LOREA: A beamline for Low-Energy Ultra-High-Resolution Angular Photoemission for Complex Materials at ALBA

Summary of the proposal prepared by:

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1.-Summary

A beamline providing ultraviolet radiation with variable polarisation in the photon energy range 7 – 50 eV is proposed. It will be optimised for angle-resolved photoemission spectroscopy measurements of the electronic structure of solids, surfaces, interfaces and nanostructures. The proposed beamline will deliver ultraviolet light with state-of-the-art resolution including an experimental end station with specific features for ultra-high (< 1 meV) energy resolution and very-low temperature (T < 1 K). The beamline will provide a versatile and competitive instrument to those scientists in the national and international research communities performing experiments on surface and bulk electronic structure and in the study of the low energy electronic properties of novel complex materials.

beamline specifications

- Photon energy: from 7 to 50 eV
- High flux: > 10^{13} ph/s/b.w. on sample
- Spot size (H) < 20 µm on sample
- Monochromator for very high energy resolution (E/ΔE > 20000@20 eV, 50000@50 eV): NIM, PGM or a combination of both
- High purity and stability of the beam at source and experimental station
- Electromagnetic quasi-periodic undulator providing variable polarization free from high energy harmonics
- End-station equipped with:

1. Analysis chamber with :

- an ultra-high-resolution electron analyzer with sub meV energy resolution and angle multidetection.
- two high-precision manipulators: one of them with sub 1 K cooling (4 degrees of freedom), the other one with sub 10 K cooling (5 degrees of freedom).

2. Pre-chamber equipped with standard preparation and characterization tools.

2.-Introduction

The development of high (meV) and ultra high (below 1 meV) resolution electron analyzers with multichannel angular detection has recently stirred the interest in angle-resolved photoemission spectroscopy (ARPES). Ultra-high-resolution (UHR) analyzers represent a major breakthrough that has allowed ARPES to mature in power and simplicity, reaching the same level as the most advanced electron microscopies. Indeed, in a similar way as real space is imaged in a microscope, now the band structure of solids, the Fourier space landscape of valence band electrons, is readily visualized on a screen with unprecedented precision.

UHR-ARPES has enormous potential in most of the fields of solid state physics. Nominally, the energy resolution can be as low as 1 meV and the angular resolution of the order of 0.1º, i.e. $\Delta k \sim 0.001 \times (E-5)^{1/2} \sim 0.01$ Å^{-1} for E = 30 eV photons. Thus, extremely accurate band structure measurements are at hand, making it possible to track most phenomena affecting the electronic structure by studying electron bands close to the Fermi energy (E_F) in the whole Brillouin zone. High and ultra-high-resolution ARPES is being already extended to research in a variety of novel systems and their underlying interactions: many-body interactions and cooperative phenomena in bulk materials, like superconductivity, magnetism and phase transitions, strongly correlated electron systems, nanoscale systems and emerging complex materials. The latter include novel unconventional superconductors, alloys, intermetallic compounds, magnetic semiconductors, f-electron systems and low-dimensional as well as self-organized systems.

The impact of UHR-ARPES in current solid state physics explains the increasing number of setups in synchrotron radiation facilities around the world. We strongly believe that ALBA must feature UHR-ARPES as well, although it must go beyond a standard system to a more specialized setup. Most of the UHR-ARPES experiments are connected to undulator beam lines that are effectively limited to photon energies beyond 20 eV. **This Proposal describes a UHR-ARPES setup exclusively dedicated to ultra-high-resolution band structure measurements using synchrotron radiation in the 7-50 eV range.** This photon energy range enlarges angular resolution and increases the probing depth range, which is especially attractive for the study of emerging complex systems with large unit cells.

It is also necessary to stress that research of complex materials requires careful in-situ sample preparation and characterization. This is a critical point that, based on our experience as frequent users of HR-ARPES in different synchrotron facilities around the world, is not being adequately addressed in most cases. Thus, we plan a flexible but powerful preparation chamber comprising different MBE sources, Scanning Tunnelling Microscopy (STM) characterization and a broad sample temperature range.

LOREA is intended to be a complement to similar experimental stations conceived for low photon energy photoemission, as 13 at BESSY, SIS at SLS, MERLIN at ALS, BaD ElPh at ELETTRA and the future ARPES beamline at DIAMOND, and as such should be a reference at the international level due to its optimization in the 7-50 eV range, encouraging external users to perform their experiments. There is a growing demand for instruments providing state-of-the-art resolution with enough flux for the investigation of an always increasing range of novel materials.

3.-Beamline layout and requirements

The main chamber should be equipped with a high-resolution electron spectrometer (Scienta R4000 or similar), with a demonstrated resolution in the meV and sub-meV range. The standard manipulator to be equipped with a He flow cryostat and a high precision sample rotation stage will be mounted on the experimental station. The standard manipulator should allow angle resolved measurements over 2π stereo radian down to T < 10 K. A user-friendly prep-chamber will be connected to the main chamber through a flexible transfer system. The prep-chamber will allow quick load-lock of MBE evaporators and in-situ calibration via a quartz microbalance mounted at the same sample stage, and will be equipped with a commercial STM for structural analysis.

A very important feature related to meV photon/electron energy resolution is the sample temperature. Thermal broadening at 10 K is approx. 1 meV. This means that when this level of energy resolution is reached, an equivalent level of sample temperatures below 5 K must be achieved. This range means an important step forward in ARPES, since most experimental setups worldwide are limited to ~10 K, and only a few (1^3 beamline in BESSY, Merlin in ALS) are reaching sub-K temperatures. This is due to the fact that achieving lower temperatures poses significant experimental problems, i.e. an excellent thermal contact must be guaranteed after sample transfer, thermal radiation shielding is needed to reach temperatures below 10 K, and a He^3 dilution cryostat is required for the sub-K range. This is a proven technology in Low Temperatures Laboratories, but its combination with the ultra-high vacuum as well as the photoemission requirements of an ARPES beamline has been achieved only very recently. We propose the construction of a specific sample manipulator designed to reach sample temperatures below 1 K and suitable for UHR measurements. Beside this, commercial solutions are nowadays available for such sample cryostats, if required.

Source and optics

The UHR requirements demand a high brilliance source, so that the use of a bending magnet is discarded vs. an undulator, the latter being able to cover the range of energies with maximum brilliance. The features required for the source can be summarized in the following points:

1.- Photon energy range : 7 eV - 50 eV using the 1st harmonic

2.- High harmonic rejection to have very good spectral purity, i.e., using a quasi-periodic undulator

3.- Variable polarization (vertically/horizontally linear polarization; circular polarization with left/right-handed helicity; all polarization rates >90%)

4.- Helicity switching. The speed of the switching does not seem to be critical, but similar Soleil devices (e.g., HU640 undulator) flip at 1 Hz.

5.- Photon flux in the range of 10^{14}-10^{15} photons/sec./0.1% b.w.

In view of the ALBA storage ring energy (3 GeV), a long electromagnetic undulator will probably be the best option due to the large magnetic period length required for the above rather low photon energy range. Indeed, in order to reach photon energies as low as 7 eV, high K values (around 8) are needed. In a configuration where the polarization ellipse does not need to be canted, the undulator may be composed of two families of coils, one producing the vertical field and the other one the horizontal field. According to the Insertion Device Group at ALBA, a period of about 400 mm is needed in order to reach 7 eV with realistic parameters (see Fig. 1), as calculated with the RADIA code. We will term this undulator as HU-400, from helical undulator.

A medium straight section (4 m long) would allocate 7 periods, while a long straight section (8 m long) would allocate 16. According to the calculations, with HU-400 a flux of 3×10^{14} Ph/s/0.1%BW in central cone can be obtained in vertical and horizontal polarizations if it is installed in a medium straight. Flux can be increased to nearly 10^{15} Ph/s/0.1%BW if the undulator can be installed in the long straight section. The theoretical on-axis brilliance and photon fluxes (H polarization) produced by the HU-400 installed in different straights of ALBA ring are shown in Figs. 2 and 3, respectively. It becomes clear that a 8 m straight section will certainly be a more attractive location due to the larger number of magnetic periods and thus enhanced brilliance of the insertion device, as required for such a high-performance beamline.

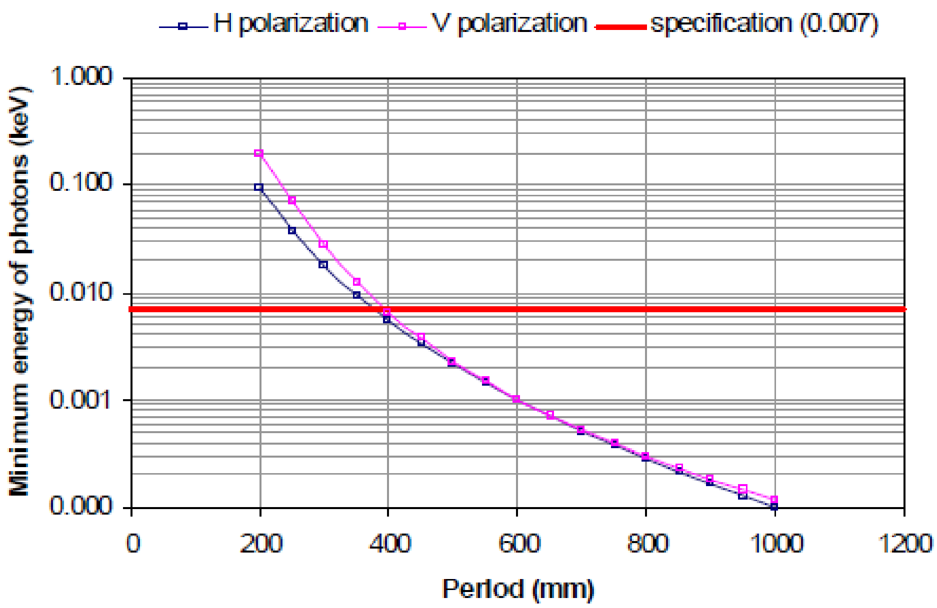

Fig. 1. Minimum reachable energy as a function of the period for an undulator with two families of coils with the following parameters: height = 25 mm, inner radius = 20 mm, outer radius = period / 4, length of straight = period / 4, current density = 10 A / mm^2 and gap = 12 mm. Courtesy of J. Campmany, ID-FE section, ALBA-CELLS.

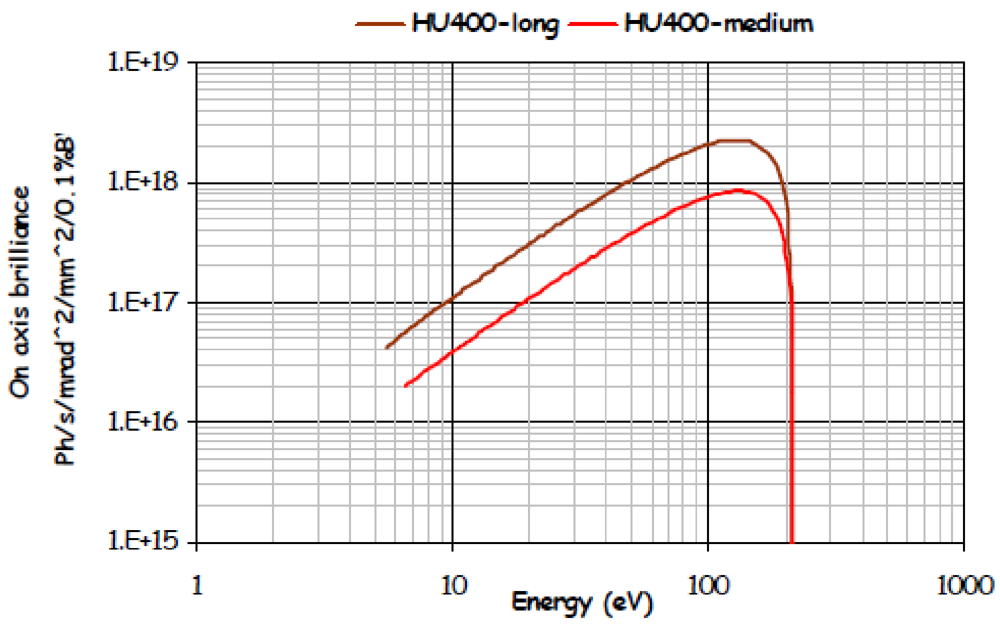

Fig. 2. Brilliance calculated for HU400 at medium (red) and long (brown) straights. Courtesy of J. Campmany, ID-FE section, ALBA-CELLS.

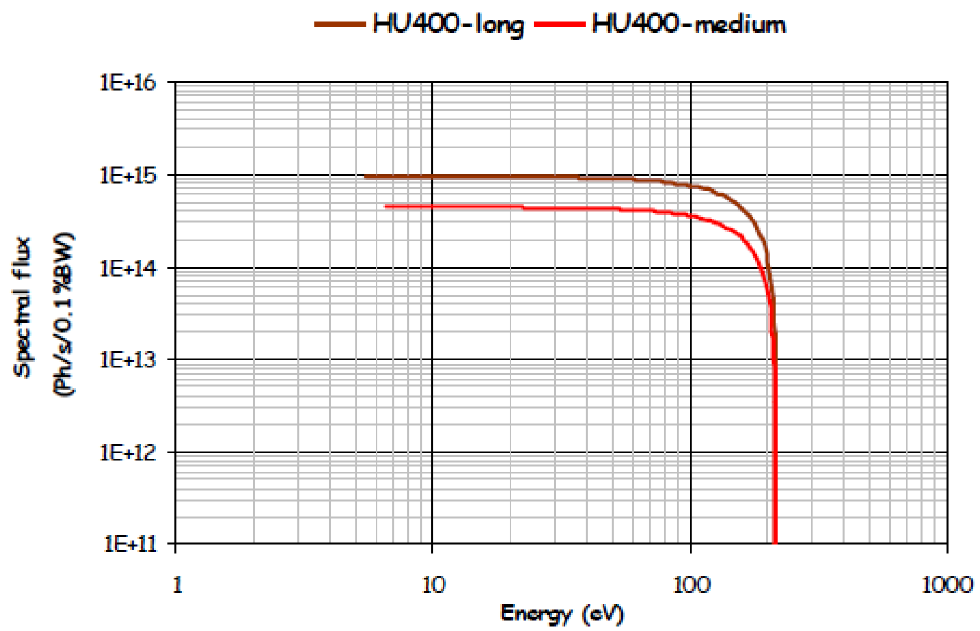

Fig. 3. Flux in central cone calculated for HU400 at medium (red) and long (brown) straights. Courtesy of J. Campmany, ID-FE section, ALBA-CELLS.

As mentioned above, a quasi-periodic undulator magnet structure would be of importance for achieving high spectral purity from the source side (see below). As a comparison, the HU640 undulator of Soleil (storage ring energy 2.75 GeV), a 640mm period 10m long electromagnetic elliptical undulator consisting of three sets of pure coils without iron yokes, provides photons in the 5-100 eV range using the first harmonic, circular as well as full linear polarization (at any orientation).

The first optical element of the beamline would have to absorb the major part of the beam power. A proper cooling system, ensuring maximum stability of the beam is needed. The energy resolution should ensure sub-meV resolution below 50 eV, i.e. $E/\Delta E > 20000$ (50000) for 20 eV (50 eV) photons. The simplest monochromators setup covering the targeted photon energy range (7-50 eV) with good resolution is a normal incidence monochromator (NIM). The use of a quasi-periodic undulator will help to eliminate higher order harmonics, which are particularly inconvenient at low photon energies. The NIM setup has significant advantages, as a demonstrated design and very high resolution at low photon energies. In turn, it has a rather low upper cut-off energy (50 eV maximum).

On the other hand, combined NIM-PGM setups reaching an extended photon energy ranges of about 4-200 eV and 10-800 eV, respectively, have been successfully installed at the 1^3 beamline at BESSY II and at the SIS beamline of the SLS. Thus, there are several design options that can fit with the target technical specifications. A final decision will be made taking into account the actual energy range provided by the undulator and the fact that the primary interest of the beamline is focused in the low energy range (7-50 eV). The sample spot size (H) should be <20 μm. As the analyzer acceptance is approx. 100 μm, bendable defocusing optics should be included in order to allow a continuous increase of the spot size up to ca. 100 μm. Defocusing, as made possible by bendable refocusing mirrors, will be mandatory when working with organic molecules in order to reduce beam damage.

Experimental end-station

The end station will be designed to obtain maximum performance for ARPES. We propose an experimental setup composed of three interconnected vacuum chambers:

(1) Analysis chamber containing the electron detector.
(2) A central preparation chamber under UHV conditions, with the usual preparation and characterization techniques, plus STM
(3) Load lock system for fast entry of external samples.

The electron detector should represent the state of the art in the field, combining high-transmittance and maximum angular resolution (i.e. Scienta R4000). In order to exploit the potential of the beamline in terms of energy and angle resolution, a crucial part is a reliable sample manipulator. As mentioned above, one original feature of the beamline is the project to build a UHV sample manipulator with a target sample temperature below 1 K. This manipulator would be specific for band dispersion studies, with ultrahigh angular and energetic resolution and will use a commercial He^3 cryostat adapted to UHV environment. A second manipulator is expected to provide a more versatile environment in terms of degrees of freedom at the sample, with a higher sample temperature, but still in the < 10 K range.

A user-friendly preparation chamber will be connected to the main chamber through a flexible transfer system. The prep-chamber will have a fast load-lock of MBE evaporators and in situ calibration via a quartz microbalance, as well as LEED and an Ar ion gun. Also an efficient gas admission system and mass spectrometer will be required. An important point is the presence of an STM stage at the preparation chamber. The STM can be chosen to be robust and stable for variable temperature measurements in the synchrotron environment. It is a unique characterization tool for the preparation of well ordered overlayers of organic molecules, but also of many other systems of interest.