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First Low-Background MX Experiments Using Closed-Circuit Helium Atmosphere in the XAIRA Beamline at ALBA

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The background of the diffraction patterns is one of the main limiting factors to the quality of macromolecular crystallography (MX) experiments, together with the radiation damage and the crystallinity and size of the crystals. In the last decade, the development of the photon-counting detectors has contributed to effectively reduce the background. Other strategies, such as the operation in vacuum or the use of helium to reduce X-ray scattering with air and maximize flux, have been shown to significantly improve the signal-to-noise ratio of diffraction images, especially at high resolutions [1-4]. However, such approaches are not widely spread due to the requirement for specific instrumentation and the difficulty of He manipulation, which compromise the use of the state-of-the-art and standard methods used in MX beamlines.
In response, XAIRA, the new microfocus MX beamline at the ALBA synchrotron light source, aims to deliver optimal diffraction images by enclosing the entire end-station in He atmosphere, including sample environment, cryostream and detector, while still maintaining compatibility with standard MX sample formats and with operation in air. The helium is recovered to an existing He purification plant nearby for sustainability and operation cost reasons. The diffractometer is based on a unique gas flow-bearing goniometer compatible with He and air, and supports fast oscillation experiments, raster scans and helical scans, while allowing a tight sample to detector distance of 70 mm. Both the detector and cryostream can use either helium or nitrogen gas. Micron-sized crystals will be localized by means of a double on-axis visualization comprising a commercial on-axis visualization system and an undrilled, high-magnification microscope for sample imaging at sub-micron resolution. X-ray-based raster scans and AI algorithms are also being developed to guide sample centering.
XAIRA is foreseen to ramp into user operation by end 2024 and aims to provide a highly stable, 3×1 µm2 FWHM size and high flux beam in the 4-14 keV range, to take further advantage of the use of He. A system of 11 interferometers pointing to the focusing optics and key diagnostics will monitor the vibrations and drifts to ensure the beam stability. The beamline optics has been presented previously [5] and includes a novel monochromator design with Si(111) channel-cut and double multilayer mounts, together with new mirror benders equipped with dynamical thermal bump and figure error correctors [6]. Here we present the first MX experiments, which take advantage of most of these instruments.
References
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I plan to submit also conference proceedings

Yes

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