



ALBA Beamline Proposal WS04

A Diffraction Beamline for Nanostructures, Thin films, Surfaces and Interfaces on Alba

A proposal prepared for the SAC February 2005

Acknowledgements

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1- INTRODUCTION:

It is proposed to build a high-resolution x-ray beamline on an ultrahigh vacuum undulator source at a 4m section at ALBA to investigate structure and magnetism at the interface and the outermost layers under well-defined and controllable environments.

The main purposes of the beamline should be the structural study of thin films and interfaces. Nowadays, there is a tendency to study how the materials properties are modified when they are confined. The final idea is to get materials with tailored properties. Thus, the study of nano-objects becomes very important not only from a fundamental point of view, in order to understand how the structural confinement influences the physical properties of the material, but also for its broad technological impact. Nanostructured systems concern physics, chemistry and biology communities, interested in their optical, magnetic, electrical and catalytic properties. The x-ray diffraction has been shown a powerful tool for structural atomic characterization of the materials. Taking into account the small amount of material that we should like to characterize (in some extreme cases below a monolayer) and the special configuration with respect to the substrate surface, some special requirement of instrumentation are needed (for example, it is necessary that the sample should have a fixed grazing incident angle with respect to the beam). Moreover, it is important not only to obtain information about the atomic structure of the material but also of the nano-order; in this way the Small Angle X-ray Scattering at Grazing Incidence (GISAXS) is recognized as a powerful tool. Thus, **the proposed beamline should combine both Small Angle at the nanometer-scale and the wide angle x-ray diffraction at grazing incidence configuration.** Three factors that are outlined in this document identify the role that X-ray diffraction will play in such studies: (i) the high energies of the X-rays to allow penetration to buried interfaces, (ii) the high flux that is required as disordered systems will produce broad, and (iii) weak scattering and the possibility of using microbeams to monitor domains of more well ordered regions on a sample. In that way it is necessary to have a very low dispersion x-ray source (low beta section).

The past few years have seen an enormous amount of activity in the development of magnetic devices for data storage, ultra-low field sensing and quantum computing applications. In such systems, a detailed knowledge of the magnetic structure, combined with the possibility of controlling the physical structure on the length scale of magnetic domain sizes and smaller (patterned magnetic nanostructures), have shown to be of critical importance. Taking into account that the study of the magnetic properties of some of these materials have a high interest, and the fact that the required instrumentation is compatible with the other beamline purposes, we propose to introduce a quarter-wave plate combined with a polarization detector for **magnetic X-ray diffraction studies of these systems at grazing incidence configuration.**

This beamline configuration is quite new, and the scientific cases that are specially adequate lie within the highlights aims of the scientific and advisory committees. Nowadays, there is no beamline with the demanded configuration at disposal of the scientist community, although it

exists a project to build a beamline with similar scientific aims at DIAMOND and SOLEIL. The XMAS beamline at the ESRF offers the possibility of studying the magnetic X-ray scattering at small angle, but the beamline configuration was not optimized for such use. The Spanish community could profit of the scientific advances that this kind of beamline could produce.

2. SCIENTIFIC CASES:

2.1 Background

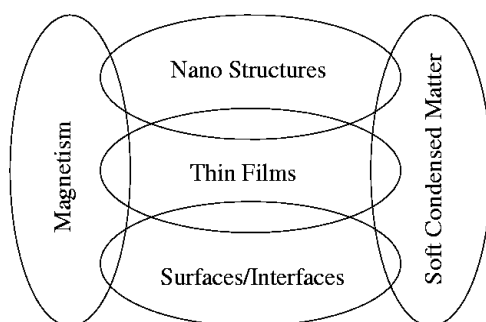
Understanding the structure of the interface between two materials is a prerequisite to answering many questions in a wide variety of scientific disciplines. The range of new scientific ideas that rely on understanding the interaction between two or more components is particularly exciting. Imposing order on relatively disordered materials, as it is found for instance in biological systems, is likely to become a significant research area in its own right. The possibility of tethering a particular chemical or biological molecule at specific sites would provide unprecedented control over reactions at the molecular level. The key to controlling this interaction is to understand the arrangement of the low dimensional structure and the influence that external parameters may have on it. The delicate balance of energies and the reduced coordination at the interface is liable to create unique effects, as has been observed in many surface science experiments studying elemental components. Its importance in areas such as the role of the surface in semiconductor devices cannot be overemphasized. For example, the bond between a semiconductor and metallic contacts will critically affect the resistance and likelihood of device failure. Extending these ideas to other environments such as buried interfaces or solid-liquid interfaces is likely to stabilize an amazing array of properties. X-ray diffraction is unique in its ability to probe such structures *in-situ*, and with high spatial and temporal resolution.

X-ray diffraction is a powerful technique for the determination of structural arrangements of low dimensional materials, such as surfaces and interfaces [1]. It can be used in a wide variety of environments including solid and liquid surfaces and solid-solid or solid-liquid interfaces, which can be probed due to the ability of X-rays to penetrate through matter. In well-ordered arrangements, the positions of the atoms can be established to an accuracy of $\pm 0.01\text{\AA}$. The power of the technique is based on two factors: the weak scattering of X-rays by matter and the brightness of modern storage ring insertion devices. The first allows simple data analysis in terms of the Fourier sum of plane waves, whereas the second means that many, often weak, reflections can be recorded, giving the high information content necessary to characterize complex structures.

In disordered systems, that will become increasingly important, the x-ray scattering will not be confined into well-defined rods but will be spread out in reciprocal space. Measuring and analyzing such diffuse scattering will enable information on the structure and disorder to be quantified. As mentioned before, three main features identify the role that X-ray diffraction will play in such studies; the high energies of the X-rays to allow penetration into buried interfaces, the high flux that

is required as disordered systems will produce broad and weak scattering and the possibility of using microbeams to monitor domains of better ordered regions on a sample. For these reasons it is necessary to have a very low dispersion x-ray source (low beta section). This configuration is not possible in a bending magnet source as it is placed at the ESRF (SPLINE); with such sources the beam size can only be reduced by means of a huge focusing of the beam, and this configuration is in a large number of cases a limiting phenomena, due to the decreasing of the x-ray diffraction resolution.

As it has been described above, the technique available with this beamline can be used by quite different research fields. In the next figure it is shown some keys themes which are expected to be prominent in the proposed beamline:



The sections that follow do not provide an exhaustive list of the measurements that will be carried out but are intended to identify the areas of high quality research that will be possible with such a flexible and powerful beamline.

2.2. The New Science

2.2.1. Nanostructures

The final goal is to develop procedures to fabricate well-ordered nanostructured materials with tailored properties for specific applications. Thus, the study of nano-objects becomes very important, not only from a fundamental point of view in order to understand how the structural confinement influences the physical properties of the material but also for its broad technological impact. Nanostructured systems concern physics, chemistry and biology communities, interested in their optical, magnetic, electrical and catalytic properties.

The self-organization processes have been observed at the surface of systems of very different character. Often the assembled systems present well defined order with periodicities at the nanometer scale. These self-assembled nanostructures potentially represent a new patterning technology, able to surpass in speed and quality the present standard methods, such as lithography, in fields as diverse as magnetic recording media or light generation in semiconductor lasers. Two methods can be employed for this aim: first, by depositing soft condensed matter layers with self-organized nanostructures on flat substrates, and, second, by using nanostructured substrates.

A. Quantum Dots.

The self-organized nanostructured substrates are created employing a wide range of self-assembly mechanisms to provide well ordered arrays of surface objects such as pits, dislocations, step bunches or pyramidal mounds. One family of techniques involves the ion bombardment of either metal or semiconductor single-crystal substrates, giving an ordered pit morphology. Whereas another uses strain driven self-organization in very thin-films or alloys. The strain-driven relaxation can take different pathways depending on the experimental system and different nanostructures as dots, wires or rings can be self-assembled. Misfit dislocations can be generated, and often in metal systems,

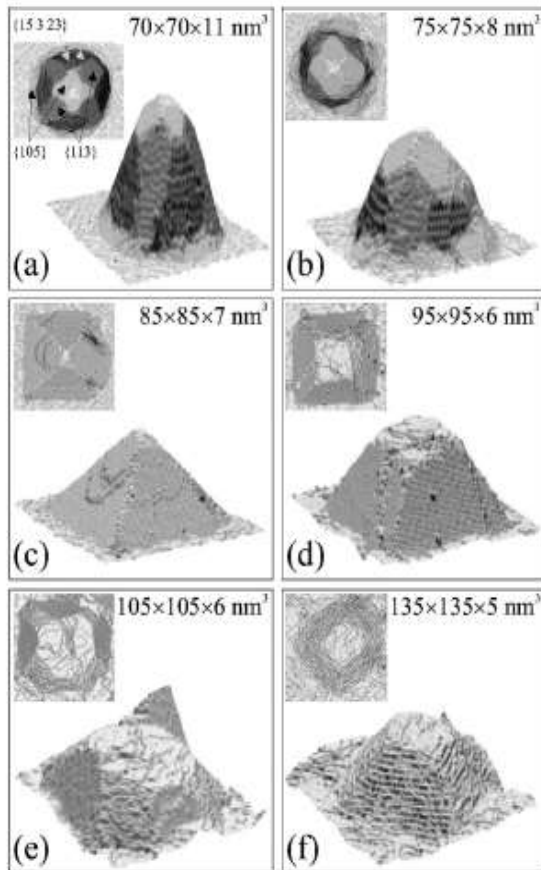


FIG. 11. Typical Ge island shapes obtained by STM during Si capping of Ge domes grown on Si(001): (a),(b), domes; (c) pyramids; (d)–(f) prepyramids. The Si coverages are 0, 1, 2, 4, 8, and 16 ML's for panels (a)–(f). From Rastelli *et al.*, 2001.

they develop into very well ordered surface patterns. On semiconductor systems a competition of relaxation mechanisms occurs, such as ripple formation, coherent 3D island growth and misfit nucleation [2]. A final technique will use crystal-lattice-mediated self-assembly to generate ordered arrays of nanoparticles over the surface of microcrystals. This variety of mechanisms will produce patterns of different length scales.

One very important power of this technique it is the fact that it is possible to study the shape and the self organization of quantum dots embedded in a matrix or covered by a capping layer. This allows to determine the sort range correlation between these entities, as well as the shape modification induced by the capping layer [3].

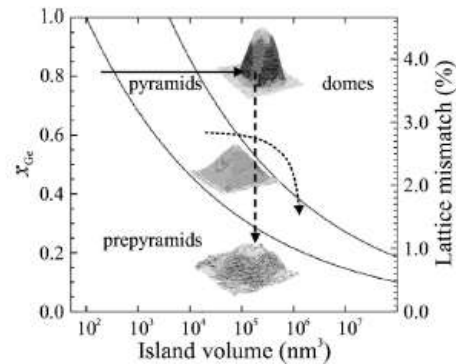


FIG. 14. Shape transition of Ge or SiGe islands grown on Si(001) during growth (solid arrow), postgrowth annealing (dotted arrow), and Si capping (dashed arrow). The solid curves represent the critical volumes for pyramids and domes. From Rastelli, Kummer, and von Kaenel, 2002, reprinted with permission from Elsevier. Copyright 2002.

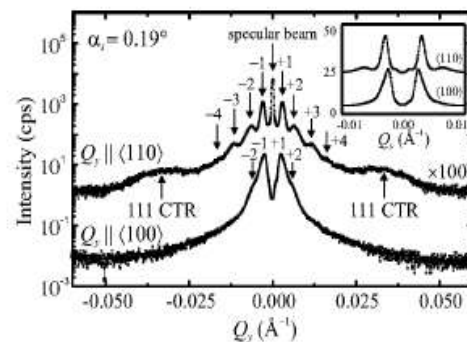
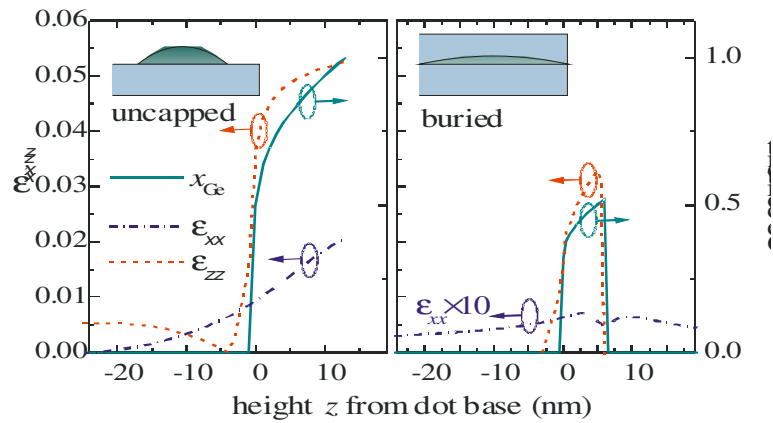
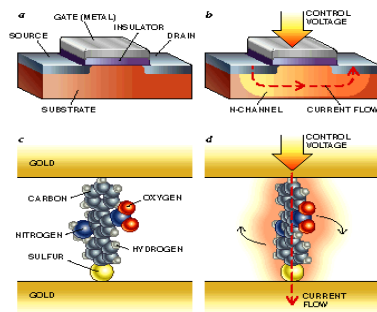
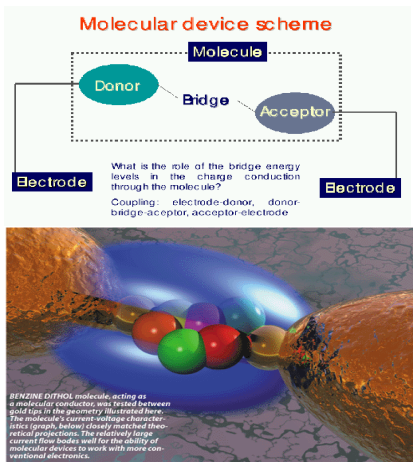


FIG. 33. GISAXS intensity distribution for two different sample orientations. Satellite peaks due to the positional correlation are visible as well as facet streaks due to island shape. From Schmidbauer *et al.*, 1998.



B. Soft-Condensed Matter Self-Organized Systems.

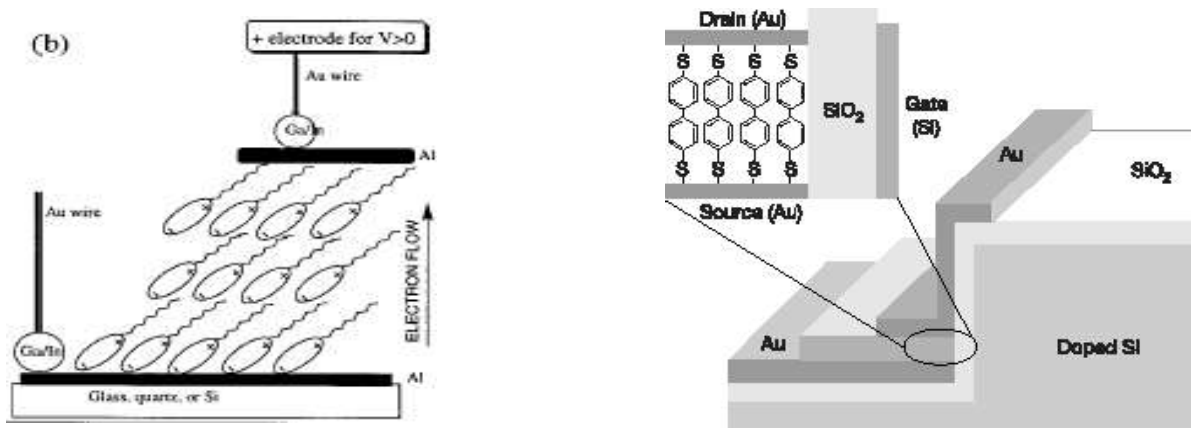
Some researchers have extensively used X-ray scattering techniques to determine the structures that can be formed by self-organization of molecules, such as long chain thiols on gold surfaces [4].



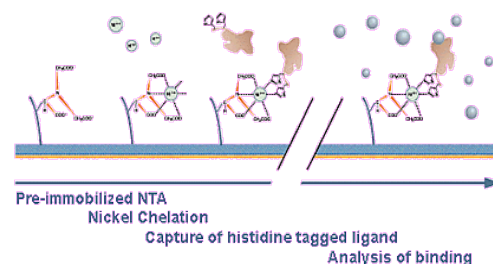
CONVENTIONAL MICROTRANSISTOR (a) has three terminals, known as the source, gate and drain. A positive voltage applied to the gate draws electrons to the insulator (b), enabling current to flow from the source to the drain. A molecule based on three benzene rings (c) was also used to switch an electric current. The center ring had asymmetric fragments, enabling it to be twisted by an electrical field (d). With a specific voltage applied, the electrical field twisted the molecule and permitted current to flow.

Such measurements are beneficial not only for the role they have in understanding the structure of the interface, but also because it aids the understanding of the self-assembly process. This is a key area for the development of devices built using a 'bottom-up' approach, which are predicted to supersede the current generation of silicon 'top-down' structures.

There are already electronic devices based in the use of the thiols or dithiols layers. For instance, a molecular rectifier and a molecular transistor devices have been presented (see figure below) [5].

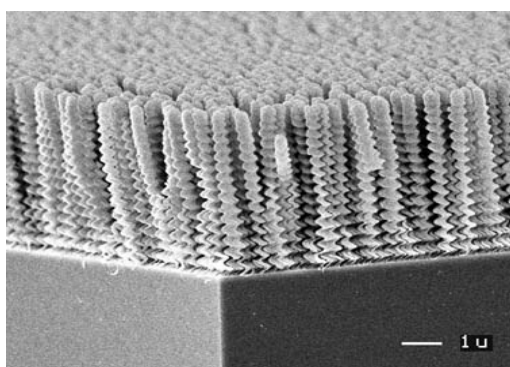


These thiols can be functionalized in order to have the possibility of connect selectively other molecules. One very interesting example is the formation of organic logic gates over the self-assembled monolayer. These devices are able to modify their conductivity (logic state) as a function of the environment conditions [6].



C. *Soft-Condensed Matter Chiral Systems.*

The creation of ordered arrangements of molecules is important in several areas of research. The substrate induced organization of the molecules to produce long-range order is an extension of the concepts of atoms forming reconstructions. It has potential benefits in the ability of the surface to selectively adsorb one enantiomer in preference to the other [7]. In many molecular systems it is very important in many molecular systems to ensure the purity of the molecules and can be very difficult to separate molecules that have the same chemical composition but differ only in the handedness of their structure. Such studies are invaluable as the effectiveness of many drugs depends on this distinction, as demonstrated by thalidomide. The ability of specific surfaces to adsorb certain molecules has therefore tremendous potential in the role of molecular purification. Recently, asymmetries in the scattering probability of polarized electrons from chiral molecules has been demonstrated [7b]. Even for unpolarized electrons, enantio-selective scattering has been predicted.



The combination of chirality and magnetism stems from Pasteur's work and is particularly appealing. In the 80's, Barron reformulated and generalized the definition of chirality given by Lord Kelvin to include motion; a chiral system is thus defined as one in which space parity is broken, while time parity is conserved [7b]. This point of view has recently been confirmed by experiments: it has been demonstrated how chirality can be introduced in a system by the so-called "magnetochiral anisotropy" effect,

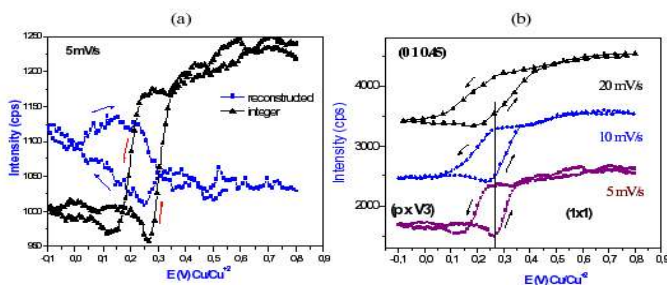
combining a magnetic field parallel to the direction of propagation of an unpolarized light beam [7b]. In this way enantiomeric excess is generated in a chemical reaction. The setup envisaged for this beamline would also allow to explore this highly suggestive subject [7c].

2.2.2. Thin films

A. *Magnetic materials*

Determining the properties and morphology of buried layers and interfaces remains an important experimental problem in solid-state science. Many of the technological end products of this science are based on thin-film devices, which consist of a series of such layers. Characterization of the physical microstructure and degree of disorder of these films is commonly carried out by reflectivity, diffraction and diffuse scattering studies. The past few years have seen an enormous amount of activity in the development of magnetic devices for data storage, ultra-low field sensing and quantum computing applications. In such systems, a thorough knowledge of the magnetic

microstructure is also required. Magnetic x-ray scattering is presently a burgeoning area able to study the magnetic structure in thin magnetic layers and more recently the induced polarization in magnetic/non-magnetic systems. Importantly the “photon-in, photon-out” nature of the experiment



Evolution of the diffracted intensity from the satellites as compared to the integer order (0 1 0.45) peak. (b) Diffracted intensity from the (0 1 0.45) reflection during voltammetric cycles at different scan rates

means that the applied magnetic field does not affect the measurements [8]. So far the studies have concentrated on transition metal and rare-earth multilayers but one expects that this will extend to actinide systems in the near future.

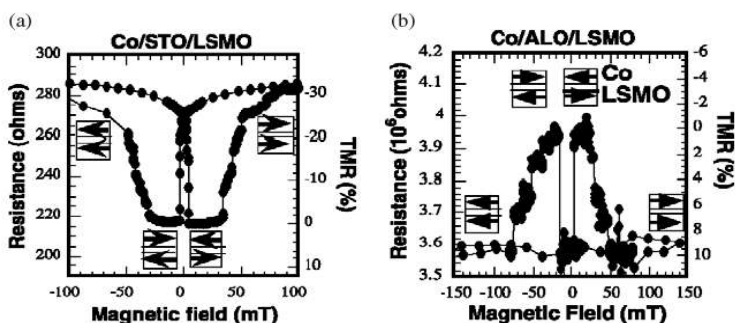
A detailed knowledge of the magnetic structure of such systems, combined with the possibility of controlling the physical structure on the length scale of magnetic domain sizes and smaller (patterned magnetic nanostructures), is thus of capital importance for the development of the field. Such structures may

be artificially created through patterning or by deposition on miscut surfaces. As device sizes are continually being shrunk the interplay between magnetic structure and physical microstructure is of ever increasing importance.

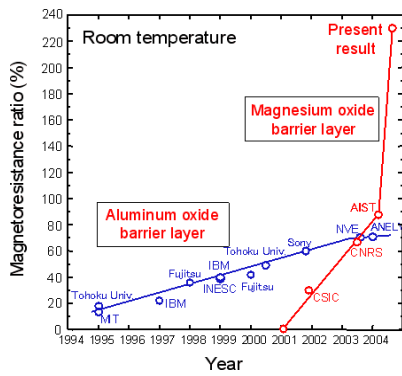
B. Buried Interfaces.

The temporal evolution in semiconductors and magnetic recording devices has followed both an exponential law (Moore’s law). Nonetheless, the continued growth in both fields is technologically limited. Improvements in both, recording and reading medias are necessary. Since the beginning of the manufacturing of magnetic hard drives in the 60s, the physical processes of recording remained the same. The increase of the areal storage density by six orders of magnitude took place by simple scaling. In spite of this continuity, researchers expect fundamental limits of this evolutionary process in the next five to ten years. The superparamagnetic effect limits the miniaturisation of the bit cell size because the stability of the magnetisation towards thermal fluctuations scales with the volume of the bit cell.

Spin Valves are the key element in giant magnetoresistive (GMR) read heads for magnetic recording disk drives. The technological trend has been associated to a decreasing in the film thickness. In the order side Magnetic Tunnel Junctions (MTJ) are attracting renewed interest due to their possible use as non volatile Magnetic Random Access Memories (MRAMs) that could replace the semiconductor



RAMs. MTJs are formed by two magnetic metals separated by a nanometer-thin insulator layer. Today’s MTJs are made of polycrystalline materials, which originate a large number of problems, of both basic and technological nature. There is much interest in growing epitaxial, single-crystal MTJs. This requires crystallographic and

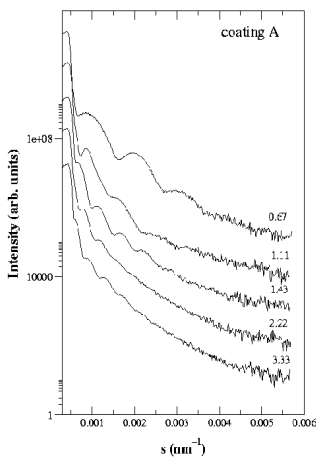


processing compatibilities for the materials involved. The decreasing in the film thickness has been so important that the interface nature from the chemical, physical and electronics point of view starts to play a fundamental role [9]. X-ray diffraction is a powerful tool for non destructive analysis of the layer structure and moreover of the physical and chemical state of their interfaces. From this point of view the evolution in the next future of both scientific fields go by the hand of the development of the structural studies by means of x-ray diffraction.

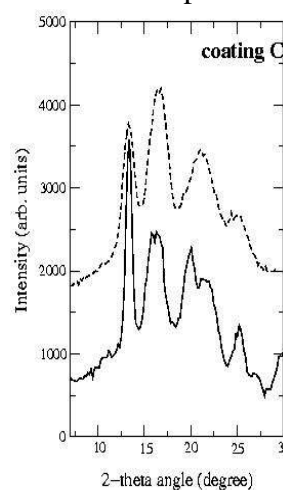
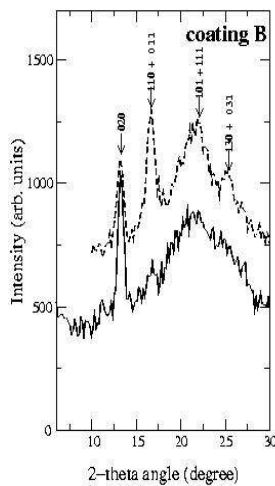
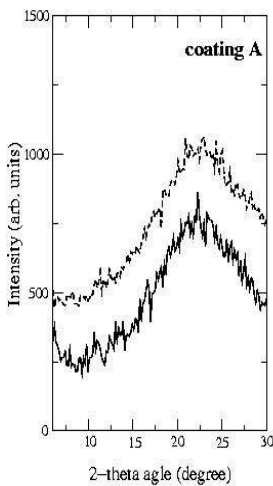
C. Polymers

A fundamental understanding of the influence of free surfaces and buried interfaces on the

properties of thin polymer films is important in many applications, including coatings, adhesion and the electronic behavior at interfaces in polymer-based optoelectronic devices. Both the free surface and the buried interface may differently affect properties such as the chain conformation, the composition of mixed systems and chain dynamics, while a combination of surface and finite size effects may also influence the character and temperature of the crystallization and glass transitions. In contrast to the extensive data available for semiconductors and other inorganic materials, indicating pronounced differences in the state of order between surfaces and bulk, very little information is available about the surface structure of polymers. Grazing incidence diffraction with synchrotron radiation is an ideal tool for such studies since the penetration depth is of the order of the molecular



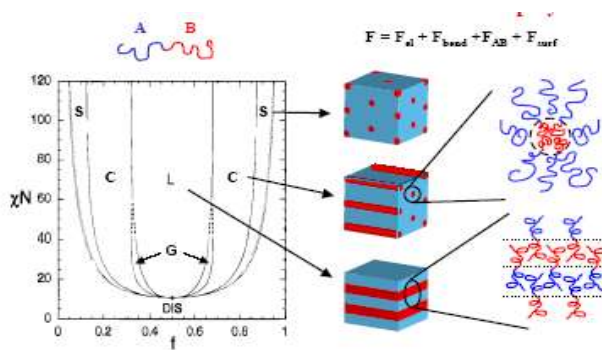
dimensions at the surface, and the surface and bulk structure can be compared by adjustment of the incident angle [10]. The scattering is weak from a molecular monolayer and the beam cross-section is small, so the high brightness of the CELLS source will greatly benefit this relatively new area of research.



Semiconducting polymers for electronic devices are a big growth area both scientifically and commercially [11]. Here polymers are used in thin films, often in multilayer structures. Since the device performance depends very largely on its interfacial properties, and as we know that electronic properties of polymers are strongly coupled to their chain conformations, we can anticipate that an understanding of the factors controlling chain ordering near

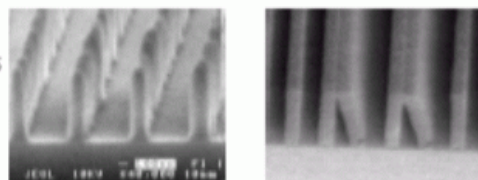
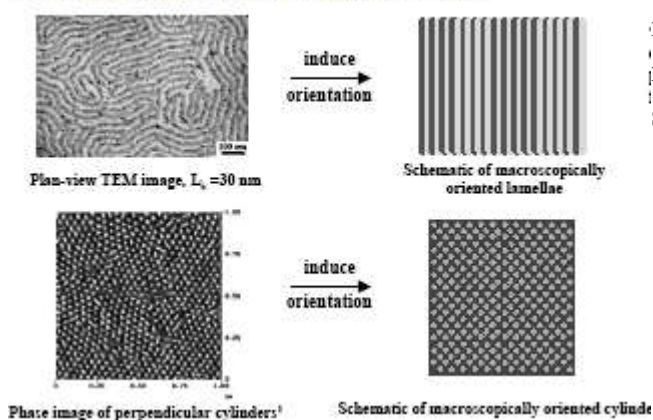


surfaces and interfaces will be crucial to optimizing device performance. Structural studies of in-situ processing of semiconducting polymer films is likely to be an important growth area for the coming decade.



The block copolymer formed by asymmetric polymers is able to form phases in the equilibrium with a self assembled morphology that can be changed as a function of the polymer blocks concentration ratio. The formation of these large size structure can be used as a chemical robust route to the fabrication of ultrahigh-density arrays of nanostructures [12]. One of the polymer block can be selectively eliminated by chemical methods. The resulting structure can be used as a mask for the formation of microelec-tronic nano-structures.

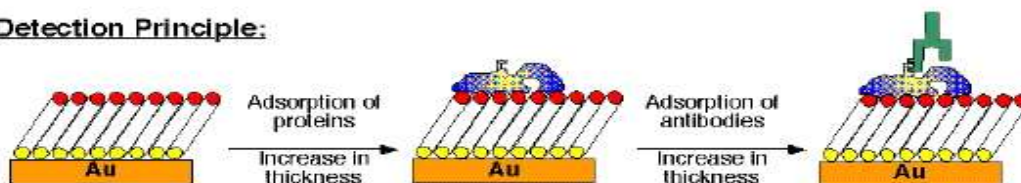
Microphase Separation of Block Copolymers in Thin Films



D. Biomolecules

The interface between biological molecules and a non-biological surface is a largely unexplored area of science, which is of relevance to important biological and medical technologies as well as future nanotechnology: medical implants, biosensors, bio-catalysis, biofouling-resistant surfaces, 'smart polymers' for controlled drug release, templates for tissue engineering and bio-electronic materials of the future i.e. bacteriorhopsodin, DNA networks [13].

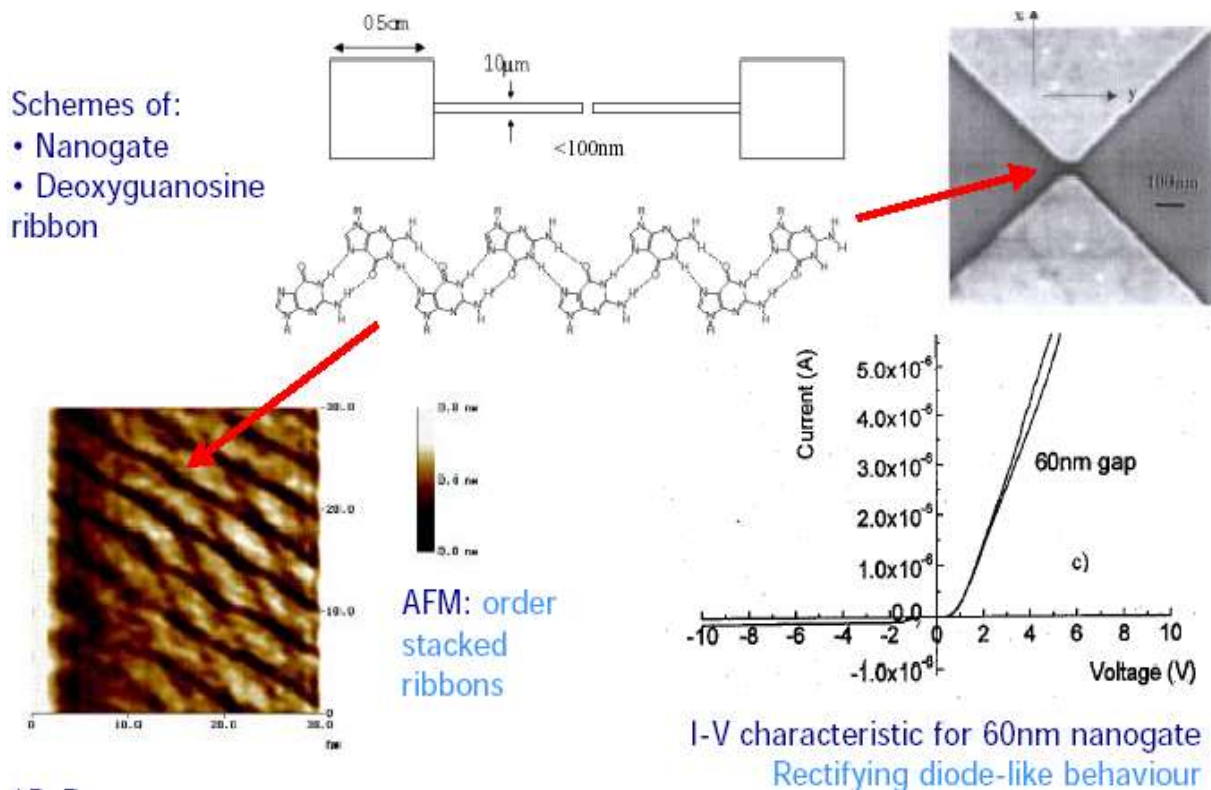
Detection Principle:



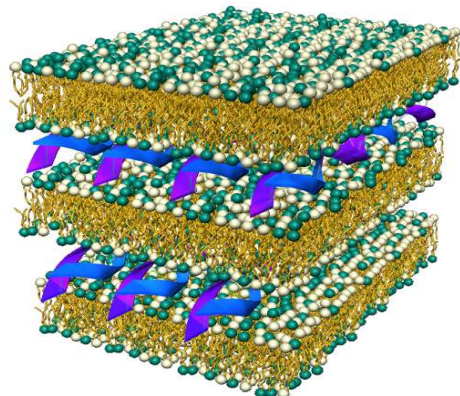
A central scientific issue is to understand and control the interactions at the interface between a solid material surface and its biological environment. In view of the hierarchy of structures occurring in proteins, these interactions need to be understood at the level of amino acids, peptide and polypeptide chains and protein molecules. Additionally, the effect of the aqueous solvent conditions and the chemical nature of the surface needs to be addressed. Vacuum-based surface techniques are

therefore not applicable and a combination of synchrotron-based surface x-ray diffraction and photon-based spectroscopies is essential.

A longer-term benefit from understanding interactions of biological molecules with interfaces, and with the aqueous environment lies in nanotechnology [14]. In the search for new functional materials it is tempting to try to exploit the intriguing peptide and protein architectures that orchestrate the catalytic and other regulatory tasks in living systems. Detailed understanding of the supramolecular interactions between biomolecules, interactions with interfaces and with the environment would thus be crucial to the design of such functional nanostructures.



Surface studies of membranes, and the molecules on their surfaces, are also hugely promising with applications for a large number of industrial processes [15]. In the food and pharmaceutical sectors,

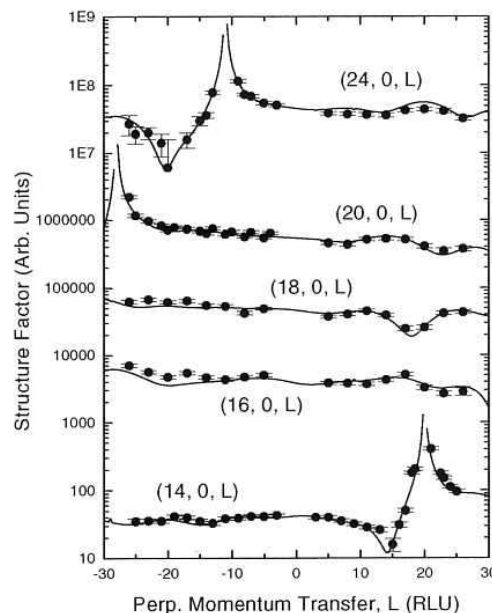
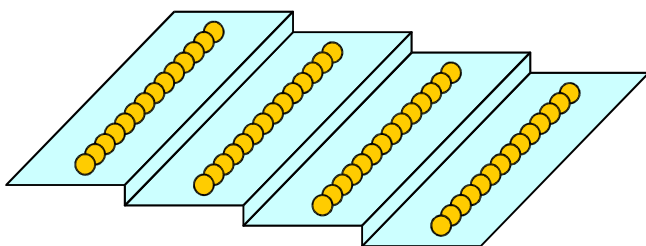


surface science is vital to understanding activities such as protein denaturation, emulsification and phase separation, binding and unbinding, and the control of interfaces. Device development and biosensors also rely heavily on information derived from surface science studies at a solid-liquid interface. Increasing numbers of diseases are now being associated with the deposition of non-crystalline deposits in organs such as the brain, heart and pancreas.

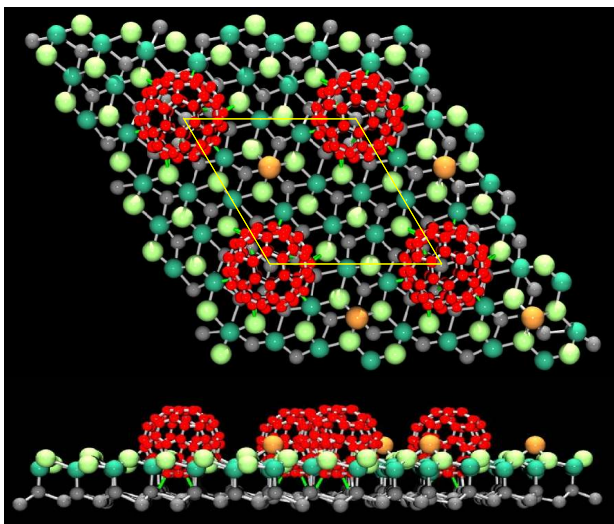
2.2.3. Surface and Interfaces.

A. Surface in UHV

In recent years, there has been significant interest in accessing the magnetic order at surfaces. Given the break in crystal symmetry at the surface one might expect to observe magnetic structures and critical behaviour different to those found in the bulk [16]. The experimental difficulty is that the surface charge scattering is typically 5 orders of magnitude weaker than the bulk scattering. For this reason, high brightness synchrotron grazing incidence X-ray scattering techniques are required to characterise the chemical structure of the surface [17]. The magnetic intensity is then further reduced by another 5-6 orders of magnitude, and so the XRMS enhancement is required to observe any magnetic contribution from the surface. Such difficult measurements will provide a significant and unique insight into surface magnetic ordering: an area of solid state magnetism that has not been exploited.



The interaction between substrates and organic or carbon based molecules induces large lateral arrangements on the substrate surface generating surface reconstructions with large unit cells. Usually, the intensities coming from these types of atomic periodicities are small, so intense X-ray beams impinging onto the sample are desirable. This fact is due to the fact that the number of reflections increase while the number of scatterers in the unit cell remains constant. The $(13^{1/2} \times 13^{1/2})$

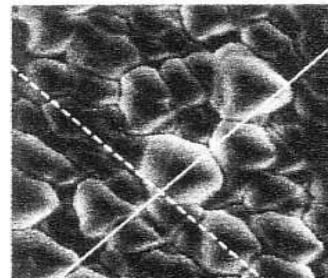
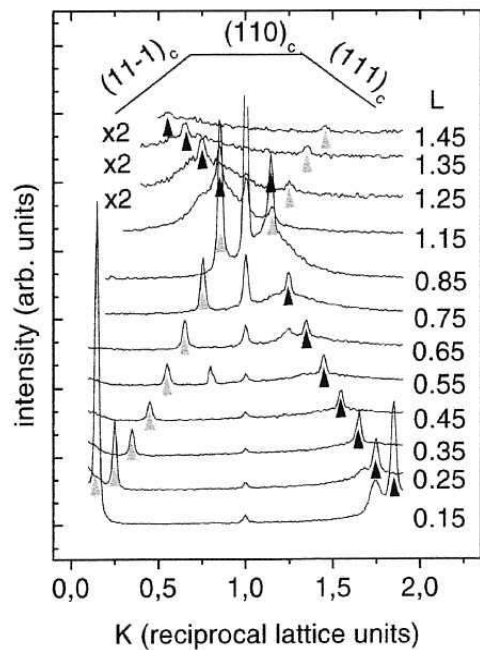


$R14^\circ$ surface structure induced by fullerene molecules onto the Ge(111) surface is an example of intermediate superstructure. Its structure determination involved the measurement of more than 2000 non-equivalent superstructure reflections with intensities sensitively lower than those containing bulk contributions. One picture showing its crystallographic structure is represented below. The surface unit cell contains one Ge-adatom and the C60 molecule is sinking into the surface, because six Ge surface atoms are missing forming nano-pits [17b].

B. Harsh environments.

For harsh environments X-ray diffraction is unique in its ability to monitor (at the atomic scale) the surface structure of materials under real-world processing conditions [18]. Such measurements will become increasingly important in future studies, where the opportunity to close the 'pressure gap'

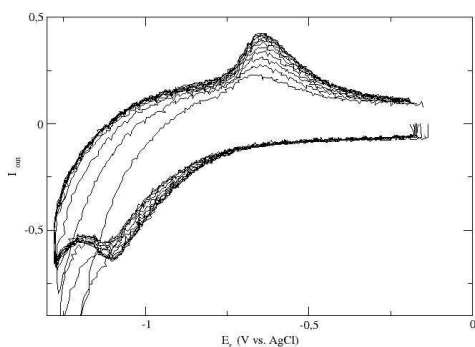
will be taken and the true processes that occur in industry will be probed, in contrast to the artificial



environments of many research studies. In addition to ultrahigh vacuum molecular beam epitaxy (MBE), processes that could be studied by this technique include metal-organic chemical vapour deposition (MOCVD) or laser ablation. These are much more prominent in technological applications because of the more rapid growth rates and more easily achieved sample environments. Some investigations at the ESRF of samples held under high gas pressures have shown the creation of microfacets at elevated pressures and temperatures. Therefore, in addition to the growth opportunities in these environments, the study of important catalytic systems (e.g. ammonia synthesis over iron) under real operating conditions will be possible.

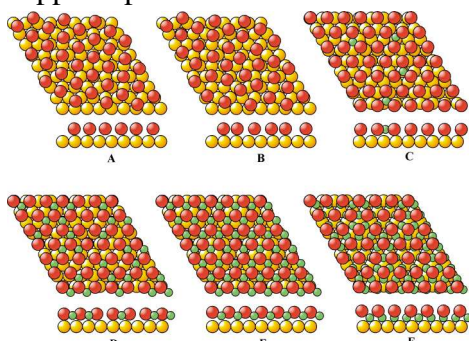
C. Solid-liquid interfaces: Electrochemistry

X-rays are able to penetrate through matter and probe the interface of interest, even in buried environments such as at the liquid-solid interface. Experiments that would exploit this feature include the study of crystalline monolayers physisorbed from multicomponent solutions onto solid substrates. Such single crystal studies improve on powder diffraction methods as the commensurate nature of the interface can be probed. The type of materials that may be studied includes liquid crystalline elastomers that combine the liquid crystal ordering within a polymeric elastomer matrix. This coupling of properties leads to some unique effects, such as 'soft elasticity' and spontaneous thermal shape changes [19].



Other research interests focus on the properties of the solid-liquid interface, and in particular between surface-adsorbed species, for example adsorbed or grafted polymers, and the interactions due to the presence of liquid layering at surfaces. This includes the way that they modify the normal interactions between surfaces, such as in colloidal stabilization by steric interactions [20]. In addition, there is interest in the dynamic behavior of molecular species -both polymers and simple liquids- when they are confined by solid impermeable surfaces to gaps of molecular dimensions. These dynamic properties are of particular importance for effects such as friction and lubrication.

Another important scientific area that relies on studies of the interface between a solid and a liquid is electrochemistry [21]. In this case, the changes in the solid-liquid interface are controlled by the applied potential. One of the most important cases is the deposit of layers or multilayers of metals or



Changes in the structure of a single Copper monolayer onto Au (111) in presence of Br- as dopant induced by the electrochemical potential

other compounds, in a process that can be considered analogous to the ordered reconstructions that occur in samples grown by molecular beam epitaxy (MBE). The high flux and careful cell design would allow the real-time study of deposition process. These studies are very useful in order to obtain tailored surfaces with very specific properties. Another important advantage of the X-rays is that they can monitor the interface during an electrocatalytic reaction, such as hydrogen oxidation, oxygen reduction, carbon monoxide adsorption and oxidation, oxide formation ..., reactions that are very important in fuel cell technology and corrosion.

D. Langmuir Blodgett films

Following the realization of Lord Rayleigh that a film of oil on water was just one molecule thick. Langmuir demonstrated that monolayers of fatty acids could be ordered on the water surface by application of lateral pressure, which triggers phase changes from a gaseous state of non interacting molecules to a "solid like" state, where the molecules interact in a rigid film. Langmuir and Blodgett demonstrated the transfer of such monolayers from the water surface to a solid substrate by slowly passing an appropriately treated substrate through the air/water interface. Films may be picked up on passing several times from air into water and vice versa, the so called Y type deposition, only on passing from water to air, Z type deposition, and on immersion from air into the water only, X type deposition. Therefore producing distinctive head to head, or head to tail, orientations of the amphiphilic molecules in a well ordered multilayer structure.

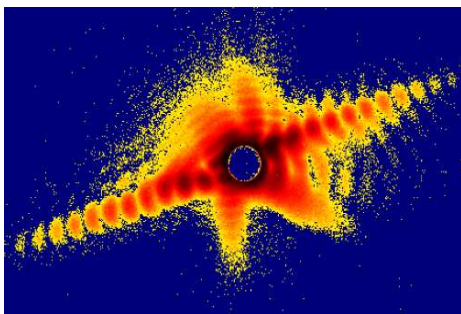
The Langmuir-Blodgett technique has demonstrated its ability to form quantum wells from organic molecules appropriately chemically-engineered to provide both a conjugated region of high electron affinity, the well, and aliphatic sidegroups, the tunneling barriers, which also act to provide the conjugated molecular constituent with its amphiphilic (hydrophobic and hydrophylic) components. Many of such molecules have been spread as Langmuir films on a subphase, and subsequently deposited on substrates as Langmuir Blodgett multilayers [22].

Control of the transfer of charge through multilayer structures offers the possibility of achieving an increase in the density of information storage, in at least one dimension, down to molecular dimensions. The presence or absence of charge in a molecular layer, that forms part of a multilayer produced by the Langmuir Blodgett technique, represents a one or zero of binary logic [23].

2.3. Opportunities with Coherence and Microbeam

The use of X-rays in diffraction has conventionally yielded the average structure of the ensemble, where the coherence length of the domains on the sample is inversely related to the width of the diffraction peaks. In such measurements, the coherence of the x-ray beam has not been a dominant factor. The advent of new-generation synchrotron sources with low source dimensions and the use of narrow bandpass insertion devices, now ensures that x-ray diffraction with coherent beams will open up a whole new range of studies. The potential of using a coherent source of x-rays in diffraction experiments has only recently been realised with some preliminary experiments carried out at the European Synchrotron Radiation Facility (ESRF) and the Advanced Photon Source (APS). Several types of measurements and analysis have been identified including the reconstruction of the shape of nanocrystals due to oversampling [24] and the determination of dynamical processes by observation of x-ray speckle [25]. The first of these requires that the size of the coherent beam closely matches that of the crystal, resulting in diffraction features with fringes arising from facets. The 'phase problem' usually associated with x-ray diffraction is overcome, as the pattern is oversampled by more than a factor of two relative to the Nyquist frequency. Inversion is therefore possible to produce a two-dimensional projection of the crystal shape.

X-ray speckle (also known as X-ray photon correlation spectroscopy) is a very powerful probe of dynamic interactions occurring within the volume of the coherent x-rays, and potentially on the microsecond timescale. It could provide detailed information on many processes including thermal roughening, evolution of growing surfaces, diffusion effects, grain boundary motion or nanocluster formation. X-ray speckle studies have attracted significant interest at 3rd generation synchrotron sources, such as the Troika facility (ID10) at the ESRF.



The feasibility of using microbeam techniques at Alba to produce a well-defined beam will ensure an extension to the range of samples that can be studied. This will include measurements of materials where the arrangement of atoms is more disordered, such as in 'real' environments like toxic atmosphere of a MOCVD reactor, in structures grown by laser ablation or in various adsorbates including biomolecules. The production of ordered nanocrystals (self assembly of nanoparticles into micron sized domains) would greatly benefit from the microbeta source option.

2.4. Analysis Techniques

Analysis of surface diffraction data has conventionally proceeded by a trial and error model refinement process, requiring a significant amount of user intervention. Such analysis can be prone to bias, and generally it is difficult to reach a globally minimised solution. Determination of surface arrangements from X-ray diffraction data is therefore frequently achieved by using a model suggested from other evidence (e.g. STM). This is unsatisfactory, not least because two different surfaces (and preparations) are involved. On the other hand, solving the structure of a surface without reference to a model, using conventional crystallographic techniques is difficult because the weak surface scattering is subject to greater error and can be dominated by the bulk. *Direct methods* extrapolate and refine phases from either a small basis set, or use a large set with random initial phases [26]. They work only if the data set is complete, free from large systematic errors in the diffraction intensities and if the structure is not too large.

Two alternative techniques may enable a more automated approach to the analysis. The first uses a Monte-Carlo (or Reverse Monte-Carlo) mechanism to invoke randomised parameter selection and change together with acceptance of a certain proportion of poor moves to jump out of local minima. The second maximum entropy (ME) method offers an alternative approach [27] and has been applied successfully to Si(7×7) and TiO₂. The formalism offers the following advantages over conventional methods

- It is robust with respect to data errors and uses the variances of the diffraction intensities in an active way.
- Bulk surface information can be incorporated.
- Likelihood estimates allow symmetry ambiguities to be resolved.
- The data need not be complete, that is reciprocal space need not be fully sampled.
- Partial structures can be used and developed.
- Likelihood allows incorrect models to be discarded.

Although this technique has many and proved capabilities, and the range of potential users is very broad due to its multidisciplinary character of this technique, the lack of opportunities of the spanish community to have access to this facility makes that it is a not as extended as it should be. In order to stimulate its use, we propose to extend the data analysis software (making it more user friendly) and to promote the access to this technique to new spanish users. This last point can be achieved thanks to some groups initiative. The general services of the UAM (Universidad Autónoma de Madrid) has placed a surface goniometer on a rotate anode that can be a starting point for some of this groups. This initial research can help these new groups to write beamtime proposals for the SPLINE (ESRF) beamline. These points should be developed during the next years in order to prepare and extend the real users community.

2.5. Expected Scientific and Technological Impact

The many different materials and processes that may be grouped under the label of ‘nanoscience’ will be important technologies in the 21st century. Key to these studies are techniques that can be

used to determine the structure at the atomic level. X-ray diffraction from such low-dimensional systems will play a crucial role in advancing these materials. This station will become the core beamlines in this area through the application of diffraction measurements to a range of *in-situ* environments.

The significance of low-dimensional systems has been recognised by a number of key institutions including the nanotechnology programme of the American government and its incorporation as a priority research area in the European Union Framework 6 programme (beginning 2003). The area of nanomaterials was recently highlighted in a report on international perceptions in Physics and Astronomy in Spain as being of ‘growing importance’ and with ‘the potential for wealth generation and new and exciting science’. The access to this technique should allow to study the behaviour of complex systems: for example, the structure and dynamics of aqueous solutions, ionic liquids, and polymers at interfaces; work in these areas could make spanish group to be competitive internationally. The UK department of health published a report entitled ‘R&D priorities for Biomaterials and Implants’ that highlighted the role that ceramic materials may play. In particular, the potential for thin film bioceramic coatings with specific chemical, structural or nanoscale topographical features is now of great interest to the medical implant device industry. Additionally the materials panel of the UK foresight exercise identified biomaterials as a high priority area, stating that ‘biomaterials are essential constituents of many medical devices that are used in direct contact with the body and the clinical performance of these devices is often related to the biomaterial properties’ [28]. The DTI sponsored initiative, ‘Building up Biomaterials’ also highlights this area and the requirement for methods to characterise biomaterials and their interfacial properties [29].

2.6. Alternative Sources

Surface X-ray diffraction facilities exist at every high energy synchrotron source around the world, including the ESRF, APS and SPring-8. The beamlines have tended to be designed to give a high flux of hard X-rays (typically 15keV) to study ordered reconstructions on single crystal samples. Access to such facilities is, however, limited due to the many international groups active in this research area. Typically, Spanish users may expect 1-2 weeks per year on such facilities. This access limits the type of experiments that can be carried out, and the studies tend to be ‘safe’ ones where success is almost guaranteed. Although this is a worthy goal, many of the most important and groundbreaking studies in this area have been made through longer coordinated experiments. One beamline (34-ID) is being developed at the APS to concentrate on coherent x-ray diffraction (CXD) [30]. However, this facility is being added to an existing station, and the range of environmental enclosures will be limited in size.

The beamline here proposed will be designed using a fully integrated approach that will encompass the entire beamline, optics, end station, sample chambers [32], detectors and analysis techniques. High energy X-rays (up to 24keV) can be produced on a medium energy source such as Alba through careful selection of the insertion device. This is likely to have consequences for the

coherence of the beam, although the quality of the source will still allow coherent diffraction studies to be made. The incorporation of microbeam source will also allow small domains to be studied on the surface, although new measurement techniques will need to be developed to compensate for the sphere of confusion of the diffractometers. Wide access for the Spanish researchers to the facility will be a key component in ensuring the success of the beamline, enabling more coordinated experiments to be undertaken, which perhaps cannot be performed elsewhere.

2.7. Beneficiaries

Beneficiaries of this facility would include the number of leading scientists working in the important fundamental areas that are associated with low-dimensional systems. The programme described above also includes enabling science that supports industrial research in the following sectors: electronics (inc. semiconductor devices), catalysis, visual displays, gas sensing, molecular electronics, polymer processing, coatings and lubricants, medical implants, biosensing and corrosion protection. Additionally studies relevant to environmental and biomedical problems will be made.

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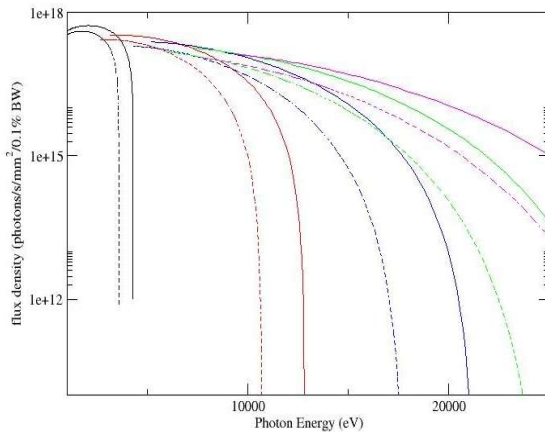
3- BEAMLIN MAIN REQUIREMENTS:

1. The beamline should be provided with a goniometer for x-ray diffraction which should have the adequate geometry to allow x-ray diffraction of material deposited on substrate. Thus, the sample surface should have a fix geometry with respect to the beam.
2. The goniometer should be open enough to install different sample environments without restrictions in the reciprocal space. These sample environments should be provided at the beamline: electrochemical cell, liquid recipe for lagmuir blodgett, furnace and cryostat, UHV deposition chamber.
3. In order to a better use of the beam divergence the goniometer should be able to easily work in vertical or horizontal configurations without restriction in reciprocal space. Vertical configuration is good when a high spacial resolution perpendicular to the surface substrate is required, or when it is not possible to set the substrate surface perpendicular to the floor (liquids, electrochemical, polymers, etc)
4. The detector arm of the goniometer should have a combination of slits+crystal analyser+NaI-scintillator mounted on a circle, to avoid diffracted beam intersection problems.
5. The beamline should have a 2D detector mounted on a mobile bank with the possibility of moving in the vertical direction, for improving the active area to study the nanostructures. It should be interesting to reach the 10Å to 1000Å range.
6. The beamline design should consider the possibility of insertion of a quarter-wave film before the sample, and a polarization analyser between sample and detector to allow magnetic diffraction experiments of the magnetic deposited materials.
7. The goniometer should be able to place high magnetic fields.
8. The beamline should have tunable energy. It is important to reach a high energy range to decrease the water absorption problem.
9. As the magnetic answer is proportional to f'' it should be necessary a large energy range to be sensitive to a large amount of materials. A range from 4.5keV to 24keV should be desirable, to reach the L edges from the element higher than $Z=53$ and the K edge of the lower elements, without the windowless problems
10. The energy precision should be of $\Delta\lambda/\lambda=10^{-4}$.
11. The beamline should have a high flux density (5×10^{17} photons/s/mm²/0.1% BW) and low divergence (to make compatible the high resolution and the high real space resolution needs for some nanostructured systems).
12. Beam size at the sample should be as small as possible without loosing the reciprocal space resolution and the beam coherence. Ideal size on the sample should be 100 x 20 micrometers (or smaller). With smaller beams, some corrections to the raw data, as area correction, are easier.

4- BEAMLIN SET-UP:

4.1- Source

The source has to deliver x-ray photons within the 4.5-24 keV energy range to fulfill the scientific



purposes of the beamline. The definitive insertion device should be studied taking into account the final synchrotron machine characteristics. However an in vacuum U20 undulator (continuous lines in figure) could, in principle, fix the desired energy range (better than an in vacuum U24 undulator dashed lines in figure). Due to the small gap needed, this undulator should work under vacuum and placed in a 4m short section of CELLS. The section is defined by its characteristic micro beta divergence source.

The total power of the U20 is estimated to 4kW. This could induce heat load problems on the monochromator. The choice of the cooling system should be studied. A water cooling system is better for stability, but it could be not efficient enough at low energy (high absorption, large incident angle). In any case, a polished and defect-free diamond window located before the first mirror (equipped with a nitrogen cooling system) could remove low energies from the white beam, without decreasing the degree of coherence of the beam and its stability.

Besides, it is important to use very few Be windows on the beam path, to reach the low energy range required (4.5keV).

4.2. Optics

Although the beamline design is not completed yet, a good starting point is the widespread 3/1 demagnification geometry, in which the monochromator to source, and monochromator to sample distances satisfy a 3/1 ratio.

The three main elements of the optics are:

- A first vertically focusing mirror, located 2 m before the monochromator; 30 cm long, about 10 cm wide, water-cooled with 3 tracks: Si, Rh and Pt to cover the full energy range.
- 2 double Si(111) and Si(311) monochromators with a sagittally-curved second crystal and water-cooled first crystal.
- A second mirror similar to the first one, without any cooling.

4.2.1. Mirrors

The mirrors act as low pass energy filters (removing high energy harmonics) by using the reflectivity properties of the metal deposited on the tracks. The first mirror is placed before the monochromator in order to reduce the heat load on the monochromator. This mirror should have meridional focusing to decrease the vertical beam divergence along the beamline. The second mirror will be placed 2m after the monochromator. Both mirrors will be removable.

However, the beam properties (shape, homogeneity) is very sensitive to the quality of the optics: local deviation of the curvature along the mirror or bad surface roughness can strongly affect the beam shape and its homogeneity. Since we want to preserve the quality of the source, short optics are proposed. The advantages of this solution are:

- To cool down the optics more easily and achieve a high thermal stability over a long period of time.
- To decrease the surface roughness in order to improve the degree of coherence and the homogeneity of the beam.
- To allow a constant radius of curvature which guarantees a single image of the source.

A wide energy range will be covered thanks to the 2 tracks of the 2 mirrors (Si and Rh). The use of the 2 tracks will be as follows:

- Si track for energies less than 15 keV ($\alpha_c^{\text{Si}} = 2 \text{ mrad}$ at $E = 15 \text{ keV}$)
- Rh track for energies less than 24 keV ($\alpha_c^{\text{Rh}} = 2.7 \text{ mrad}$ at $E = 24 \text{ keV}$)

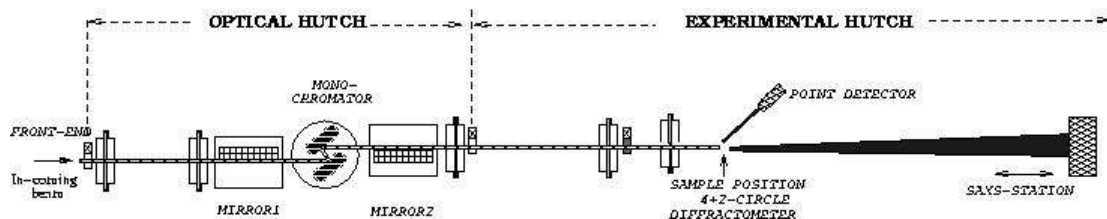
4.2.2.- Monochromator

The monochromator will be located at 27 m from the source. For energies less than 20 keV, two double Si (111) crystals will be used with a sagittally-curved second crystal to achieve the horizontal focusing. For higher energies, a Si (311) crystal can be used in case of high flux requirements. Thanks to the diamond filter (removable), a water-cooling system should be sufficient to evacuate the heat load, which is mainly due to the low energies. We think this would avoid the thermal instabilities due to a nitrogen-cooling system.

4.3. Experimental station set-up

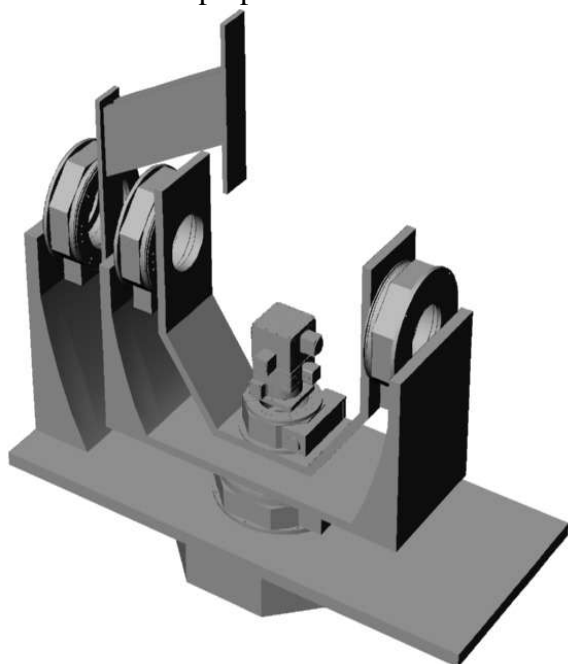
This preliminary beamline setup is based on the hypothesis of around 50m long beamline, where the distance source-wall is 15.5m. With a 3:1 geometry, the optics placed at 27m would give a focusing distance of 9m at which it should be placed the goniometer. Note that the definition of the optics element is, at this moment, not finalized by calculations, and the exact placement of the instruments is only tentative. This calculation should also specify the available final flux. A separated preparation room will be necessary, for the beamline control.

An sketch of the beamline is shown here below:



4.3.1.- Goniometer

The proposed goniometer is a tentative design which recovers all the instrumental requirements needs for the scientific aims proposed at this project. It has the 2-circle freedom for the detector arm. The detector arm of the goniometer should have a combination of slits+crystal analyser+ NaI-scintillator mounted on a circle to avoid diffracted beam intersection problems. In order to a better use of the beam divergence the goniometer should be able to easily work in vertical or horizontal configuration without restriction in reciprocal space. Vertical configuration is good when a high spacial resolution perpendicular to the surface substrate is required, or when it is not possible to set the substrate surface perpendicular to the floor (liquids, electrochemical, polymers, etc). The



goniometer should be open enough to install different sample environments without restrictions in the reciprocal space. These samples environment should be provided at the beamline: electrochemical cell, liquid house for Lagmuir Blodgett, furnace and cryostat, UHV deposition chamber. The spatial resolution would be of (+/- .002 r.l.u.) as maximum. The motor speed should be optimized in order to reduce the travelling times. The maximum time should be set at 60 second per each complete motor turn.

4.3.2.- 2D detector

Following the improvement of synchrotron sources, detectors have shown since the 90s an important evolution. X-ray detectors made of CCD cameras are now the state of the art and will gradually replace "image plates" or gas detectors for many applications. However, if these cameras appear as a real progress and are now widely used in laboratories or at synchrotron for protein crystallography, they do not fulfill all requirements due to their limited dynamical range, their saturation and blooming, and the required demagnification optic.

New detectors are currently developed using hybrid pixels: they consist in a detector in which incoming photons are directly converted to electron clouds associated to dedicated electronic chips. Such detectors are characterized by energy discrimination and wide dynamical range (10^6 photon/s/pixel). As no mechanical shutter is needed, these detector arrays can be used for real time experiments in the millisecond range.

The beamline should have a 2D detector mounted on a mobile bank with the possibility of moving

in the vertical direction for improving the active area to study the nanostructures. It should be interesting to reach the 10Å to 1000Å range.

4.3.3.-Magnetic and chiral scattering devices

The incident linear polarized radiation can be converted into circular polarization using a quarter phase plate. This technique is the only way to look at highly anisotropic magnetic materials for which the direction of the sample magnetization cannot be reversed. The plate assembly is situated upstream of the diffractometer. The diamond crystal is mounted on a Huber goniometer and should be driven to the quarter wave condition with two circles. The rotation stage which moves the crystal to the Bragg condition, should have an accuracy of 10^{-4} degrees. Orthogonally mounted to this circle a second circle should be placed to set the optical axis of the diamond at 45 degrees to the incident and plane polarization with an accuracy of ± 10 arcseconds. These two circles are positioned upon two translation stages giving horizontal and vertical adjustment within 10µm.

A polarization analyzer could be placed at the detector arm to complete the magnetic scattering set-up. This set-up is fully suitable for detecting the change in the x-ray beam polarization induced by the scattering of chiral structures.

5. ESTIMATED BEAMLINER COSTS

	Price (in k€)
Source	
Insertion device + front-end	190
Beamline & Optics	
Other equipment (Slits cooled + flight tubes + pumps + etc)	390
Mirrors and Mechanisms	305
Monochromator System	230
Infrastructure	
Hutches+fluide+wiring+Safety	480
Experiment	
Multi-axis Diffractometer (with analysers)	530
Sample environments	155
Detectors	350
SAXS table+tube	190
Magnetic scattering devices	60
Total	2880

ANEXE I. USERS:

I.1 Project Supporting Scientist.

An extensive list of publications of the spanish scientific community in the topics related with this beamline will be too long (more than four hundred) for being listed in this document. In fact, some relevant publications has been included as reference in the description of the scientific cases. It is important to notice that some of the project proposers have a large experience in similar beamlines not only as users but also as beamline scientist. Their compromise to have an active participation as well in the design as in the beamline construction under requirements of the ALBA scientist warranties the implication of the supporting and potentials users in the beamline development.

Dr M.J. Capitán Aranda	Inst. Estructura de la Materia	CSIC
Dr. J. Álvarez Alonso	Dpto. Física de la Materia Cond.	UAM
Dr. J. J. de Miguel Llorente	Dpto. Física de la Materia Cond.	UAM
Dr. X. Torrelles Albareda	Ins. Ciencias de Materiales Barcelona	CSIC
Dr. Enrique Herrero	Dpto. Química Física	Univ. Alicante
Prof. Juan M. Feliú	Dpto. Química Física	Univ. Alicante
Dr. Alfonso Cebollada	Inst. de Microelectrónica de Madrid	CSIC
Dr. Jorge M. Martínez	Inst. de Microelectrónica de Madrid	CSIC
Dr. Miguel A. Rodríguez Pérez	Dpto. Física de la Materia Condensada	Univ. Valladolid
Prof. José A. de Saja Sáenz	Dpto. Física de la Materia Condensada	Univ. Valladolid
Dr. Rafael Andreu Fondacabe	Dpto. Química Física	Univ. Sevilla
Dr. Juan J. Calvente Pacheco	Dpto. Química Física	Univ. Sevilla
Prof. Enrique Fatás	Dpto. Química Física	UAM
Dr. Concepción Alonso	Dpto. Química Física	UAM
Dr. Miguel Clemente	Inst. Ciencia Molecular	Univ. Valencia
Dr. Javier Díaz	Dpto. Física de la Materia Condensada	Univ. Oviedo
Prof. Fausto Sanz	Dpto. Química Física	Univ. Barcelona
Dr. Mercedes Perez-Mendez	Inst. de Polímeros	CSIC
Dr. Julio Camarero de Diego	Dpto. Física de la Materia Condensada	UAM
Dr. Germán Castro	Inst. de C. Materiales de Madrid (SPLINE)	CSIC (ESRF)
Dr. Jose A. Martín Gago	Inst. de C. Materiales de Madrid	CSIC
Dr. Maria F. Lopez	Inst. de C. Materiales de Madrid	CSIC
Dr. Maria Alonso	Inst. de C. Materiales de Madrid	CSIC
Dr. F. Pigazo	Inst. de C. Materiales de Madrid	CSIC
Dr. F. Javier Palomares	Inst. de C. Materiales de Madrid	CSIC
Dr. Carlos Prieto	Inst. de C. Materiales de Madrid	CSIC
Dr. Alicia de Andrés	Inst. de C. Materiales de Madrid	CSIC
Dr. Esther Barrena	Max-Planck-Institut für Metallforschung	Stuttgart
Dr. Carmen Ocal Moncayo	Ints. de C. Materiales de Madrid	CSIC
Prof. Federico Soria	Inst. de C. Materiales de Madrid	CSIC
Dr. M. Eugenia Dávila Benítez	Inst. de C. Materiales de Madrid	CSIC

Dr. Juan de la Figuera Ballón	Dpto. Física de la Materia Condensada	UAM
Prof. Rodolfo Miranda Soriano	Dpto. Física de la Materia Condensada	UAM
Dr. Amadeo L.V. de Parga	Dpto. Física de la Materia Condensada	UAM
Dr. Leonardo Soriano	Dpto. Física Aplicada	UAM
Dr. Juan José Hinarejos Murillo	Dpto. Física Materia Condensada	UAM
Prof. Clara Conde	Dpto. Física de la Materia Condensada	Univ. Sevilla
Dr. M ^a Ángeles Gómez Rodríg.	Ints. Ciencia y Tecnología de Polímeros	CSIC

I.2 Potential users:

This is a non exhaustive study about the Spanish potential users. There are other research groups within the Catalysis, Biophysic, Medical, etc fields that are not recorded here due to the huge community list that should implies.

A. Nanostructures.

It can be consulted the web pages: <http://www.nanospain.org/nanospain.htm>, that coordinates the research in nanoscience in Spain

Instituto de Microelectrónica de Madrid	CSIC-Madrid
Centro Nacional de Microelectrónica	CSIC-Barcelona
Instituto de Microelectrónica de Sevilla	CSIC-Sevilla
Dpto. Nanociencia Molecular y Materiales orgánicos	Inst. Cien. Mat.-Barcelona-CSIC
Nanoestructuras en superficies	Unv. Autonoma Madrid-CSIC
Grupo procesado técnicas láser	Inst. óptica CSIC.
Propiedades de transportes, ópticas y magnéticas	Inst. Ciencias Mat. Madrid-CSIC
Lab. Nanotecnología Aplicada	Univ. politécnica de Cartagena
Lab. Magnetoópticas y láminas delgadas	Univ. Oviedo
Ing. Física y de Superficies	Ins. Ciencias Materiales Madrid-CSIC
Dpto. Óptica	Univ. Complutense de Madrid
Dpto. Física Materia Condensada	Univ. Autónoma Madrid
Ing. Química y de Alta presión	Univ. Valladolid
Fac. Farmacia	Univ. Santiago de Compostela
Dpto. Física teórica y atómica molecular y nuclear	Univ. Valladolid
Dpto. Ingeniería electrónica	Univ. Autónoma Barcelona
Fac. Física- Dpto. ECM	Univ. Barcelona
Física de Bajas temperaturas	Inst. Ciencias Materales Aragón
Ciencias experimentales	Univ. Jaume I
Farmacia y tecnologia farmaceutica	Univ. Navarra
Dpto. Física Aplicada	Univ. Politénica de Cataluña
Inst. de sistemas optoelectrónicos y microtecnologia	Univ. Politénica de Madrid
Física de Materiales	Univ. Autónoma de Madrid
Física Aplicada	Univ. Castilla la Mancha
Física Aplicada	Univ. de Vigo
Dpto. Física	Univ. de Murcia
Catálisis Aplicada	Inst. Catálisis y Petroquímica- Madrid-CSIC
Ins. Ciencia Molecular	Univ. Valencia

Dpto. Física	Univ. Carlos III
Grupo propiedades mecánicas de sólidos	Univ. Sevilla
Dpto. Física de Materiales	C. Internacional de física de donostia CSIC-UPV
Genética molecular	Inst. Biología molecular- Barcelona-CSIC
Lab. Magnetismo	Univ. Cantabria.
Grupo Magnetismo y mat. magneticos	Universidad del País Vasco
Materiales Porosos Funcionales	Inst. Nac. del Carbón CSIC
Electrónica y tecnología de Computadores	Univ. Granada
Espectroscopia vibracional y procesos multif.	Inst. Estructura de la Materia-CSIC
Grupo de electrónica	Univ. Salamanca
Física Aplicada	Univ. Autónoma Madrid
Inst. Magnetismo Aplicado	Univ. Complutense Madrid
Combustibles Fósiles	CIEMAT-CSIC
Centro de innovación en biotecnología	Univ. Rovira y Virgili
Conservación y Calidad de los alimentos	Inst. Agroquímica y tecnología de alimentos
Estructura de Macromoléculas	Centro Nacional de Biotecnología-CSIC
Ciencia y tecnología del medio ambiente	Univ. Católica de Avila
Dpto. Materiales	C. de estudios e Inv. Tecnocas de Guipuzcoa
Centro de Inv. y desarrollo de la Armada	Ministerio de Defensa
Física Aplicada	Univ. Alicante
Química Bioorgánica	Inst. Investigaciones Químicas-CSIC
Química Analítica supramolecular	Univ. Córdoba
Dpto. Física	Univ. Publica de Navarra
Unidad de Aplicaciones de nanomateriales	Fundación Labein
Área de longitud	C. Español de Metrología
Dpto de Láser e Imagen	Asociación indus. de óptica, color e imagen
C. Ingeniería Avanzada de superficies	Asociación de la Industria Navarra
C. de Investigaciones en bioelectrónica y nanobiociencia	Parque Científico de Barcelona
Ingeniería Química y tecnol. del Medio Ambiente	Univ. Zaragoza
Dpto. tecnología de surfactantes	Inst. Inves. químicas y ambientales de Barcelona
Dpto. Química Orgánica	Univ. Autónoma de Madrid
Inst. Biología Molecular y Celular	Univ. Miguel Hernández
Química Macromolecular	Univ. del País Vasco

B. Polymers.

The spanish groups that works into this field and could profit of the science developed in this beamline, thus could be considered as potential users can be found in the web pages: <http://www.ucm.es/info/rsequim/gep/> (PRESIDENTE: Dr. José Manuel Pereña Conde, Madrid). In the association there are a total of 157 subscriptions shared in the centers:

Inst. de Ciencia y Tecnología de Polímeros	ICTP-CSIC	www.ictp.csic.es
Instituto de Materiales Poliméricos-POLYMAT	Universidad del País Vasco	www.sc.ehu.es/polymat
Centre Català del Plastic	Univ. Politècnica de Catalunya	www.ucp.edu/ccp
Dpto. Física Macromolecular.	IEM-CSIC	www.iem.csic.es
Esc. Técn. Sup. de Ingen. Indus.	Univ. Politècnica de Madrid	www.etsii.upm.es
Instituto de Estudios Biofuncionales.	Universidad Complutense de Madrid	

Dpto. Química Aplicada	Universidad de Navarra
Dpto. Física Aplicada. (Ferrol)	Universidad da Coruña
Dpto. Química Inorgánica	Universidad de Zaragoza
Dpto. Química Analítica-orgánica	Universidad Pública de Tarragona
Dpto. Química Inorgánica	Universidad de Oviedo
Dpto de Conser. y Calidad de los Alimentos	IATA-CSIC
Dpto. Química Orgánica	Universidad de Alcalá de Henares
Dpto. Física Aplicada	Universidad de Santiago de Compostela
Dpto. Química Física	Universidad Politécnica de Cartagena
Dpto. Física Materia Condensada	Universidad de Valladolid
Dpto. Físico-Química	Universidad San Pablo Ceu
Dpto. Ciencia y Tecnol. Polímeros	Universidad del País Vasco
Dpto. Física Materia Condensada	Universidad de Sevilla
Dpto. Termodinámica Aplicada	Universidad Politécnica de Valencia
Dpto. Química Física	Universidad de Murcia

However, not all these groups works in polymers area are related with thin films polymer field that are the scientific cases described in the present project.

C. Electrochemistry

The Spanish groups that works into this field and could profit of the science developed in this beamline, thus could be considered as potential users can be found in the web pages: <http://www.upct.es/electroquimica/index.htm> (PRESIDENTE: Dr. Toribio Fernández Otero, Cartagena). In the association there are a total of 234 subscriptions shared in the centers:

Dpto. de Química (Electroq)	Univ. Autónoma Madrid
Dpto. de Química Física.	Univ. de Murcia
Dpto. Química Física	Univ. Alicante
Inst. Const. y Cemento	CSIC
Dpto. de Química Física	Univ. Salamanca
Dpto. de Química Física	Univ. Sevilla
Dpto. de Química Física	Univ. Santiago
Área de Química Analítica	Univ. Burgos
Dpto. de Química Física.	Univ. de La Laguna
Dpto. Química Analítica	Univ. del País Vasco
Dpto. de Química Física	Univ. de Córdoba
Dpto. de Ciencia de Materiales	Univ. Complutense Madrid
Dpto. Química Orgánica	Univ. de Alcalá de Henares
Facultad de Ciencias	Univ. de Valladolid
Dpto. de Química Física y Analítica	Univ. de Oviedo
Centro Nac. Invest. Metalrgicas (CENIM)	CSIC
Dpto. de Química Ingeniería	Univ. Barcelona
Facultad de Ciencias	Univ. de Extremadura
E.U. de Formación Profesorado EGB	Univ. de Extremadura
Escuela Politécnica Superior de Alcoy	Univ. Politécnica de Valencia
E. U. Politécnica de Alicante	Univ. Politécnica de Alicante
Inst. de Química Física "Rocasolano"	CSIC
Dpto. de Química Física	Univ. Autónoma de Barcelona

Dpto. de Ciencias Analíticas
 Dpto. Química Orgánica
 S. E. Acumulador
 Centro de Electroquímica y materiales Inteligentes
 Dpto. de Química Física
 Dpto de Ingeniería de la Construcción.
 Lab. Bioquímica y Análisis Clínicos
 E. U. de Ing. Técn. Industrial
 Dpto. de Ingeniería Química
 Dpto. de Química, C-IX
 Dpto. Química Física
 Inst. Energías Renovables CIEMAT
 Dpto. de Física Aplicada C-IV
 Unidade Ciencias Exactas
 Dpto. Enxeria Química

 Facultad de Ciencias.
 Dpto. de Química Fundamental e Industrial
 E. U. Ingeniería Técnica Industrial.
 Dpto. de Ingeniería Química
 Instituto Químico de Sarriá

Univ. Nacional de Educación a Distancia
 Univ. del País Vasco.
 Tudor S.A. Guadalajara
 Univ. Politécnica de Cartagena
 Univ. de Murcia
 Univ. de Alicante.
 Univ. de Oviedo
 Univ. Extremadura
 Univ. Politécnica Cataluña. Barcelona
 Univ. Autónoma de Madrid
 Univ. de Malaga
 CSIC
 Univ. Autónoma de Madrid
 Univ. Algarve
 Univ. Vigo
 IBERCOL,S.L. (Valencia)
 Univ. de Castilla-La Mancha
 Univ. Santiago (La Coruña)
 Univ. Cádiz (Algeciras)
 Univ. Politécnica de Cataluña
 Barcelona

E. Magnetism.

This is a non-exhaustive list of spanish groups working in this scientific field

Group	Contact person	Address
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E. Surfaces and Interfaces

Dpto. de Física de la Materia Condensada.	Univ. Autónoma de Madrid
Dpto. de Física Aplicada	Univ. Autónoma de Madrid
Dpto. Intercaras y Crecimiento	Inst. Ciencias Mat. Madrid-CSIC
Dpto. Física e Ingeniería de Superficies	Inst. Ciencias Materiales Madrid
Dpto. Física de Materiales	Univ. Complutense de Madrid
Grupo Interdisciplinar sistemas complejos	Univ. Complutense de Madrid- Univ. Carlos III Madrid
Dpto. de Superficies e Intercaras	Inst. de Ciencias de Materiales de Sevilla-CSIC
Dpto. Física Aplicada I.	Univ. del País Vasco
Dpto. Cristalografía y química del estado sólido	Inst. Cienc. Mat. Barcelona-CSIC

F. Chiral Molecules.

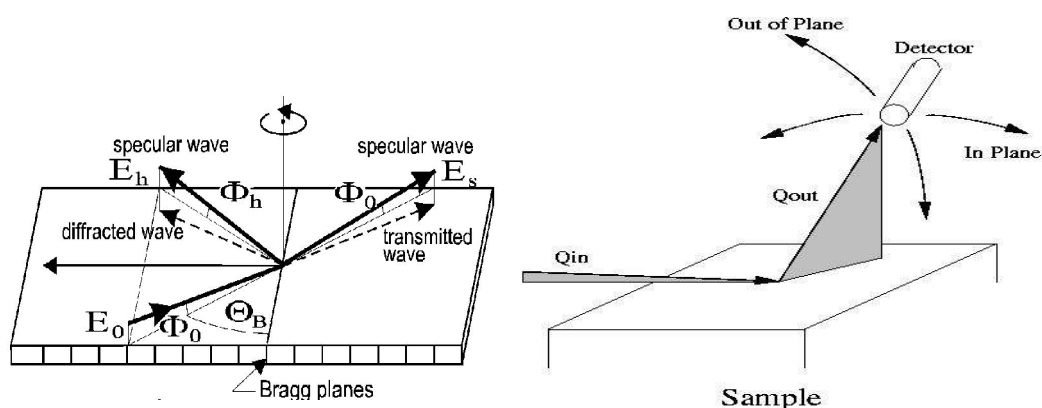
Important research groups can be found all over Spain; a representative but not exhaustive account includes Barcelona (Figueredo, Font, Ortuño, Bosch, Amat), Madrid (Martínez, Vilar, Fraile), Santiago de Compostela (Quinoa, Riguera), Zaragoza (Mayoral), Alicante (Nájera, Yus), Sevilla (Fuentes, Fernández), Oviedo (Gotor), Valladolid (Pedrosa), Tarragona (Claver), Castellón (Carda), Granada (Izquierdo, Plaza), etc.

ANEXE II. TECHNICAL OVERVIEW:

In order to give an idea to future users about the different information that could be obtained in the beamline here proposed, we will briefly describe the different x-ray diffraction techniques pointed out along this proposal:

II.1. Grazing Incidence X-ray Scattering

This corresponds to the more traditional x-ray diffraction techniques which gives information about the atomic structure of the material. The possibility of fixing the incident angle with respect to the substrate surface allows to enhance the diffracted signal coming from the outermost layers. The structural information that it can be obtained depends on the degree of structural dependence that the substrate impose on the deposited film. If there is a high degree of dependence it will correspond to a single crystal film, and the analysis should be like a single crystal but with respect to the substrate. In the more extreme case the study of the scattered signal perpendicular to the surface gives information even about the last atomic layer. If the dependence is medium it should correspond to a powder but with a preferential crystallization growth directions; in that case it should be possible to study in that case the film texture. In the case of no-dependence it should be like a powder film.

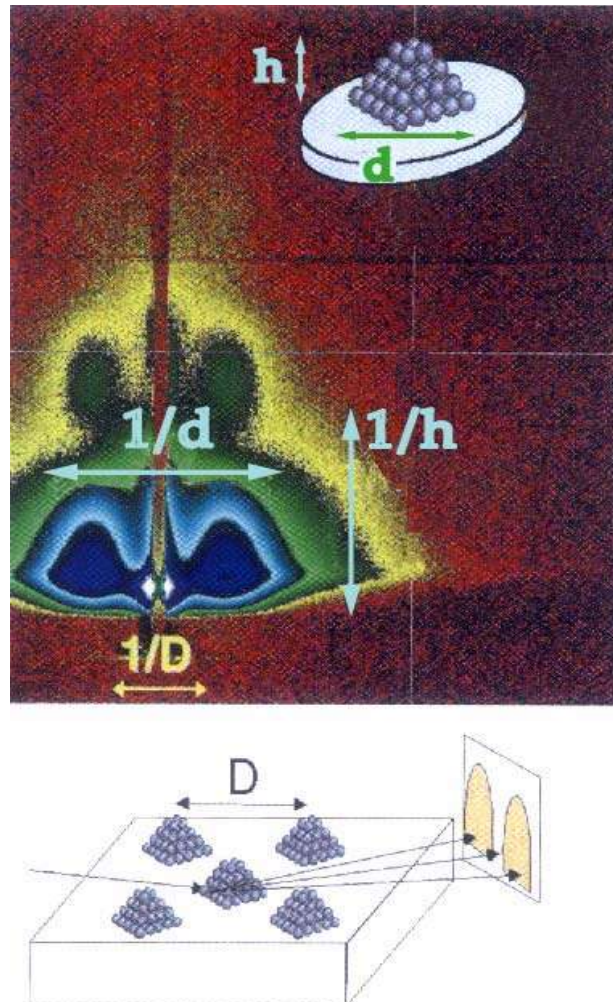


The possibility of tuning the energy in a large energy range (4.5keV to 30keV) should allow to play with the atomic scattering contrast, due to the jump in the atomic scattering factor observed around the absorption edges (Anomalous X-Ray Scattering).

II.2. Grazing Incidence Small Angle Scattering

The Small Angle X-ray Scattering (SAXS) technique is sensitive to heterogeneities in the electron density on a mesoscopic scale ($10\text{-}10^3 \text{ \AA}$), so it is very suitable to the studies of particles distribution study. If the SAXS experiments are carried out at or near the total reflexion of the material (GISAXS) it gives mainly information about the nanostructures at the outermost layers of the material. Thus, it is possible to study nanostructures either deposited on a flat surface, either formed at the surface (quantum dots), or embedded in the matrix of a thin film layer, and it does not require the matrix sample and/or deposit to be crystalline. The 2D diffracted intensity gives information

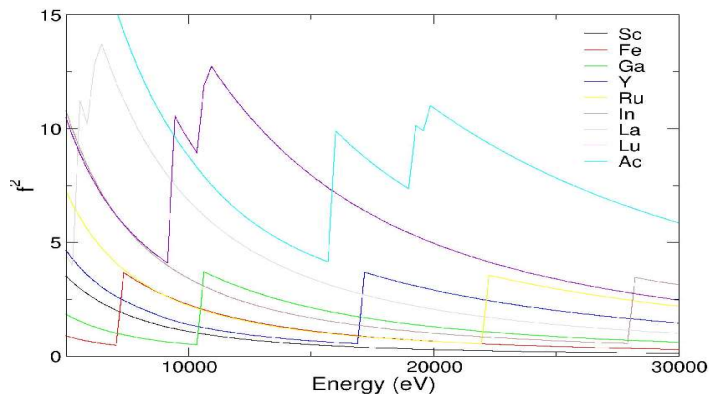
about spatial anisotropic distribution of the objects and their shape as it can be observed in the next figure. To obtain information about the average lateral size, height and separation between islands or the surface quality is straight forward. Thus, it is possible to use this technique to determine *in situ* and in real time the morphology of islands or films under real deposition/evaporation conditions, from the very beginning of the growth.



II.3. Grazing Incidence Magnetic and Chiral Scattering

Significant advancement has been made in the study of fundamental magnetism across the periodic table from the transition metals to the rare-earth compounds and the actinides. These advances have benefited substantially from the development of magnetic x-ray scattering. Traditionally, the technique of choice for the study at an atomic level of detail of magnetic structures, correlations and excitations has been magnetic neutron scattering. Pioneering measurements of non-resonant magnetic x-ray scattering, in 1972 by de Bergevin and Brunel, showed that photons could be used to study magnetic systems. They have shown a change in the intensity of the x-ray diffracted by ferromagnetic or ferrimagnetic material when the external magnetization is reversed. The differences in the x-ray diffracted signal are directly proportional to the atomic factor f^2 . It is important to notice that this atomic factor changes around their absorption edges (see next figure) and this effect is more dramatic at the L-edge. The resonant magnetic scattering profits of this

phenomena to increase the magnetic diffraction signal. Nowadays, the high flux of third generation synchrotron sources makes both resonant or non-resonant x-ray magnetic diffraction techniques routine. However, a beamline with an energy range from 4.5keV to 30keV reaches the L-edge of the atoms with Z higher than 53 and the K edge of the lower ones.



In recent years, there has been significant interest in accessing the magnetic order at surfaces. Given the break in crystal symmetry at the surface one might expect to observe magnetic structures and critical behavior different to those found in the bulk. The experimental difficulty is that the surface charge scattering is typically 5 orders of magnitude weaker than the bulk scattering. For this reason, high brightness synchrotron grazing incidence X-ray scattering techniques are required to characterize the chemical structure of the surface. The magnetic intensity is then further reduced by another 5-6 orders of magnitude and so, one requires the x-ray resonant magnetic scattering enhancement to observe any magnetic contribution from the surface. Such difficult measurements require the flexibility of the beamline and will provide a significant and unique insight into surface magnetic ordering: an area of solid state magnetism that has not yet been exploited.