

## Applied crystallography at ALBA Synchrotron

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ALBA is a third generation synchrotron facility constructed and managed by the consortium CELLS (www.cells.es) and it includes a 3 GeV storage ring with a relatively low horizontal emittance, 4.6 nm×rad. ALBA synchrotron is the largest Spanish research infrastructure that started operation with official users in May 2012.

I will divide the talk in three parts: i) a succinct general description of the facility; ii) a brief overview of the operating beamlines and those under construction; and iii) a summary of applied crystallographic studies that are being carried out at our synchrotron.

I will start with a very brief description of our facility including milestones, staff structure, general parameters, and our accelerator complex: linac, booster and the storage ring.

Secondly, I will introduce our seven operating beamlines. 1) BL13-XALOC: macromolecular crystallography, 2) BL04-MSPD: high-resolution and high pressure powder diffraction, 3) BL11-NCD: non-crystalline diffraction for small (and wide) angle X-ray scattering experiments (SAXS/WAXS), 4) BL29-BOREAS: soft X-ray magnetic circular dichroism and scattering; 5) BL24-CIRCE: photoemission spectroscopy (with near ambient pressure capabilities, NAPP) and microscopy (PEEM), 6) BL22-CLAESS: X-ray absorption and emission spectroscopies, and 7) BL09-MISTRAL: soft X-ray full-field cryo-microscopy.

Three additional beamlines are being currently built. 8) BL01-MIRAS: infrared micro-spectroscopy, to become operational in November 2016; 9) BL20-LOREA: angle resolved photo-emission spectroscopy, to become operational in December 2018; and 10) BL-MICROFOCUS-MX: microfocus for macromolecular crystallography, which will become operational in 2020. A scheme of the ten beamlines are given in Figure 1.

Thirdly, I will describe selected crystallographic works that are being carried out at our beamlines. These studies range from single crystal investigations of macromolecules at BL13-XALOC, to powder diffraction studies at BL04-MSPD, or bio- small angle scattering at BL11-NCD.

BL13-XALOC has an optics design based on an in-vacuum undulator, a Si(111) channel-cut crystal

monochromator and a pair of mechanically bendable KB mirrors. This allows several operation modes including a focused configuration, where both mirrors can focus the beam at the sample position to 52 μm × 5.5 μm FWHM (H×V) and a defocused configuration that can match the size of the beam to the dimensions of the crystals. The endstation includes a high-accuracy single-axis diffractometer, a removable minikappa stage, an automated sample-mounting robot and a photon-counting detector that allows shutterless operation. Several examples of data collections and crystal structures will be presented.

BL04-MSPD powder diffraction beamline has a superconducting wiggler as photon source which allows a very broad energy range, 8-50 keV. The energy of the photons are selected using a Si(111) double crystal monochromator. Furthermore, MSPD has two endstations. The first endstation is devoted to high-resolution and high-speed powder diffraction. The detector system for high-resolution is a multycrystal analyzer setup coupled to point detectors, whereas the detector for high-speed data collection is a Mythen-II. Several examples of *in-situ* experiments will be presented. The second endstation is a microcrystal diffraction setup based on a KB mirror which results in a beam size close to 15 μm and a CCD detector system. Several types of experiments can be carried out including single-microcrystal like data collection in thin samples. However, this endstation is optimized for high-pressure powder diffraction studies in diamond-anvil-cells, DACs, where heating and cooling equipments are available (electrical resistance heating!). Examples of high-pressure studies using DACs will be presented.

Finally the capabilities of BL11-NCD for bio-SAXS will be presented. Here, it is possible to corroborate the structures determined by macromolecular crystallography of crystals for the same system(s) in solution. Aggregation effects as well as flexibility behavior, etc., may be characterized.

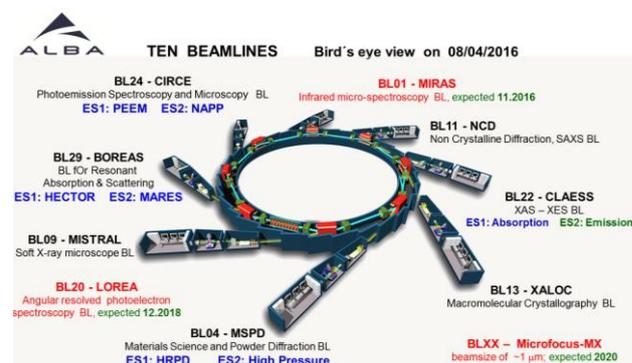


Figure 1. Overview of ALBA synchrotron beamlines as 08<sup>th</sup> of April, 2016.