SwissMX: Fixed Target vector scanning diffractometer for Serial Crystallography at SwissFEL

Claude Pradervand*, Isabelle Martiel, May Marsh, Ezequiel Panepucci, Thierry Zamofing, Jan Hora, Wayne Glettig, Meitian Wang, Robert Kälin, and Bill Pedrini

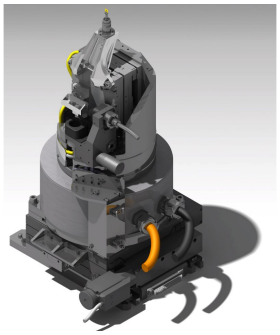
Paul Scherrer Institut, Switzerland

**claude.pradervand@psi.ch*

X-ray Free Electron Lasers (XFELs) are currently pushing the limits of protein X-ray crystallography for atomic-resolution structure determination of macromolecules beyond the possibilities offered at third generation synchrotron sources [1]. In order to study micrometer-sized crystals at an XFEL, two methods for sample delivery have emerged, either based on injectors for liquid or viscous media or on fixed targets. In the fixed-target method, the protein crystals are deposited on a solid support, which is scanned through the beam to expose new crystals at each pulse. To maximize the hit rate, efforts have gone in the direction of solid supports with grids or wells, on which the protein crystals are prepositioned [2], [3]. This allows scanning the crystals though the x-ray beam on a regular grid. This method is however not suited for all types of protein crystal preparations. Our approach is to offer also the possibility to use solid support membranes without wells, with the crystals in random position. The individual crystals can be pre-located and the solid support chip is then transferred, by an automated sample delivery system, to the diffractometer, where the crystals can be scanned in an arbitrary pattern to address the crystals at their random positions.

We designed and built a dedicated diffractometer that will make it possible to collect serially diffraction patterns at up to 100 Hz on many small crystals ($< 5\ \mu$m) by scanning the sample support in a continuous, arbitrary motion. It also allows the more traditional, synchrotron-like data collection modality by means of helical scans on large single crystals. The diffractometer installed inside a chamber, which allows operation not only in air but also in helium atmosphere, thus making measurements with photon energies down to 5.0 keV possible. Both room-temperature and cryogenic conditions are possible.

We present the design of the diffractometer and chamber and first measurements done at the Swiss Light Source.



SwissMX Diffractometer

References

[1] Schlichting, I., IUCrJ, 2, 246-255 (2015)

[2] Roedig, P., Nature Methods 14, 805-810 (2017)

[3] Oghbaey S., Acta Cryst. D72, 944-955 (2016)