantum Conductance in Nanometer Sized Contacts.
- Wave Transport through Surface Corrugated Waveguides.
- Conductance Distributions in Disordered Wires.
- Intensity Correlations and Fluctuations in Random Media.
- Electromagnetic Field-Particle Interactions in Waveguides.
- Electrodynamic interactions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



Conductance of a smooth contact versus opening angle and cross section [Torres et al., Phys.Rev.B 49 16581 (1994)]



Field Intensity pattern for a single-mode waveguide with a small particle in different positions.
[Gómez Medina et al., Phys.Rev. Lett. 86, 4275 (2001)]



Conductance distributions for bulk disordered wires. $\beta = 1$ ($\beta = 2$) indicates the presence (absence) of time-reversal symmetry. Continuous lines correspond to P(g) obtained from the Monte Carlo solution of the Dorokov-Mello-Pereira-Kumar equation with N=6. Results for surface disordered wires are shown for comparison (after García-Martín et al., Phys Rev.Lett. 87,116603 (2001)). Symbols represent the numerical calculations based on the Anderson model for different configurations.
[Froufe-Pérez et al., Phys.Rev. Lett. (2002) in press]

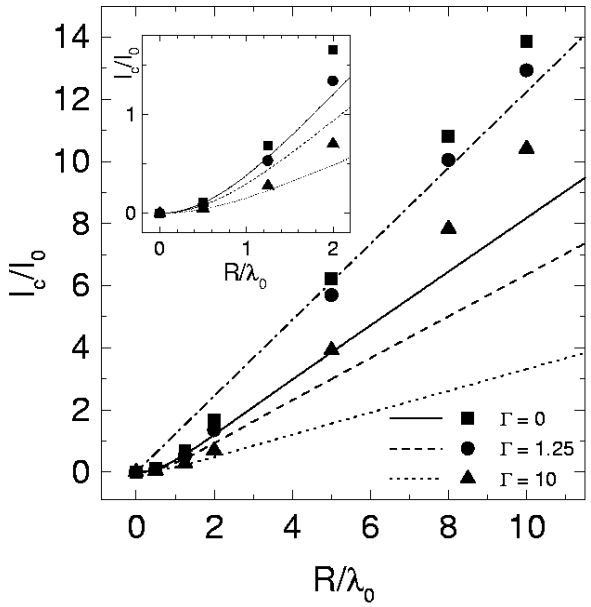
For additional information, please contact Juanjo Sáenz at email: juanjo.saenz@uam.es .

QUANTUM DYNAMICS AND COHERENCE

Prof. Fernando Sols.
Dr. Heiner Kohler, Dr. Sigmund Kohler.
Ph. D. students: Miguel Rey, Elsa Prada, Brian J. Power.

We perform theoretical research in the two broad areas of mesoscopic electron transport and dilute quantum gases, with a general interest in macroscopic quantum phenomena and quantum dissipation. Specifically, we study electron transport in normal, superconducting, and hybrid normal-superconductor structures, with emphasis on Fermi pumps, Josephson links and the general theory of superconducting transport. Within the physics of atomic Bose-Einstein condensates, we investigate the Josephson effect and macroscopic quantum interference phenomena. Below we describe a sample of recent research.

Quantitative theory of the critical current in a wire. We study superconducting transport in homogeneous quasi-one-dimensional wires in the cases of both equilibrium and nonequilibrium quasiparticle populations, using the quasiclassical Green's function technique. First we consider narrow superconductors with arbitrary current densities and impurity concentrations ranging from the clean to the dirty limit. Local current conservation is guaranteed by ensuring that the order parameter satisfies the self-consistency equation at each point. For equilibrium transport, we compute the current, the order parameter amplitude, and the quasiparticle density of states as a function of the superfluid velocity, temperature, and disorder strength. Nonequilibrium is characterized by incoming quasiparticles with different chemical potentials at each end of the superconductor. We calculate the profiles of the electrostratic potential, order parameter, and effective quasiparticle gap. We find that a transport regime of current-induced gapless superconductivity can be achieved in clean superconductors, the stability of this state being enhanced by nonequilibrium. Allowing for arbitrary wire width, we study the structure of the Meissner effect in a current-carrying cylindrical wire with any amount of disorder following a numerical procedure that is exact within the quasiclassical approximation. A distribution of current is found that is non-monotonous as a function of the radial coordinate. For high currents, a robust gapless superconducting state develops at the surface of both clean and dirty leads. Our calculation provides a quantitative theory of the critical current in realistic wires.



Critical current I_c as a function of radius R for three different values of disorder strength Γ. Discrete points are the result of the exact calculation. Lines are obtained from the approximation that the critical current is reached when the current density at the surface equals the uniform value for a narrow wire at its critical current. The dash-dotted line gives the prediction from the phenomenological Silsbee's rule, according to which the critical current is reached when the magnetic field at the surface equals the thermodynamic critical field of the superconductor. Inset: Magnification of the small R quadratic behavior (narrow wire limit)

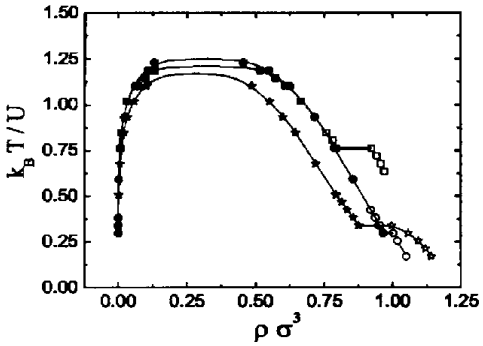
Ref. J. Sánchez-Cañizares, J. Ferrer and F. Sols. "Nonlinear and nonlocal Meissner effect in superconducting wires". Phys. Rev. B 63, 134504 (2001).

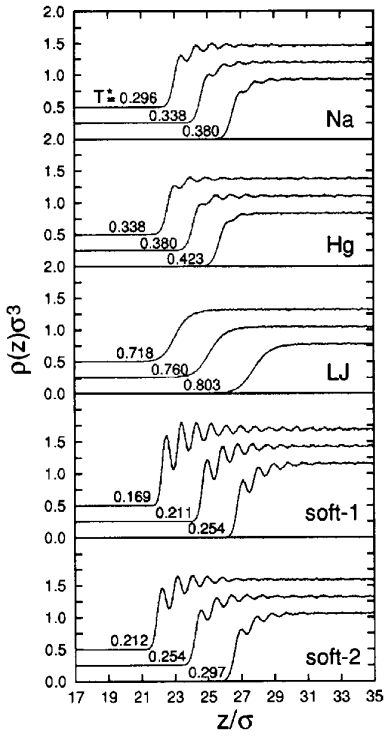
STATISTICAL MECHANICS AND COMPLEX SYSTEMS

Prof. P. Tarazona, Prof. E. Velasco
PhD students: R. Checa, D. de las Heras and F. Penna

In the last two years we have been involved in the study of a number of topics related to the microscopic structure and phase behaviour of a variety of systems of particles, focusing on both their bulk and surface properties.

One of our most relevant works, as far as surface properties are concerned, involves the surface structure developed at the liquid-vapour interfaces of some metals, e.g. Hg and Ga, which have been generally attributed to the metallic character of the corresponding fluids. We have proposed an alternative explanation, not based on many-body electronic effects but on a (simpler) low-temperature effect. The above surface effects would then be visible because of the low triple point of the system, which allows to access the low-temperature region and hence to unravel genuine equilibrium surface oscillations. This scenario is feasible even in systems where interactions have a pairwise character. Using computer simulation techniques, we have been able to conclude that there are (at least) two mutually excluding generic properties that a pair potential must have in order to give rise to a low triple-point temperature for the system: (i) a relatively soft repulsive part at short distances, typical of alkali metals; (ii) a very hard repulsive part at short distances, together with a flat attractive well at intermediate distances, typical of metals like Hg.





Our simulations show that, for these systems, the ratio of triple-point temperature to critical temperature is very low with respect to that in the case of van der Waals fluids. This means that for low temperatures the liquid-vapour interface is stable, exhibiting density oscillations along the normal direction. Fig.1 shows temperature vs. density phase diagrams for a number of model potentials that meet one the two criteria mentioned above (represented by stars and circles), along with the phase diagram for a Lennard-Jones potential (squares), which does not satisfy any of them, both somehow constructed so as to give similar critical-point temperatures. As can be seen, the triple point is located at very low temperatures relative to the corresponding temperatures for the Lennard-Jones potential, a typical van der Waals system. Fig.2 shows the corresponding density profiles along the normal direction for the models referred to in Fig.1. The correlation between a low triple-point temperature and the appearance of surface oscillations is evident. For further information see Ref. 1.

Also, using computer simulation, we have studied two further topics related to the properties of these interfaces. On is the one the relation between the occurrence of surface oscillations and the location of the Fisher-Widom line, which separates states with oscillating decaying behaviour in the positional correlations of the system from states with purely monotonic decay. But, what is more important from an experimental point of view, we have investigated how the oscillatory structure disappears with the system size and the role played by capillary waves in this respect. Our results show that the temperature dependence of the oscillations is clearly dominated by capillary waves, the effects associated with the Fisher-Widom line having a minor, if not negligible, role. Additional details can be found in Ref. 2.

1. E. Velasco, P. Tarazona, M. Reinaldo-Falagán and E. Chacón, *J. Chem. Phys*. **117**, 10777 (2002)
2. P. Tarazona, E. Chacón, M. Reinaldo-Falagán and E. Velasco, *J. Chem. Phys*. **117**, 3941 (2002).

AB-INITIO SIMULATIONS OF MATERIALS

Prof. Emilio Artacho, Prof. José María Soler.
Dr. Maria Victoria Fernández, Dr. Oscar Paz. Ph. D. Student: Eduardo Anglada.

The main research line is: Ab initio order-N methods and realistic quantum mechanical simulations of complex systems.

Compared to materials-simulation methods based on classical potentials, the main advantage of ab initio methods (based on first-principles density functional theory, without any adjustable parameters), are their generality, reliability, and accuracy. They involve the solution of Schrödinger's equation for each electron, in the selfconsistent potential created by the other electrons and by the nuclei, and they can be applied to a huge variety of systems and properties. The ex-ponential increase in computational power, combined with the development of new algorithms and more efficient methods, has allowed their application to in-creasingly large and complex systems. Today it is possible to treat one hundred atoms in a workstation, and several hundred in a supercomputer. However, the fact that the CPU time scales as N^3 , with N the number of atoms, has pre-vented an even faster progression, and that the most interesting systems and properties, from a technological point of view, are still out of the reach of these methods.

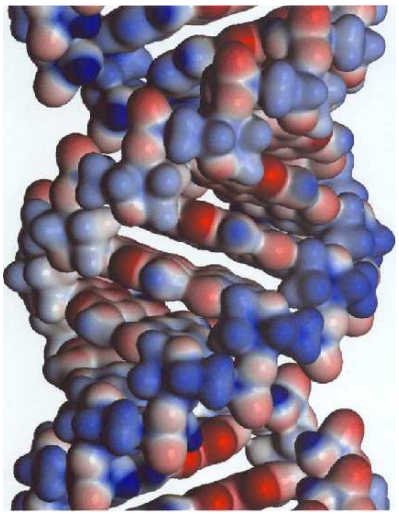
Recently, it has been realized that, with a transformation of the electronic extended states into an equivalent local representation, it is possible to obtain the same results with a cost of CPU and memory which scales as N instead of N^3 . During the last few years, we have developped a program, named SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) which is at the forefront of these so-called order-N methods. It is a general-purpose code, which can treat efficiently crystalline and amorphous solids, liquids, surfaces and molecules, either metallic, insulating or semiconducting. It is able to address very large systems, of the order of one thousand atoms in workstations, and up to a hundred thousand atoms in supercomputers. Besides structural, mechanical, electronic or magnetic properties, it routinely calculates the atomic forces, using them to relax the structure or to perform ab initio molecular dy-namics. These characteristics make it extremely competitive to address a large variety of problems in the forefront of materials science, chemistry, geology, biol-ogy, and pharmacology. Thus, appart from the code development itself, we have started a large number of collaborations with both Spanish and foring groups to study problems like

Electrons in DNA. Although the biological importance of DNA is obvious, recently it has been considered as a building block to make new electronic devices, connecting gold nanoclusters. In this context, it is critical to determine its ability to conduct an electrical current but different conductance measurements differ in more than ten orders of magnitude, from wholly insulating to superconducting. In collaboration with an experimental group in the Autonomous University of Madrid, we have calculated the electronic structure of a chain of dry poly(dG)-poly(dC), which is considered the most favourable sequence for electrical conduction. However, we have found that the extremely narrow width of the valence band, and its sensitivity to variations of structure or sequence, essentially rule out band-like conductivity.

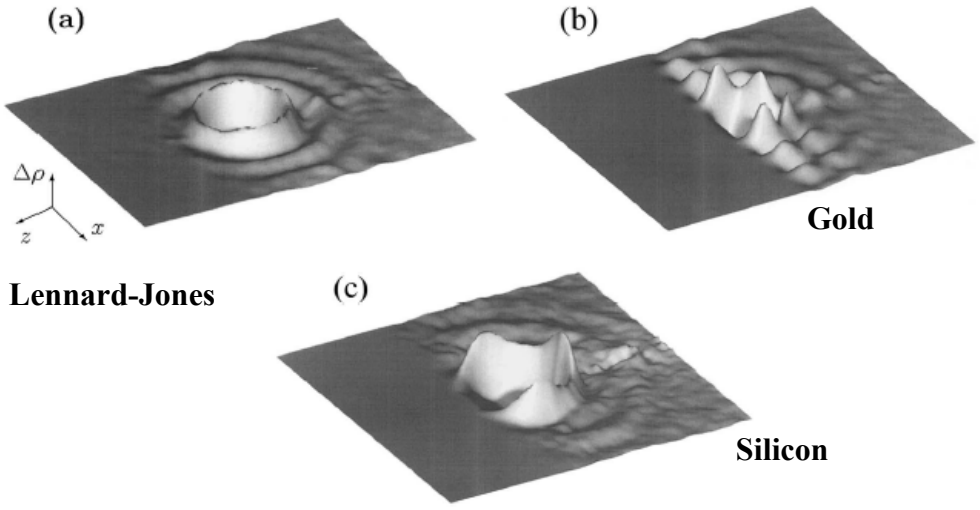
Local structure and bonding in the liquid silicon surface. Using ab initio molecular dynamics, we have studied the local structure of a liquid silicon surface, comparing it with other liquid surfaces (the Lennard-Jones fluid and gold) simulated with classical potentials. The pair distribution function shows preferential in-plane bonds, leading to the formation of a surface layer and to density oscillations as a function of depth.

Monatomic gold wires. Despite the fundamentally non-directional character of its metallic bonding, we have found that monatomic gold wires may adopt a relatively rigid zig-zag structure, produced by the quantized longitudinal and transversal electron states.

Amorphous gold nanoparticles. Combining an extensive structure search, using classical potentials and genetic algorithms, with ab initio calculations to validate selected low-energy structures, we have determined that the most stable geometries of many gold nanoclusters is essentially amorphous. Furthermore, we have linked the tendency of gold towards amorphization to its metallic bonding.



• Fig.1. Surface of constant electron density of a molecule of dry DNA in the A conformation. It has eleven base pairs (715 atoms) repeated periodically. The color represents the selfconsistent electrostatic potential obtained from the density functional calculation. Red corresponds to negative regions (oxigen and nitrogen) and blue to positive ones (hydrogen).



• Fig. 2. Pair distribition function in three liquid surfaces: a) the Lennard-Jones fluid; b) gold, simulated with an embedded atom potential; c) silicon, simulated by ab initio molecular dynamics. x and z directions are parallel and perpendicular to the surface, respectively.
Soler, and E. Artacho, Phys. Rev. Lett. 85 (2000) 4992-4995

INTERACTING ELECTRONS IN NANOSCALE WIRES

Prof. Alvaro Martín-Rodero, Prof. Alfredo Levy-Yeyati.
Ph.D. students: Enrique Vecino, Laura de la Vega

The research lines are:

Electron transport in mesoscopic systems
- Mesoscopic Superconductivity
- Current fluctuations in quantum coherent conductors
- Transport in quantum dots
- Atomic-size contacts and atomic chains
- Hybrid nanostructures

Strongly correlated electron systems
- Kondo effect
- Metal-insulator transition
- Approximation methods for strongly correlated systems

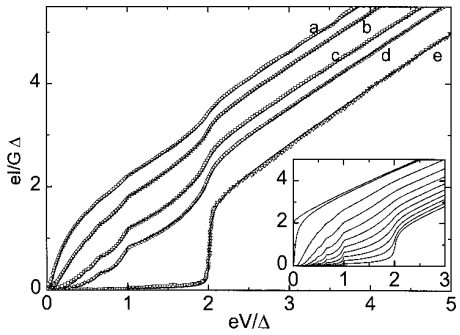
Conduction through single-atom contacts

The electrical conductance properties of individual atoms have been revealed. By combining theoretical model calculations and a series of experiments on various types of single metal atoms, it is shown that the electrical resistance of single atoms is determined by the chemical properties of the particular atom.
The electronics industry has been capable of continuously reducing the size of the components on computer chips for the last three decades. The width of electrical connections on mass-production items such as memory chips approaches already sizes only 500 atoms wide. This suggests that atomic scale devices are within reach. Although we do not expect this to be realised in the foreseeable future, it is important to understand how the properties of conductors change as their size is reduced from the every-day macroscopic scale down to the atomic level, and at which scale changes are to be expected. Using techniques based on the scanning tunneling microscope it is now possible to manipulate individual atoms and measure their properties.

Indeed, the conduction properties at the atomic scale are very different from every day experience. It turns out to be possible to send an extremely strong current, in excess of 10 microamperes through a single atom contact, corresponding to a current density of 1.5×10^{14} A/m^2. By comparison, the electrical wiring for the 220V home electricity supply has fuses, which melt at 16 Ampere. If the wires would be able to carry the same current per area of the cross section of the conductor as atom size contacts, they would be able to carry 400,000,000Ampere. This illustrates that the mechanism, which determines the resistance of the microscopic contact, is entirely different from the mechanism responsible for the resistance in ordinary wires. The latter is usually described in terms of scattering of electrons (as *particles*) at impurities and defects in the metal. In contrast, for atomic size contacts the resistance is determined by the wave character of the electrons and requires a quantum mechanical description. This shows up very clearly in the measured values of the resistance for single atom contacts, which for simple monovalent metals is always close to the quantum value of resistance. This fundamental unit is given by $h/2e^2$= 12.9 kOhm, and is thus completely given in terms of two fundamental physical constants, Planck's constant h and the electron charge e.

In a publication in Nature [394,154 (1998)] we have shown that the chemical valence determines the electrical resistance of an atom. Gold has a valence of one, and we say that this gives the atom a single `channel' for conductance. This channel has the above-mentioned resistance of 12.9 kOhm. An atom of the metal lead (Pb) is a better conductor and has three conduction channels, while in daily life Pb is a ten times poorer conductor than gold. An atom of the metal niobium has even five conduction channels.

In order to establish the number of conductance channels for each of the atoms we used a special property of superconducting contacts. When the contacts are cooled below the superconducting transition temperature, and a voltage is applied over the contact, the current is seen to rise by a series of characteristic steps (Fig. 2). By analysing these steps we were able to count the number of conduction channels for each type of atom.



Measured current-voltage characteristics (symbols) of five different configurations of a Pb sample at 1.5 K using STM and best numerical fits (lines). The inset shows a series of theoretical curves for a single conductance channel and various transmission probabilities of the electrons through the channel. The characteristic steps allow us to determine how many channels contribute to the current.

More recently we have analyzed different transport properties of atomic size conductors including:
Shot noise in superconducting state [PRL 82, 4086 (1999)]
Supercurrent [PRL 85, 170 (2000)]
Dynamical Coulomb blockade [PRL 87, 046802 (2001)]
Fractional Shapiro steps in superconducting contacts under microwave radiation [PRL 88, 157001 (2002)]

PROPAGATION OF CLASSICAL WAVES IN PERIODIC MEDIA

Prof. José Sanchez-Dehesa.
Ph. D students: Fernando López-Tejeira, Jorge Bravo-Abad, Lorenzo Sanchis, Andreas Håkansson

Research interest:

Elastic wave propagation in phononic crystals
Acoustic devices based on sonic crystals
Light propagation in photonic crystals
Optical devices design by genetic algorithm

The propagation of classical waves in periodic media is the main subject in the group. With regards to the topic of sound propagation in sonic crystal (periodic distributions of sound scatterers in air) we have demonstrated the existence of frequency gaps at which the propagation is forbidden [Phys. Rev. Lett. **80**, 5325 (1998)]. This effect can be used to construct efficient sound shields. Also, we have shown that these system can be used to fabricate refractive devices for airborne sound, such as lenses and interferometers [Phys. Rev. Lett. **88**, 023902, (2002), and Fig. 1] whose behaviour is analogous to their counterparts for light waves. If the cylinders are coated by a soft sheath and embedded in a hard medium, the final system possesses subfrequency gaps, and elastic wave propagation shows Fano like resonance features in the transmission spectrum [Phys. Rev. Lett. **88**, 225502 (2002)].

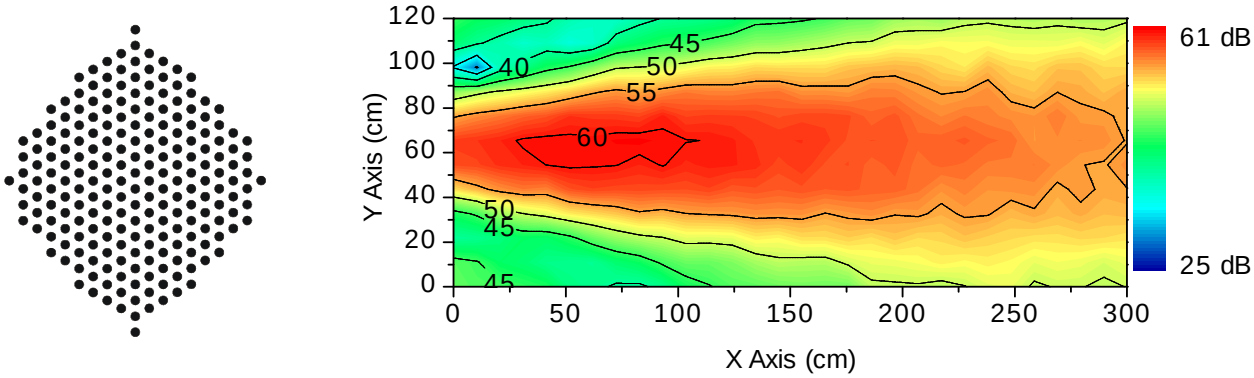


Figure 1. Map of the sound level (in dB) along with the sketch of the acoustic lens based on a two-dimensional sonic crystal (SC). The sketch is drawn to scale. The lens-like sample measure 1.2 m of width. We have used SC with a triangular lattice of 4 cm diameter cylinders, the pitch being 6.35 cm. The pressure map has been taken at a frequency of 1700 Hz, which is well below the first gap that starts at 2300 Hz.

In the field of light propagation in media with periodic modulation of its refractive index (photonic crystals), our efforts are focused in the topic of artificial opals. These consist of a fcc lattice of silica spheres in air, and also in two-dimensional structures of dielectric rods are studied. Both systems are analysed for the sake of their application in optical devices [see, for example, Phys.Rev. B**64**, 245113 (2002); Phys. Rev. B**65**, 185110 (2002), Phys. Rev. B**65**, 245111 (2002)]. With such purpose we are currently applying genetic algorithms in the design. Particularly, we have designed an optical lens that can be employed as a spot size converter with a reduction ratio 11:1, and a f-number as low as 0.47. (see Fig. 2)

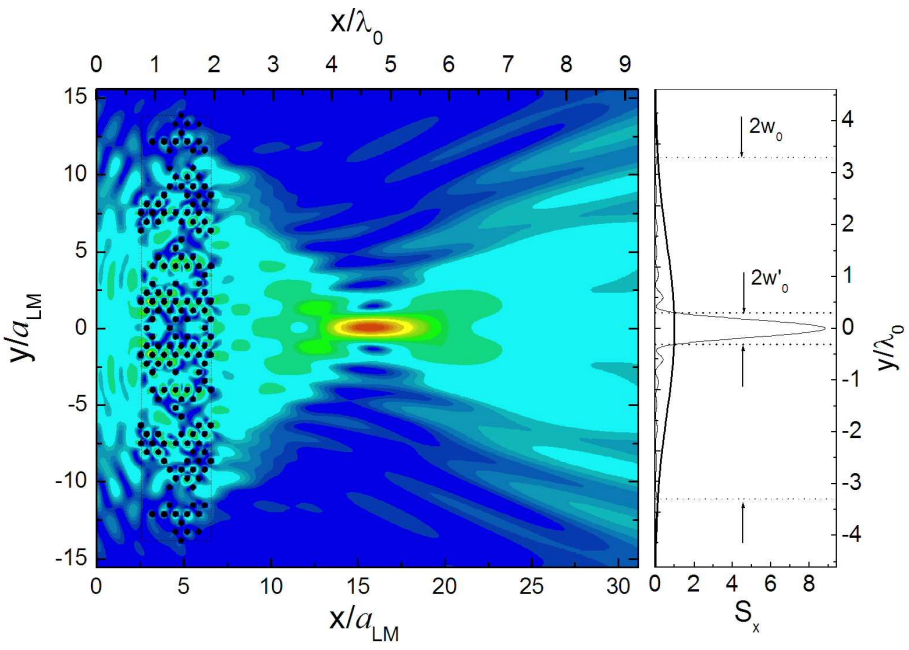


Figure 2. (left panel) Focusing effect produced by a spot-size converter (lens) designed by genetic algorithm. It shows the pattern of the electric field modulus produced by the scattering of a Gaussian light beam of width $2w_0$ that impinges from the left to the lens. This consists of an array of Si cylinders (black dots) in silica background. The length scales are given in terms of the lattice parameter employed in the design of the lens, a_{LM}, as wells as in terms of the working wavelength of the lens λ_0. A scale colour is used, red (blue) colour means maximum (minimum) intensity.
(right panel) The x-component of the Poynting vector is represented at the focal point (x_f=4.60 λ_0) (thin line) as well as along the y-axis at x=0 (thick line).

Collaborations: Francisco Meseguer (UPV-CSIC); Cefe López (ICMM-CSIC); Javier Marti (ITACA-UPV); Felipe Ramos-Mendieta (Univ. Sonora, México).

ELECTRONIC AND ELECTROMAGNETIC THEORY FOR NANOSYSTEMS, SURFACES, HETEROSTRUCTURES AND ORGANIC MOLECULES

Prof. Fernando Flores
Prof. Francisco José García-Vidal, Prof. José Ortega, Prof. Rubén Pérez
Dr. Pavel Jelinek. Ph.D. Students: Jose Manuel Blanco (TA), Pilar Fernández de Pablos (TA), Blanca Biel, Cesar González, Hector Vázquez

Simulation methods (electronic properties) of complex systems.

Density Functional Theory (DFT) provides the standard approach to the calculation of electronic properties. Codes where DFT is implemented in a plane wave basis, like the CASTEP package used in our group, provide an accurate but very computationally demanding tool. Our group works in the development of alternative efficient approaches based on the use of a local orbital basis. We have collaborated in the development of Fireball, an efficient DFT implementation in a local orbital basis. In order to improve the efficiency of the code and the description of the exchange and correlation effects with local orbital basis, we have also developed an alternative formulation of DFT in terms of the orbital occupancies(DFT-OO).

Exchange-Correlation Energy as a function of the orbital occupancies: Implementation on First Principles Local Orbital Methods. *P. Pou, R. Oszwaldowski, R. Pérez, F. Flores y J. Ortega. Int. J. Quantum. Chem.* ***91*** *151 (2002).*

Further developments in the local-orbital density-functional-theory tight-binding method. *J.P. Lewis et al., Phys. Rev. B* ***64*** *195103 (2001).*

Local-density approach and quasiparticle levels for generalized Hubbard Hamiltonians. *P. Pou, R. Pérez, F. Flores, A. Levy Yeyati, A. Martín-Rodero, J.M. Blanco, F.J. García-Vidal y J.Ortega. Phys. Rev. B* ***62*** *, 4309-4331 (2000).*

Correlation Effects. Kondo Effect.

The development of the DFT-OO method is strongly linked with the implementation of ab initio Green's functions methods to treat correlation effects in solids and molecules. Our approach is based on the dynamical mean field approximation (DMF) and the self-consistent replacement of the exchange-correlation potential of the DFT-OO method by an appropriate self-energy. Recent applications include Kondo efect and the understanding of ferromagnetism in Fe and Ni.

Electron Correlation Effects and Ferromagnetism in Iron. *P. Pou, F. Flores, J. Ortega, R. Pérez,y A. Levy Yeyati.J. Phys: Condens. Matter* ***14*** *L421 (2002); A. Levy-Yeyati et al., Phys. Rev. Lett.* ***83*** *, 600 (1999).*

Transport in Nanostructures.

Transport properties can be efficiently formulated in terms of a local orbital basis, and thus linked with the first principles methods that we have developed for the calculation of the electronic properties. Our approach is based on the combination of Green's function techniques and the Keldish non-equilibrium formalism. Applications of that formalism range from the theoretical analysis of Scanning Tunneling Microscopy (STM) images, Ballistic Electron Emission Microscopy (BEEM) --with special attention to the calculation of electron lifetimes-- and mechanical and transport properties of metallic nanocontacts.

N. Mingo et al, Phys. Rev. B ***54*** *, 2225 (1996); F.J. Garcia-Vidal et al, Phys. Rev. Lett.* ***76*** *, 807 (1996) ; K. Reuter et al, Phys. Rev. Lett.* ***81*** *, 4963 (1998); P.L. de Andres et al, Prog. Surf. Sci. 66 , 1 (2001) ; P. Jelinek et al, Phys. Rev. B RC submitted (2002); P. F. de Pablos et al, Phys. Rev. B* ***66*** *075411 (2002).*

Surfaces and interfaces. Organic compounds.

We have also used the theoretical techniques mentioned above to study different surface and interface problems. We first mention the recently discovered $\sqrt{3}\times\sqrt{3}\leftrightarrow 3\times 3$ two-dimensional phase transition on Sn/Ge(111). We have shown that this phase transition is associated with a soft phonon. In a recent paper in collaboration with Prof. García-Michel's group, we have analyzed the surface phonons of this system finding out that the phase transition is of the order-disorder type.
As a second example, we have studied the atomic geometry of the passivated Se/GaAs(100) surface, and its metallization. We have found that the Schottky barrier formation depends crucially on the reactivity of this surface with the deposited metal atoms. We finally mention that we have started to analyze the interface formation of thin organic films on metals or semiconductor surfaces. In the case of the metal/PTCDA--molecule interface we have analyzed how the metal-surface/organic-molecule interaction is enough to create an electrostatic dipole responsible of the Schottky barrier, and to define a Charge Neutrality Level for the PTCDA molecule.

Surface Soft Phonon and the $\sqrt{3}\times\sqrt{3}\leftrightarrow 3\times 3$ phase transition in Sn/Ge(111) and Sn/Si(111). *R. Perez, J. Ortega and F. Flores Phys. Rev. Lett. 86 , 4891 (2001).*

Metallization and Schottky barrier formation for Se passivated GaAs(100) surfaces. *B. Biel, I. Benito, C. Gonzalez, J.M. Blanco, J. Ortega, R. Pérez, and F. Flores Appl. Surf. Sci.* ***190*** *, 475 (2002).*

Dipole formation at metal/PTCDA interfaces: role of the CNL. *H. Vazquez, R. Oszwaldowski, P. Pou, J. Ortega, R. Pérez, and F. Flores. (in preparation) (2002).*

Mechanical Properties from first principles

Mechanical properties of materials are controlled by the breaking and remaking of bonds at the atomic scale. We have shown that carefullly designed large-scale first principles simulations, where the quantum nature of atomic bonding is properly described, provides useful information on long standing mechanical problems.
Applications range from tip-sample interactions involved in nanoindentation, polishing and the operation of scanning probes (STM and Atomic Force Microscopy (AFM)), to the understanding of brittle fracture in Silicon. Much of the recent effort is focused on understanding image contrast in Dynamic AFM, operated in the frequency modulation (FM) mode.

Dynamic Atomic Force Microscopy Methods.*R. García y R. Pérez. Surf. Sci. Rep.* ***47*** *197-302 (2002).*

Interplay between Nonlinearity, Scan Speed, Damping and Electronics in Frequency Modulation Atomic Force Microscopy. *M. Gauthier, R. Pérez, T. Arai, M. Tomitori y M. Tsukada. Phys. Rev. Lett. 89 146104 (2002).*

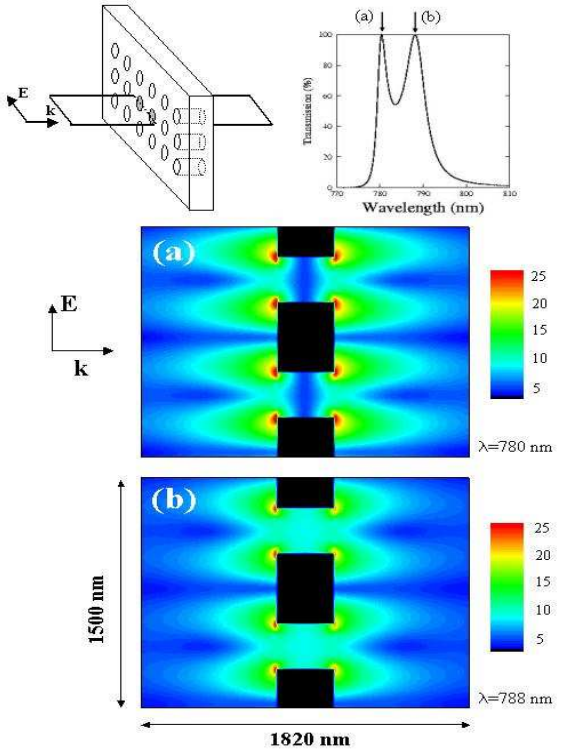
Can Atomic Force Microscopy Achieve Atomic Resolution?. *M. R. Jarvis, R. Pérez y M. C. Payne. Phys. Rev. Lett. 86 1287-1290 (2001).*

Directional Anisotropy in the Cleavage Fracture of Silicon. *R. Pérez y P. Gumbsch. Phys. Rev. Lett 84, 5347-5350 (2000).*

OPTICAL PROPERTIES OF NANOSTRUCTURED METALS

Prof. F.J. García Vidal
Dr. Esteban Moreno Soriano

We perform theoretical research in the area of optical properties of metals that are structured in the nanometer scale. In the last few years there has been a renewed interest in exploiting the dielectric response of metals to make photonic materials. Very recently, it has been discovered that transmission of light through subwavelength hole arrays made in a metal film can be orders of magnitude larger than expected from standard aperture theory. This extraordinary transmission effect has many potential applications in subwavelength lithography, near field microscopy, optical modulators, flat panel displays, among others. In Refs. [1] and [2] we have demonstrated that the enhancement of transmission is due to tunnelling through surface plasmons (see Fig.1) formed on each metal-dielectric interface. Different regimes of tunnelling (resonant through a kind of ``surface plasmon molecule´´, or sequential through two isolated surface plasmons) are found depending on the geometrical parameters defining the system.



The plot illustrates the effect of the surface plasmon molecules. The x-axis depicts the propagation of light. The y-axis runs along a cut of the periodic array of holes (the cut considered is represented schematically in the upper left panel). The upper right panel shows the wavelengths (780 and 788 nm) at which light is transmitted through the metal. Two separate cases are shown in (a) and (b), corresponding to the two different plasmon molecule levels: the symmetric (b) and antisymmetric (a) linear combination of surface plasmons at both interfaces. It is worth noticing the huge enhancement of the fields at the surfaces, by a factor of order 500 in intensity.

[1] L. Martín-Moreno, F.J. García-Vidal, H.J. Lezec, K.M. Pellerin, T. Thio, J.B. Pendry y T.W. Ebbesen, Phys. Rev. Lett. ***86****, 1114 (2001).*
[2] A. Krishnan, T.Thio, T.J. Kim, H.J. Lezec, T.W. Ebbesen, P.A. Wolff, J.B. Pendry, L. Martín-Moreno y F.J. García-Vidal, Opt. Comm. ***200****, 1 (2001).*

SOLID STATE LASERS

Prof. J. García Solé
Prof. L.E. Bausá, Prof. C. de las Heras, Dr. D. Jaque García, Dr. J.A. Sanz García.
Ph. D. Students: M.O. Ramirez, J.J. Romero.

The research activity of our group is related to the growth, characterisation and laser oscillation of new crystals activated with optical ions with potential applications to develop new laser sources.

As it is well known the word LASER refers to Light Amplification by Stimulated Emission of Radiation. A laser system consists in three basic parts: a laser medium (solid, liquid or gas), a cavity and a pumping (optical, electrical...) system. The production of stimulated emission of light occurs into the laser medium, which can then be considered as the heart of laser. Solid State Lasers are those in which the medium is a dielectric crystal containing a certain amount of the so called "activators" (ion or colour centres). In fact the first laser, known as Ruby laser and discovered by Maiman in 1960, was a solid state laser consisting in an Al_2O_3 crystal doped with a small amount of Cr^{3+} ions. The intense red coherent light produced by this laser is related to specific electronic transitions of the Cr^{3+} ions.

Since this discovery, the number of Solid State Lasers has dramatically increased due to different requirements from industry and science to produce coherent and monochromatic light in different wavelengths of the electromagnetic spectrum and with different characteristics. Nowadays, hundreds of activated laser crystals have demonstrated laser operation and this number is continuously increasing.

Our group investigate crystals activated with rare earth (Nd^{3+}, Yb^{3+}, Tm^{3+},.....) and/or transitions metal ions (Cr^{3+}, Cr^{4+}, Ti^{3+}, ...) which have potential applications as new lasers.

The present interest is focussed into the study of non-linear laser crystals (mostly niobates and borates) doped with rare earth and transition metal ions devoted to develop new compact (diode pumped) solid state lasers which can generate visible and/or ultraviolet radiation by the so called "Self-Frequency-Conversion" processes.

Figure 1 show, as a relevant example, how coherent green light is produced from a $YAl_3(BO_3)_4$ (YAB) crystal doped with Nd^{3+} ions by the so called "Self-Frequency-Doubling" process. In this process the infrared laser light generated by the Nd^{3+} ions ($\approx$1 μm) is converted into green light of double frequency ($\approx$ 0.5 μm) by means of internal second harmonic generation (inside the YAB laser host crystal).

Other nice interaction processes can be obtained when the appropriate crystal is used, giving rise to different visible and ultraviolet wavelengths. For instance, our group has recently discovered that the same crystal of figure 1 can be used to produce a Red (R), Green (G) and Blue (B) laser based on different self-sum-frequency processes inside the crystal. RGB laser sources are of interest in applications such as optical printing and laser displays.

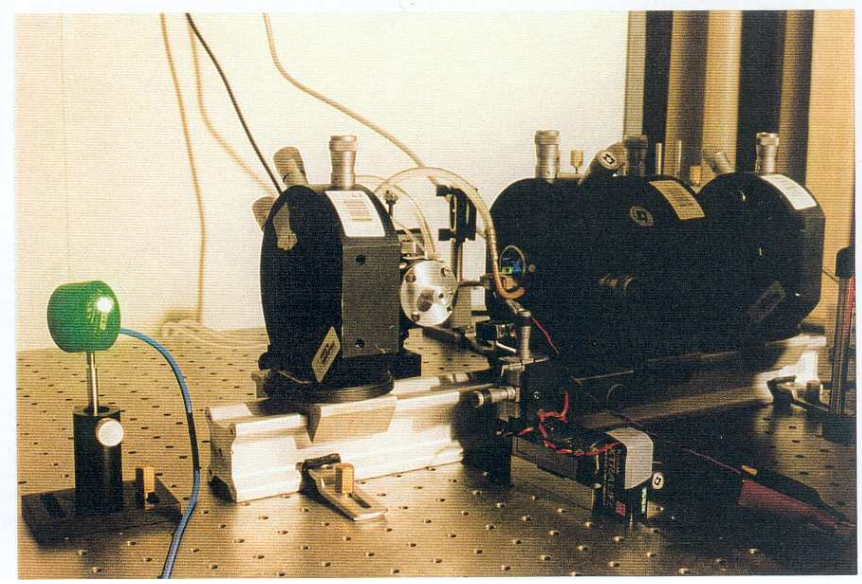


FIGURE 1. Generation of green coherent light from a $YAl_3(BO_3)_4$:Nd^{3+} laser crystal.

Our research in new laser crystals involve three defined and inter-related aspects:

i) Growth of crystals and preparation of laser elements.-

Some of the crystals (principally $LiNbO_3$) we investigate are grown in our laboratory by the Czochralski method while other crystals are obtained in the frame of a variety of scientific cooperations with different laboratories in the world. We also have the facilities needed to prepare laser elements: Cutting, polishing and spectral coating facilities.

ii) Characterisation by advanced optical spectroscopy.-

Grown crystals are investigated by basic and advanced optical spectroscopic techniques (laser site selective spectroscopy, time resolved spectroscopy,...) using our continuos and pulsed laser source facilities. Information on basic processes, such as active centres symmetries, energy transfer phenomena, excited state absorption, ..., can be obtained.

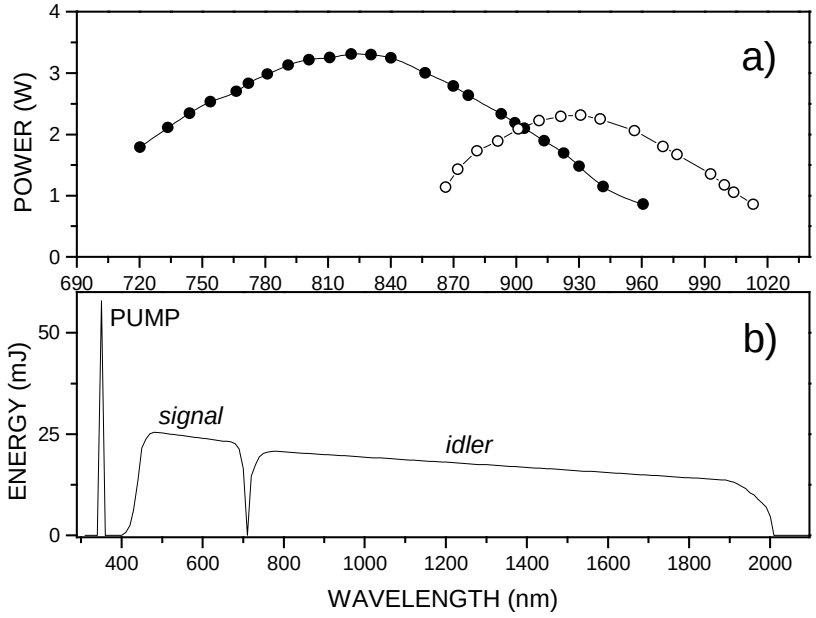


Figure 2 shows the laser excitation/pumping spectral range that can be covered by means of our Optical Parametric Oscillator (OPO) and our Ti-Sapphire tunable laser.

iii) Laser oscillation experiment.

Laser oscillation is the last step in the research of a new laser medium. These experiments permit to establish the viability of this medium for a particular application. However, in addition, these experiments permit to access new physical basic research problems.

THE PHOTOREFRACTIVE EFFECT. PHENOMENA, MATERIALS AND APPLICATIONS

Prof. Fernando Agulló-López, Prof. Luis Arizmendi, Prof. Mercedes Carrascosa.
Dr. Josefa Limeres, Ph. D. Student: Gabriel Fernández Calvo.

The group has investigated many topics related with the photorefractive effect, either concerning its basic properties as nonlinear optical effect, or the materials and applications. The photorefractive (PR) effect is a peculiar nonlinear optical effect that consists of a change in the refractive index induced by inhomogeneous low intensity illumination of a photoconductor and electrooptic material. In typical PR experiments, a sinusoidal pattern, obtained by the interference of two plane waves, is used. As a result, a sinusoidal diffraction grating, or phase hologram, is recorded in the material. PR media have been proposed for several holographic applications, such as interferometry by real-time holography, optical storage, interconnects, etc. In the last few years the main research lines have been the following ones:

Material nonlinearities:

The physical mechanism of the PR effect involves the redistribution of charge in the material that gives rise to a spatially varying internal electric field. Then, this internal electric field leads to the generation of the corresponding refractive index pattern via the electrooptic effect. The former process consists of three steps 1) optical and/or thermal excitation of carriers from the filled traps, 2) migration of the free carriers in the conduction (or valence) band, and, finally, 3) subsequent recombination of the free carriers at the acceptor sites.

All these three processes, free charge generation, transport and recombination, take place themselves through a non linear mechanism inside the material that give rise to interesting new effects. Among them we have extensively studied two phenomena:

a) *Nonlinear grating cross-talk and spatial frequency mixing.* When more than one holographic grating is recorded in a photorefractive material the non linear PR response leads to the mutual coupling of the involved gratings and to the generation of new components with k vectors that are linear combinations of the ones intentionally recorded [1]. These crosstalk phenomena have been extensively investigated in various photorefractive materials (BSO, $BaTiO_3$ and $LiNbO_3$). In fig. 1 we show the diffraction efficiency η of the numerous combinational gratings observed when writing two photorefractive gratings in $LiNbO_3$ [2].

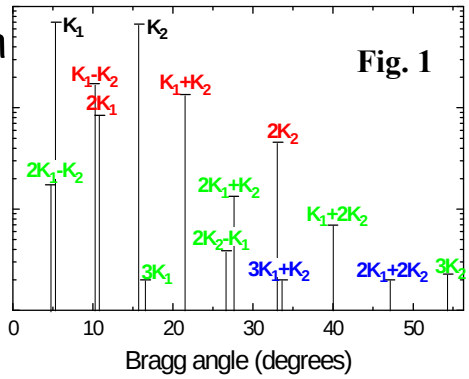


Fig. 1

b) *Charge singularities and associated quasi-discontinuities of the refractive index change.* To enhance the photorefractive effect in non ferroelectric photoconductive materials and AC electric field is applied to the crystal during illumination . In this configuration we have found that material nonlinearities give rise to very narrow charge peaks and consequently to quasi-discontinuities of the refractive index change. This interesting effect gives rise, in turn, to unusual properties of beam propagation under these conditions [3]. (See Fig. 2).

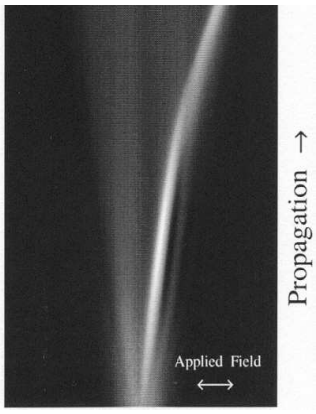


Fig. 2

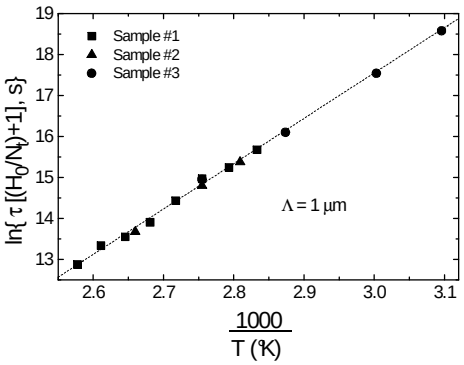
Spatial solitons and nonlinear propagation of beams. Spatial optical solitons are self-trapped light beams than propagate in nonlinear media and preserve their spatial profile by virtue of the balance between diffraction and nonlinear optical focusing. PR materials exhibit an extraordinary scenario for the investigation of such nonlinear phenomena, and several types of spatial solitons have already been predicted and demonstrated experimentally in slow ferroelectric materials. Our group has shown that soliton propagation is also possible in fast PR materials (BSO,BTO,BGO,AsGa,CdTe,etc) placed in a strong and rapidly oscillating AC field [4]. These spatial solitons rely on a different mechanism than the one usually encountered in slow ferroelectric materials. Namely, they induce a refractive index quasi-discontinuity and propagate attached to it in similar fashion as a nonlinear surface wave does along an interface.

Photorefractive thin films. In this case we address the theoretical modelling of the effect when the thickness of the active material is low (1-10 μm). Relevant edge effects have been found and different kind of materials have been investigated such as semiconductor, multiple quantum wells or organic films [5].

Photrefractive effect in periodically poled $LiNbO_3$. Periodically poled ferroelectrics can be considered as new photorefractive materials combining suppression of long scale variations of the refractive index (suppression of optical damage) with a strong photorefractive effect at high spatial frenquencies. We have investigated different aspects of the photorefractive effect of these materials in both behaviour regimes [6,7].

Linear detection of phase changes by holographic methods. Investigation of possible industrial applications of fast cubic PR materials has been carried out (sensors). We have shown theoretically that a full vectorial approach to describe beam coupling in cubic PR materials placed in a strong and rapidly oscillating AC field predicts the possibility of linear detection of fast signals. Our theoretical results have been supported by experiments that have given direct confirmation of linear phase-modulation detection [8].

Long-lifetime photorefractive holograms via thermal fixing. We have studied very deeply the process of thermal fixing of volume hologram via ionic charge screening of the electronic charge distribution of the recorded hologram, and the subsequent developing process [9]. In particular we investigated the decay times of fixed holograms recorded in $LiNbO_3$:Fe at different temperatures in the range 60 – 130 °C for samples with different oxidation state $[Fe^{3+}]/[Fe^{2+}]$ and hydrogen concentration [10]. In the figure it can be observed how the decay times, weighted using a theoretically predicted factor depending on these concentrations, follow a unique straight line. Our results demonstrate that in our $LiNbO_3$:Fe samples, the hydroxyl ions are the charge carriers responsible for thermal fixing of holograms. By control of the Fe impurity concentration, the oxidation state, and the concentration of OH^- ions, we can obtain fixed volume holograms with very high diffraction efficiency (~100%) and with a lifetime longer than 10 years, suitable for practical holographic devices.



Characterization of material parameters using photorefractive holographic measurements. Hologram diffraction efficiency behavior with temperature and illumination is used to determine some bulk material parameters. The electronic photo and dark conductivities are obtained from the decay lifetimes. Through the decay times of fixed holograms we have also determined the ionic OH^- diffusion coefficient in the c-axis direction of $LiNbO_3$ crystals and its activation energy [10]. This coefficient has a value of $D_H = (1.4 \times 10^{-3}\ cm^2\ s^{-1}) \exp[-(0.95\ eV)/k_BT]$.

[1] J. Limeres, M. Carrascosa, L. Arizmendi, F. Agulló-López y P. Andersen, Phys. Rev. B. (2002), in press. **[2].** E.M. de Miguel-Sanz, J. Limeres, L. Arizmendi and M. Carrascosa, , J. Opt. Soc. Am. B 16, 1658-1663 (1999). [3] G.F. Calvo, B. Sturman**,** F. Agulló-López, M. Carrascosa Phys Rev. Lett. 84, 3839 (2000).**[4]** - G.F. Calvo, B. Sturman, F. Agulló-López, M. Carrascosa,. Submitted to Phys. Rev. Lett. **[5]** E.V. Podivilov, B. I. Sturman, G.F. Calvo, **,** F. Agulló-López, M. Carrascosa y V. Pruneri, Phys Rev B 62, 13182-13187 (2000).**[6]** M.Goul´kov, S.Odoulov, I.Naumova, F.Agulló-López, G.Calvo, E.Prodilov, B.Sturman and V.Pruneri, , Phys. Rev. Lett. 86, 4021 (2001). **[7]** G.F. Calvo, F. Agulló-López, M. Carrascosa and L. Solymar, J. Opt. A : Pure Appl. Opt. 3, 413 (2001)**[8].** K. Paivasari, A.A. kamshilin, B. I. Sturman, G.F. Calvo, F. Agulló-López and M.Carrascosa, Appl. Phys. 90, 3135 (2001).**[9]** E.M. de Miguel-Sanz, J. Limeres, M. Carrascosa and L. Arizmendi,J. Opt. Soc. Am. B, 17, 1140 (2000). **[10]** E.M. de Miguel-Sanz, M. Carrascosa and L. Arizmendi, Phys. Rev. B 65, 165101 (2002).

PHOTOVOLTAIC MATERIALS

Prof. Máximo León
Prof. José Manuel Merino, Dr. Julio Ramiro.
Ph.D. students: Adolfo López, Elvis Hernández, Gregorio Albornoz.

Research Lines:

Cu- and Ag-chalcopyrites, ABC_2 (A = Cu, Ag; B = Al, Ga, In; C = S, Se, Te)
Ordered defect compounds, AB_xC_y ($2 \le x \le 5$, $3.5 \le y \le 8$)

Our group has a large experience both in multinary compounds synthesisation and thin film deposition with several evaporation techniques (thermal, "flash", e-beam) among which the "flash" evaporation method has been extensively used to deposit $Cu(Ga,In)Se_2$ thin films for $Mo/Cu(Ga,In)Se_2/CdS/ZnO$ solar cells fabrication. By this method we have achieved an efficiency close to the 6% (active area ~ 1 cm^2) in $CuInSe_2$ and $CuGa_{0.25}In_{0.75}Se_2$ based solar cells (Fig. 1) [*Thin Solid Films* **361-362** (2000) 22-7].

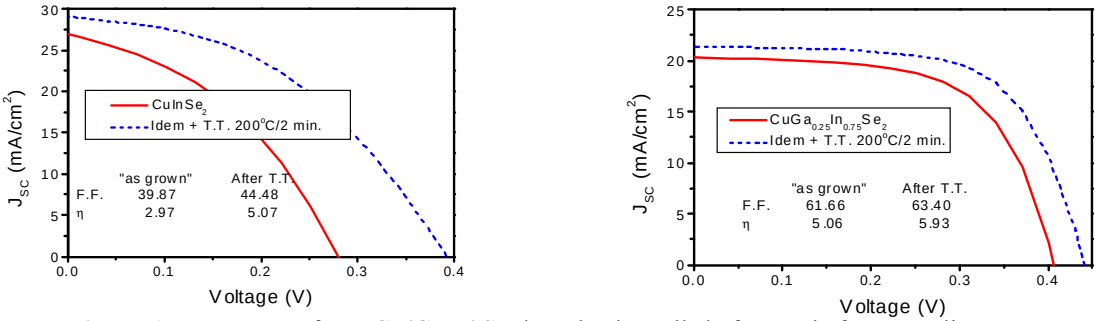


Figure 1 I-V curves of two $Cu(Ga,In)Se_2$ based solar cells before and after annealing

By X-ray powder diffraction and Rietveld refinement of the diagrams we have studied several $CuGa_{1-X}In_XTe_2$ synthesised compounds determining their structural parameters as well as for different $CuInSe_2$ compounds with compositions close to the stoichiometric one. In the former case we have observed that the lattice parameters depend linearly on the In and Ga contents [*J. Vac. Sci. Tchnol. A* **11**(5) (1993) 2430-6] while in the latter we have observed that the Cu-content strongly affects the structural parameters such as the fractional coordinate of the Se atom, x[Se], and the interatomic distances (Fig. 2) [*J. Appl. Phys.* **80**, (1996) 5610 6]

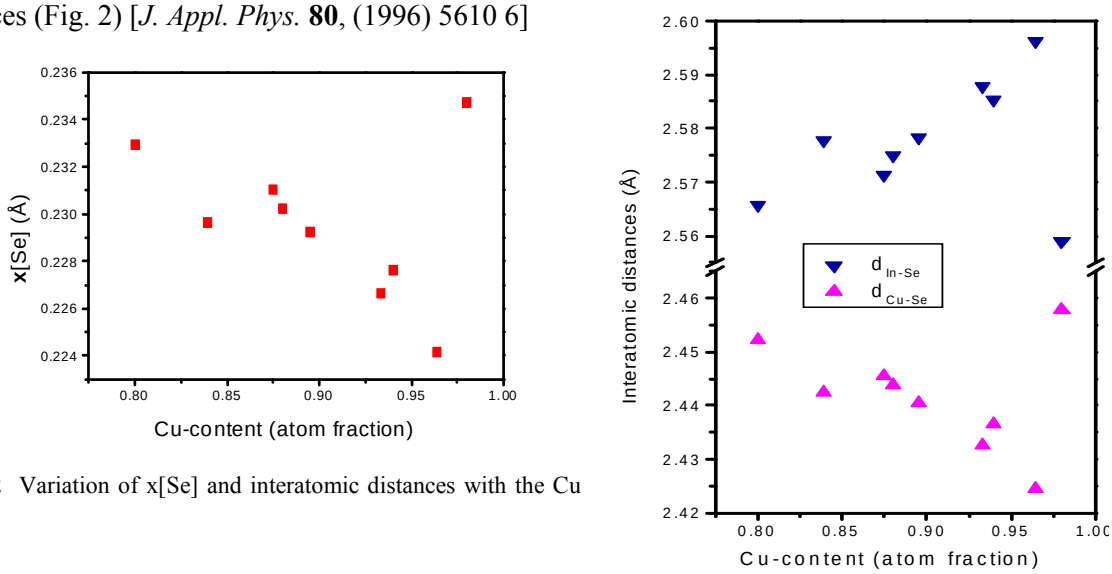


Figure 2 Variation of x[Se] and interatomic distances with the Cu content

Considering Jaffe and Zunger's band structure calculations in chalcopyrite compounds, we have calculated the bond ionicities, f_i, of several $CuBC_2$ (B = Al, Ga, In; C = S, Se, Te) compounds. To evaluate these ionicities, we have estimated the effective number of Cu valence electrons and proposed a new set of Cu-C bond susceptibilities. Also, the $f_{i,Cu-C}$ bond ionicities were found to increase with the atomic fractional coordinate of the C atom, x[anion], indicating that the anion position is a good estimation of the Cu-C bond ionicity (Fig. 3) [*Phys. Rev. B* **61**(15) (2000) 10211-5].

More recently, we have started to study the phase transitions in $CuInSe_2$, $CuIn_3Se_5$ and other related compounds with synchrotron radiation. Heating and cooling cycles at different speeds were carried out in a ceramic oven from room temperature to ~1000°C and 2D diffraction images were recorded with an on-line MAR image plate. Figure 4 depicts the experimental procedure to take the diffractograms. All the diagrams are being now analysed by means of a Rietveld refinement to identify and study the different phases appearing during both heating and cooling cycles.

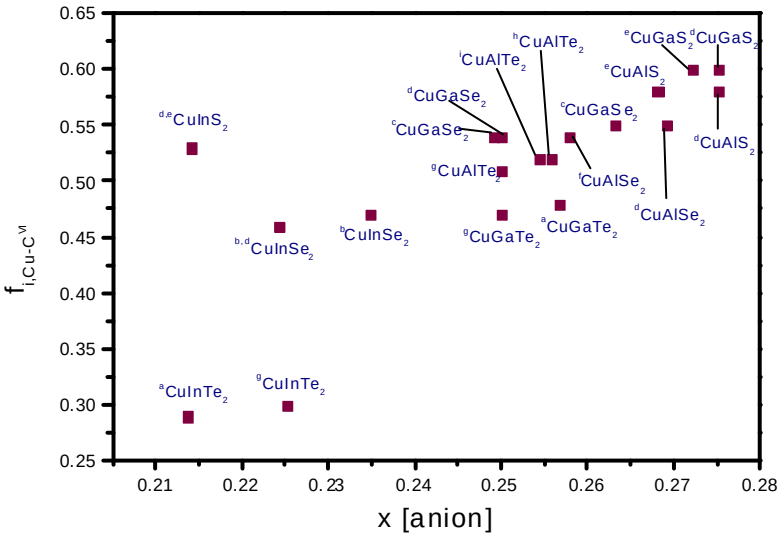


Figure 3 Cu-C bond ionicities vs. the anion fractional coordinate values.

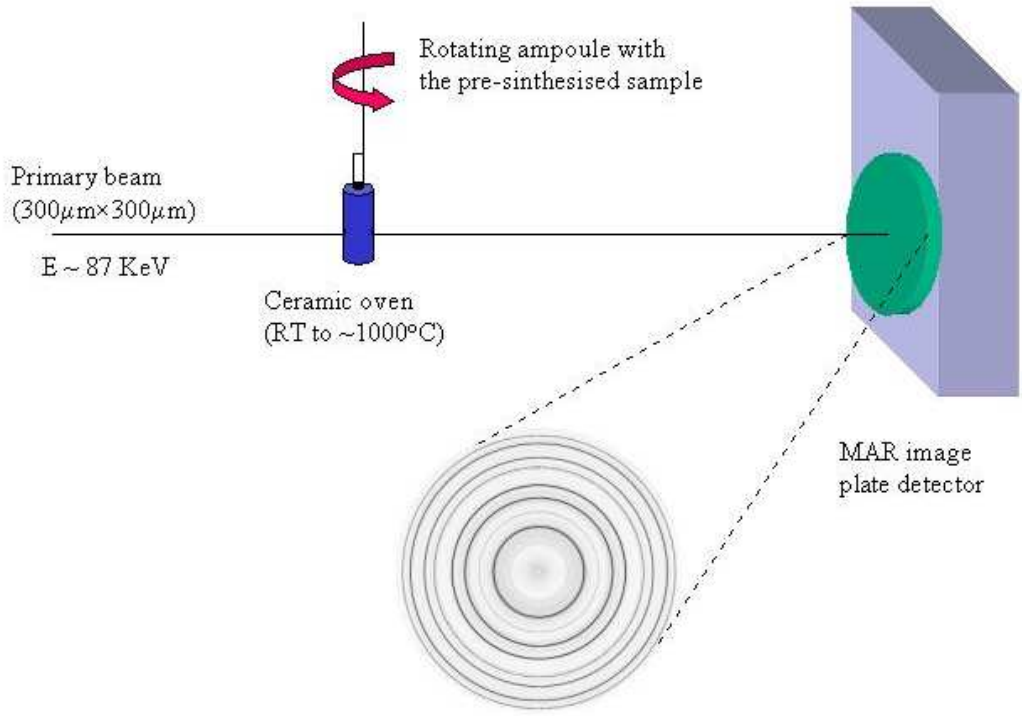


Figure 4 Esquematic drawing for the phase transitions experiment

ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY OF SOLIDS

Prof. Fernando J. López
Prof. David Bravo. Dr. Agustín Martín (UPM)

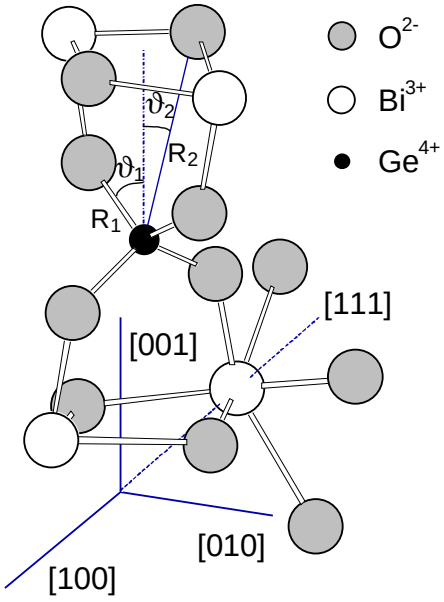
The Technique

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. It is to be noted that a great part of the commonly accepted models for point defects in solid state physics have been proposed or confirmed through magnetic resonance experiments.

The EPR laboratory is used by various Departments of Physics and Chemistry sections of the Faculty of Sciences at the Universidad Autónoma de Madrid. The equipment consists of a Bruker ESP 300 E spectrometer, working in the X-band. Also, different cryostats for measurements in the 5 K-600 K temperature range are available as well as systems for illumination of the sample inside the spectrometer.

Research lines

Study of materials for solid state lasers.



Solid state lasers are widely used in various scientific areas as material processing, spectroscopy, medicine, communications, displays, photonics, etc. For all of these applications two types of laser are particularly useful: tunable lasers and microlasers adequate for "integration" in an optical circuit.. Both types of laser consist on a single crystal host having good optical and thermal characteristics doped with one or more laser-active impurities. The impurities are transition metal ions as Cr^{3+}, V^{2+}, Ti^{3+}, etc. or rare earth ions as Nd^{3+}, Er^{3+}, Dy^{3+}, Yb^{3+}, U^{3+}, etc. The hosts are double oxides ($LiNbO_3$, BGO, BBO, etc.) or halide compounds (LICAF, LISAF). However, the precise structure of the emitting centers is not yet well known in many cases. The determination of that structure is of capital interest for the optimization and application of these lasers. For example, the Cr ion is a typical laser-active impurity in solid-state lasers but its valence and local symmetry in the lattice determine its emitting properties. So, Cr^{3+} coordinated with six O^{2-} ions gives laser emission in the VIS range but Cr^{4+} coordinated with four O^{2-} ions gives laser emission in the IR range.
Therefore, it is essential to know the valence state of the laser-active ions, their position in the crystalline host, the symmetry of the surroundings and the possible associated defects. Such information can be obtained by means of the EPR spectroscopy. Moreover it is necessary to determine the stability of the laser-active centers under thermal treatments and under very intense light irradiation.
In this research a wide variety of hosts are studied: $Bi_4Ge_3O_{12}$ (BGO); $Bi_4Si_3O_{12}$ (BSO); β-BaB_2O_4 (BBO); congruent or stoichiometric $LiNbO_3$ co-doped with Mg, Zn or Hf; $YAl_3(BO_3)_4$ (YAB); $KTiOPO_4$ (KTP); $RbTiOPO_4$ (RTP); $LiCaAlF_6$ (LICAF); $LiSrAlF_6$ (LISAF). In these materials a

variety of impurities: transition metal ions and rare earth ions have been studied and various centers identified. As an example, the Cr ion in BGO crystals has been identified both as Cr^{3+} in the Bi^{3+} site and as Cr^{4+} in the Ge^{4+} site. The figure shows a partial scheme of the BGO structure where the two cation sites available for impurity occupation are observed.

Study of materials for microelectronics

Amorphous silicon oxide SiO_2 and silicon nitride SiN_x:H are the most extensively used dielectrics in the microelectronics industry. The requirements of ultralarge scale integration technology have stimulated the development of low thermal processes for the deposition of SiO_2 and SiN_x:H. Among these, the electron cyclotron resonance (ECR) plasma method shows interesting features as low hydrogen incorporation into the films and reduced damage. Unfortunately, the electrical properties of plasma deposited films are worse than for thermally grown ones. However, rapid thermal annealing (RTA) treatments have been found to improve the properties of films.

These materials are prepared in the Universidad Complutense de Madrid. In our laboratory the EPR technique has been used to measure the density of defects (dangling bonds) and their evolution with the RTA treatments. We have observed that the remaining H in the samples can passivate the Si dangling bonds and that for high temperature RTA the H is released. Moreover, the EPR technique allows to determine the types of dangling bonds in the sample.

For SiN_x:H films the structure of Si-dangling bonds depends on film composition. In the Ni-rich films they are of the form $\cdot Si \equiv (N_3)$, whereas in the Si-rich films are of the form $\cdot Si \equiv (Si_3)$. On the other hand, films with similar N/Si ratio containing oxygen show predominantly dangling bonds of the form $\cdot Si \equiv (SiO_2)$. In the SiN_x:H films the density of defects is strongly correlated to the H content of the sample.

Also SiO_x:H films have been studied. For this material, it is ascertained that the RTA treatments change the proportion of different type of defect E' ($\cdot Si \equiv (O_3)$) and D ($\cdot Si \equiv (Si_3)$) and that RTA at high temperature promotes the formation of almost defect free SiO_2 matrix containing highly defective Si nanocrystals.

Collaborations

The above mentioned research is carried out in cooperation with other research groups of the Department and other institutions, among which are: Univ. Rovira i Vigili, Tarragona, Univ. Complutense de Madrid, Instituto de Ciencia de Materiales, CSIC Madrid, Hungarian Academy of Sciences, Budapest, Russian Academy of Sciences, Moscow

HARD COATINGS AND NANOSTRUCTURES

Prof. Jose M. Sanz,Prof. Eduardo Elizalde, Prof. Leonardo Soriano, Prof. Carmen Morant.
Dr. Pilar Prieto, Ph.D. Students: Carlos Quirós, Gonzalo G. Fuentes, Jorge Gómez García, Luis Fernández, Marta Sánchez

Research activity:

a) Development of thin film and coatings and surface modification by ion beam bombardment; b) synthesis of new materials with catalytic activity; and c) study of nanostructured materials. The research in these three main lines has been complemented by a more fundamental research related to the application of chemical and structural characterization techniques to systems like thin films, surfaces and nanoparticles. In particular, we have used photoelectron spectroscopies (XPS/AES), REELS, AFM and techniques that use synchrotron radiation like XAS and resonant photoemission.

a) **Development of thin film and coatings and surface modification by ion beam bombardment**

This research line is based on the projects : "Hardness enhancement by compositionally modulated structure of Ti/TiN/TiCN/CN multilayer films" (MAT99-0201) and "Development and application of new carbon nitride coatings in cutting tools" (BE97-4845) . TiN, TiC, CNx, Ti(C,N) films and CNx/TiCNx/TiN/Si multilayer structures were deposited by dual-ion beam sputtering (DIBS). The mechanical properties and the tribological behaviour seem to depend on their stoichiometry and microstructure. Under appropriate deposition conditions, coatings with high hardness, low friction coefficient, high wear resistance and good adhesion were obtained.

b) **Synthesis of new materials with catalytic activity**

In the project "Porous Inorganic catalytic films and membranes for pollution removal applications" (ENV4-CT97-0633) we developed thin film membranes either porous and/or dense with catalytic activity for the removal of pollutants, mainly NO_x, from the exhaust gases of combustion plants. We used plasmas and/or ion beams for the preparation of SiO_2 and ZrO_2 membranes. To determine the role plaid by the carbon species on the catalyst surface and the chemical characteristics of the active species in the selective reduction of NO, a systematic study by photoemission has been carried out.

c) **Nanostructured materials (**PB96-0061 and CAM 07N/0006/99 Projects)

We worked in the line of controlling the microstructure of nanostructured materials through the preparation methods. In particular, TiO_2 nanoparticles (< 5 nm) embedded in a surfactant have been studied by XPS and EXAF spectroscopies.

FERROELECTRIC MATERIALS

Prof. Julio A. Gonzalo ,
Prof. Carmen Aragó, Dr. Manuel I. Marqués.

In the Laboratory of Ferroelectric Materials, Department of Materials Physics, C-IV (UAM), research in ferroelectrics is being carried out for the last twenty years. Many applications of ferroelectric materials come from their pyroelectric (infrared detectors, energy converters), and piezoelectric (transducers) 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), periodically poled crystals (LN) with alternating refracting index, and electronic emission from ferroelectrics catodes can be obtained.

RESEARCH PROJECT

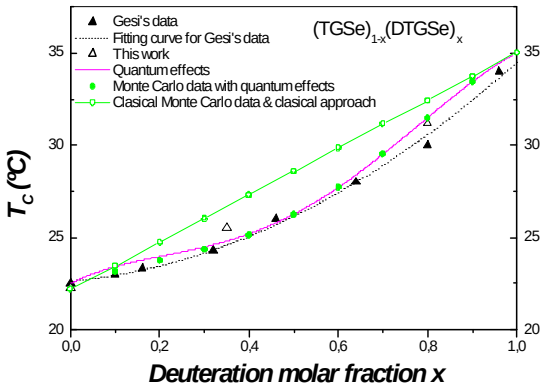
"Desplazamientos atómicos y grado de orden-desorden en transiciones ferroeléctricas mesoscópicas" (DGICyT, 2001-2003)

RESEARCH LINES

Switching transient in conexion with domain structure (crystals and ceramics) is studied in ferroelectric crystals of the TGS/DTGS family. As a growing voltage is applied to the sample, three different zones can be distinguished in the field dependence of the switching current intensity. An effective field microscopic approach, based on the evolution of the ferroelectric domains, has been shown to describe this behavior.

Also the characteristics of phase transitions are examined (order-disorder, displacive, mixed in character). It is well known that hydrogen bonded ferroelectric materials undergoing a second order transition are supposed to have an order-disorder character. In the same way, materials with first order transitions, such as the perovskites, are traditionally considered of displacive character. In last years, some intends of clasification of ferroelectric materials similar to that intended for ferromagnetics have been made using a ratio called the Rhodes-Wolfarth parameter. It has been studied the way in which the deuteration in TGS family crystals, and the composition in PZT ceramics affect the ferroelectric transition order and its character.

Since 1998, work on numerical simulations of phase transitions by Monte Carlo methods is being carried out.



Composition dependence of transition temperature in partially deuterated TGSe. The experimental data are compared with the results obtained by means of MonteCarlo simulations both in a classical and quantum approach.

Collaboration with other research groups in our Department to grow new ferroelectric crystals (SBN, LT) and to study ferroelectric domains structure in connection with nonlinear optical properties (Second Harmonic Generation in SBN60: Nd) is under way.

EXPERIMENTAL TECNIQUES

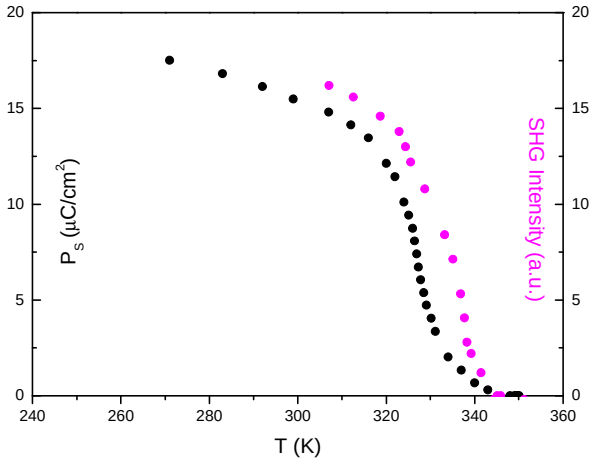
In order to observe the hysteresis loops of the ferroelectric materials, a classical DDP bridge, connected to an oscilloscope, is being used. The acquisition of the spontaneous polarization data and its analysis is fully automated. In all measurements a control of temperature (with a precision of 0.1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

Switching pulses on ferroelectric crystals are driven by a bipolar rectangular voltage that can be amplified until +/-1000V. The length of the pulses is of 500 μs 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.

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.

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 10.5μF.

A Brillouin spectrometer may be used to investigate temperature and pressure induced phase transitions, and a birefringence measurement device of high precision is being set up to provide a more complete overview of the relationship between ferroelectric an optical properties.



Comparison between temperature dependence of the spontaneous polarization (obtained from pyroelectric charge release) and the intensity of second harmonic generation.

THIN FILMS AND NANOSTRUCTURES

Prof. J.M. Martínez-Duart,
Prof. R.J. Martín-Palma, Prof. M. Hernández, Dr. M. Manso,
Ph.D. Students: V. Torres-Costa, M. Arroyo-Hernández.

Main research lines: Nanostructured silica, porous silicon, and interaction biomaterials-human cells.

Due to its particular structure, which confers this material many interesting properties, porous silicon (PS) is currently used for many applications in a wide variety of fields ranging from optoelectronics to biomedical applications. For this reason, detailed structural characterization of PS is mandatory in order to improve our understanding of the physical mechanisms responsible for the different behaviour of PS with respect to bulk silicon, its light emitting properties among them. In particular, since PS shows quantum size effects, the quantitative determination of the size of the crystallites that compose PS, as well as their relative orientation, morphology, etc. is of great significance. Properties such as emission light, intensity, quantum efficiency, spectral response, etc., of the different optoelectronic PS-based devices will depend on the characteristics of the silicon nanocrystals. High-resolution transmission electron microscopy and digital image processing are used in our group to investigate in detail the structure of PS. We have found that PS is composed of rounded Si nanocrystals with characteristic sizes between 21 Å and 80 Å, embedded into an amorphous matrix and with no preferential orientation [Fig. 1, from R.J. Martín-Palma, L. Pascual, P. Herrero and J.M. Martínez-Duart, Applied Physics Letters 81(1), 25-27 (2002)].

In addition, Porous Silicon Multilayer Stacks (PSMS) are formed by a periodic variation of the current density during the electrochemical formation process on silicon wafers under a constant level of illumination. From these structures, cross-sections are prepared for their study by Transmission Electron Microscopy (TEM). The images obtained (Fig.2) show several PS layers with periodic variations of porosity and thickness according to the formation parameters. In addition to this, reflectance measurements of PSMS in the infrared range led us to conclude that the control of the formation parameters of the PSMS makes possible the design of various optical devices such as interference filters, dielectric mirrors, etc.

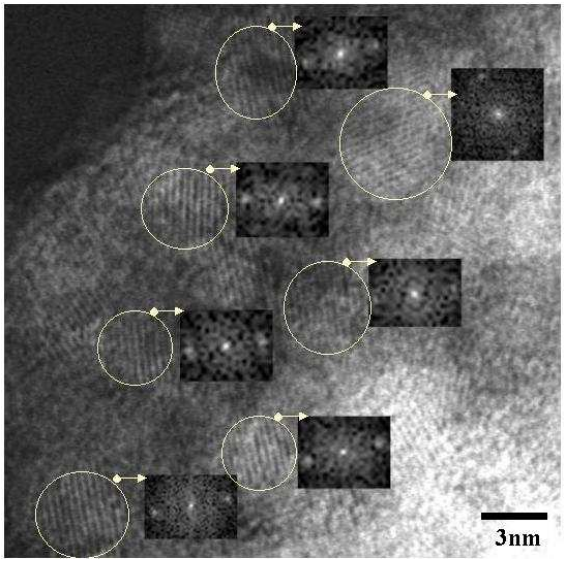


Fig. 1. Structure of the individual Si grains that compose porous silicon.

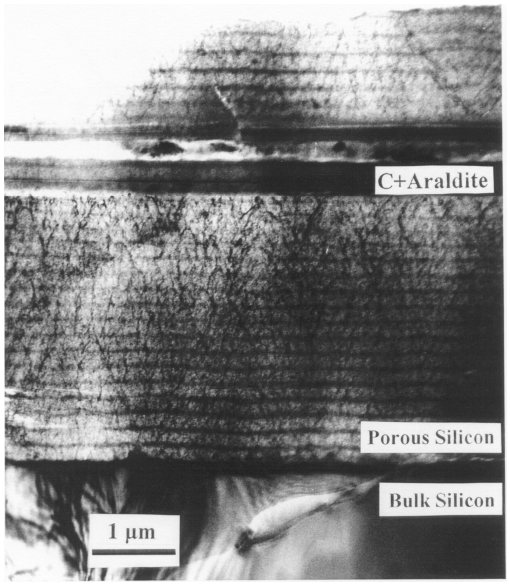


Fig. 2. TEM cross-section image of twofaced multilayer structures composed of 38 PS layers.

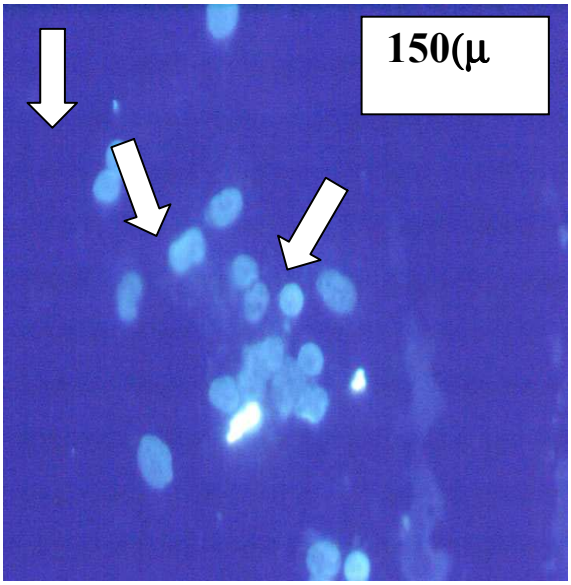


Fig. 3. Fluorescence micrograph showing the behavior of human MSCs seeded onto hydroxyapatite coatings.

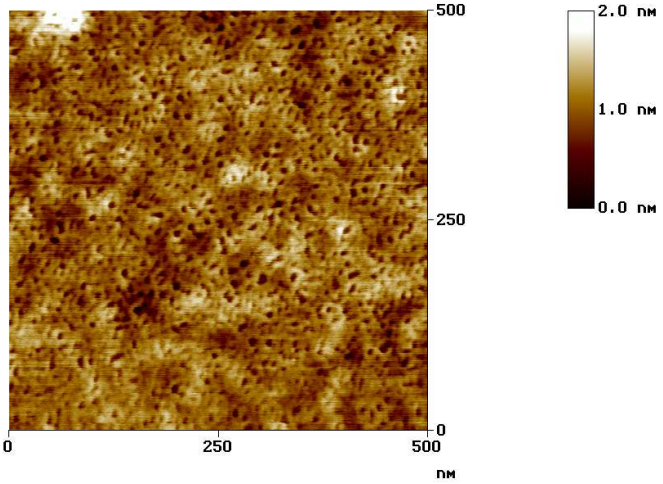


Fig. 4. Nanoporous silica thin film grown by Pulsed Electron Beam Evaporation.

The bioactivity of several surfaces of biomaterials have been investigated by physical and biological techniques. Fig. 3 shows hydroxyapatite (HAP) coatings formed by the aerosol-gel technique from different kinds of phosphate precursors. This ceramic outlayer should act as a bioactive ceramic in contact with bone tissue, allowing a rapid integration of the coated prostheses. In the case of HAP surfaces, we observed the evolution of human mesenchymal stem cells (hMSCs) onto different coatings by means of fluorescence techniques. From the different experiments, it was estimated that about 65% of the seeded cells were adhered to HAP surfaces (see Fig. 3). As it can be observed, the hMSCs exhibit a tendency to form colonies. Furthermore, hMSCs on HAP surfaces showed proliferation signals since cell nuclei were systematically observed to form pairs. In fact, the adherence and density of hMSCs on HAP was very similar to that observed on *in-vitro* generated osteoclasts on whale dentin by using staining techniques [from M. Manso *et al.*, Biomol. Eng. (2002)].

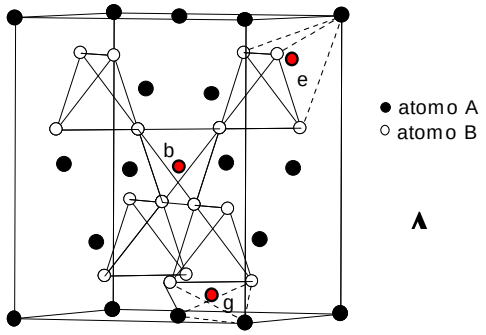
In reference to our studies of nanoporous materials, Fig. 4 shows an AFM image of nanoporous silica thin film, grown by using Pulsed Electron Beam Evaporation technique on silicon <100> substrates. The surface roughness of these films is only of 0,25 nm. Many pores appear scattered on the surface. The typical imaged pore dimensions are in the range 4 – 10 nm for their diameters and 0,2 – 1 nm for the imaged depth. The depth estimations are in excellent agreement with the values obtained from X-ray measurements of these nano- and meso- porous arrays. [from M. Hernández *et al.*, Thin Solid Films, Vol 402/1-2, (2002) pp. 111 – 116]

LABORATORY OF MATERIALS FOR ENERGETIC APPLICATIONS

Prof. Carlos R. Sánchez
Prof. Isabel Jiménez Ferrer, Prof. Francisco Fernández Rios,
Ph.D. Students: Antonio Pascual Salvador, Julio Bodega Magro.

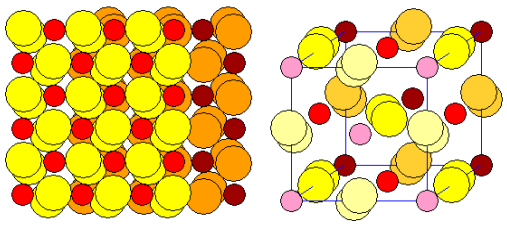
The aims of this laboratory stretch from the preparation of materials useful for energetic applications to their characterisation and optimisation in experimental devices. Two fields are being researched: metallic hydrides as hydrogen storage materials and metallic dichalcogenides thin films for photovoltaic and thermoelectric applications. The group has been working in these fields for the last 15 years. Along this time, a wide experience in the preparation of materials has been developed: metal alloys (mechanical alloying, arc melting, thin films...) and thin films of metallic dichalcogenides (flash and thermal evaporation, sulfuration, screen printing...), as well as, in characterisation techniques (structural, compositional and morphological).

In relation to the hydrogen storage in metals, at the moment, we are involved in the study of storage and kinetic properties of low weight materials based on magnesium. Experimental facilities have been developed to serve the study of hydrogen absorption/desorption processes, both by electrolysis of water and from hydrogen gas and also for their characterisation.

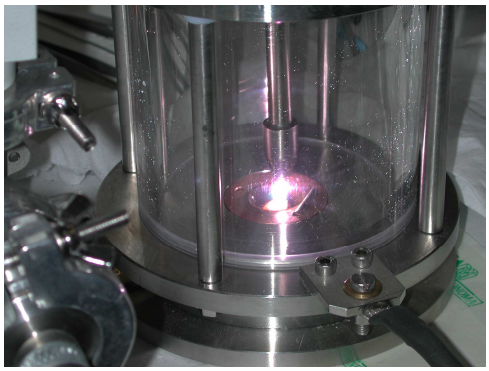


Unit cell of cubic C-15 Laves phase.
Interstitial places of H atom in red.

With respect to the metallic dichalcogenides, the research is centred in Iron disulfide (pyrite) although other metallic sulfides are also been investigated (NiS_2, TiS_3, TiS_2). The interest in FeS_2 is due, besides its adequate properties, to the low toxicity of its components and the facility to get it as p- or n-type semiconductor. At this moment, our research is focused in the metal diffusion across the pyrite film in order to get a controlled doping of the films.



Pyrite is often described as having a modified halite structure, in which, iron atoms alternate with pairs of covalently-bonded sulfur atoms. The pairs of atoms are skewed in alternate directions, so pyrite has lower symmetry than halite.



Preparation of an intermetallic alloy in an arc furnace machine.

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

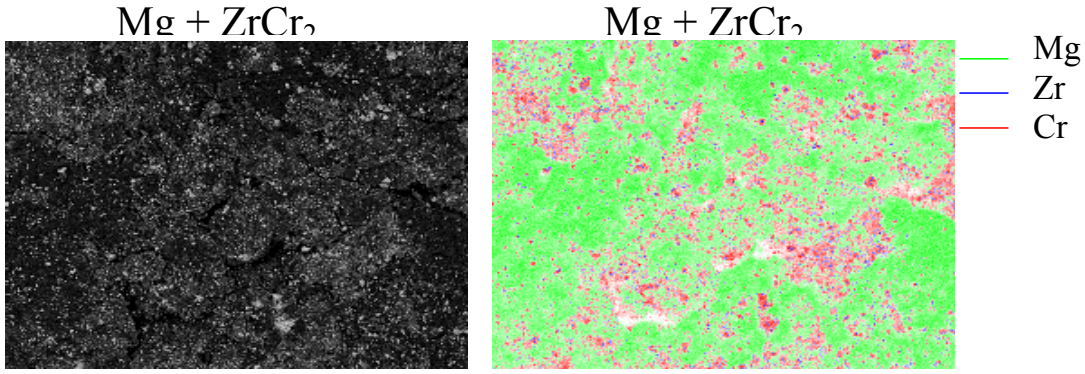
- Thermal and Flash evaporation equipment, in which it is possible to prepare thin films formed by up to four different elements in vacuum and in a controlled atmosphere.
- A vacuum closed space system in a controlled temperature furnace to make sulfuration of metallic films.
- Planetary ball mill system, hydraulic press (up to 15 Ton), arc furnace machine used for the synthesis of intermetallic alloys.
- Facility for solid-gas reaction synthesis of metal hydrides at H_2 pressure up to 60 bar.
- Facility for electrochemical synthesis of metal hydrides with in-situ measurement of hydrogen

concentration in the metal.

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

- 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
- Profilometer system of thickness measurement for thin films.

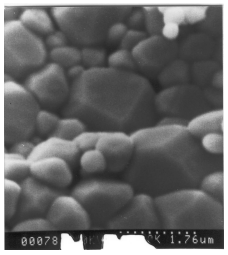
The structural characterisation is usually done by XRD, available in the SIDI service at Autonoma Univ. SEM and EDAX facilities are also provided by this service.



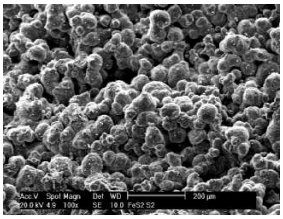
BSE (backscatterined electrons, left) and EDX (energy dispersive of X-ray, right) images of an alloy surface formed by Mg an ZCr

The group has also access to Ion Beam techniques (R.B.S., E.R.D) and Neutron spectroscopies techniques (difraction, INS, QNS, etc).

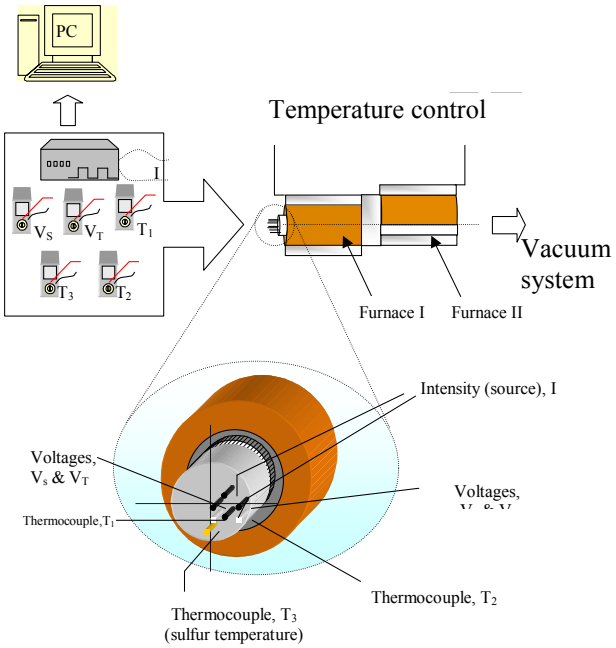
At last, electrical and thermoelectrical properties of thin films are investigated by means of a system developed in our laboratory, which allows the "in situ" measurement of these parameters during the film formation process.



SEM micrograph of a FeS_2 thin film obtained by sulfuration of Fe films at 600ºC



SEM micrograph of polycrystalline FeS_2 obtained at 450ºC from Fe and S powder



Experimental setup for the "in situ" measurements of electrical and transport properties

CRYSTAL GROWTH LABORATORY

Prof. Ernesto Diéguez
Dr. Maria Dolores Serrano, Dr. Verónica Bermúdez, Dr. Jose Luis Plaza.
PhD Students: David Callejo, Victoria Corregidor, Rebeca Martínez, Carmen Ruiz

Experimental and numerical simulation of bulk GaSb single crystals, grown by Bridgman method

Pure and doped single crystal GaSb substrates have been grown with the Bridgman technique, with a size of 12/24mm diameter, and 40/60mm length. The dopants used in the above research have been: Zn, Te, Mn, In, Er, Nd y Gd.

The effect of dopants has been studied with chemical analysis, luminescence and mechanical techniques. A feed-back between the experimental results, crystal growth process and the simulation of the growth experiments has been done, in order to improve the quality of the crystals.

A strong effort has been done on the simulation of the growth process by Bridgman method and the experimental results obtained in the doped crystals. More specifically the heat and momentum transfer numerical analysis in a vertical Bridgman Growth technique, and the modelling of the solute segregation by using free-surface techniques has been studied.

The elastic and plastic properties of the material produced during crystal growth process has been determined and compared with that predicted by the Haasen model. A prediction of dislocations evolution during crystal growth has been established, which will improve the crystal quality of the material.

Growth and characterization of bulk high resistivity CdTe crystals.

The growth of pure and doped bulk CdTe crystals has been performed by the Bridgman technique and by the Markov method. The objective was to achieve high resistivity CdTe material, carried out by means of different dopants. The following dopants have been studied: Zn, Mn, V, Ge, Ga, Cl.

The energy level position in the band-gap for eight elementary defects has been theoretically deduced and compared with experimental results. In general two types of defects reactions have been discussed, being responsible for Cadmium vacancy creation defects. Moreover, it has been shown that the most probable candidate for the native deep-level donor is a tellurium antisite.

A deep analysis has been carried out in the compensation mechanism of CdTe crystals by doping with Ga. A resistivity map along the whole length of the samples shows a resistivity value up to 10^9 Ω.cm. In this particular a compensation mechanism has been studied for CdTe:Ga. A Te antisite defect is supposed to give a stable compensation and a tolerance for variation in shallow impurity concentrations.

CdTe films were grown by physical vapor deposition on different substrates, like glass, alumina or sapphire. They were characterized by X Ray diffraction and shows a preferential (111) growth direction. The I-V curves were performed and the resistivities obtained are in the range of 10^6 Ω.cm.

Engineering and characterization of periodic poled lithium niobate structures doped with rare earth ions.

Periodically Poled Lithium Niobate crystals (PPLN) doped with Yb, Nd, Er, and Hf either pure or co-doped with Mg have been obtained. The period of the structures was varied from 4 to 20 microns. It has been found that tailoring the growth conditions, it means the pulling to rotation rate ratio during off centered Czochralski growth, the periodic structures can be modulated as desired. To understand the formation of the PPLN structures, crystals codoped with Hf and Hf:Er where grown. Results are summarized as: i/ a variation in the Li/Nb ratio along the periodic structure has been measured, and has been related with the compositional gradient created by the high temperature gradient along the solid-liquid interface during growth; ii/ the dopant concentration is constant along the periodic structure; and iii/ to preserve the PPLN structure is necessary to cool the crystal following a quenching procedure.

PPLN crystals have been characterized regarding their nonlinear optical properties showing

that: i/ a continuous wave self-OPO based in a PPLN structure doped with Yb^{3+} has been demonstrated. The wave length of the device can be adjusted by adjusting the spatial period of the structure; ii/ based in previous results a OPO-chip has been created; iii/ a frequency converter has been developed to convert the tunable laser emission of a Ti:sapphire (750-850 nm) laser allowing for laser radiation in 440-475 nm and 485-505 nm.

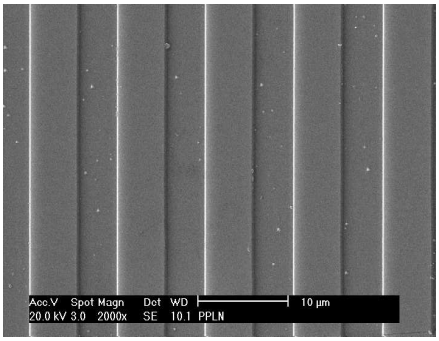


Figure shows a typical Periodic Structure obtained during off centered Czochralski crystal of a Yb doped Lithium Niobate crystal.

Growth and characterization of new borates laser materials

New borates $YAl_3(BO_3)_4$ rare earth doped has been grown by the Solution Growth. The conditions for solid-state synthesis have been defined, and crystals doped with Y, Er and Nd have been grown.

Analysis by X-ray diffraction techniques has been carried out, and a carefully study about the lattice parameter has been developed. The distribution coefficient of the Rare Earth impurities has been studied. The crystals are analyzed by optical methods.

Experimental and numerical simulation of GaSb thin films grown by Liquid Phase Epitaxy technique.

A Liquid Phase Epitaxy (LPE) equipment has been developed for the growth of semiconductor thin films. In particular the characteristics of the equipment have been fitted to the growth of binary and ternary allows belonging to the III-V groups. The main material to be grown is GaSb due to their potential properties to be used in optoelectronic, thermophotovoltaic cells and communications industry. However the versatility of the LPE will allow for the growth of semiconductor allows based in II-VI growth.

The growth in the LPE equipment is carried out inside a quartz tube, with controlled atmosphere, where the source material is inside a mobile graphite boat, which is displaced over several substrates. The system of thermocouples allows control temperature better than 0.5ºC. In figure 1 can observed an electronic microscope image of the preliminary films grown with this equipment, where microcrystals can be obtained. Using computer simulation with FIDAP code, the simulation of the LPE process is carry out, in order to compare the experimental with the simulated results.

Visiting scientists: Dr. Vladimir Babentsov, Dr. Edward Kokanyan , Dr. Nikolai Sochinski,. Edgardo Saucedo

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MOLECULAR NONLINEAR OPTICAL MATERIALS

Prof. Fernando Agulló-López,
Ph.D. Students: Gema Rojo, Guillermo Martín Fuchs.

Organic and polymeric (molecular) materials are recently receiving much attention since they are very promising for nonlinear optical (NLO) applications and devices. They have several advantageous features over their inorganic counterparts such as design flexibility, low dielectric constant, low cost, etc. Our group has been carrying out an extensive research program on the nonlinear behaviour of molecular materials along three main lines: a) highly conjugated compounds related to the family of phthalocyanines (Pc), b) organometalic compounds based on Fe and Mo complexes and c) polyphosphazenes as examples of inorganic polymers. The major effort has focused on Pcs, in collaboration with the Department of Chemistry of UAM and the group of prof. Zyss (Paris). In addition to interesting third-harmonic spectroscopy experiments , the group has followed several synthetic strategies to optimize the second-order NLO response of those compounds, including peripherical substitution (push-pull) and intrinsic modification of the macrocycle (e.g. subphthalocyanines). Significant susceptibiliy values have been achieved and useful criteria for the optimization of the response has been established. It has been obtained that the NLO response of the SubPcs can be described as purely octupolar in the macrocycle plane but having a permanent dipole moment in the perpendicular direction.

The studies of organometallic compounds have been performed in cooperation with the Department of Inorganic Chemistry of the University Complutense (Madrid). Measurements carried out both in solution and films have provided for the first time meaningful information on the molecular response (in comparison with previous powder experiments). Finally, the work on polyphosphazenes containing the NLO chromophore (similar to the DO3) were carried out in cooperation with the University of Oviedo. Guest-hosts as well as side-chain systems were investigated. A new synthetic route has led to compounds with high glass-transition temperature T_g and so having good thermal stability. The relaxation processes have been investigated by optical absorption and second-harmonic generation.

References:

G de la Torre, T. Torres and F. Agulló-López, *The phthalocyanine approach to second harmonic generation*, Adv. Mater. 9, 265 (1997).

G.de la Torre, P.Vazquez, F.Agulló-López and T.Torres, *Phthalocyanines and related compounds: organic targets for nonlinear optical applications*, J.Mater.Chem. 8, 1671 (1998). (Feature article).

GROUP OF NON-LINEAR OPTICAL WAVEGUIDES

Prof. José M. Cabrera
Prof. Dr. Mercedes Carrascosa, Prof. Angel García-Cabañes
PhD. Students: Gonzalo de la Paliza, Olga Caballero, Angel Alcázar de Velasco.

SUBJECTS AND EXPERTISE

The Group started with the subject of non-linear optical (NLO) waveguides about thirteen years ago. Focusing mainly on proton exchanged (PE) $LiNbO_3$ waveguides, the following topics are covered:

1.Preparation of PE-waveguides by:
- 1.1 Inmersion in an acid melt at high temperature and presuure
- 1.2. Under acid vapor atmosphere at high temperature and presuure
- 1.3. Inmersion in liquid water or under water vapor at high-pressure high temperature.

2.Characterization of optical waveguides by the following techniques:
- 2.1. Structural characterization of the guide layer by high-resolution X-ray angular spectroscopy, ion beam methods and micro-Raman spectroscopy.
- 2.2. Index profiles by optical mode analysis, either from angular spectra or optical field measurements with the near- and far-field configurations.
- 2.3. Propagation and insertion loss measurements by beam atenuation and interface reflectivity.
- 2.4. Non-linear optical coefficients measurements of the waveguide material by using the method of the strong-absorption regime.
- 2.5. Electro-optical (EO) measurements of the waveguide EO coefficients by a modified Mach-Zehnder interferometric technique.
- 2.6. Photorefractive and optical damage measurements using guided beams inside the guide material, by the holographic and single beam methods, as well as dark and light conductivity measurements.

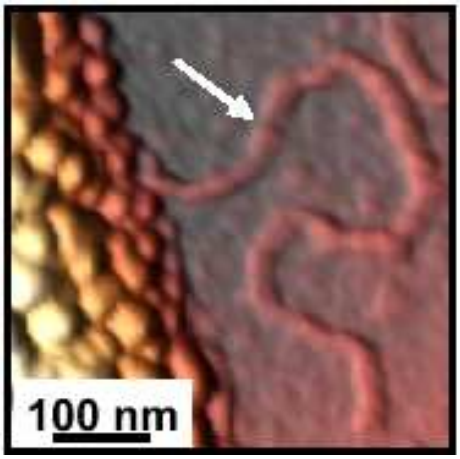
3.Application of the photorefractive fixing technique to a highly selective Bragg reflector inside the waveguide (filter bandwidth in the picometre range).

MAJOR ORIGINAL ACHIEVEMENTS

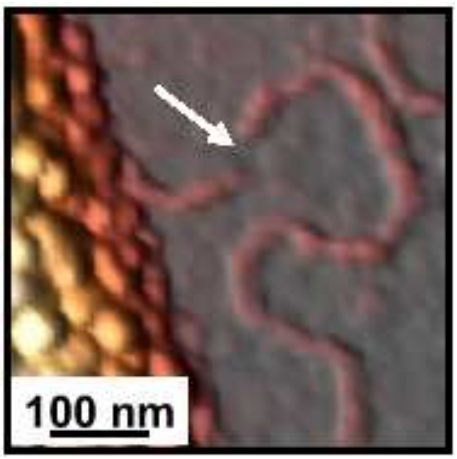
1.Identification of the $Fe^{2+} \rightarrow Fe^{3+}$ conversion during PE-treatment (the Fe^{2+}/Fe^{3+} ratio is a clue parametre in the photorefractive behaviour of $LiNbO_3$ waveguides).
2.Demonstration of an holografic method for determining the hydrogen concentration in $LiNbO_3$ for values within the range 10^{13}-10^{19} H/cm^3.
3.Development of a very narrow-band interference filter in bulk photorefractive $LiNbO_3$.
4.Preparation and full characterization of a stable, highly homogeneous phase (κ_2-phase) of the PE-material which is simultaneously NLO active, with very low optical damage and high index jump.
5.Theoretical and experimental implementation of a high-absorption regime method for the measurement of second harmonic generation coefficients of the waveguide material, even profiling the value along the guide index profile.
6.Development of a modified Mach-Zehnder interferometric methods for high precision measurement of electro-optic coeficients, about a factor ten better than best current measurements.
7.Experimental explanation of the short lifetime of photorefractive gratings in PE-waveguides in terms of surface ionic charges. Development of a simple technique to eliminate those charges and its negative effects.

NEW MICROSCOPIES LABORATORY
LABORATORIO DE NUEVAS MICROSCOPÍAS

Prof. Arturo M. Baró
Prof.Jaime Colchero; Prof. Julio Gómez Herrero; Prof. José María Gómez Rodríguez,; Prof. Javier Méndez Pérez-Camarero.
Phd Students: Iván Brihuega, Óscar Custance, Adriana Gil Gil, Cristina Gómez Navarro; Fernando Moreno Herrero; Nicoleta Nicoara; Pedro José de Pablo Gómez.



SFM image of a DNA molecule connected to a gold electrode.

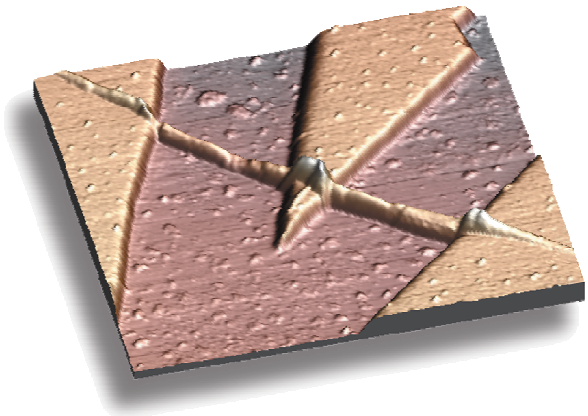


The molecule after being cut using an SFM

Research Lines

1. Scanning force microscopy (SFM):

Electrical tranport in molecules.



Carbon nanotubes belongs to the fullerens' family. These cylinder-like molecules can be seen as folded graphene planes with a minimum diameter of 1 nm. By using a Scanning Force Microscope we have measured the electrical current transport as a function of the voltage drop along the nanotube length. These characteristics have allowed us to obtain the resistance of the nanotube. In addition, we have been able to distinguish between contact resistance and intrinsic resistance of the nanotube. In the latest case, we have established a relation between the experimental resistivity obtained from our experiments and the defects along the nanotube. Finally, a number of predictions indicate that the current vs. voltage characteristic of a nanotube may change along the nanotube length from semiconductor to metal type and vice versa. These kind of phenomena have been also detected in our experiments.

DNA is the most relevant molecule in biology since life is based on it. However, little is known about the electrical transport properties of the DNA molecules. These properties are important, first from a biology point of view, because is known that electron transport plays an important role in the mechanism of damage and repair under external radiation. Second, because if the DNA is a conductor

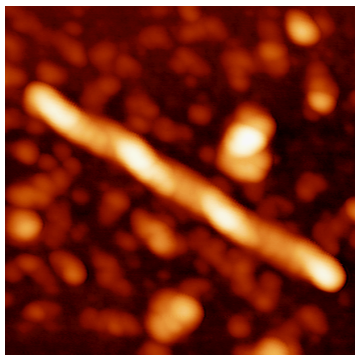
or can be modified to be a conductor, then it can be used to fabricate nanodevices. A number of works have been published suggesting that DNA can support electrical transport. In our group we have shown the regular DNA is not a conductor and therefore in order to be used in electrical circuits is should be modified.

Proteins and DNA interactions

SFM studies of DNA-protein complexes have been done in the direction to localize protein-binding sites in gene promoters. SFM appears as a powerful and complementary tool to the standard biochemical techniques. SFM can compete with biochemical techniques in terms of simplicity, cost and speed.

Biopolymers structure characterization

The Paired Helical Filaments (PHF) are an aberrant structure present in Alzheimer patients. They are mainly made of a protein called tau, and the exact arrange of this protein in the polymer is not yet understood. We have used the SFM to characterize the structure of this type of polymers.



Fundamental studies on SFM.

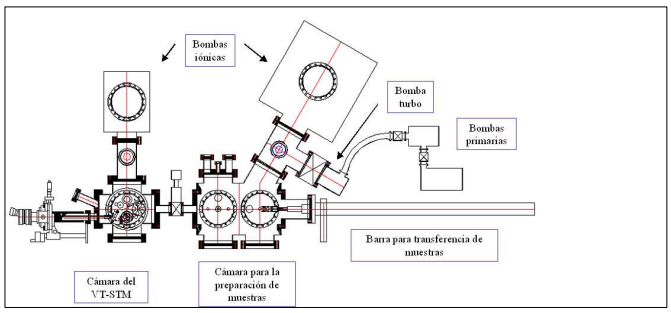
We have developed and studied a number of scanning modes for SFM: Jumping Mode, Dynamic modes, 3D modes, Electrostatic and Magnetic Force Microscopy. In order to obtain a better understanding of SFM we have carefully studied the tip-sample interaction.

2. Scanning Tunneling Microscopy (STM):

STM instrumentation.

We have fully designed and built the first variable temperature ultra-high-vacuum scanning tunneling microscope available in Spain. This variable temperature STM, connected to a continuous flow liquid He ultra-high-vacuum cryostat, allows imaging at sample temperatures in the range of 40K to 400K.

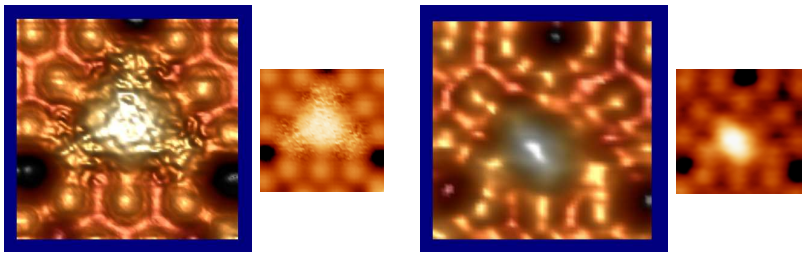
Variable temperature STM (40-400K)



Ultra-high-vacuum system ($5x10^{-11}$ Torr)

Diffusion at the atomic scale of metal adsorbates on semiconductor surfaces.

The detailed knowledge at the atomic scale of adsorption and diffusion mechanisms of single adatoms on highly reconstructed semiconductor surfaces is of fundamental importance in a great deal of current and future technological processes. In particular, recent works have unveiled the potentiality for next generation devices of self-organization of nanoclusters on Si(111)-(7x7) surfaces. Although the identification of stable adsorption sites and diffusion pathways and energy barriers is crucial for the understanding of the formation of such nanoclusters, there is still a lack of both theoretical and experimental information. In our group we have performed a variable temperature scanning tunneling microscopy study of the surface diffusion of single Pb and Sn adatoms on Si(111)-(7x7) surfaces working in a temperature range between 40K and 400 K. A careful analysis of Pb/Si(111)-(7x7) has been carried out, yielding valuable information on the atomistic mechanisms and energetics of this prototype system.



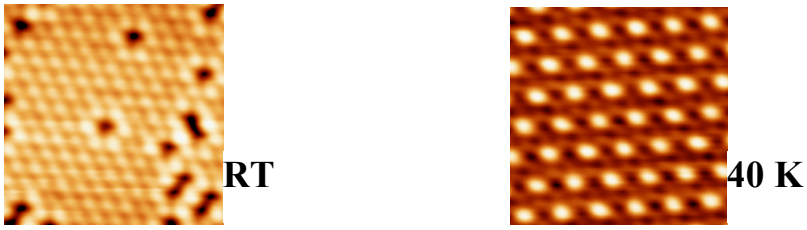
Si(111)-7x7 at room temperature *Si(111)7x7 at low temperature (40K)*

Phase transitions on low dimensional metal-semiconductor systems.

Structural and electronic phase transitions on metal-semiconductor surfaces are subjects of fundamental interest. By means of variable temperature UHV scanning tunneling microscopy and spectroscopy, several phase transitions have been analyzed on Pb/Si(111), Sn/Si(111) and Pb/Si(001) systems.

Adsorption and growth properties of organic molecules on surfaces.

The adsorption and growth of PTCDA molecules on inorganic substrates is under current investigation by means of UHV STM and STS and SFM in air. This fundamental research is included in the DIODE European Union Network for the future design of organic-inorganic devices.



Pb/Si(111)-(√3x√3) ⇔ (3x3) phase transition

LASUAM (Laboratorio de Superficies de la UAM)

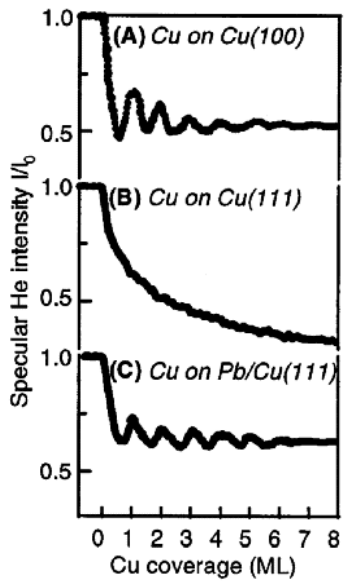
Prof. Rodolfo Miranda,
Prof. Juan J. De Miguel, Prof. Amadeo L. Vazquez de Parga, Dr José Mª Gallego, Dr. Juan de la Figuera, Dr.Julio Camarero, Dr. Jose E. Prieto, Dr. Daniel Farias, Dr. Juan J. Hinarejos, Dr. Roberto Otero, Dr. Vincent Cross, Dr. M.C.G. Passeggi Jr.
Ph.D. Students: Miguel A. Niño, Fabian Calleja.

Lines of Research:

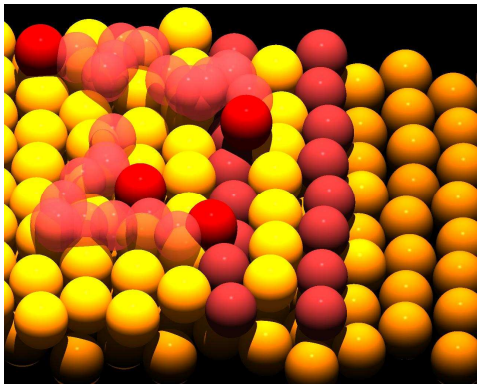
a) New concepts on heteroepitaxial growth: The use of surfactants

The recent advances in techniques of materials fabrication have resulted in many types of nanostructured materials with custom-made properties. Novel physical properties, such as oscillatory magnetic coupling or giant magnetoresistence, are revealed when "classic" materials are produced in the shape of thin films or superlattices with high enough structural perfection or when brand new materials are synthesized.

Following the discovery at the Surface Physics Laboratory of the role of surfactants on modifying the mode of growth of thin metallic films, an important effort has been devoted to explore the consequences and mechanisms of surfactant action. The surfactants employed now are single monolayers of some materials (e.g. Pb) that float at the surface during the growth of thin films, trilayers or superlattices, producing films much flatter than without them. It has been found by He scattering, computer simulations and STM experiments that the layer of surfactant modifies the diffusion of the deposited atoms, mostly on the terraces of the substrate, in such a way that nucleation of new islands is delayed and the growth changes from 3D to 2D (layer-by-layer). In order to understand the details it was necessary to determine the energies associated to the different atomic processes that may take place during diffusion on a growing surface. The resulting crystalline structure of the grown systems has been determined by quantitative LEED



The figure shows the intensity of a beam of He atoms specularly reflected from a surface during evaporation under MBE conditions. The oscillations have monolayer periodicity and signal that the epitaxial growth takes place layer by layer. Notice that layer by layer growth is induced on Cu(111) by the presence of a monolayer of Pb acting as a surfactant.



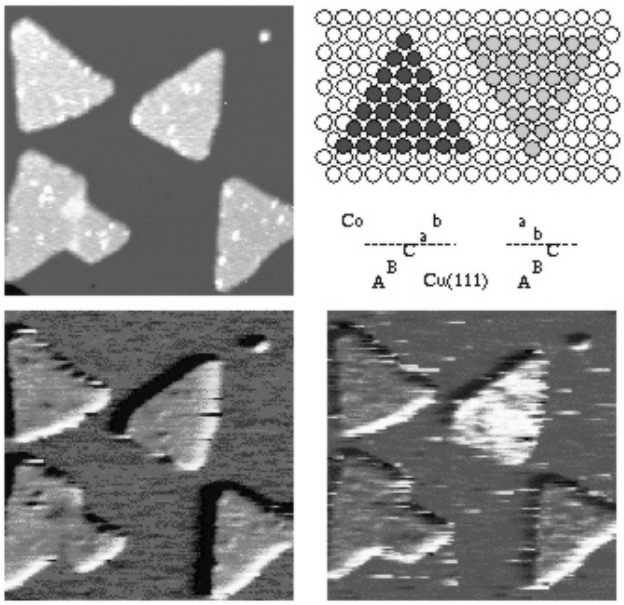
The figure shows a snapshot from a computer simulation of the movement of Cobalt atoms in the vicinity of a step of Cu(111). The Co atoms arriving from the upper terrace descend the step by exchanging place with a Cu atom at the step. The Co atoms arriving at the steps from the lower terrace form an atomic "wire". Both observations are in agreement with STM images of the same system.

b) Scanning Tunneling Spectroscopy of confined systems

Spatial confinement of electrons by adequate energy barriers within regions, whose size is smaller than certain critical lengths, results in discrete energy states. It can then be envisaged that a suitable array of potential barriers could tailor the electronic states. Adjusting the physical dimensions of the confinement region modifies these electronic states. Typically, the wavefunctions are modified if the size of the confinement region is of the order of the electron wavelength, say the Fermi wavelength. For metals this implies that we have to control the size of the materials at the nanometer scale, while for semiconductors, only 200 nm are required. In order to play this "wavefunction engineering "game, a careful exploration of different scenarios need to be done. In the past years we have found that magnetic superlattices constitutes a prototype systems to reveal new physics (and applications).

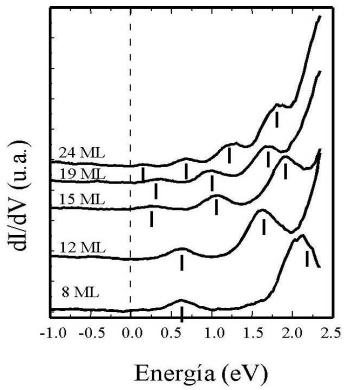
Some years ago it became feasible to grow metallic superlattices with the required level of accuracy and the electron states created, known as Quantum Well States (QWS), were discovered to be involved in new physical phenomena such as the oscillatory magnetic coupling and the related Giant Magnetoresistence. In magnetic superlattices the QWS are spin-polarized because the reflection amplitudes at interfaces are spin-dependent. They move in energy as the thickness of the spacer changes. As they cross the Fermi level, the total energy of the systems oscillates with their contribution changing the relative energy of the magnetic configurations (parallel and antiparallel) of the adjacent magnetic layers.

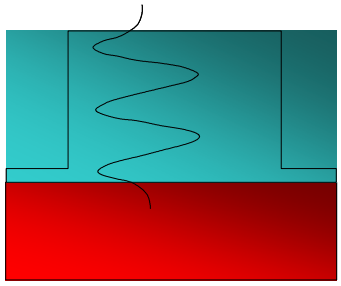
We have characterized by means of local spectroscopy with the STM the influence of another set of electronic states namely the states associated to a stacking fault at the Co/Cu interface and found that they are responsible for the enhanced transmission of hot electrons across this interface. This effect might be relevant to increase the performance of a new type of spin transistors. Furthermore, the difficulties in determining the actual barriers that keep the electrons confined has been analyzed.



The upper left part of the figure shows an STM topographic image of triangular Co islands deposited on Cu(111) indicating that the islands have two different orientations. The model at the right illustrates that the orientation depends on whether a stacking fault is present at the Co/Cu interface or not. The two lower images are spectroscopic images proving that electrons are more easily injected into the faulted island (bright) due to the presence of empty electronic states associated to the stacking fault. The occupied states (at the left) are evenly distributed between the faulted and the unfaulted islands.

The figure shows the Quantum Wells States (QWS) of electrons confined on Pb nanocrystals of different thickness. The nanocrystals were grown on Cu(111) and the QWS were detected locally by Scanning Tunneling Spectroscopy. The lower figure shows schematically the confinement of the Pb electrons inside the nanocrystals by the work function on the vacuum side and by the gap along (111) in the Cu bulk.





c) Magnetic properties of low dimensional systems

Physical systems in which some of the dimensions are smaller than the characteristic lengths relevant for magnetism (domain wall size, exchange length, etc) display a low dimensional behaviour. This is easily realized by growing epitaxial films with thickness in the few monolayers range. Following our early discovery of the dependence of the Curie temperature on the thickness of an ultrathin magnetic film, we have determined that also the coercivity depends on the thickness of the film. Magnetic anisotropy is another property that changes substantially for very thin films. In fact, the influence of the surface anisotropy can induce a reorientation of the magnetization direction, in such a way, that the easy direction of magnetization is perpendicular to the surface for very thin films, rotating abruptly upon increasing the thickness and eventually leading to a magnetization in the plane of the film, as dictated by the shape anisotropy. The different contributions to the anisotropy can be obtained experimentally. To this end, an improved morphology of the film (obtained thanks to the use of surfactants) has found to be essential.

d) Probing gas-surface potential energy surfaces with diffraction of hydrogen molecules:

An understanding of the dissociative chemisorption of molecules on solid surfaces is fundamental in order to get a detailed picture of the basic steps involved in many surface chemical reactions. The possibility of carrying out high-dimensional dynamical calculations has renewed the interest in diffraction studies with molecular beams of hydrogen molecules. These calculations have shown that information regarding the dissociative chemisorption potential can be obtained not only by measuring the fraction of molecules that stick to the surface, but also, and perhaps more precisely, by analyzing diffraction of molecules over a wide range of incident energies and with an angular resolution high enough to allow investigation of rotationally inelastic transitions.

The diffraction of H_2 molecular beams from surfaces is in principle quite similar to diffraction of He, the only major difference being the possibility of rotational-state transitions in the case of molecular scattering. At low surface temperatures, this occurs mainly via an inelastic process, in which the incident molecules convert part of their translational energy into rotational energy. This leads to the appearance of additional diffraction peaks in the angular distributions, which are called rotationally inelastic diffraction} (RID) peaks. We have recently investigated the diffraction and rotational transitions of D_2 scattered from NiAl(110) at incident energies between 88 and 157 meV. An important conclusion of our work is that the behaviour exhibited by these transitions as a function of incident energy is independent of angle of incidence.

ELECTRONIC AND ATOMIC STRUCTURE OF SURFACES AND INTERFACES

Prof. E.G. Michel
Dr. P. Segovia, Ph.D. Students: J. Lobo, A. Tejeda

Our research is focused on the description of the electronic and atomic structure of low dimensional systems, mainly solid surfaces and interfaces. To this aim we use basically two experimental techniques: Angle-resolved Valence-band Photoemission Spectroscopy (ARUPS) and Surface X-ray Diffraction (SXRD).

Photoemission experiments are done at our home laboratory, using an angle-resolving electron energy analyzer mounted on a UHV goniometer and a discharge lamp. We also use different Synchrotron radiation facilities as HASYLAB (Germany), LURE (France), and ELETTRA (Italy). SRD is done mainly at the ESRF (Grenoble).

Our research topics include:

Quantum well states: these electronic states are formed in thin films due to the confinement of electrons in the vertical direction. They specially important because they are behind the transmission of the oscillatory magnetic interaction in magnetic superlattices. They are also observed in thin metallic films on semiconductors, where they play a role in determining the morphology of the growing film (electronic growth).

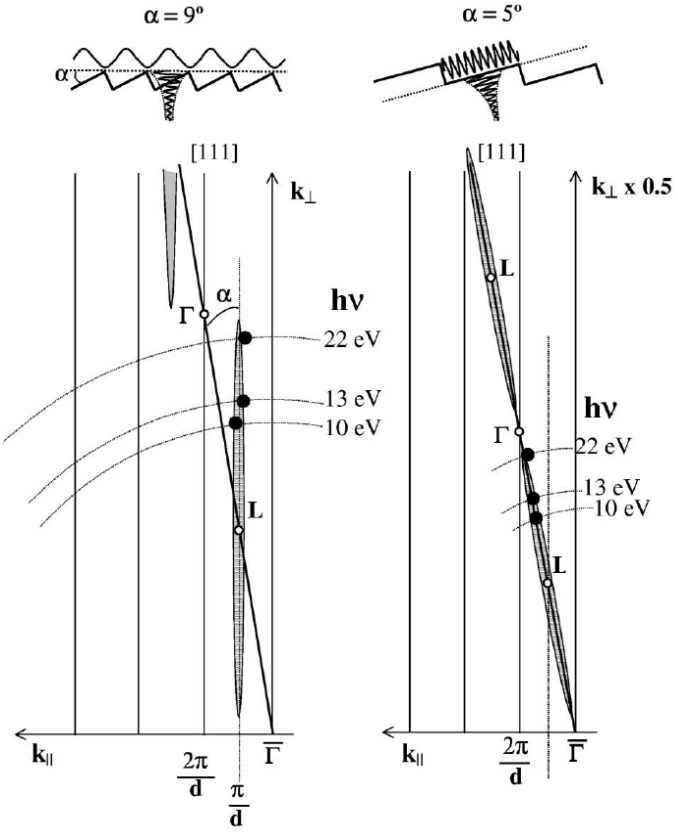
Metal-insulator transition and electronic effects in structural surface phase transitions: the origin of metallicity in many surface systems is still an unsolved problem. The metallic character can be probed very efficiently using ARUPS, since this technique allows to track the origin of the electronic states behind metallization.

Charge-density waves (CDW) in surfaces: electron-phonon coupling (besides other effects) can give rise to the stabilization of a charge density wave in the bulk. This phenomenon has been actively searched in surfaces since many years. A surface CDW state involves structural and electronic effects that are beyond existing theoretical models, and it is an interesting playground to test several different electronic properties.

Low-dimensional systems (quantum wires, quantum dots) : low dimensional materials (1D and 0D) exhibit fascinating electronic properties, but good experimental model systems are difficult to conceive. We have used noble metal surfaces prepared as regular arrays of linear, monoatomic steps of the (111) orientation as model systems for lateral nanostructures. The main reason is that they posses the well-known p_z-like surface state, that can be readily detected by photoemission. These electrons scatter strongly at step edges, leading to confinement within terraces and superlattice effects. Vicinal surfaces are obtained by cutting a single crystal with a small deviation of the surface normal with respect to the (111) plane ("miscut" angle). As shown in the left, we find two type of steps at Cu(111) vicinal surfaces, depending on the local packing at the edge, i.e. (100)-like steps and (111)-like steps. A variety of surfaces is produced by simply changing step density and type.

All our vicinal Cu(111) surfaces, from 5º to 11º miscut, displayed a clear two-dimensional surface band in angle-resolved photoemission, very similar to the band measured in flat Cu(111). The variety of vicinal surfaces prepared made it possible to examine the transition from a surface state modulated by the (111) plane of the terraces to a surface state modulated by the average, stepped surface . The transition is determined by a Fourier analysis of the surface state in the three-dimensional reciprocal space, that allows to distinguish the confinement plane of the surface state (Phys. Rev. Lett. 84, 6110 (2000)). The data points in the right represent the bottom of the surface band measured at different energies in angle-resolved photoemission and plotted in momentum space.

They line up perpendicular to the terrace for 5º miscut surface and perpendicular to the surface plane for 9º miscut surface. Thus, the transition occurs at about 7º miscut (d=1.7 nm terrace width).



Description of the photoemission experiment from a vicinal surface using an electron diffraction model. The dots are three-dimensional k values obtained from the ARUPS data. The cigar-shaped shaded hatched regions represent the spread of the surface state wave function in k space. The corresponding wave function in real space is indicated on top. A characteristic switch of the orientation occurs at a critical miscut angle of about 7º.

THE SEMICONDUCTORS GROUP AT THE UAM (SEMICUAM)

Prof. Jose M. Calleja, Prof. Luis Viña, and Prof. Herko van der Meulen (experimentalists).
Prof. Carlos Tejedor (theoretician). Dr. M. Dolores Martín, Dr. Lukasz Klopotwski.
Ph.D. Student: Jaime Sánchez Páramo, Diego Porras, José Ignacio Perea, Miriam del Valle, Dipankar Sarkar, Alberto Amo.

The semiconductors group at the UAM (SEMICUAM) has been working on the electronic structure and on the optical properties of semiconductor low-dimensional structures for the last 20 years. It is composed by experimental and theoretical groups working in close collaboration. In the years 2000-2001 the group has worked in the following topics:

1. Optical and magneto-optical properties of low-dimensional electron systems.

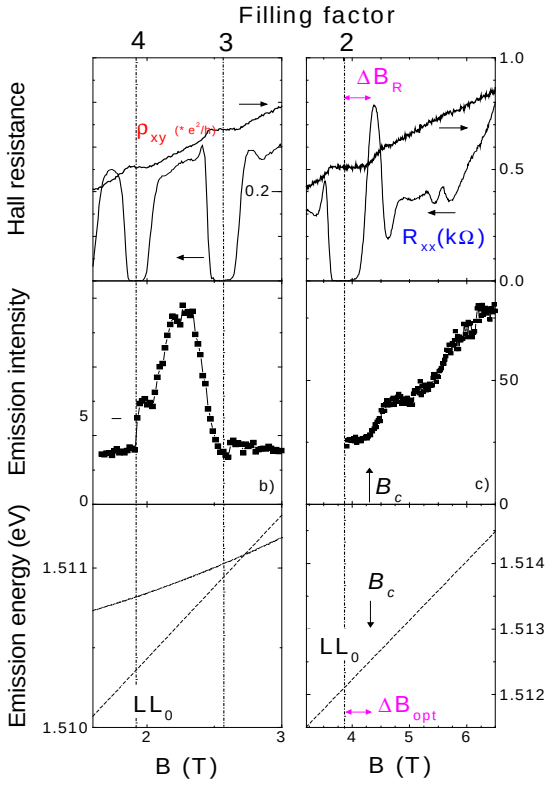


Figure 1

The influence of many-body processes in the optical properties of two-dimensional electron systems has been studied in modulation-doped GaAs-based quantum wells and heterostructures. These studies include the determination of the role played by hole-localization on the optical response of the electron system. The application of an external magnetic field at low temperatures (300 mK) reveals the appearance of distinct anomalies in the emission spectra around integer values of the filling factor. As an example, the simultaneous measurement of the emission intensity and the longitudinal and transverse resistances shown in Fig. 1 for a GaAs/AlGaAs heterojunction reveals the correlation of the optical anomaly (the kink in the lower curve below ν=2) and the onset of extended stated at the Fermi level.

In order to look for manifestations of Luttinger liquid behavior in one-dimensional systems, the group has studied the elementary electronic excitations of an extremely diluted ($2x10^5$ electrons/cm) electron gas formed in cleaved-edge-overgrown GaAs quantum wires, in collaboration with Lucent Technologies. The energies and intensities of the intraband plasmon and the collective peak at the single-particle energy have been detected using inelastic light scattering. As preliminary results are inconclusive, this work is still underway.

2. Spin dynamics in quantum wells and microcavities

Time-resolved photoluminescence has been used to study the spin relaxation mechanisms in semiconductor quantum wells as a function of exciton density and temperature. Different spin components are resolved using circularly polarized photoluminescence: exciting with a σ^+-polarized light pulse, the co-polarized (σ^+, +1) and cross-polarized (σ^-, –1) emission are observed, as shown in Figure 2; a rate equation analysis allows also the estimation of forbidden (dark states) excitonic populations (dashed lines). Time resolution as short as 2 ps is reached using the up-conversion detection technique. Special attention has been paid to the spin dependent excitonic interactions, which have been studied under resonant and non-resonant excitation conditions at liquid helium temperatures. In the former case, a pure exciton gas is created, whereas in the latter the excitons are

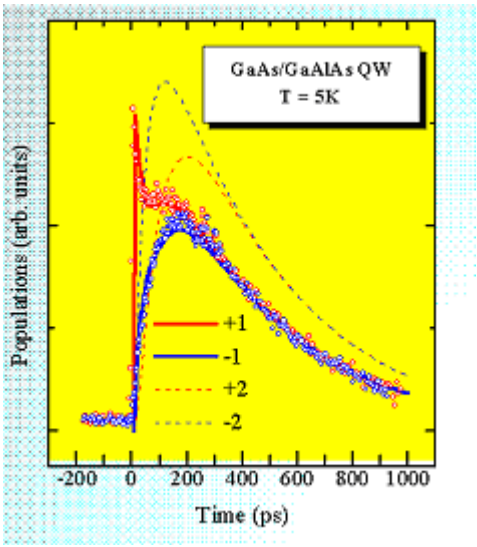


Figure 2

surrounded by a charged electron-hole plasma. In double quantum well structures, the distance between electrons and holes comprising the excitons could be externally tuned by applying an electric field perperdicular to the well planes. The interactions are studied as a function of excitation intensity, excess energy, spin polarization and electron-hole separation

The dynamics of coupled exciton-photon modes (polaritons) has also been studied in semiconductor microcavities. The degree of circular polarization of the photoluminescence, which reflects the spin properties of the polaritons, depends strongly on the excitation power-density and an abrupt increase occurs when the emission becomes stimulated. Furthermore, it is observed that a finite time is needed to reach the highest value of spin orientation, in contrast with the case of excitons in quantum wells where the spins are aligned instantaneously after a pulsed excitation. The faster emission dynamics of the polaritons that undergo stimulated emission, as compared with that of the polaritons with opposite spin, produces a very fast and efficient reversal of the polarization in the non-linear emission regime.

This laboratory has received recently a superconducting magnet to perform time-resolved magneto-luminescence measurements at fields up to 8 T and temperatures down to 2 K.

3. Quantum dots in high magnetic fields: spin textures and Kondo physics

Quantum dots in high magnetic fields are an excellent laboratory to study many-body effects in both transport and spectroscopy experiments. We have concentrated in the theoretical analysis of topological spin excitations of a quantum dot.(see Figure 3) Two kind of excitations appear: one family of excitations having skyrmion-like character and being localized at the center of the dot and another one localized at the edge and being responsible for the quantum dot reconstruction when the conditions of the system are varied. From our analysis we have concluded that an experimental manifestation of the existence of such highly correlated states is a peculiar chess-board aspect of the conductance of the system due to a Kondo-like effect.

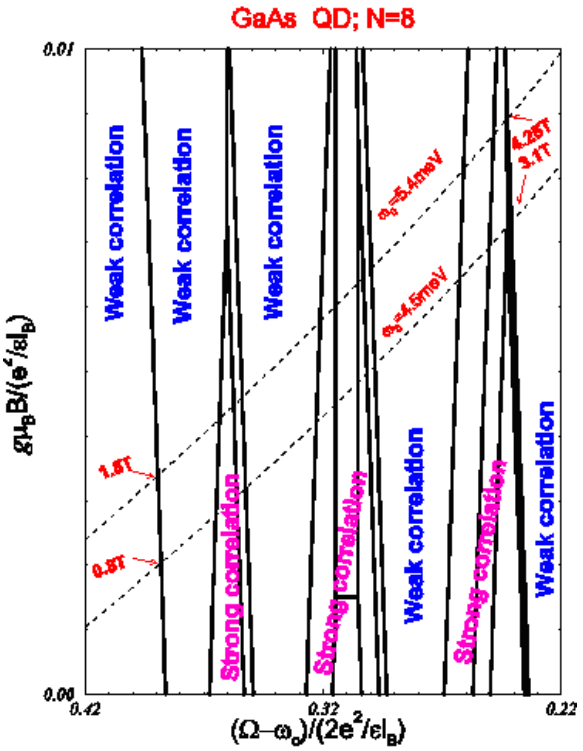


Figure 3

4. Bose-Einstein condensation of excitons and polaritons

Since both excitons and polaritons have quasi-bosonic character, these particles can condense in a macroscopic coherent state. Such a condensation has never been experimentally observed. We have been developing different theoretical approaches to determine what should be the most adequate conditions to study condensation. In the case of excitons, we have analyzed two aspects of the problem: the importance of the spin degree of freedom in the condensation, and the coherence of the light emitted by the exciton condensate. In the case of polaritons, we have developed a theoretical description of the stimulated light emission experimentally observed in microcavities. In a next step, Bose-Einstein condensation is studied by solving Bloch-like equations for both polariton populations and electrical polarization as the order parameters.

5. Optical characterization of GaN-based structures

In collaboration with the ETSIT of Madrid we have investigated the influence of strain and growth conditions of several semiconductor structures based on III-group nitrides. In particular, optical emission and Raman scattering have been successfully used to determine the role of the Si-doping on GaN films the degree of strain relaxation associated to dislocation formation. Also AlGaN and GaN nanocolumns have been studied by SEM, cathodoluminescence and Raman scattering to determine important parameters, as the absence of strain, the Al content in ternary systems and the origin of the different optical emission lines observed. Finally the study of InGaN multiquantum wells have been started.

ADVANCED MATERIALS FOR INTEGRATED GUIDED OPTICS

Prof. F. Cussó, Prof. G. Lifante,
Dr. E. Cantelar, Dr. J.A. Sanz-García. Ph. D. Student: M. Domenech.

The Advanced Materials for Integrated Guided Optics (AMIGO) group focuses its activity in the achievement of photonic devices in waveguide configuration.

The areas of activity cover a broad range of interest, which includes: 1) Crystal growth. 2) Spectroscopic characterisation. 3) Planar and channel waveguide fabrication. 4) Waveguide characterisation. 5) Modelling and simulation of waveguide devices. 6) Integrated lasers and amplifiers. 7) Non-linear devices. 8) Integrated optical sensors.

1) Growth of rare earth-doped $LiNbO_3$ monocrystals. The laboratory has the facilities for Czochralski growth and experience in growing rare-earth doped $LiNbO_3$ single domain and PPLN.

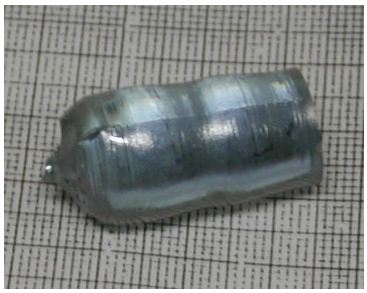


Fig. 1a) LNB:Nd^{3+}

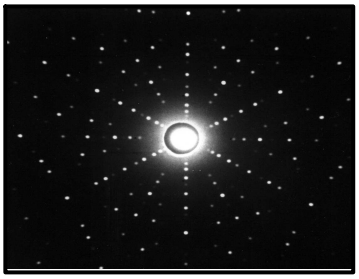


Fig. 1b) Lauegram of a LNB monocrystal

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

3) Planar and channel waveguide fabrication. Zn-diffused LNB and ionic-exchange in glasses are areas of currest activity. Ion-implantation appears as an emergent area of interest in connection with the Parque Tecnológico de la Comunidad de Madrid. Adapting silicon microelectronics technology, optical channel waveguides are also fabricated.

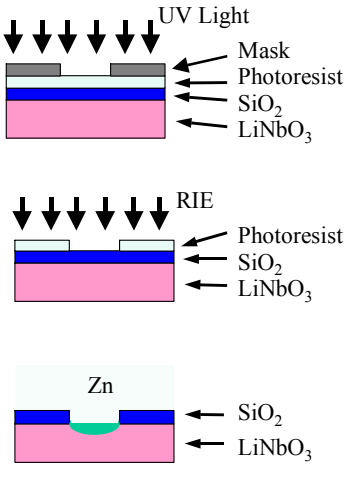


Fig. 2a) Channel waveguide fabrication

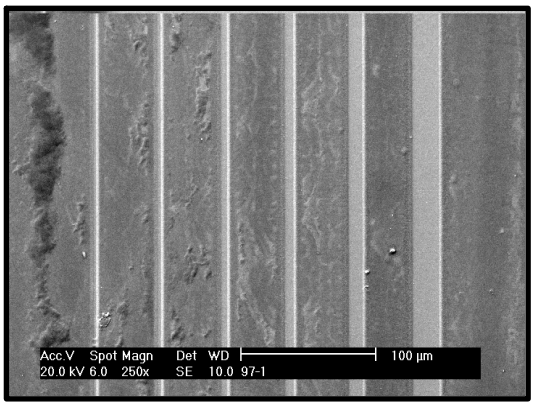


Fig. 2b) SEM of LNB channel waveguides

4) Waveguide characterisation. Waveguide evaluation (modal spectra, modal fields, attenuation and spectroscopy) are routinely operated in the AMIGO laboratory

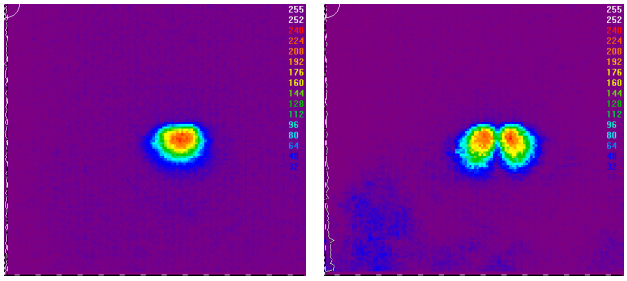


Fig. 3a) Modal intensities of a channel waveguide

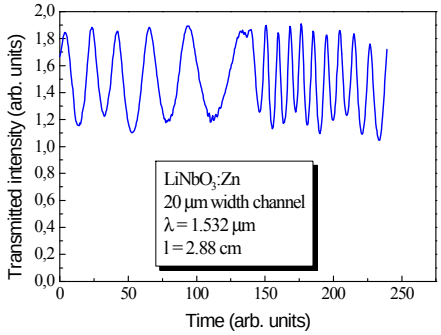
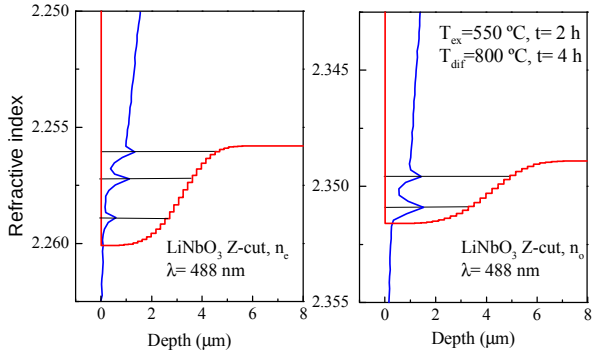
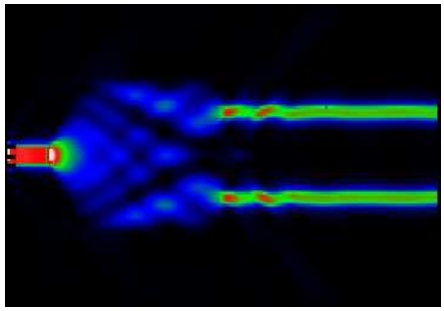


Fig.3 b) FP evaluation of losses

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

Fig.4a) Modelling of waveguide RI profiles Fig. 4b) Simulation of a 3dB MMI





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

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

8) Integrated optical sensors. Integrated Mach-Zehnder interferometers are under development for opto-chemical-sensors fabrication.

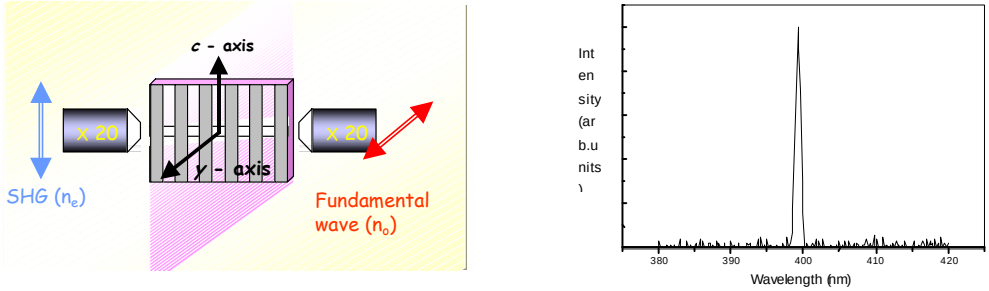


Fig. 5) Experimental set-up (left) and SHG output (right) in PPLN channel waveguides.

BIOFUNCTIONALIZED SOLID SURFACES

Dr. Marisela Vélez

The design of soft biocompatible and bio-functional interfaces on solid surfaces is a fast developing highly interdisciplinary field with numerous scientific and practical applications. Practical aspects include 1) the fabrication of ultra thin matrices for the immobilization of enzymes, cell-receptors or hormone-receptors in non-denaturating environments, 2) the design of mimetic of tissue surfaces to immobilize cells in a stress-free way and to study the effects of pharmaceuticals on cellular behaviour, or 3) the self-assembly of high electrical resistance membranes on electro-optical devices for the design of smart biosensors.

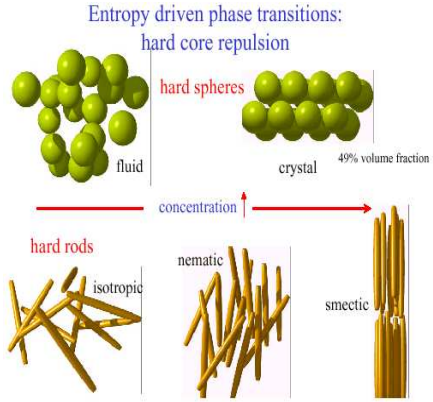
The main interest of my laboratory is to reconstitute membrane proteins into surface supported membranes in order to study biologically relevant membrane processes with the help of surface techniques such as the atomic force microscope and other single molecule analytical techniques being developed in this campus (optical tweezers and single molecule fluorescence) . The methodological challenge is to separate the lipid membrane from the solid surface by ultra thin and soft polymer that will mimic the intracellular environment and provide enough space for the inserted membrane proteins and prevent them from interacting directly with the solid support.

Soluble proteins can also be immobilized on surfaces while retaining their activity, allowing the use of single molecule techniques as the atomic force microscope and single molecule fluorescence to characterize the biophysics of relevant biological processes of individual molecules.

The main biological systems with which we are currently working are:

1) The septal complex involved in bacterial cell division [BMC2002-04617-C02-02 project, "Functional interactions in the bacterial septal complex: influence of the membrane lipid environment" in collaboration with the group headed by Dr. Germán Rivas, at the Biological Research Center, (CIB, C.S.I.C.)]

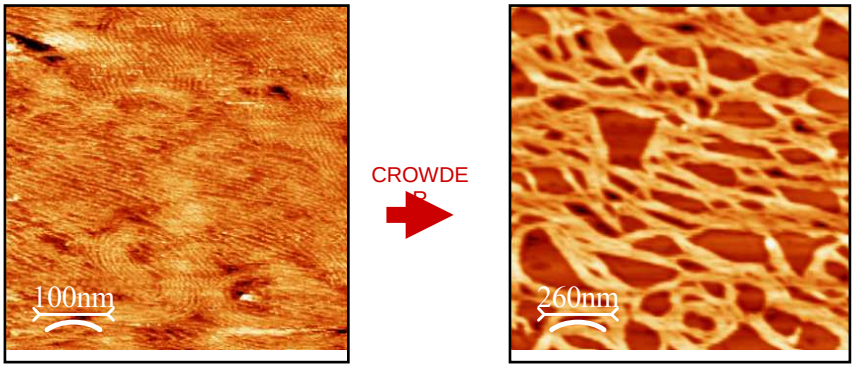
We are currently studying the effect of crowder molecules and surfaces on the polymerisation of the protein FtsZ, the prokaryotic analogue of tubulin and one of the most important molecules in the formation of the septal ring.



Crowding-induced polymer network formation predicted by excluded volume theory

2) Membrane proteins involved in the asymmetric lipid distribution between the two leaflets of a bilayer (flipases). (Collaboration with The Laboratoire de Physico-Chimie des Membranes Biologiques, headed by Prof. Philippe F.Devaux, through the co-tutorial of the PhD. Thesis of graduate student Iván López Montero)

3) Biophysical characterization of the functional cycle of cytosolic chaperonin CCT [Collaboration with Prof. José María Valpuesta and Prof. José L. Carrascosa from the National Biotechnology Center (CNB, C.S.I.C.) and Prof. Carlos Bustamante, from the University of California, Berkeley]



APPLICATIONS OF QUANTUM CHEMISTRY METHODS TO THE SOLID STATE: STRUCTURE AND SPECTROSCOPY OF LANTHANIDE, ACTINIDE, AND OTHER HEAVY-ELEMENT IMPURITIES IN IONIC CRYSTALS.

Prof. Luis Seijo and Prof. Zoila Barandiarán

The interest on the f^n and $f^{n-1}d$ local electronic states of lanthanide and actinide impurities in ionic crystals like, for example, $Cs_2NaYCl_6:Ce^{3+}$ or $Cs_2ZrCl_6:U^{4+}$ (Fig. 1), has been growing in the last few years.The electronic transitions which occur upon visible and UV excitation to the high energy f^n and $f^{n-1}d$ levels are involved in a variety of phenomena of technological interest which are not always fully understood. The $f^{n-1}d \rightarrow f^n$ emission transitions of rare earth doped materials make them usefull as solid state lasers and scintillators. Recently, due to environmental reasons, lanthanide impurities are being ivestigated as possible multiphoton emitting systems, in an attempt to replace Hg-discharge by (higher energy) Xe noble gas discharge in fluorescence lamps.[1] For this type of application the knowledge of the relative energy position of the higher f^n and lower $f^{n-1}d$ levels is a basic information. Also recently, up-conversion emission, which has been widely demonstrated and studied in lanthanide doped crystals, is being investigated in trivalent and tetravalent actinide impurities.[2,3] The investigation of the actual energy transfer mechanism which occurs during the two-photon absorption process, ultimately leading to the emission of higher energy light, is neither simple nor complete. It certainly demands a detailed knowledge of a very large manifold of excited states, which, depending on their spectroscopic parameters (equilibrium distance, vibrational frequency, relative energy), are candidates to be intermediate states in the non-radiative and radiative energy transfer processes. Furthermore, the spectroscopic properties which depend on the $f^{n-1}d$ manifold of states, vary considerably with the host crystal, since the chemical environment (even beyond first neighbours) affects notably the more exposed *d* electronic structure.

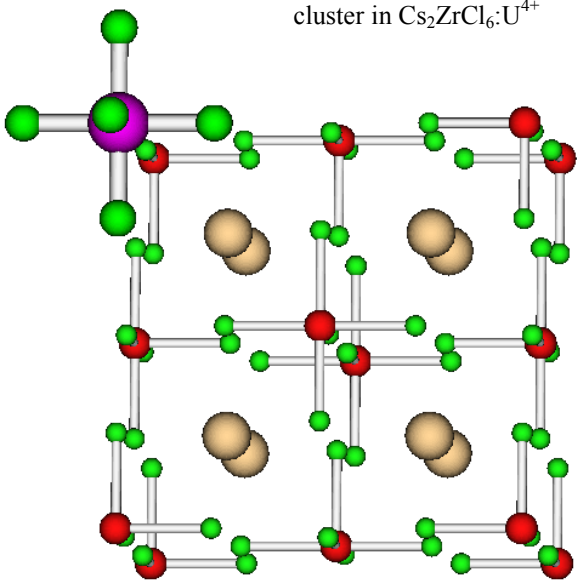


FIG. 1. $(UCl_6)^{2-}$ defect cluster in $Cs_2ZrCl_6:U^{4+}$

Theory and experiments become particularly complementary in this context. In fact, on the one hand, high precision of nowdays spectroscopic techniques allows for the accurate determination of electronic transition energies and local vibrational frequencies. However, the assignments of the spectral signals beyond the fn manifold through the usual fitting procedures based on the Crystal Field Theory parametric Hamiltonians demands such large amount of parameters that it becomes impractical and only the onset and range of the $f^{n-1}d$ bands can be identified. On the other hand, the measurement of the local distortions produced by the impurity in the host is far more difficult for the ground electronic state and can not be measured for any of the excited states. This limitation is important since the f-element – ligand equilibrium distance is expected to vary notably from the f^n to the $f^{n-1}d$ manifolds.

Quantum chemistry methods applicable to local defects in the solid state have been dessigned in our group, whose results can be either used together with experimental spectroscopic data to help to understand these complex systems and their properties, or can be used to add efficiency to the experimental research by investigating a priori structural and spectroscopic properties of systems which, in many cases, are very difficult and dangerous to handle experimentally. For this to be possible, the accuracy of the results must be not far from that attained through experiments and this

can only be assured if the methods treat very accurately, the following interactions: Relativistic effects including spin-orbit coupling must be considered. Simultaneously, valence electron correlation has to be dealt with trough multiconfigurational expanssions of the molecular defect wavefunction based on multireferences, using very flexible gaussian type basis sets. These two requirements are met by the ab initio model potential method (AIMP) developped in our group (see Ref. 4 and references therein), which is an effective core potential method that can include spin-orbit relativistic effects and can be combined with a variety of quantum chemical correlation methods to calculate the potential energy surfaces of the ground and excited states of the cluster defect usually defined as the f-element impurity plus its first neighbours: $(UCl_6)^{2-}$ in $Cs_2ZrCl_6:U^{4+}$. The effects of the embedding host crystal must be considered as well. The AIMP method has been formulated also as an embedding technique4 useful to describe the quantum mechanical effects of a set of host lattice ions which are described by Hartree-Fock wavefunctions occupying crystal sites. These wavefunctions (which are calculated in advance, through embedded ion calculations in the perfect host) originate the AIMP embedding operators which are added to the defect cluster Hamiltonian.

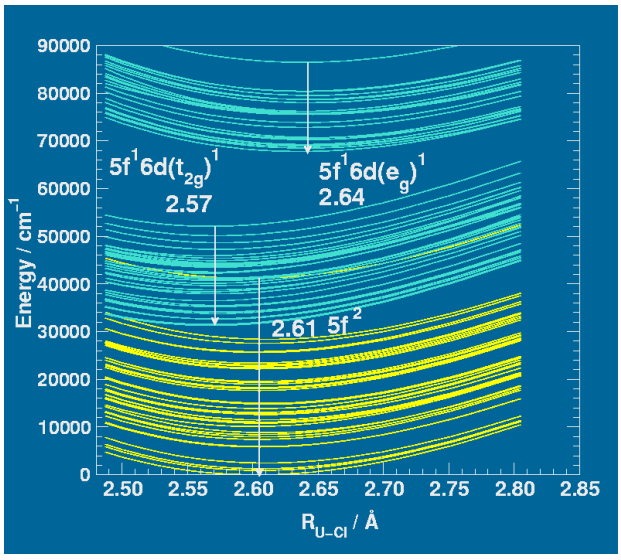


FIG. 2. $5f^2$ and $5f^16d^1$ $\Gamma_{g,u}$ manifold of $Cs_2ZrCl_6:U^{4+}$

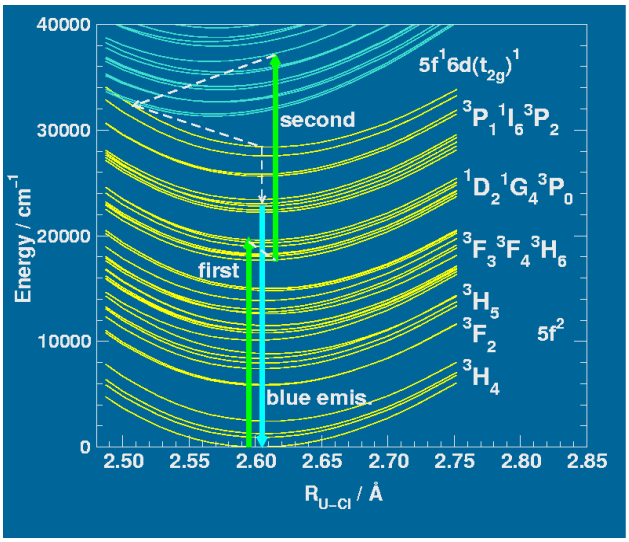


FIG. 3. Green to blue up-conversion mechanism in $Cs_2ZrCl_6:U^{4+}$

The whole crystal is thus described as a generalized antisymmetric product involving the multiconfigurational cluster electronic wavefunction and the external ion Hartree-Fock wavefunctions. The cluster–host interactions which are therefore considered include electrostatic interactions (both short and long-range type), exchange interactions and linear independency (to fulfill Pauli principle). The method has been widely tested and applied to the calculation of the structure and spectroscopy of transition metal impurities in ionic hosts (see Ref. 4 for a review of the core/embedding AIMP method and its results in gas phase molecules and local properties of solids in the bulk and at the surface). It has also been tested in $Cs_2ZrCl_6:Pa^{4+}$,[5] and work is in progress in $Cs_2YNaCl_6:Ln^{3+}$ (Ln=Ce–Lu), $Cs_2ZrCl_6:U^{4+}$, and $Cs_2YNaCl_6:U^{3+}$. Core AIMP parameters and (gaussian type) valence basis sets are available for the chemically relevant elements of the Periodic Table (up to Z=103); those corresponding to lanthanide and actinide elements have been presented and tested in Ref.6. Embedding AIMP parameters are also available for a variety of halide and oxide cryatals. The results that can be obtained and their accuracy can be illustrated for $Cs_2ZrCl_6:U^{4+}$.Green to blue upconversion has been demonstrated experimentally for this system and it has been explained as the result of a two-photon absorption process involving only f electronic states. We have modelled this system as described above and have calculated the potential energy surfaces of all f^n and $f^{n-1}d^1$ electronic states associated to the octahedral (UCl6)4- cluster embedded in the AIMP representation of the Cs_2ZrCl_6 host. The results appear in Fig. 2 (the assignment of the electronic states has been omitted). The calculated U–Cl equilibrium distances are

found to be common to a number of cluster electronic (spin-orbit) states grouped in what can be called the *f2, f1d(t2g)1,* and *f1d(e2g)1* superconfigurations (Fig. 2).
The comparison of the *f -f* spectrum (difference of energy minima) with available experimetal data is very good, the largest error being some 1500 cm-1. A di_erent possible interpretation of the green to blue upconversion is suggested by our results which can be followed in Figure 3. It involves a first green *f - f* absorption withing the *f2* manifold, followed by a non-radiative relaxation, a second green absorption which involves a dipole allowed *f - d* excitation, followed by a non-radiative relaxation down to the *f* manifold where blue light can be emitted.

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LOW TEMPERATURE LABORATORY
LABORATORIO DE BAJAS TEMPERATURAS (LBT – UAM)

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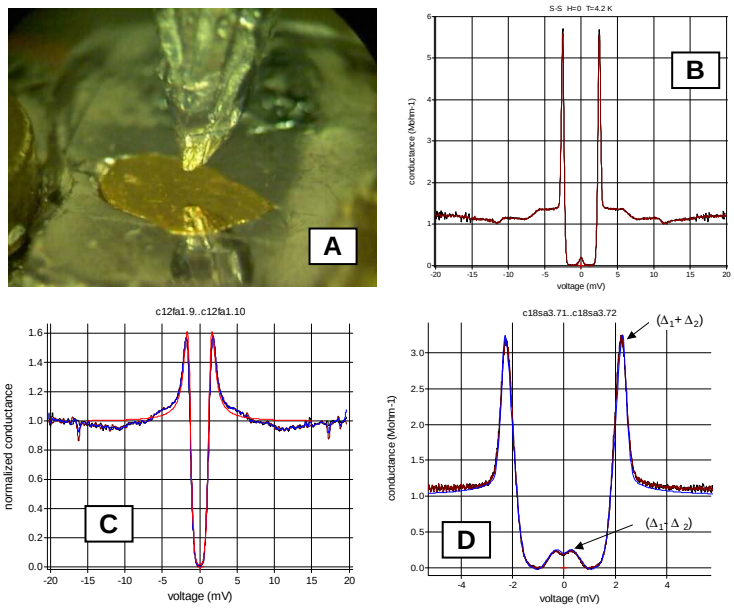
Prof. Farkhad Aliev, Prof. Nicolás Agraït, Prof. Arkadi Levanyuk, Prof. Miguel Angel Ramos, Prof. José Gabriel Rodrigo, Prof. Gabino Rubio-Bollinger, Prof. Raúl Villar, Dr. Hermann Suderow, Dr. César Talón.
Ph.D. Students: Maria Crespo, Rocío Grande, Ruben Guerrero, Pastora Martinez, Juan José Riquelme

The research activities in the Low Temperature Laboratory – UAM (LBT – UAM) were, in the past, oriented to the study of the thermal properties of solids, mainly of disordered ones, with calorimetric, dilatometric and thermal transport techniques. Following the invention of the STM the laboratory acquired a good experience in the behaviour of piezoelectric ceramics at low temperature, which permitted the construction of different LT-STM. Today, 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 atomic chains and contacts. A promising field is the combination of all this know-how with nanolitographic techniques to produce nanostructures, which can be fabricated now in the UAM. Other important research lines at LBT-UAM are devoted to the study of magnetic multilayers involving low frequency noise and magnetic tunneling experiments, and the study of polimorphic alcohols combining calorimetric, x-ray difraction and neutron spectroscopy experiments.

Superconducting STM tips

Continuous indentation-retraction cycles of the STM tip against the sample result in the creation of a nanostructure between tip and sample, the connective neck. In particular using superconducting (SC) materials, sharp nanotips result after the rupture of a lead nanobridge (S-S). The creation of these nanotips is done in-situ at low temperature.
The X-Y positioning device in our LT-STM/S unit allows a complete characterization of the nanotip (both in S-S and N-S tunneling configurations) and its use for the topographic and spectroscopic study of other superconducting materials. These capabilities are shown in the following figures, where a composite sample made of three different samples (Au, Pb and $NbSe_2$) is studied. The tip DOS is checked on gold (N-S) and lead (S-S) regions.



Figures:

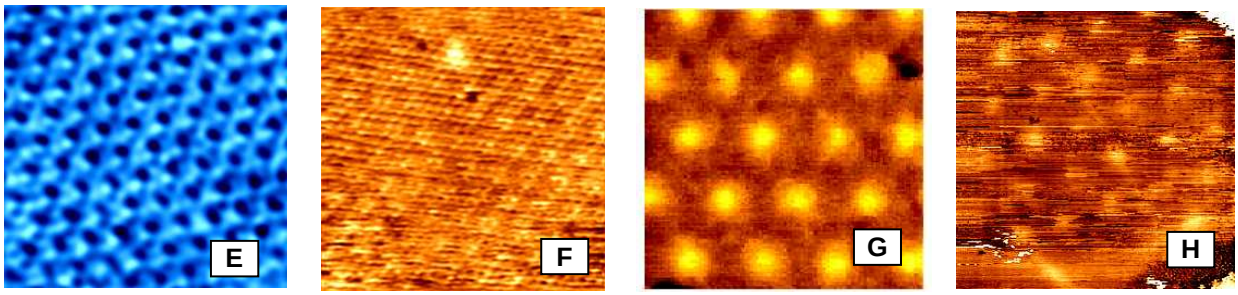
***A**: Actual SC tip and multi-sample configuration.*

*Tunneling curves obtained with the SC tip on Pb (**B**), Au (**C**) and $NbSe_2$ (**D**).*

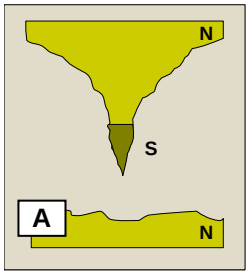
***E**: Atomic resolution on $NbSe_2$ with a Pb tip.*

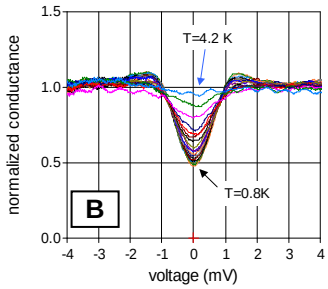
***F**: Observation of CDW and atomic defects in $NbSe_2$ with a Pb tip.*
*Vortices in $NbSe_2$ with Au tip (**G**) and Pb tip (**H**).*

These data are obtained at 4.2 and 2 K.



The superconducting nanotips can also be used to investigate the behaviour of the superconducting state at these extreme confinement geometries. We have created Pb nanotips that present superconducting properties (detected measuring the DOS) under magnetic fields as high as 2 Tesla, more than 30 times higher than the bulk critical field for lead.





Figures:
***A**: Schematics of the SC nanotip (note the bulk normal electrodes).*
***B**: Tunneling curves obtained in this tip geometry versus temperature under a magnetic field of 2 Tesla.*

Scanning Tunnelling Spectroscopy at very low temperatures.

Recently, the experimental capabilities of the laboratory have been considerably extended by a dilution refrigerator, which gives us the possibility to make experiments at very low temperatures (0.03K) and under very high magnetic fields (10 T). The experimental set-up has been partically developed in the laboratory in order to decrease significantly the necessary time for cooling down, to increase the versatility of the set-up and to insure an electromagnetically clean environment. In addition the system has been properly isolated from vibrations. Two Scanning Tunnelling Microscopes have been installed in this dilution refrigerator and in a previously available ^{3}He system capable to reach 0.3K and 13 T. These systems offer the possibility to make measurements of the local electronic density of states (tunneling spectroscopy) with an extremely high resolution in energy (4μV at 0.05 K).

Ultra high resolution spectroscopy in high and intermediate T_c superconductors: Multiband superconductivity, Gap anisotropy and Pairing interaction

The recently discovered superconductor MgB_2 has caused a veritable rush in the scientific community, due to the relatively large (40K) critical temperature and the simplicity of its chemical formula. Only one month after its discovery we succesfully made the first tunneling spectroscopy measurements in this material. At this time, the only experimental data available were the magnetic susceptibility, the resistivity and the isotope effect. Our measurements inspired several theoretical calculations, where the scenario of multiband superconductivity (different values of the superconducting gap in different sheets of the Fermi surface) was proposed. Nowadays, this scenario has been widely confirmed by all kinds of experiments, including our subsequent measurements on single crystals of this material, made in collaboration with ISTEC in Japan.

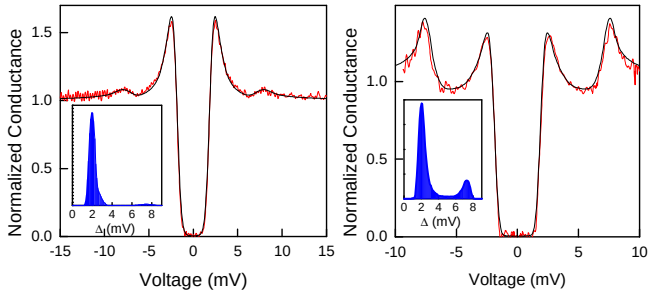


Figure 1. Conductance curves obtained in MgB_2 showing different contributions of the two bands to the total conductance. (Left: 2K, single crystal. Right: 0.6K, single grain)

On the other hand, we could also adress successfully the question about the symmetry of the superconducting wave function and the pairing interaction in borocarbide materials ($RENi_2B_2C$) thanks to the very high resolution in energy of our experiments (made in high quality single crystals grown in Ames and in Grenoble). We have demonstrated for the first time the presence of a highly anisotropic pairing interaction, driven by Fermi surface nesting, together with a highly anisotropic gap. This challenges present theories of superconductivity. The clear observation of coexistence of nearly ferromagnetic, and antiferromagnetic order and superconductivity in these compounds is another subject which we are exploring now in detail.

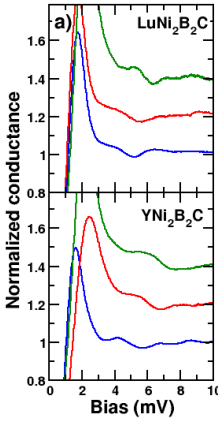


Figure 2: The low energy phonon features measured in the tunneling spectroscopy of the non magnetic Y and Lu borocarbides (T_c = 15.6 and 16.5 K)

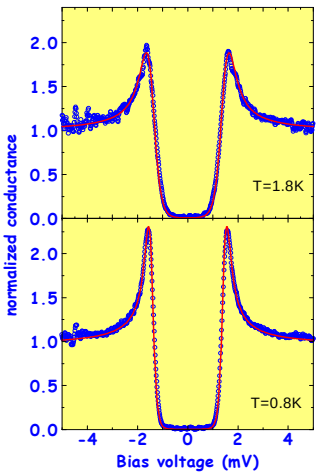


Figure 3: Tunneling conductance of TmNi2B2C (Tc=11K). At 0.8K, superconductivity and antiferromagnetism coexist.

Spectroscopy of superconducting materials with very low critical temperatures

Many materials having very low critical temperatures (between 1 and 2 K), as the heavy fermion superconductors (UPt_3,URu_2Si_2,$PrOs_4Sb_{12}$), are very interesting from the fundamental point of view, because much new physics is expected to evolve from precise studies of their superconducting properties. The sucessful measurement of these materials needs a first test in well known superconductors as Al. In a different context, this opens the possibility to study spin injection effects into superconductors, which are not present in other well known materials with higher T_c (as Pb) due to an increased spin orbit interaction.

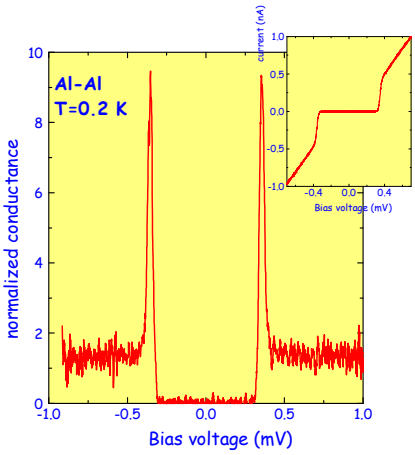
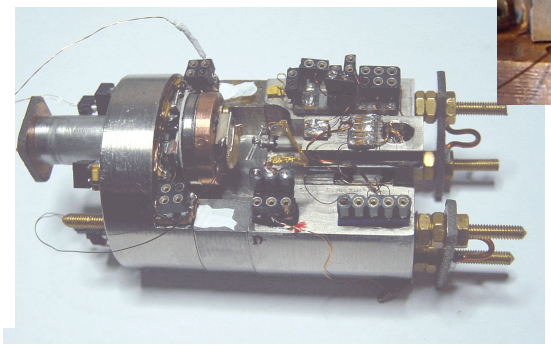


Figure 3: Tunneling conductance of an Al-Al junction made with an STM

Local tunneling spectroscopy in mesoscopic systems

Nanolithography based on the scanning electron microscope (SEM) makes possible the fabrication of metallic structures with well controlled sizes and shapes with a resolution of the order of 50 nm. At this length scale, intermediate between the atomic and the macroscopic worlds, the electronic transport properties start displaying features associated with the quantum nature of the charge carriers. The basic concept behind these phenomena is the quantum coherence of the electrons over the scale of the

In order to study with atomic resolution the electronic quantum states giving rise to the mesoscopic phenomena, we have designed and built a low temperature AFM/STM with spectroscopic capabilities. This microscope consists of a quartz tuning fork which acts as a force sensor, and a xy table with a lateral range of several milimeters.

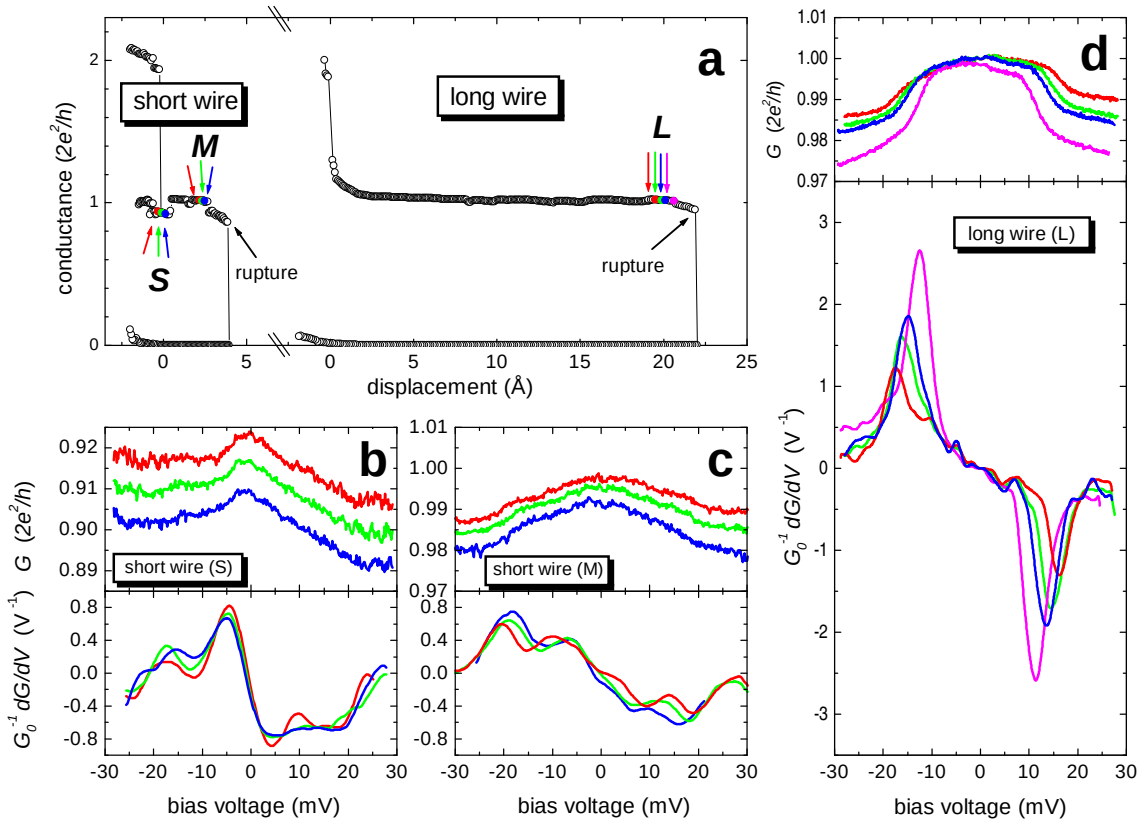


Atomic contacts and atomic chains: mechanical and transport properties

Using STM techniques we fabricate freely suspended atomic chains of single gold atoms at liquid helium temperatures. These chains, which form spontaneously during the fracture of gold nanocontacts, form very stable metallic wires. Using a very senstitive force sensor we can resolve the force evolution during the formation of the chain, where the individual atomic-rearrangement events for addition of atoms to the chain can be clearly identified. We find that the bond strength of the chain is about twice that of a bulk metallic bond.

Electronic transport in these chains is ballistic and takes place through an almost completely open conductance channel giving a conductance very close to $2e^2/h$. The variation of the differential conductance with voltage reflects the electron-phonon interaction and allow to study the vibrational modes of these chains. We find that the frequency of longitudinal phonons and the magnitude of the electron-phonon interaction can be tuned by varying the tensile force on the chain.

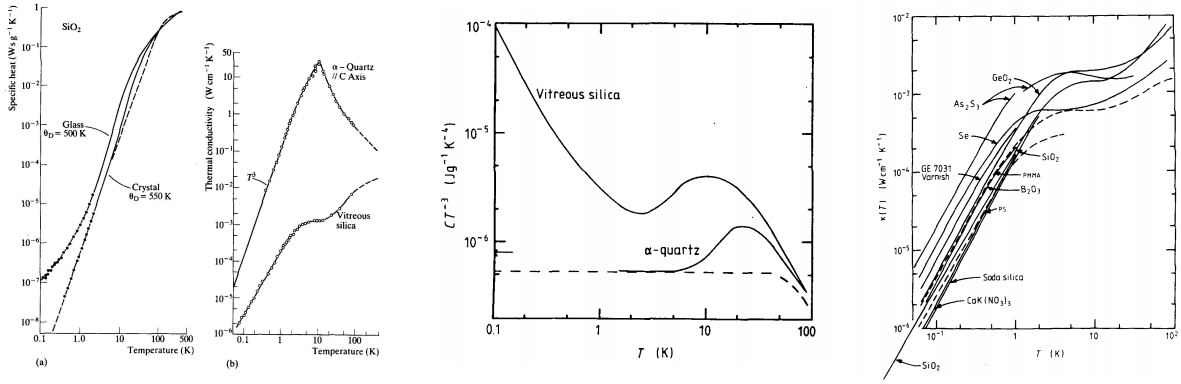
Conductance (a) and force (b) during formation and rupture of a gold atomic chain at 4,2 K. (c) Computed force using DFT. [Rubio-Bollinger et al. PRL 87, 026101 (2001)]



Differential conductance and its derivative vs voltage for atomic chains of different lengths, showing the electron-phonon interaction. [Agraït et al, PRL 88, 216803 (2002)]

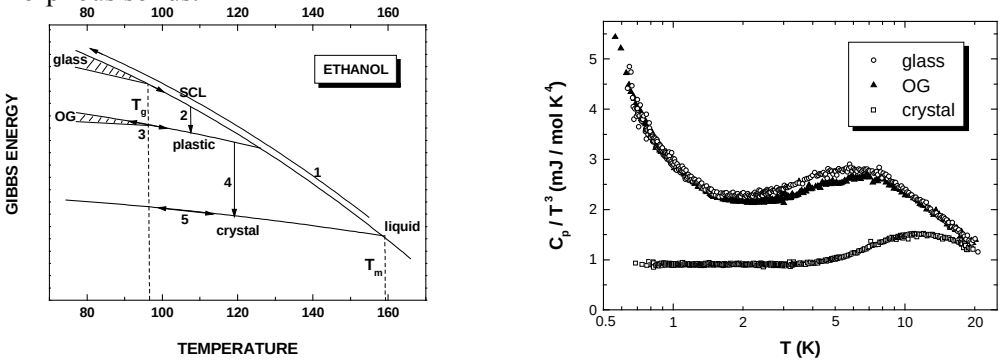
LOW-TEMPERATURE PROPERTIES OF GLASSES AND DISORDERED SOLIDS

Since 30 years ago, it is well known that glasses or amorphous solids exhibit *universal* thermal properties at low temperatures, which are in turn very different from those of crystalline solids. Below 1 K, the specific heat C_p of dielectric glasses is much larger and the thermal conductivity κ orders of magnitude lower than the corresponding values found in their crystalline counterparts (see Figure below, left). C_p depends approximately linearly and κ almost quadratically on temperature. This is in clear contrast to the cubic dependences observed in crystals for both properties, well understood in terms of Debye's theory of lattice vibrations. Above 1 K, C_p still deviates strongly from the expected dependence $C_{Debye} \propto T^3$, exhibiting a hump in C_p/T^3 which is directly related to the so-called *boson peak* observed by neutron or Raman vibrational spectroscopies (see Figure below, right). In the same temperature range the thermal conductivity exhibits an ubiquitous *plateau*.



The research line on *Low-temperature properties of glasses and disordered solids*, aims to deepen in our understanding of abovementioned properties universally exhibited by non-crystalline solids at low temperatures. This subject remains a matter of widely interest and vivid debate, in conjunction with the more general problem of the very nature of the glass-transition phenomenon and the glassy state itself. Both issues continue to be among the major unsolved problems of condensed matter physics.

Following investigations on archetypical glasses such as boron oxide and how these properties depend on the thermal history of the glass, more recently we have focused on hydrogen-bonded molecular systems, namely simple alcohols, which present the peculiarity of being liquid at room temperature and have been hence seldom studied at low temperatures. Specifically, we have measured during last years the low-temperature specific heat of different alcohols (normal and fully-deuterated ethanol, 1- and 2- propanol, and glycerol) in their different -ordered or disordered- phases. Ethanol exhibits a very interesting polymorphism (see Figure below, left) presenting three different solid phases at low temperature: a fully-ordered (monoclinic) crystal, an orientationally-disordered (cubic) crystal or "orientational glass" (OG), obtained by quenching a plastic crystalline (rotator) phase, and the ordinary structural (amorphous) glass obtained by supercooling the liquid fast enough. Very interestingly, both the standard transition glass↔supercooled liquid (SCL) and the dynamic transition OG↔plastic crystal, are found to occur at the same temperature $T_g \approx 95$ K and have comparable discontinuities in specific heat By measuring and comparing the low-temperature specific heat of the three phases (see Figure below, right), in the "boson peak" range (2-10 K) as well as in the tunneling-states range below 1K, we have been able to provide a quantitative confirmation that "glassy behavior" is not an exclusive property of amorphous solids.



MAGNETICAL DYNAMICS AND NOISE IN MAGNETOELECTRONIC SYSTEMS AND NANOSTRUCTURED SUPERCONDUCTORS

Our currently run projects mainly involve studies of the low frequency noise and complex magnetic dynamics in magnetic multilayers, magnetic tunnel junctions and structured superconducting films. Below we describe two of our recent findings.

By using direct (magnetization) and indirect (magnetoresistance) we studied low frequency magnetic domain wall dynamics in epitaxial antiferromagnetically coupled multilayers (Fe/Cr) and magnetic tunnel junctions (Co/Al2O3/Py) [Fig.1]. Analysis of complex (below 10000Hz) magnetic susceptibility shows that at T less than 10K a high temperature hysteretic low field peak in the magnetic losses transforms to a non-hysteretic dip, indicating a possible qualitative change in the dynamics of the DWs. We relate the observed non-trivial response to possible quantum nucleation and depinning of the domain walls. The frequency dependence of the dissipation at small non-zero magnetic fields, at lowest temperature (T=2K), may be reasonably well fitted by the expression that describes the losses of a damped oscillator with a single relaxation time of about 0.0003 sec

We have studied the low frequency (3Hz-177Hz) complex magnetization dynamics in Co/Al2O3/Ni80Fe20 magnetic tunnel junctions (MTJs) at temperatures between 4.2K and 300K. The measurements are carried out by using two different experimental techniques. The first method probes directly magnetic properties via DC magnetization and AC susceptibility, while the second one measures AC magnetization dynamics of the ferromagnetic electrodes near the cross area, which is related to the tunnelling resistance. By comparing data obtained by the two methods, we conclude on the difference between the domain walls pinning mechanism in the interface and in the bulk. We also studied the variation with AC drive amplitude and frequency of the interface related magnetic losses layer near the coercive field of permalloy. We observed a weak frequency dependence and a pronounced nonlinear behavior of the losses as a function of AC excitation amplitude

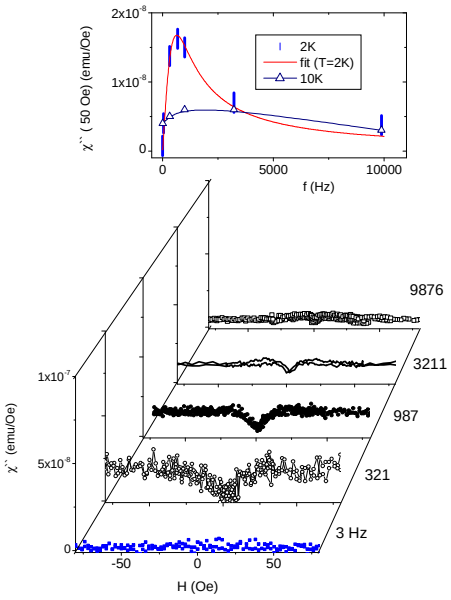


Fig.1. Low frequency losses in Fe/Cr multilayers at 2K [Aliev et al., PRL, v. 88, p.187201 (2002)]

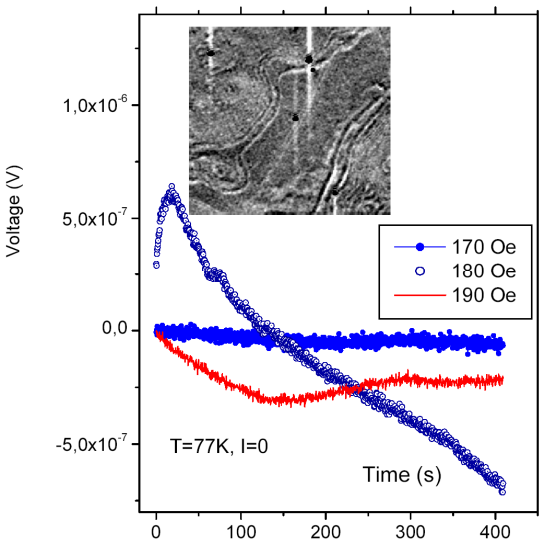


Fig.2 Detection of the extended domain wall in [Fe/Cr]10 multilayer(see RT MFM image in the inset) via noise transport measurements J.M.@M.M, v.240, p.165 (2002)

THEORETICAL STUDIES ON MIXED-STATE PROPERTIES OF TYPE II SUPERCONDUCTORS: ELASTICITY-DRIVEN INTERACTION BETWEEN VORTICES

Prof. Arkadi P. Levanyuk
Ph.D. Student: Andrés Cano

It is well known since long ago that the elastic strain induced by vortices in superconducting materials is a key point in the understanding of phenomena such that vortex pinning, vortex motion, correlations between vortex and crystal lattices... We have focused our attention in the attractive interaction between vortices that arises as a result of the vortex-induced strain, what is the basis of almost all above mentioned phenomena.

Although vortex-induced strains has been the subject of numerous studies, we have found that it has been considerably underestimated until now. It is because it was assumed that vortex cores, considered as cylindrical inclusions of the normal phase, were the only sources of strain. However, we have demonstrated that, in type II superconductors, the main source of vortex-induced strain is the non-core region. Moreover, the corresponding non-core-induced attraction between vortices proves to be stronger than the previously considered core-induced one, at least by a factor $\ln^2\kappa$ (the Ginzburg-Landau parameter κ can be up to 1000 in some materials).

Experimental implications of the resulting new situation have been explored. Because the leading contribution to the vortex-induced strain is the non-core one, it should be taken into account first of all when discussing, for instance, orientation of the vortex lattice with respect to the crystal lattice. It is shown to be also important when interpreting the thermal anomalies of the transition between the superconducting and the mixed states.

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MATERIALS MICRO-ANALYSIS USING IONS BEAMS (CMAM)

Prof. Fernando Agulló-López, Prof. Aurelio Climent-Font, Dr. Gastón García, Dra. Mª Teresa Fernandez,
PhD students: Carlos Pascual, Oscar Espeso, Olga Enguita

Research lines:

Interacion ion-matter.
Stopping force studies for several projectiles: H, He, C, N, Si in insulating and conducting materials of interest in microelectronics (Ti, Si, SiO_2, silicides, Si_3N_4, Al_2O_3, etc.

Characterization of wave guides using TOF-ERDA
Characterization using the detection of the time of flight of elastically recoiled atoms, of $LiNbO_3$ subjected to proton interchange and Zn diffusion.
Design and construction of a time of flight station at CMAM.

Characterization of archaeological materials using ion beam techniques
Ion beam techniques like PIXE y RBS, including microbeam, are used to study archaeological artifacts: metallic threads coated with gold, bronzes, cheramics, etc. Construction and assembly of a microbeam line at CMAM.

Characterization of atmospheric aerosols using PIXE
Elemental composition study of the urban aerosol with PIXE. Apportionment of the contaminant sources. Assembly of an experimental line optimized for the study of aerosols using PIXE at CMAM.

Study BCN materials with TOF-ERDA techniques
TOF-ERDA techniques are quite suitable for the determination of depth profiles of samples composed by light elements.

Research done in collaboration with: Instituto de Ciencia de Materiales de Madrid, CSIC., Rossendorf Research Center, Dresden, Germany, Centro Nacional de Aceleradores, University of Sevilla. LAMEL Institute, Bolonia, Italy. University of Jyvaskyla, Finland. Lund University, Sweden. Helsinki University, Finland. University of Florence, Italy. Universidad Nacional Autónoma de Mexico. Departamento de Calidad Ambiental, Ayuntamiento de Madrid. Franco Lucarelli, University of Florence, Italy.

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Coordinator: L. Viña

- "Methods of measuring distance dependent interactions with the Atomic Force Microscope". ***Prof. Suzi Jarvis***. Research Center for Atom Technology. Tsukuba. Japan.

- "Superfluidity, Phase coherence and the new Bose-Condensed Alkali Gases". ***Prof. A. J. Leggett.*** MacArthur Professor. University of Illinois at Urbana-Champaign.

- "Enhancement of various Optical Processes due to Group-velocity anomaly in Photonic Crystals". ***Prof. Dr. Kazuaki Sakoda***. Research Institute for Electronic Science. Hokkaido University. Japan.

- "Experiments with single atoms and photons: An exploration at the heart of Quantum Physics". ***Prof. Serge Haroche.*** Professeur de Physique à l´Universié Pierre et Marie Curie et à l´Ecole Normale Supérieur. Paris. France.

- "Superconductivity in Granular Platinum at very low Temperatures". ***Dr. Reinhard König***. Physikalisches Institut. Universität Bayreuth. Germany.

- "Fractional Charges and other Tales from Flatland". ***Prof. Horst L. Stoermer, Nobel Prize in Physics 1998***. Dpto. Physics Columbia University. New York, NY and Bell Labs, Lucent Technologies. Murray Hill. NJ.

- "El laboratorio del acelerador Peletron del IFUNAM". ***Prof. Alicia Oliver***. Instituto de Física. Universidad Nacional de Mexico.

- "Recent results from the CDMS (Cryogenic Dark Matter Search) Experiment". ***Prof. Blas Cabrera***. CDMS collaboration. Stanford University. USA

- "Microcavidades de semiconductores: de las aplicaciones a la física". ***Prof. Emilio. E. Mendez***. Dept. of Physics and Astronomy. State University of New York at Stony Brook. NY, USA.

- "Descubrimiento de un "Famoso" comportamiento tipo Ferromagnético y Superconductor del Grafito". ***Prof. Dr. Pablo Esquinazi***. Dpto. Superconductivity and Magnetism. Fakultaet fuer Physik und Geowissenschaften. Universitaet Leipzig. Germany.

- "Physics near the Mott Transition". ***Prof. P.B. Littlewood***. Head of the Theory of Condensed Matter Group. Cavendish Laboratory. Cambridge, UK.

- "Spectroscopy in Electron Wonderland: Quantum liquids and Phase Transitions". ***Prof. A. Pinczuk.*** Dpts. of Applied Physics and of Physics. Columbia University, New York, NY and Bell Laboratories. Lucent Technologies.

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Coordinators: L. Viña and A. Levy Yeyati

- "Towards Solid State Quantum Bits". ***Prof. Daniel Esteve***. Quantronics Group. SPEC-CEA Saclay, F91191 Gif-sur-Yvette. France.

- "Surface Physics and Computer Simulations". ***Prof. Dirk O. Boerma***. Nuclear Solid State Physics Materials Science Centre. Groningen University. Nijenborgh 4, 9747 AG Groningen, NL.

- "The Flux-line Lattice in High-temperature Superconductors". ***Prof. Ernst Helmut Brandt***. Max-Planck Institut für Metallforschung. Stuttgart. Germany.

- "Time-reversed Acoustics". ***Prof. Mathias Fink***. Laboratoire Ondes et Acoustique. ESPCI, University Denis Diderot Paris 7.

- "Nuclear Microscopy and its Aplications in Biology and Medicine". ***Prof. Geoff W. Grime***. University of Oxford. UK.

- "Hidden symmetries in the cuprates". ***Prof. Robert B. Laughlin. Nobel Prize in Physics 1998.*** Stanford, USA.

- "Quantum Dots single Photon Source". ***Prof. A. Imamoglu***. UC Santa Barbara. USA.

- "Towards Mesoscopic Physics with cold Atoms: From Wires to Atom Chips"**.** ***Prof. Jörg Schmiedmayer.*** Physikalisches Institut. Universität Heidelberg. Philosophenweg 12. Heidelberg. Germany.

- "Electrons in lateral Semiconductor Superlattices". ***Prof. Ulrich Roessler***. Institut für Theoretische Physik. Universität Regensburg. Germany.

- Course "Ion-Solid Interactions and Simulation". ***Prof. Dirk O. Boerma***. Nuclear Solid State Physics Materials Science Centre. Groningen University. NL.

- "What Problems of Physics and Astrophysics seems to be beginning of the 21^{th} Century". ***Prof. V.L. Ginzburg.*** Lebedev Institutu, Russia.

- "Toward DNA Nanoelectronics?"**.** ***Prof. Danny Porath.*** Chemistry Dpt., Hebrew University in Jerusalem and Center for Nanoscience and Nanotechnology, Tel-Aviv University, Israel 69978.

INTERNATIONAL SUMMER SCHOOLS "NICOLÁS CABRERA".

VII International Summer School "Nicolás Cabrera" (2000)

IMAGING AND MANIPULATION OF MATTER AT NANOMETER SCALE

Sponsored by: MEC and CAM, UAM

Organizing Committee:
Directors: F. Flores / M. Salmerón
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PROGRAM

- Theory of STM and AFM.
- Atomic and Molecular Manipulation
- Chemical Reactivity at the Nanoscale level.
- Friction.
- AFM and Biology
- Nanowires and Nanocontacts in normal metals and superconductors.
- Theory and experimens of BEEM.
- SNOM.
- Kondo effect and Superconductivity.

LECTURERS

- N. Agrait, Universidad Autónoma de Madrid. Spain
- A. Baratoff, University of Basel, Switzerland.
- A. Baró, Universidad Autónoma de Madrid. Spain
- L.D. Bell, Jet Propulsion Lab., Caltech, USA
- F. Besenbacher, CAMP-Univ. of Aarhus, Denmark.
- D. Eigler, IBM Almaden Research Center, USA
- C.F.J. Flipse, Eindhoven Univ. Tech., The Netherland.
- H. Gaub, Ludwig-Maximiliam-Univ. Munchen, Germany.
- J.K. Gimzewski, IBM Zurich, Switzerland.
- H. von Kanel, ETH Zurich, Switzerland.
- J. Krim, North Carolina State University, USA.
- M.C. Payne, University of Canbridge, U.K.
- A. Martín Rodero, Universidad Autónoma de Madrid. Spain
- B. Persson, Forschungszentrum Julich, Germany.
- M. Persson, Chalmers Univ. Technology, Sweeden.
- H. Rieder, Frei Universitat Berlin, Germany.
- P. Sautet, Scole Normale Superieur Lyon, France.
- P. Joyez, CEA Saclay, France.
- S.Weiss,LawrenceBerkeleyNationalLab.USA.

VIII Internatinal Summer School "Nicolás Cabrera". (2001)

WHERE PHYSICS AND BIOLOGY MEET:
Molecular motors,
Biomembranes
Electron transfer in biological system.

Sponsored by: UAM, MEC, SBE (Sociedad de Biofísica de España), Fundación BBVA

Directors: N. Agrait / M. Vélez

LECTURERS

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- C. Bustamante. UC Berkeley
- R. Cross. Marie Curie Research Institute
- L. Dutton. Univ. of Pensilvania
- Evans. Univ. of British Columbia
- Keller. Univ. of New Mexico
- G. Mclendon. Princeton University.
- J.N. Onuchic. UC San Diego
- M. Sansom. Oxford University.

IV SCIENTIFIC MEETING FOR YOUNG RESEARCHERS

November 12, 2000. Colegio Mayor Luis Vives, Madrid.

- "Spin dependent exciton-exciton interaction in "hot" and "cold" 2D exciton gases controlled by electric field". Günter Aichmayr
- "Spatial distribution of the propagation intensities of waves in guides with surface disorder". Antonio García Martín.
- "Dynamical effects in low coating phases in the system Pb/Si (111). Oscar Custance
- "Characterization and developing in Silicon nanostructures for optoelectronic devices". Raúl José de Palma.
- "Anomalous magnet-optical properties in a bidimmentional electron gas". Herko van der Meulen.
- "Energy detection and fly time in the elastic dispersion: TOF-ERDA line in the UAM acceleration". Oscar Espeso Gil
- "High doses implantation of Boron, Carbon and Nitrogen ". Lucía Barbadillo.
- "Non-lineal and non-local Meissner effect in superconductor wires". Javier Sanchez Cañizares.
- "Nanolithografic service". Prof. Gabino Rubio
- "The UAM Accelerator". Prof. Aurelio Climent.

V SCIENTIFIC MEETING FOR YOUNG RESEARCHERS.

November 30, 2001. Miraflores de la Sierra, Madrid.

Invited Conference: "Grabbing the Cat by the Tail: Studies of DNA packing by single ϕ29 Bacteriophage particles using optical tweezers". Carlos Bustamante. University of California, Berkeley & Howard Hughes Medical Institute.

- "Biocompatibles structures and solid surfaces functionalitation". Miguel Manso.
- "Modification methods in the growth of Cu (111) magnetic thin films". Daniel Farias.
- "Quantum conductance in semimetal nanocontacts of Bismuth". Jose Gabriel Rodrigo.
- "High hard Titanium Carbonitrides growth by sputtering assisted by low energy ion beams". Gonzalo G. Fuentes.
- "Application of differential PIXE and SEM-EDX to the study of arqueometric metallically covered". Olga Enguita.
- "Spatial solitons in fast photorefractive materials". Gabriel F. Calvo.
- "Stimulated emission and Bose_Einstein condensation of polaritons". Diego Porras.
- "Exchange energy and correlation in function of the orbital occupation numbers: total energy calculation and quasiparticles". Pablo Pou.

INTERNATIONAL SYMPOSIUM

"PHYSICS AT THE DAWN OF THE 21st CENTURY "

March 26-27, 2001. Fundación Ramón Areces. Madrid

Description

Six prominent physicists address a broad audience to speak about some of the most burning questions in Physics at the beginning of the new century.

Speakers

Sir Harold W. Kroto (Sussex), Nobel Prize for Chemistry 1996
Jean-Pierre Hansen (Cambridge)
Robert H. Austin (Princeton)
Robert B. Laughlin (Stanford), Nobel Prize for Physics 1998
Carl E. Wieman (Boulder), Nobel Prize for Physics 2001
Gerard 't Hooft (Utrecht), Nobel Prize for Physics 1999

Organization

Fundación Ramón Areces
Instituto Universitario de Ciencia de Materiales "Nicolás Cabrera"
Universidad Autónoma de Madrid.

Program

- "Arquitecture of the microcosmos", Sir Harold W. Kroto, University of Sussex.
- "Statistical mechanics of supramolecular aggregates from complex fluids to bimolecular assemblies", Jean Pierre Hansen. University of Cambridge.
- "Biological physics in the 21st century", Robert H. Austin, Princeton University.
- "Riding the storm of condensed-matter physics in the fabulous valley of silicon", Robert B. Laughlin, Stanford University.
- "Bose Einstein Condensation: quantum weirdness at the lowest temperature in universe", Carl E. Wieman, University of Colorado.
- "Where do we stand in elementary particle physics", Gerard 't Hooft, University of Utrecht.

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Center for Microanalysis of Materials (ion-beam accelerator), run by INC.

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