Poster

Scientific opportunities for SSX in MX beamlines at ALBA

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ALBA is a 3-GeV synchrotron radiation facility located near Barcelona, Spain, servicing worldwide academic and industrial users with ten operating beamlines and four more in construction. Two of these beamlines are dedicated to macromolecular crystallography (MX): BL13-XALOC, a flexible beamline in operation since 2012, and BL06-XAIRA, a microfocus beamline currently under commission. Each of these two beamlines has a distinct and complementary role in ALBA's serial crystallography (SSX) program.

BL13-XALOC is a multipurpose MX beamline covering the 5.2 – 22 keV energy range, with photon fluxes up to $2.5 \cdot 10^{12}$ ph/s and a beam size adjustable between 50×7 μm^2 and 300×100 μm^2 [1]. The beamline is equipped with a high viscosity extrusion injector [2], which has already been available to users for several beamtime cycles. The injector has been successfully used to obtain high quality radiation-undamaged SSX data out of slurries of microcrystals (15 - 30 μm in size) from five different soluble proteins, at room temperature [3]. The transition from single crystal oscillation MX to SSX is highly facilitated thanks a three-axis motorized stage where the injector is mounted [4]. Noteworthy, time resolved SSX approaches have also been implemented, currently based on laser-controlled reaction activation [5], with other strategies being developed. In addition, the recent upgrade of the beamline detector to a Dectris Pilatus 3 X has reduced the acquisition time and unlocked studies of processes with time scales down to ~10 ms.

On the other hand, BL06-XAIRA microfocus beamline (4.0 – 14 keV), scheduled to host the first user experiments by October this year, is designed to provide a highly stable micrometric X-ray beam of 3×1 μm^2 FWHM at 1 Å wavelength, adjustable down to 1×1 μm^2 and up to at least 10×10 μm^2 [6], aiming to support a broad range of microfocus MX experiments. In addition to a vertical single-axis diffractometer for oscillation data collection from samples on pins, meshes and small chips, the beamline will be fitted with a dedicated fast sample rastering stage to optimally perform fixed-target SSX experiments from large chips. Another distinctive element of the beamline is a chamber enclosing the whole end station, which allows experiments to be performed either in air or in helium atmosphere, and both at room temperature or under cryogenic conditions. The helium environment can drastically reduce the background noise, thus increasing data quality for the whole energy range, but also prevents flux loss at low energies, providing the optimal conditions for anomalous phasing and elemental analysis experiments. Moreover, with the combination of a flux at sample position over $3 \cdot 10^{13}$ ph/s, provided by an inhouse-designed dual (Si(111) channel cut + double multilayer) monochromator, and a Dectris Eiger2 XE 9M photon-counting detector capable of acquiring data at frame rates of 1 kHz, the beamline will be able to host time-resolved SSX experiments in the millisecond regime.

These implementations at the MX beamlines are complemented with the microcrystal-growing facilities available at the synchrotron BioLab. This way, ALBA users are offered two serial data collection approaches as routine methods for room-temperature structure determination of proteins and their complexes.

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