SU8 beam-line transfer from Super-Aco to Soleil: A low-energy light source for electronic and structural studies in Condensed matter.

ABSTRACT

The present proposal is concerned with the transfer of the SU8 beamline connected to Super-Aco to the Soleil storage ring. During the last three years, this beamline has been operative at LURE covering the needs of a wide Soft X-ray Synchrotron Radiation community in several scientific fields, such as Physics, Chemistry, and Material Science. The well fitted experimental station connected to a high performance beamline, has permitted to carry out alternatively basic and applied research in the area of corrosion, carbon-derived materials, catalysis, polymers, microelectronics, magnetic materials, metallic alloys, superconductors, and new artificial compounds. The electronic structure of solid materials has being deeply studied in the core level and valence band region, together with a complete determination of the Fermi surface topology. Moreover, the electronic studies of materials have been "in situ" habitually completed with structural analyzes using Photoelectron Diffraction and Soft X-Ray absorption. Presently, the whole set-up is restrained because of the low flux, low energy resolution and large source size. However, its installation in a third generation storage ring as Soleil will ensure a natural and successful evolution toward a ultra-high performance and competitive beamline for the incoming years.

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1.- INTRODUCTION

1.1.- Historical evolution of the SU8 beamline at Super-Aco

Since 1991, the current French-Spanish collaboration at LURE has successfully assumed a two fold role in the area of Synchrotron Radiation (SR) activities: i) the reception and care of users and, ii) the development of an in-house scientific research. The initially, highly specialized one-technique beamline was developing its capabilities up to become, nowadays, in a interdisciplinary and high performance beamline (SU8). It has shown to be capable to satisfy the exigencies of a growing European Scientific Community related with the use of low-energy synchrotron radiation. The existence of this beamline has been so far conceived for Spain as the counterpart, in the area of low-energy, to the Spanish participation at the ESRF.

During the past ten years, the well home-fitted end-station connected to Super-Aco has utilized more than 120 runs of available radiation per year. The operation runs have been distributed into three different undulator beamlines (SU6, SU7 initially and lately SU8), depending on the user demands. Every year, more than 90 scientists have performed experiments at the Station. Of these about 80 % came from France and Spain and the rest from Europe (mainly Italy and Germany). The scientific projects cover experiments in solid state physics, surface physics, materials science, chemistry and physical chemistry. Figure 1 shows schematically the geographical localization of the European groups that have contributed to the development of the SU8 beamline and in a direct or indirectly way to the conception of this document.

The SU8 beamline is currently dedicated to the study of the electronic properties of solid systems using integrated Photoemission (PES), Absorption (XAS in detail: NEXAFS) and High-Resolution Angle Resolved Photoelectron Spectroscopy (ARPES). This last technique has been in-house further developed in order to perform studies of Fermi surface topology throughout large portions of the reciprocal space. The instrumentation associated to these basically electronic techniques has been closely linked to those related to a typical structural technique as Photoelectron Diffraction (PED) in its different detection modes (energy and angular scans).

In essence, the SU8 beamline at LURE, has provided light with many useful properties to the experimental scientists. With it, chemists have performed studies of chemical reactivity at a new level of precision, and materials scientists have tackled questions that can lead to new concepts in semiconductor devices. Indeed, due to the specially designed Experimental Station, it has been unique in performing such experiments and plans are afoot in Triste, USA and Switzerland, to build similar facilities in the near future.

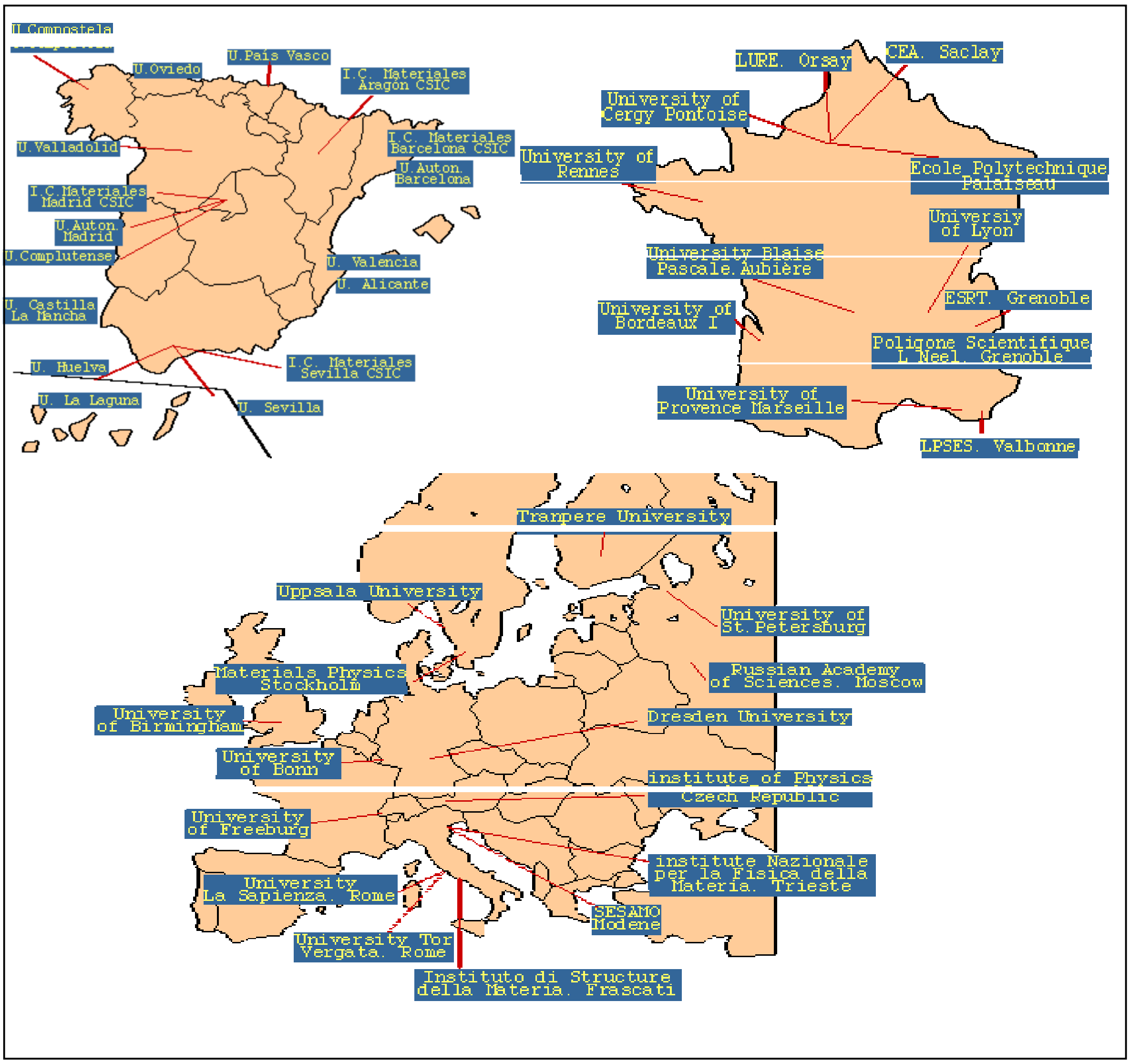

Figure 1. Geographical localisation of the European groups related with the SU8 beamline. One time every two years, most of the Universities and research centres indicated in this figure visit the SU8 beamline at LURE to perform their experiments.

1.2.- Available instrumentation

The existing SU8 beamline is basically constituted by two elements: an undulator-wiggler as a source, which ensure an elevated flux of photons and a high performance varied line spacing (VLS) plane grating monochromator (PGM), in order to ensure a high spectral resolution at the end experimental station. The combination of these two essential elements has provided a source of intense and well-conditioned ultraviolet and soft x-ray radiation, which can range from 16 to 950 eV. The insertion devise has been designed for the beamline taking into account the characteristics of the 800 MeV Super-ACO storage ring of LURE. Its first harmonic is produced around 15 eV and its general characteristics are listed in table I. The possible adaptation at Soleil of this existing insertion device has been considered. The results of this analysis give rise the third scenario described at the end of this proposal.

Technology	Hybrid
Period length	100 mm
Minimum gap	39 mm
Maximum gap	250 mm
Number of periods	21
Total number of full size poles	(21 x 2) x 2
Total number of poles	(22 x 2) x 2
Total length of magnet assemblies	2 200 mm
Average peak field at T = 20 °C	> 0.45 T

TABLE I: Technical specification of the existing insertion devise of the SU8 beamline at Super-Aco

It is important to notice that the existing insertion device is not able to provide variable polarisation and its first harmonic if it is connected to Soleil ring is as high as 65 eV. The optical configuration is defined by a monochromator with six plane holographic gratings and three spherical mirrors inside (see their specifications in the scheme of Figure 2). The nine optical elements of the monochromator can be easily interchangeable under vacuum in order to select the photon energy. In order to keep a high luminosity, the length of the monochromator has been designed larger than 6 m. As pre and post-focusing optics, toroidal mirrors, in astigmatic mode have been chosen, leading to the existing layout of the SU8

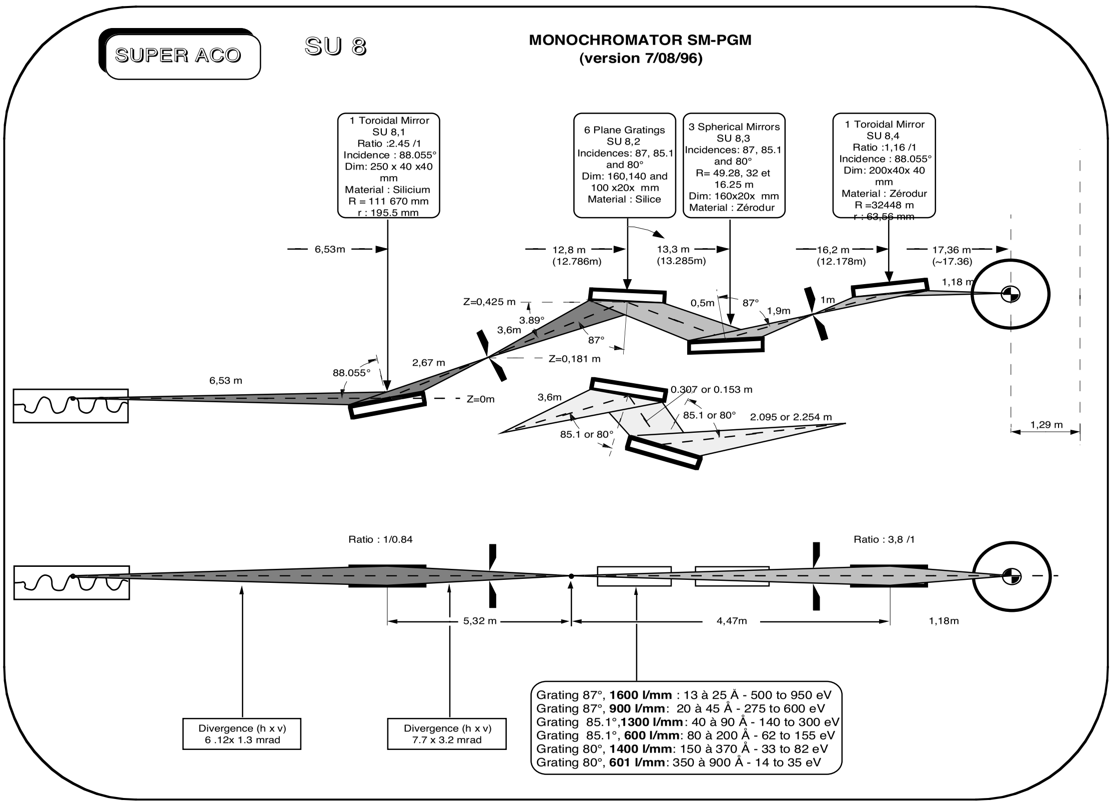

Figure 2. Layout of the SU8 beamline at Super-Aco.

1.3.- User community

The Orsay-Madrid group associated to the SU8 beamline has successfully assumed the role of reception and care of users together with the development of an in-house scientific research. Every year, more than 20 research groups mainly from Europe have performed experiments at the Station. The scientific projects have covered experiments in a wide scientific field. The SU8-beamline group has provided active involvement in the user projects. In particular, they not only have assisted in the evolution and utilization of the specific beamline-developed techniques, but they have in addition act as the primary partner of their scientific projects. For those less skilled SR users, the SU8-staff has provided a close assistance. Figure 3 shows the evolution of number of runs demanded every year in green and the total runs admitted by the international committee, since 1991. We can observe a great increase of demanded runs when the SU8 beam line was available to users, in 1998.

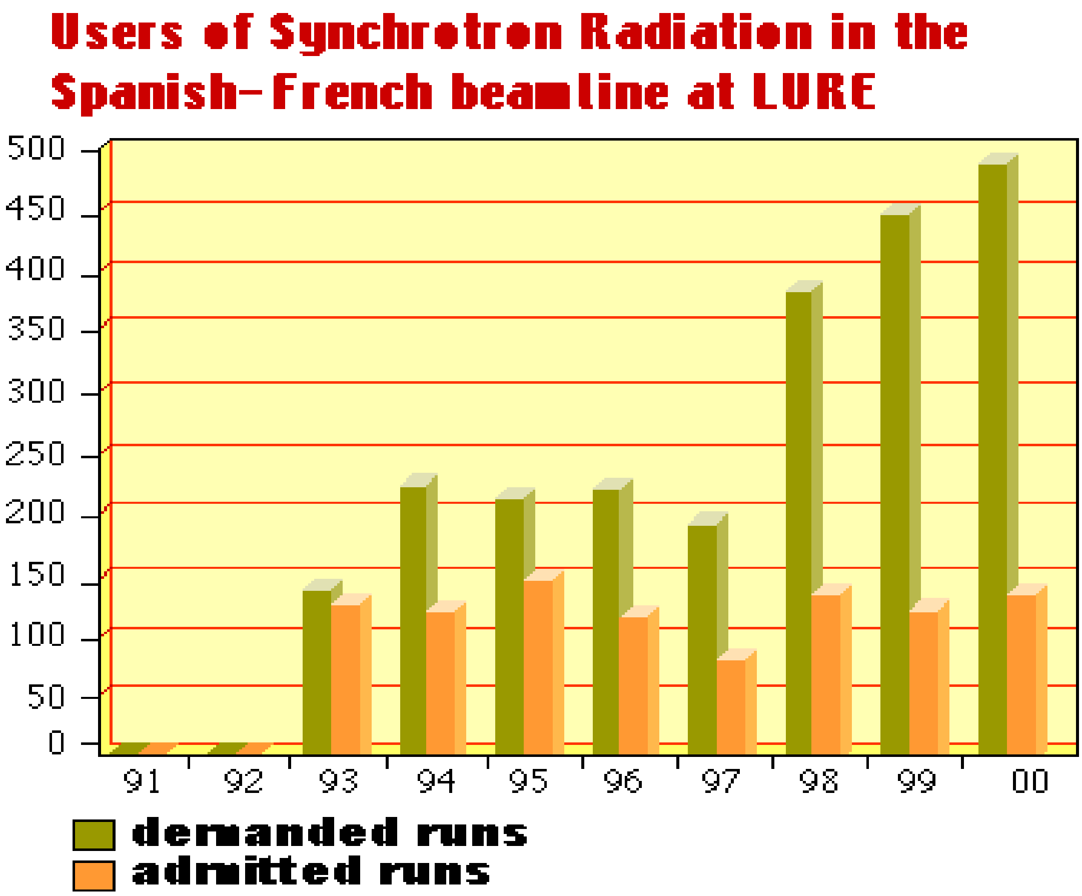

Figure 3. In green the total runs demanded by the scientific community is indicated. Yellow bars show the used runs, which limited by the Synchrotron radiation delivered by Super-Aco, every year.

1.4.- Limitations and needs of the existing set-up

Although, the present beamline is well adapted to the Super-Aco storage ring, it needs to be up-dated in order to be compatible with a 3rd generation storage ring as Soleil. In the second part of this proposal, we will treat specifically all the changes needed, however, at this point, we will list the main limitations to be taken into account:

1.- The insertion device: The undulator may be changed accordingly to the new ring.
2.- The pre- and post-focussing mirrors to collimate the light should be changed.
3.- The refrigeration system should be reinforced in order to support the higher power dissipated by the new source.
4.- One of the grating (the lowest photon energy) should be changed in order to avoid the second order contributions, which will be higher in Soleil than Super-Aco.
5.- The end-station should be modernised.

2.- TRANSFER OF THE SU8 BEAMLINE FROM SUPER-ACO TO SOLEIL. Scientific Case

2.1.- Introduction

The development of SR sources during the last 10-15 years has opened up major new areas of science by creating a high brightness and wide range tunable source of X-rays. This is particularly dramatic in the energy range of the soft X-ray (SXR) and vacuum ultra-violet (VUV) radiation, where almost no useful laboratory sources (continuum or line) are available. Opening up these areas, however, has exposed the need for new high performance beamlines capable to provide substantially higher photon fluxes and spectral resolution at the sample.

In the VUV/SXR spectral range, which for our present purposes we will define as covering photon energies from 15eV to 1000 eV, all experiments can be broadly classified as spectroscopy. An important underlying problem exacerbating the need for the **higher photon fluxes** is the fact that the majority of experiments performed in this spectral region involve the study of very small quantities of matter, often in high state of dilution. In the case of solid state and materials science, much of the interest is in the outermost two or three atomic layers (Surface Science), and even when the object of investigation is the bulk electronic structure, many of the methods of detection (e.g. photoemission) actually probe only the outermost few atomic layers. Added to these small sample masses is the difficulty that many physically important processes have low cross-section.

A basic limitation in many experiments in the VUV/SXR spectral range is therefore the number of the photons at the sample. In many cases, however, there are at least two other related problem; **sample size and spectral resolution**. In most current studies of condensed matter, light spot sizes on the sample have dimensions of order millimetres and it is impossible to investigate any microscopic inhomogeneities. The implied focusing can only be achieved if the photon source is of much increased brilliance. Brilliance can also be of prime significance in making substantial gains in spectral resolution without loss of flux. Major gains are therefore only achievable using **undulator sources** which provide much enhanced brilliance as well as increased usable integrated flux.

Within the broad energy range of 15-1000 eV defined above, it is important to consider the detailed **science/photon energy interrelationship** because, as we shall see bellow, the use of undulator source creates a far stronger relationship between the machine energy and the possible photon energies than is the case for simple bending magnet sources.

As remarked above, the **low energy end of the photon energy** range from 15-50 eV is the one of primary interest in valence electronic level spectroscopy. In the case of studies of solids and surfaces, the most powerful methods of investigation are based on Angle Resolved Photoemission (ARPES), which through the conservation of energy and reduced momentum allows direct E-k band mapping of occupied valence bands. For such studies the minimum energy required to photoemit from a solid correspond to the work function (typically 4-5eV) so the lowest useful energy lies in the range of 5-16 eV. In order to map bands, it is then necessary to vary the final state energy over one or two bulk Brillouin zones, leading to upper useful energies in the 50-150 eV range.

The **upper end of the nominal energy range** (150-1000eV) is of interest mainly for core level studies, particularly, though not exclusively, of solids. Experiments fall into two rather different categories. In one, aimed at the investigation of electronic or "chemical" structure by high resolution core level Photoemission (PES) measurements of "chemical" energy level shifts, or high resolution near edge absorption spectroscopy, the requirement is for high sample flux at high spectral resolution but a fixed, or only narrow range tunable, energies. In the second category, of wide energy range scanning experiments, are EXAFS (Extended X-ray Absorption Fine Structure or SEXAFS for surfaces) and scanned energy mode Photoelectron Diffraction (PED), two techniques aimed at determining local geometrical structure, particularly at surfaces. In both types of experiments a key consideration is the 1s core level binding energies of the elements in the first full row of the periodic table. Higher atomic mass elements all have core levels with binding energies in the 50-500 eV energy range which can be used for at least some such studies. For the first row elements, the 1s level is really the only true core level, and in view of the chemical significance of many of these elements, accessing these levels is of great significance. Of particular note are the 1s levels of C, N and O with binding energies of approximately 280eV, 400eV and 530eV. Near Edge (NEXAFS) studies of these levels can be achieved with photon energies of no more than about 600eV, although EXAFS or photoelectron diffraction from O 1s requires energies up to 800-900eV. Other levels of great interest for electronic structure studies, in the 500-1000eV energy range, include the 2s and 2p (the first p-states!) of the first transition series elements.

In particular, the present and future activities developed at the SU8 beamline cover most of the above mentioned scientific interests. The intense activity carried out during the last few years has involved rather different and complex scientific projects. For that reason, it is almost impossible to describe all the advantages and benefits that they will report if the SU8 beamline could be transferred to Soleil. In the follow then, we will concentrate on a few selected scientific cases, which are closely associated to the more implicated groups concerned with the beamline.

2.2.- Scientific case and new physics associated to the project:

2.2.A.- Angle Resolved Photoemission and Fermi Surface imaging"

If in a simple photoemission (PES) experiment, in addition to measure the kinetic energy of the photoelectrons, it is possible as well, to determine precisely the emission direction, PES becomes in a more complete technique namely, Angle Resolved Photoemission (ARPES). This technique allows measuring the dispersion of the electronic bands as a function of the k vector of the reciprocal space. This is the most direct source of information to characterize the electronic structure of any material.

During the last few years at LURE, the SU8 group has developed an alternative method to the traditional ARUPS, which allows to determine directly contours of the FS of any ordered metallic material. This technique, basically consists in scanning automatically large portions of the reciprocal space at a fixed photoelectron energy. In this way we can record two dimensional images of photoelectrons intensity as a function of the wave vector parallel to the surface. Initially, this technique was used studying bidimensional systems, in which the electronic states do not disperse as a function of the k vector perpendicular to the surface. However, recently we have applied this technique in combination with a tuneable light source as a synchrotron radiation using the SU8 beamline at LURE. Selecting the photon energy, it is possible to determine bidimensional images of the FS at different $k_{\perp}$. The detection of successive bidimensional images for several photon energies gives rise the complete determination of the 3D- Fermi Surface.

The SU8 beamline activities in this field are so far very successful, however the energy and spatial resolution is limited. As a natural development of these studies, at SOLEIL the end-station may be equipped with a Scienta type electron analyzer in order to have a level of energy resolution at the end-station comparable to the resolution provided by the beamline. In addition, the study of Fermi surface topology may be accomplished admirably, if the photoelectrons could be discriminated in spin. Following this line, the insertion device proposed for the SU8 at SOLEIL (in scenario I and II) consists of two undulators capable to provide photons of variable polarisation to perform Spin-resolved circularly polarised photoemission. The Scienta type analyser will be enhanced with a spin discriminator after the lens responsible of the energy analysis. The additional instrumentation required to do operative these developments is detailed in scenario I and II.

Case I. <u>Electronic properties and Fermi surface topology of High Tc superconducting materials: As an example Bi2212</u>

The normal state of the high Tc superconductors is one of the most debated question in solid state physics as it is an important step to understand high Tc superconductivity (Fig. 4). There are a number of theories proposed to explain the normal state electronic structure based on the experimental results on the Fermi surface. ARPES, has been widely used for the experimental determination of the Fermi surface and the super-conducting gaps.

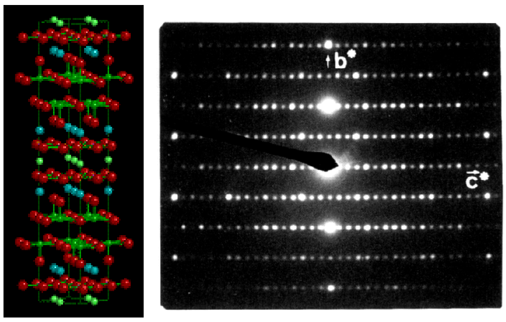

Figure 4. Structure and Diffraction pattern of a Bi2212 crystal. Those samples are the prototypical systems in superconducting materials due to their crystal perfection.

However, the task of measurement of the Fermi surface is quite tedious by using the standard approach based on the measurement of several energy distribution curves (EDCs) at each emission angle to get a single point of the FS. Using this method only few points of the FS can be measured in each experimental run and it is possible to overlook relevant features of the FS. A new approach has been used to map the FS of quasi-two dimensional systems by measuring directly the total PES intensity by full angle-scanning. As we have described in the last report of LURE, we have taken-up the task to measure the complete FS combining this novel method with the high intensity of the synchrotron radiation emitted by an undulator source and we have succeed to map the FS over a large k-space covering a very large extended Brillouin zone with high contrast, (see Fig. 5).

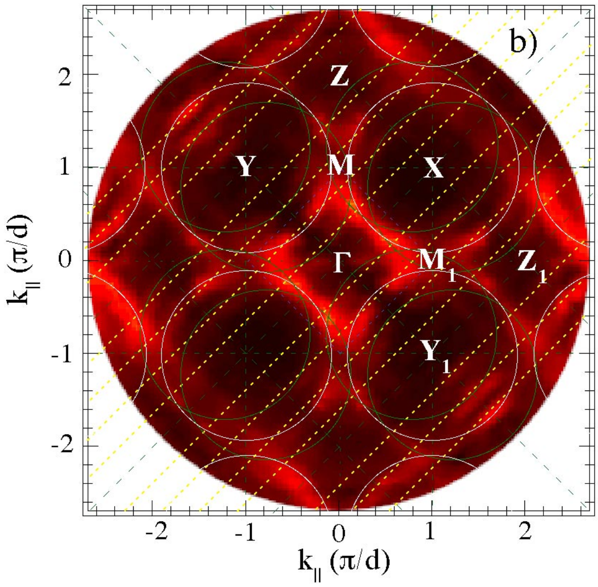

Figure 5. The figure shows large portions of the Fermi surface of a Fermi Surface of $Bi_2Sr_2CaCuO_{8+\delta}$ crystal at the optimum doping with Tc=91 K, (measured at the SU8, September 2000).

At the present a large network of labs from Europe (ARPES measurements), Japan (growth of samples) and USA (theoretical calculations) is collaborating in the context of this project together with the SU8-beamline group (the concerned groups are listed below). This extensive collaboration has just started, however, it has reached important results in the field. Complex experimental Fermi surface maps measured at different photon energy have been well reproduced by extensive first principle theoretical calculations suggesting the existence of phase separation or bilayer splitting at optimal doping.

Concerned groups:

- ***P. Pfeuty and F.Onufrieva***
  Laboratoire Léon Brillouin ,CEA-Saclay, (theory group).

- ***Ivanna Mrkonjic and Slaven Barisic***
  Department of Physics, University of Zagreb. (Theory group)

- ***Matti Lindroos.***
  Tampere University of Technology, Tampere, Finland, (Theory group)

- ***Arun Bansil and Robert Markiewicz***
  Physics Department, Northeastern University, Boston, 02115. USA, (Theory group).

- ***Stuart Abell and Guang Yang***
  School of Metallurgy and Materials, Birmingham University, England, (Sample Growth).

- ***Genda Gu***
  Physics Deparment, Brookhaven National Geographic, USA, (Sample Growth).

- ***S. Tajima and N. Koshizuka***
  Superconductivity Resaerch Laboratory, ISTEC, Tokyo, Japan, (Sample Growth).

- ***Isidoro Rasines and Juan Campa***
  Instituto de Ciencias de Materiales de Madrid (ICMM), (Sample Growth).

- ***Maria-Carmen. Asensio and José Avila***
  LURE-CSIC, (Photoemission group).

Case II. Spin-resolved Electronic structure and Fermi surface topology of Colosal Magnetoresistence: Manganites

Colossal magnetoresistance (CMR) describes the property of materials whose conductivity can be dramatically increased by the application of a magnetic field. It is believed that a strong coupling of electrons to the lattice is essential to explain the magnitude of the CMR effect. In this scenario, the electrons (or holes) are trapped by local lattice distortions, and these polarons, i.e.the localized holes and the surrounding lattice strain, inhibit the flow of current. However, there is not a clear picture explaining how these polarons interact with the magnetic fluctuations that lead to ferromagnetic order and metallic conductivity at high magnetic field or low temperature. The low dimensionality of these compounds enhances the temperature range over which charge and magnetic fluctuations can be studied, and makes them easier to separate from other dynamic processes.

At low temperatures, properly doped manganites exhibit ferromagnetic metallic or nearly metallic behavior, while at high temperatures they exhibit a paramagnetic insulating behavior. It should also be remembered that the manganites belong to the class of materials where electron correlations are deemed important, a problem that has challenged the condensed matter physics community for over 50 years. A complete experimental determination of the electronic structure of these materials together with the Fermi surface topology discriminated in spin can be essential for the comprehension of these fascinating materials. The European activity in this area is very intense, many groups in France and Spain are now a days leading the development of new methods to growth ordered samples and their application to applied fields. Below, we mention only those have already manifested their interest in the use of the SU8 beamline.

Interested groups in the development of this subject at the SU8 beamline:

- ***M. Velazquez, A. Revcolevschi, J.P. Renard, C. Dupas.***
  Laboratoire de Physico-Chimie de l'Etat Solide, and Institut d'Electronique Fondamentale, Departament MMS, Universite de Paris-Sud

- ***A. Fert***
  Unité Mixte de Physique CNRS-Thales, Domaine de Corbevill, 91404 Orsay, France et Université Paris-Sud, 91405 Orsay, France

- ***J. Rodriguez-Carvajal, M. Daoud-Aladine , L. Pinsard-Gaudart.***
  Laboratoire Léon Brillouin, CEA/Saclay and Service de Physique Statistique Magnetisme et Supraconductivite, DRFMC, CEA/Grenoble.

- ***Ricardo Ibarra, Berta Landa***
  Instituto de Ciencias de Materiales de Aragon-CSIC, Spain.

- ***Josef Fontcuberta, Jose Navarro***
  Instituto de Ciencias de Materiales de Barcelona, Bellaterra, Spain

- ***Jose Luis Martinez, Alicia De Andres, Mar Garcia-Hernandez, Geli Vozmediano and Francisco Guinea**.*
  Instituto de Ciencia de Materiales de Madrid-CSIC.

Case III. <u>Low dimensional systems</u>

Layered transition metal dichalcogenides (TMDC´s) of type TX_2 (T is the transition metal and X= S,Se,Te) and graphite substrates are of fundamental interest from both fundamental and applied points of views. They are consider as prototype systems of reduced dimensionality, where covalently bound sandwich units of X-T_X structures are separated each other by only weak van der Waals interlayer interactions. Depending on the transition metals involved, they exhibit metallic or semiconducting behaviour. They include wide bandgap insulators, semiconductors, metals, and superconductors. We focus our attention in low-dimensional oxide conductors that present a insulator-metal transition driving by a charge density wave (CDW). The existence of a CDW is associated to the existence of parallel regions of the Fermi surface connected by a nesting vector. In this case, the determination of the FS is the key to understand the electronic properties of these materials.

There are many groups working intensively in this field in Europe. We mention below some of them, however, a further development of the SU8 at Soleil with the possibility of spin

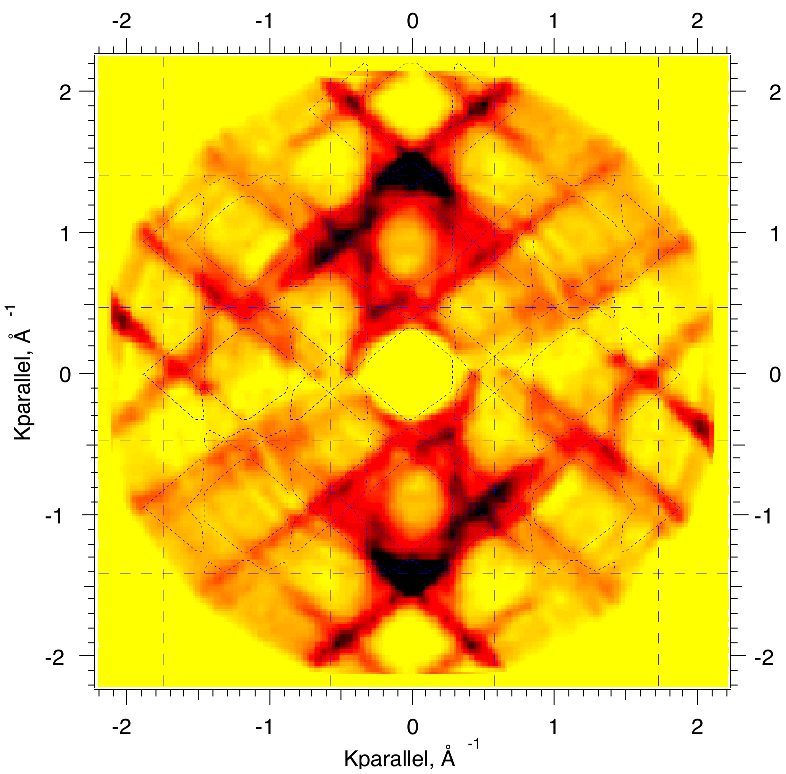

Figure 6. Fermi surface of the Low dimensional conductor Mo_4O_{11}. The parallel sections of the Fermi surface show the existence of a nesting vector responsible of the metal-insulator transition. The experiment result is compared with theoretical calculations made by Prof. Jean Paul Pouget and his group.

Concerned Groups:

- ***H. Guyot, J.Y. Veuillen, G. Foucaudot, J. Marcus***
  CNRS, LEPES, Grenoble, France
- ***Sylvie Drouard, P. Labbé, D. Groult***
  CRISMAT-ISMRA (Laboratoire de Cristallographie et Sciences des Materiaux), 14050 Caen
- ***Pascale Foury, Jean-Paul Pouget***
  Laboratoire de Physique de Solides, Faculté des Sciences d'Orsay, Universite Paris-Sud
- ***Stéphane Jobic***
  Laboratoire de Chimie des Solides, Institut des Matériaux de Nantes.
- ***S.L. Molodtsov, F. Shiller, T. Gantz, C. Laubschat,***
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- ***M. Richter***
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Case IV. Tridimensional Fermi surface of metastable magnetic and alloy phases.

A comparison between the electronic band structure of different transition metal surface systems, especially between different crystal structures of the same metal and between different metals with the same crystal structure, is of special significance for understanding the behavior of low dimensional systems and find the next between their structure and their electronic and magnetic properties. Attention is focused on the experimentally observed consequences of spin-orbit coupling; this interaction causes the band structures and FS of these metals to depend on the magnetization vector, and it can result in the formation of "Spin-hybridized" sheets of the FS.

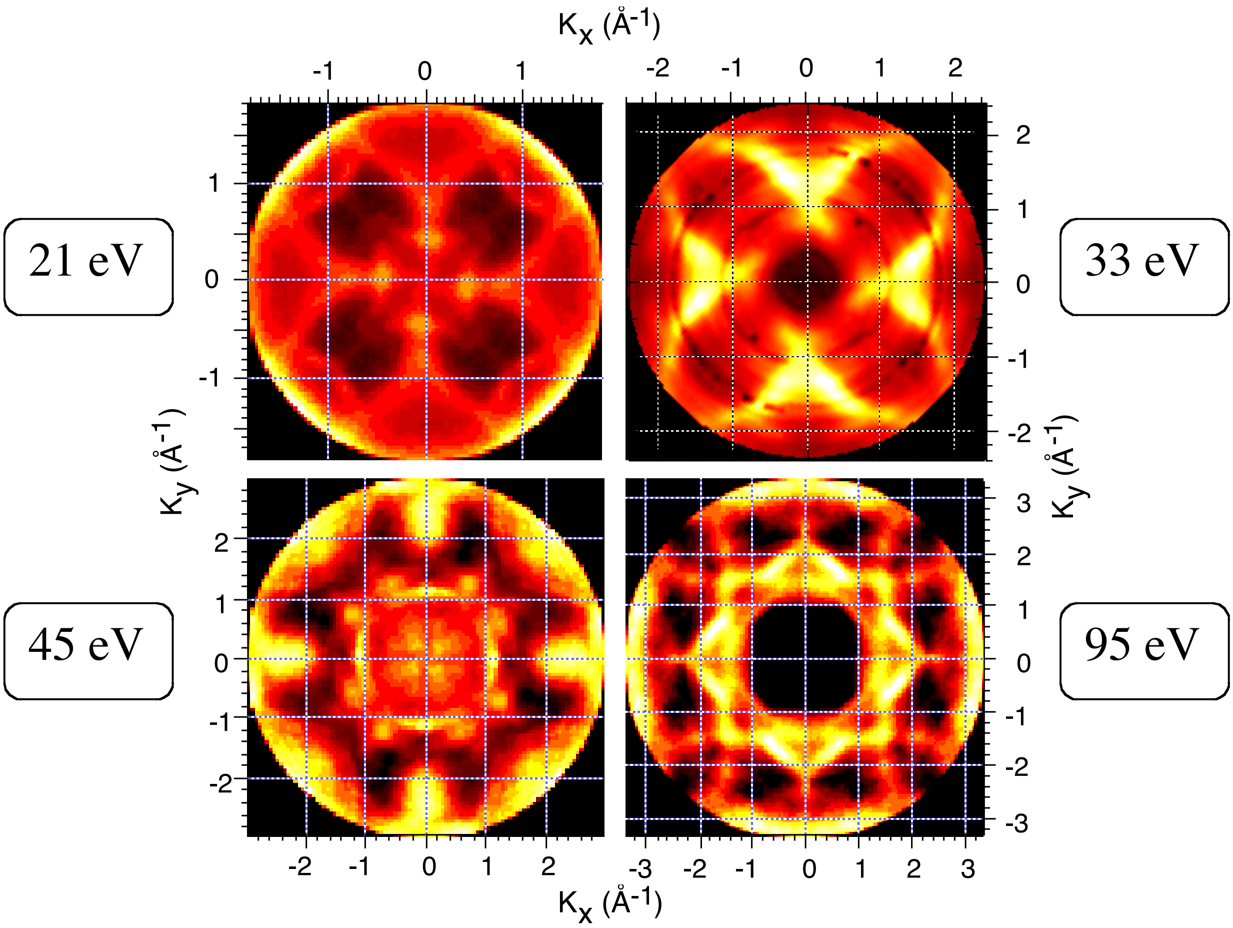

Figure 7. Experimental Fermi Surface determination of a 3D metastable magnetic material as Co(100)-fcc

Among the more traditional metastable magnetic phases, we could mention the bulk Co FCC grown on cooper substrates . In the nature, cobalt is stable, at room temperature in a HCP structure. The dHvA data of this phase has been recently reviewed in detail, in order to get an accurate description of the FS of this material. The SU8-beamline group has already done the first determination of the Fermi surface of this phase summing-up both spins (up and down). In Figure 7 we can see some of the results. We are convinced that this type of studies could be highly improved using an undulator that can supply high flux of polarised photons. With those developments, we plan to extend this type of studies to alloy compounds as those extensively studied by CEA-LURE group, (see below).

Concerned groups:

- ***N. Barrett***
  SPCSI-DREAM-DSM, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France

- ***M.C. Asensio, J. Avila, M. Izquierdo***
  LURE and ICMM-CSIC

Case VI. <u>Electronic properties of Surfaces, interfaces and nanostructures</u>

Interest in nanotechnology is growing rapidly. Now it is possible to arrange atoms into structures that are only a few nanometers in size. A particularly attractive goal is the self-assembly of nanostrustures, which produces large amounts of artificial materials with new properties. Looking at it from a general perspective, one finds that there are three independent length scale in physics that converge onto the single digit nanometer regime. Quantum mechanics, electrostatics, and magnetism conspire to produce a common length scale in the single-digit nanometer regime. These three length scales determine the operation of electronic devices, such as a quantum well laser, a single electron transistor, and a magnetic hard disk.

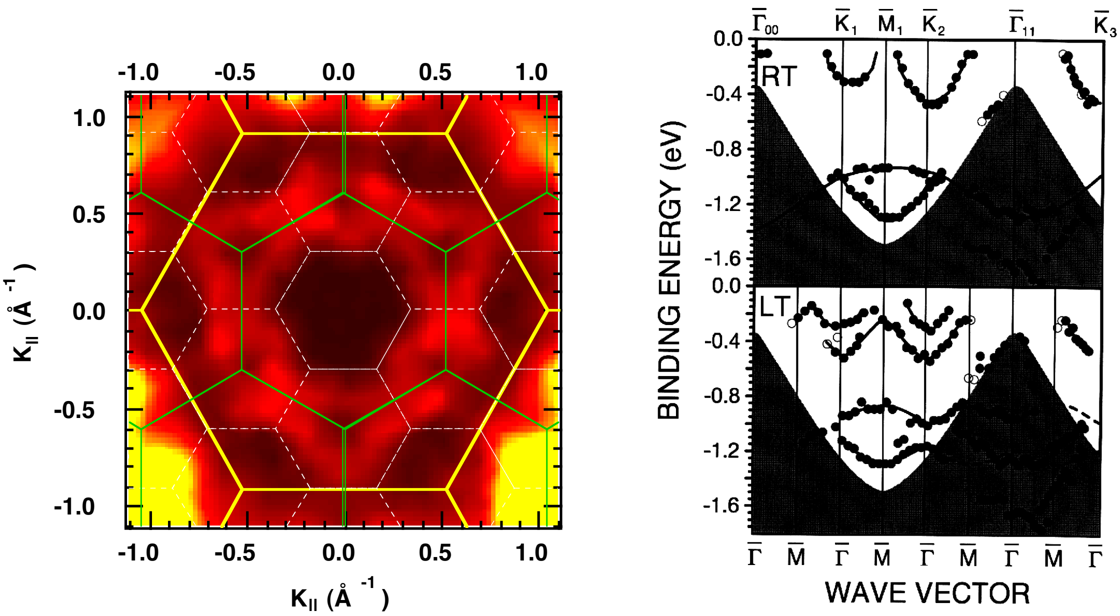

Figure 8 (left panel) Fermi surface of (√3x√3)R30° reconstruction of Pb on Ge at RT and (right panel) experimental band structure of the same phase, PRB 57,14758(1998).

In this field, a very active research has been conducted by several laboratories at the SU8 beamline. As an example, figure 8 shows part of the important contributions produced by the Marseille-Rome-Madrid collaboration in the field of phase transitions of Sn(Pb) on Ge single crystals. These results can be effectively improved with a Scienta analyser as a detector and a variable polarisation source.

Groups concerned:

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  LURE and ICMM-CSIC

Case VII. Oxide materials and interfaces oxide/oxide

The study of oxide/oxide interfaces has been a hot topic in the last few years since most of the applications of thin films are governed by interface phenomena, i.e. wetting, adhesion, reactivity, etc., specially as the film becomes thinner. In this field, the extensive work done by the SRSIM-DRECAM group at Saclay has allowed to grow magnetite films with thickness from 0.5 to 25 nm on alumina substrates by atomic-oxygen-assisted MBE. Fe_3O_4 is predicted theoretically to be a half metal ferromagnet, meaning that electrons at the Fermi level are full polarised. Fe_3O_4 nanometric layers are thus good candidates for being used as magnetic electrodes of tunnel spin-valve devices. However, a complete electronic structure determination of those materials as a function of the growth parameters is needed. These and other complex oxide systems are of current interest to be studied by photoemission. Bellow we mention some of the groups interested in this subject.

Concerned groups:

- ***Susana Gota, Martine Gautier-Soyer***
  SRSIM-DRECAM, CEA Saclay, Bât.462, 91191 Gif-sur-Yvette (France)
- ***L. Soriano, J.M. Sanz***
  Departamento de Física Aplicada, Universidad Autónoma de Madrid, Spain
- ***A.R. Gonzalea-Elipe, A. Fernandez, A. Caballero, J. Jimenez, J.C. Sanchez, J.J. Alonso, F. Yubero***
  Instituto de Ciencia de Materiales de Sevilla and Universidad de Sevilla. Spain

Case VIII. Intermetallic and Rare earth compounds

Discovery of superconductivity in the quaternary systems Y-Pd-B-C (T_c=23K) and Y-Ni-B-C (T_c=15K) is one of the most important events of the past decade in the field of intermetallic superconductivity research. In particular, in the nickel-based series RNi_2B_2C, the replacement of yttrium by other rare earth induces a broad variety of low temperature behaviours. While $LuNi_2B_2C$ is superconducting at 16.5K, $LaNi_2B_2C$ does not show any superconducting transition. The compounds with R=Pr, Nd, Sm, Gd and Tb do not superconduct and exhibit several magnetic structures, on the other hand, $CeNi_2B_2C$ is an intermediate valence compound while $YbNi_2B_2C$ is a heavy fermion compound and none of them is superconducting. In some of these compounds superconductivity coexists with antiferromagnetism with rather high values of transition temperatures. This is a rather unique behaviour as very often magnetism destroys superconductivity. Despite the strong chemical implication needed to develop this field, the electronic characterisation of these families of compounds is essential to the research groups involved in this area, because the information obtained can be used as a guide to design new materials with improved properties.

Concerned groups :

- ***E. Alleno, C. Mazumdar, C. Godart.***
  LCMTR-CNRS, ISCSA, 2-8, rue Henri Dunant, 94320 THIAIS, France

- ***Dr. B. Chevalier,Dr. A. Demourgues,Dr. F. Fourgeot***
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2.2.B. PHOTOELECTRON DIFFRACTION AT SOLEIL

Photoelectron diffraction (PED) is a powerful technique for the geometric structure determination of surfaces and interfaces. In a PED experiment, the photoemission from core-levels of surface atoms is measured with respect to emission angle and excitation energy. The photoelectrons from an emitter atom undergo interference effects due to scattering with neighboring atoms, leading to angle and energy-dependent intensity fluctuations, i.e. diffraction patterns. Typically, so-called diffractograms are measured, i.e. hemispherical intensity maps around the surface for constant kinetic energy. The diffraction pattern is strongly dependent on the local atomic structure around the emitter. By comparing the experimental diffraction to theoretically simulated patterns for different structural models, the atomic structure around the emitter can be determined. A decisive advantage of PED compared to other diffraction techniques, is that it is chemically specific. In recent developments of the PED technique, direct holographic inversions of large PED data sets have been made, thereby directly obtaining the atomic structure.

The power and usefulness of the PED technique has been dramatically enhanced by the new third generation synchrotron radiation sources. Their very high photon flux and brilliance allow fast data adquisition of very large PED data sets, combined with high energy resolution. Another advantage is the possibility to choose different kinetic energies. At high kinetic energy, single-scattering dominates, leading to the co-called forward-focussing effect and making the analysis simple. At low kinetic energy, multiple scattering became important, which makes the diffraction pattern more sensible to the whole 3-dimensional structure around the emitter. An additional advantage is that at low kinetic energy the surface sensibility is increased, allowing the separation of the core-level signal from the substrate into bulk and different surface components. In particular, the method namely, Scanned Energy

Photoelectron Diffraction (PhD) relies on the coherent interference of the direct photoelectron wavefield, emitted from an atom within the adsorbate , with components elastically scattered by surrounding atoms, specially in the substrate. By scanning the photon energy, and measuring the emitted intensity in specific directions, the resulting intensity-energy spectra contain information on the local structural environment which can be elucidated by comparison with the results of model calculations.

At second generation synchrotron sources, the low photon flux and so the low data adquisition efficiency is a serious limitation, that forced us to work with less reactive surfaces and/or take very small data sets. But our results nevertheless proved the power of low-energy PED for structural determination of surfaces. To continue this kind of project it is essential to dramatically improve the instrumentation for low-energy PED. The SU8 beamline is specially fitted to perform PED experiments with an wide flexibility, which permits its use to a broad range of materials. The transfer of this beamline to Soleil, will allow a further development of PED taking advantage of a variable polarized excitation source.

Case I. Adsorption Site Determination of N, O and C-derived species on semiconductor surfaces using Photoelectron Diffraction

The adsorption and thermal decomposition of small molecules on semiconductor surfaces is of current interest for both, fundamental interest and technological importance. In order to get a precise understanding of the interaction between molecules and surfaces, it is necessary to know the influence of the surface morphology on its reactivity. In particular, the attention has been focussed on the passivation of III-V semiconductor (Rennes' group) and thermal nitridation of Si substrates, where different nitriding species, such as , NO, NH_3, and N_2H_4 , have been extensively investigated (Roche's group). An analogous situation characterizes the adsorption of simple hydrocarbons on semiconductor surfaces. The reactivity of silicon surfaces to these molecules is of considerable importance with regard to a whole range of catalytic reactions used in the exploitation of fossil fuels. However, their structural description remains almost unexplored.

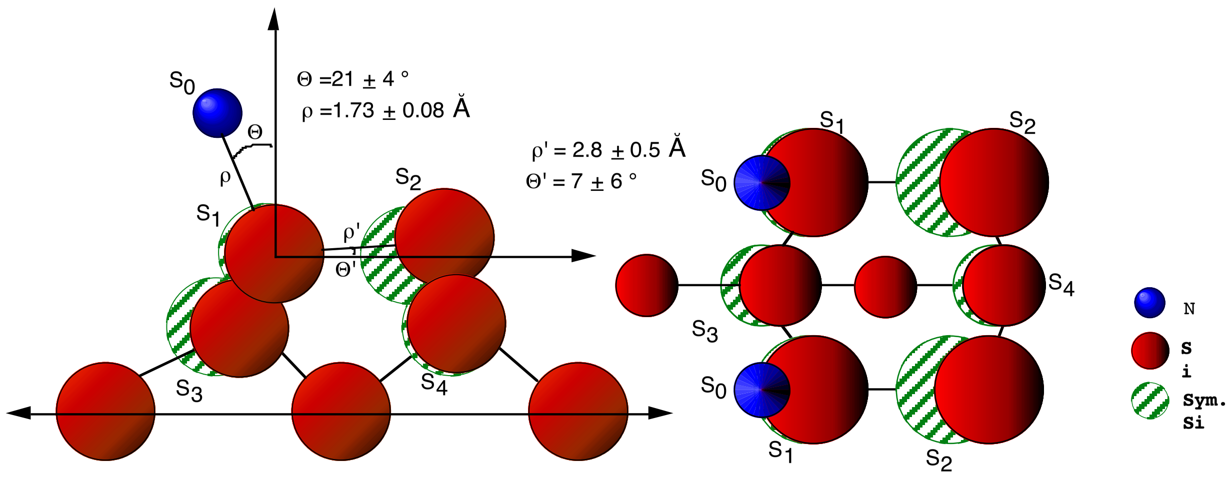

Figure 9 shows the PhD results obtained in the case of the adsorption of NH_3 on Si(100)2x1 at the SU8 beamline, PRL 79,673 (1997).

The current activities in this area at LURE have developed a traditional trial-and error PhD procedure and a modern direct analysis method. The combination of both protocols and a sophisticated data acquisition software developed at the SU8 beamline has allowed to resolve several structures. Figure 9 shows the adsorption site and bond distance obtained in the case of the adsorption of NH_3 on Si(100)2x1. Possible geometry changes due to thermal dissociation could be also investigated. Among the specific objectives, several French groups concerned with this structural studies have focussed their work for the next few years, on the adsorption geometry determination of atoms, small molecules and hydrocarbons and their thermal dissociation products on semiconductor substrates.

Concerned groups:

- ***G. Jezequel, F. Solal***
  Equipe de physique des Surfaces et des interfaces
  UMR PALMS/EPSI, Bat 11 C, Campus de Beaulieu, Universite de Rennes
- ***M. Rochet***
  Chimie-physique matiere et rayonnement, Université P. et M. CURIE (PARIS 6)
- ***Maria Grazia Proietti***
  Instituto de Ciencias de Materiales de Aragon-CSIC, Zaragoza.
- ***M.C. Asensio, J. Avila, M. Davila***
  LURE and ICMM-CSIC
- ***H.Ascolani, S. Bengio***
  Dept. Colisiones Atomicas, Centro Atomico Bariloche, Argentine.

2.3.- Description of the new SU8 beamline at Soleil

Due to the fact that SuperAco is a second generation storage ring, the whole setup (beamline plus end station) cannot reach the highest energy and angular resolution, demanded now a days to perform state-of-the-art photoemission experiments. The photon flux is too low which results in a poor count rate when the performance is pushed to the design limits. The present situation with a low count rate is a consequence of the existing single channel detection system and the fact that the synchrotron light is not a 3rd generation type source. The possibility to transfer the beam line to SOLEIL has opened up a very interesting future for the SU8 beamline.

2.3.1.- The source

As mentioned before, the insertion device existing at Super-Aco is an hybrid undulator, which has been designed in order to provide a high flux for an energy range of 16 eV to 950 eV at the 800 MeV storage ring. Its first harmonic is produced around 15 eV. As the energy of the Soleil storage is 2.7 MeV, a study has been persuaded in order to design an insertion device ables to provide high flux of photons in the same energy range. Given the technical requirements, the insertion device design group of Soleil suggests the installation of two different undulators: one for low energy range and the other one for medium energy. The first one, a electromagnetic undulator, with a total length of 3.6 m and a 300 mm period for low energy range up to 200 eV, with a K = 6.77. The second ondulator, standard permanent magnet undulator, with a total length of 1.8 m and a period of 80 mm, covers a range of energy from 0.2 keV up to 0.9 keV. Both of them can provide variable polarized photons. The scenario of only one undulator to cover the whole range of energy (10-1000 eV) and provide variable polarization is not suitable. For the low energy undulator, the table II shows the main characteristics (total power, power at the slit, power at the chamber) for a typical undulator with 300 mm of period at 10 eV.

Period (mm)	Polar	Kx	Kz	+/- K/γ (mrad)	Total Power (W)	Power Slits (W)	Power Chamber (W)	Max Density Chamber (W/mrad2)	ΔT(°)
300	V	6.77	0	+/-1.26	500	314	166	765	140

Table II. Low energy electromagnetic undulator

The characteristics of the second undulator have been selected in order to overlap both unduladors at around 0.2 keV of photon energy. The Table III shows their technique specifications.

λ(mm)	K	+/-K/γ (mrad)	B(T)	N	P(W)
80	2.80	+/-0.52	0.378	22	615

Table III. Permanent magnet undulator operative for an energy range of 0.2-0.9 keV.

Figure 10 shows the total delivered power at 15m from de source of both undulators. For a 90% of maximun flux, the beam dimension at 15 m from the source is of 4mm (hor.) x 2mm (vert.), which corresponds to the position of the first mirror. The power for this opening at 15 m of the source is only 80 W. The divergence cone of radiation for the lowest energy is of 0.23 mrad, so 3.45 mm at 15 mm. Due to the fact that the variable polarizability is operative, the diaphragm should be 4mm x 4mm, which corresponds to a total power of 135W.

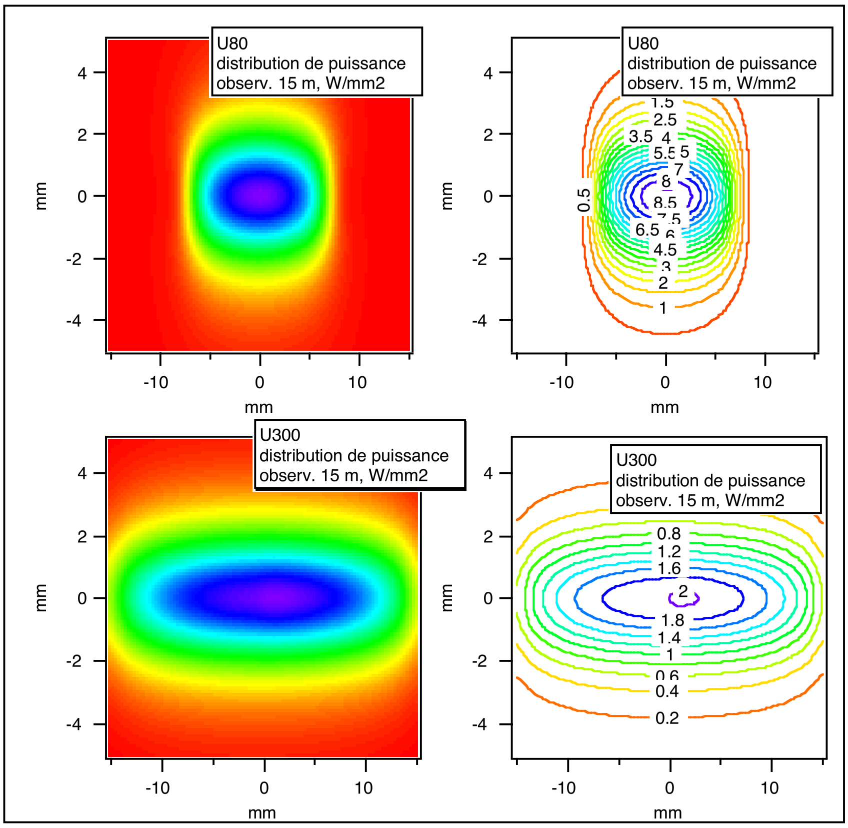

Figure 10. Power distribution delivered by the beam at 15 m from the source at different gaps apertures. Part a) and b) correspond to undulators U80 and U300, respectively.

2.3.2.- Optical configuration

The plane grating monochromator (PGM) of SU8 was designed to provide a high photon energy resolution in the energy range 15-900 eV. However the transfer of SU8 to SOLEIL will result in an improvement of the performances. This very favorable experimental situation can be achieved at a low cost since the monochromator and one of the end stations are already available. Only a few modifications in the beam line should be carried out to adequate the beamline to the characteristic of the SOLEIL's beam. The scheme of the beamline at Soleil is pictured in Figure 11 .

The modifications respect to the actual SU8 beamline at LURE are the following:

i) Change the **M1** pre-focusing mirror to a **spherical mirror.**
ii) Improve the **refrigeration** system of M1 due to the higher power delivered by the source
iii) Change the **lowest energy grating** in order to avoid the second order contributions.
iv) Improve the actual system of **refrigeration of gratings**.
v) Change the actual M3 post-focusing mirror by two post-focusing mirrors: A **parabolic** mirror **M3** (for horizontal focusing) and a **spherical M4** (for a vertical post-focusing).
vi) The **holding chamber** of the post-focusing mirrors should be changed in order to place the two new mirrors (M3 and M4).

2.3.3.- End Stations

In the initial version of the SU8 beamline project at Super-Aco, the end station has been designed with a movable platform that accommodates two independent experimental chambers. It enables the photon beam to be directed to either experimental chamber **without breaking the vacuum**. One of the chamber sites is outfitted with the existing ARPES system suited to perform angle resolved photoemission and photodiffraction experiments, investigating well ordered massive solids, surfaces and interfaces, addressed mainly to **basic science research**. The second site can be occupied by a chamber equipped with partial and total yield electron detectors and a fix high-resolution energy analyzer to perform absorption (through NEXAFS and SEXAFS measurements) and high resolution photoemission experiments on solid state. Figure 12 shows the perspective view of the implantation of the platform in the experimental hall, as well as the movement that allows changing the end stations. Due to the limited space available at Super-Aco, this platform has not be installed at LURE. However, it has already built and it is eventually ready to be placed at SOLEIL.

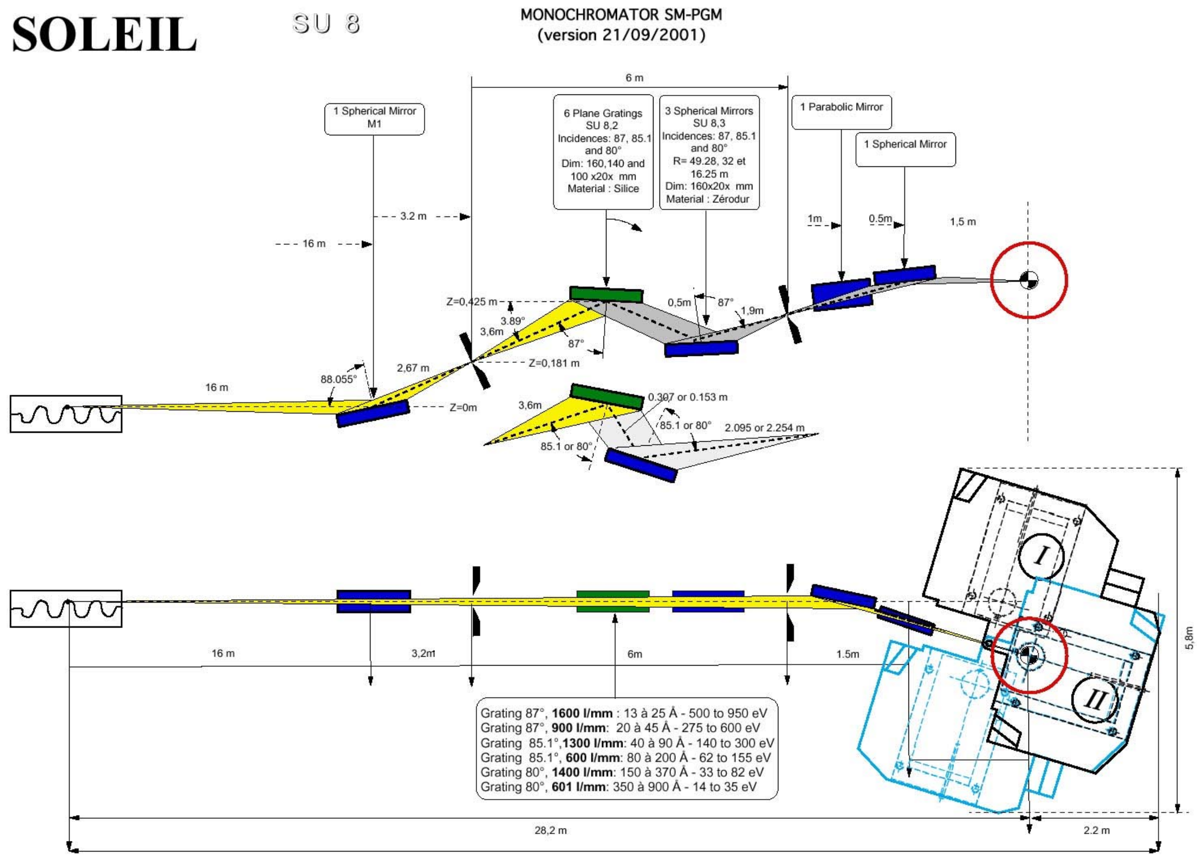

Figure 11: Layout of the SU8 beamline at SOLEIL

The second end Station (Section II) is planned to be equipped by an Ultra High Vacuum chamber with a fix high resolution hemispherical analyzer (SCIENTA Type Analyser), with a multichannel detector. If the SU8 beam line is positioned in a medium straight section of Soleil storage ring, the length of the beamline from the first mirror up to the end station is 26.2 m, totally compatible with the standard 39 m length available for each line at Soleil. The transversal dimensions of the platform are also well fitted at the Soleil hall. The whole system requires 5.5m wide, where 9 m are available.

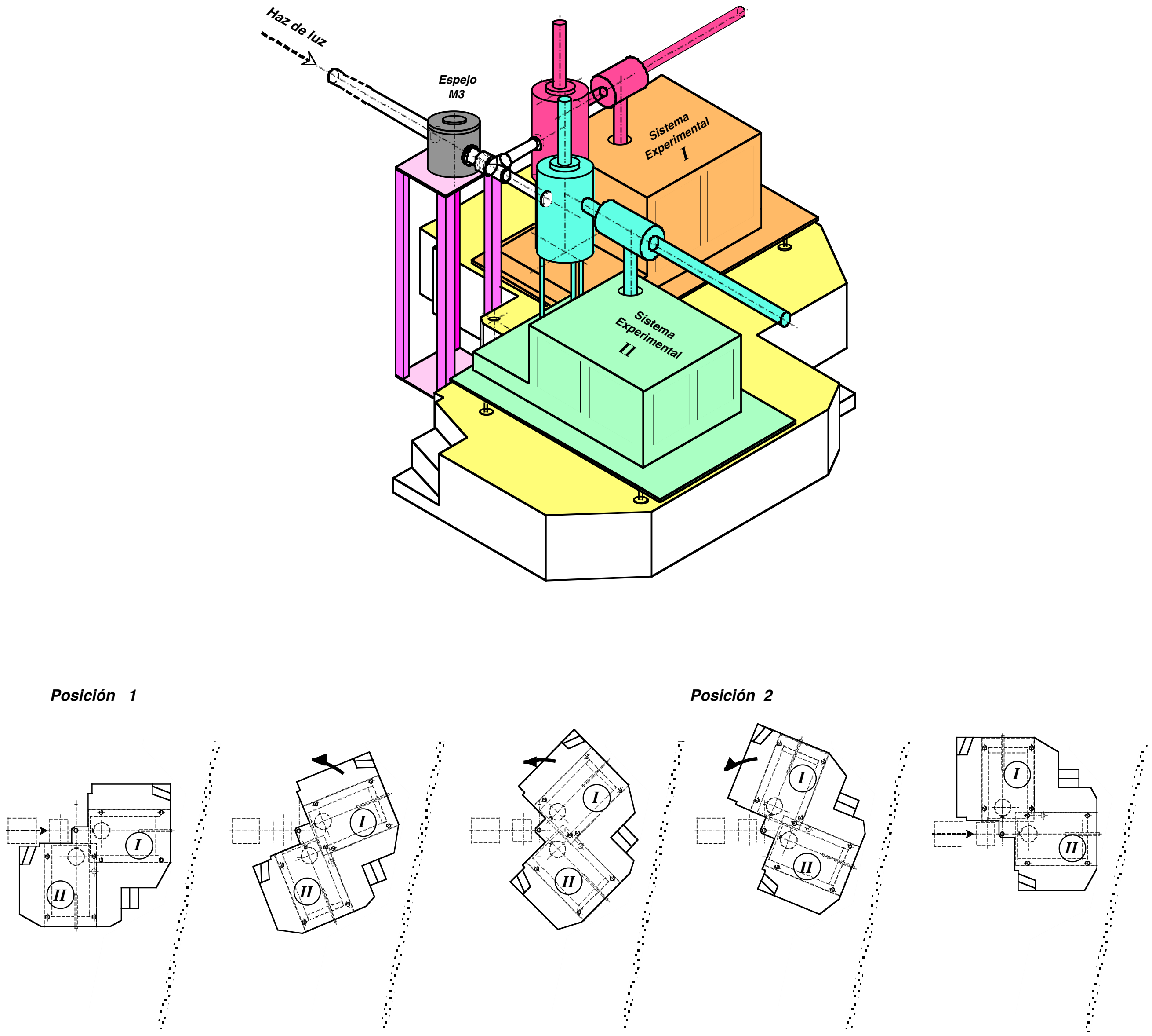

Figure 12: The scheme of the platform with the two end-stations is shown in the top part of the figure. The platform movement permitting the alternative positioning of Station I and II in line with the beamline is depicted in the bottom of the figure.

3.- SYNOPSIS OF THE PROPOSED SCENARIOS

3.1.- Technical Characteristics

SCENARIO I: With two end stations

Station I: Angle Resolved Photoemission and Diffraction of ordered materials.
Station II: Absorption Spectroscopy and High-Resolution Resolution Photoemission.

Source Characteristic
Two insertion devices of 300 mm. and 80mm. of period. The energy range covered by the source will be from 15 up to 1000 eV with variable polarized light.

Optical elements
A focusing spherical mirror (M1) to re-image the source at the first slit.
Monochromator: Varied line spacing (VLS) design in which the mechanically ruled gratings operate in the converging light from spherical mirror. In order to cover the whole required energy range from 16 to 900 eV, six diffraction gratings are coupled to three spherical mirrors (one mirror for each two gratings).
A horizontal refocusing parabolic mirror (M3) and a vertical refocusing spherical mirror (M4) image the exit slit at the centre of the chamber.

Detectors
Multichannel detector, bidimensional detectors, total and partial electron yield, hemispherical high-resolution electron analyser with spin-discriminator.

Beam line control
Automatic control of the beamline, undulator gap and end stations by a high performance personal computer.

<u>SCENARIO II:</u> With only one end station

Station : Angle Resolved Photoemission and Diffraction of ordered materials with the possibility of a High-Resolution Resolution electron analyzer.

Source Characteristic
Two insertion devices of 300 mm. and 80mm. period undulator. The energy range covers by the source will be from 10 up to 1000 eV and with variable polarized light.
Optical elements
A focusing spherical mirror (M1) to re-image the source at the first slit.
Monochromator: The same as scenario I.

Detectors
Multichannel detector, bidimensional detectors, total and partial electron yield, hemispherical high-resolution electron analyser with spin-discriminator.

Beam line control
Automatic control of the beamline, undulator gap and end station by a high performance personal computer.

SCENARIO III: With only one end station using SU5 and SU8 Ondulators from SuperAco

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Scenario III takes into account the possibility to use SU5 and SU8 undulators, existing already at SuperAco. Two main problems have been found for this scenario. The more important one is the energy of the first harmonic in both undulators, which is as high as 65 eV. With low this energy limit more of the scientific cases detailed in this proposal cannot be performed, because they need photon energy lower than 65 eV. The other difficulty is the conception of the SU8 undulator, which is not able to change the vector polarization.

Station : Angle Resolved Photoemission and Diffraction of ordered materials with the possibility of a High-Resolution Resolution electron analyzer. Notice that the use of these techniques will be operative only for hv > 65 eV.

Source Characteristic
Two insertion devices of 100 mm.(SU8 undulator) and 250mm. period (SU5) undulators. The energy range covered by the source will be from 65 up to 1000 eV. The only variable polarized light will be delivered for the energy range covered by the SU5 undulator.

Optical elements
A focusing spherical mirror (M1) to re-image the source at the first slit.
Monochromator: The same as scenario I.

Detectors
Multichannel detector, bidimensional detectors, total and partial electron yield, hemispherical high-resolution electron analyzer.

Beam line control
Automatic control of the beamline, undulator gap and end station by a high performance personal computer.

3.2.- Budget of the three envisaged scenarios

SCENARIO I

Source (U300 and U80)	3 MF
New Spheric mirror M1	0.2 MF
New refrigeration system for M1	0.3 MF
New Lowest energy graiting R1	0.2 MF
New Refrigeration system for the monochromator	0.4 MF
New post-focusing parabolic mirror M3	0.2 MF
New post-focusing spherical mirror M4	0.2 MF
New chamber for post-focusing mirrors	0.5MF
Implantation of SU8 at SOLEIL	1MF
Implantation of the platform at soleil	0.2 MF
High resolution analyzer	
(SCIENTA 2002+ Spin Detector)	1.5 MF
Second experimental station	2 MF
Total:	9.7 MF

SCENARIO II

Source (U300 and U80)	3 MF
New Spheric mirror M1	0.2 MF
New refrigeration system for M1	0.3 MF
New Lowest energy graiting R1	0.2 MF
New Refrigeration system for the monochromator	0.4 MF
New post-focusing parabolic mirror M3	0.2 MF
New post-focusing spherical mirror M4	0.2 MF
New chamber for post-focusing mirrors	0.5MF
Implantation of SU8 at SOLEIL	1MF
High resolution analyzer	
(SCIENTA 2002+ Spin Detector)	1.5 MF
Total	7.5 MF

SCENARIO III

Source (SU5 and SU8)	--- MF
New Spheric mirror M1	0.2 MF
New refrigeration system for M1	0.3 MF
New Lowest energy graiting R1	0.2 MF
New Refrigeration system for the monochromator	0.4 MF
New post-focusing parabolic mirror M3	0.2 MF
New post-focusing spherical mirror M4	0.2 MF
New chamber for post-focusing mirrors	0.5MF
Implantation of SU8 at SOLEIL	1MF
High resolution analyzer	
(SCIENTA 2002+ Spin Detector)	1.5 MF
Total	4.5 MF