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Convergent beam X-ray crystallography and 3-D diffraction imaging using multilayer Laue lenses

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Highly-converging X-ray beams created by multilayer Laue lenses (MLLs) [1] bring new opportunities for X-ray crystallography and 3D diffraction microscopy. Our recent MLLs achieve a numerical aperture (NA) of ~ 0.02 at a photon energy of 17.5 keV (or 0.71 Å wavelength), meaning that beam converges onto the focus over an angular range of 40 mrad or 1.3º. When the crystal is placed downstream of the focus, there is a correlation between position in the beam and the angle of incidence of a ray. The crystal selects Bragg reflections from the supplied range of angles, at particular locations of the crystal (slices, in the case of a single crystal). In this configuration, the diffraction data provides a mix of crystallography and (tomographic) microscopy. We are particularly interested in developing convergent-beam diffraction as a way to obtain fully-integrated Bragg reflections in single exposures (to reduce the number of patterns required in serial crystallography at free-electron laser sources) and to obtain structure factors of high accuracy by observing and accounting for spatial variations in crystals, such as their shape, strain, or defect structure. Additionally, using the mapping between position and incidence angle, 3-D microscopic images of the diffraction efficiency of the crystal was obtained from the same data set. The simple experimental setup and data collection strategy offers advantages such as ample operational space and easy adjustment of the spatial resolution by changing the geometry. The convergent beam diffraction (CBD) scheme, with further development in progress is potentially applicable to multi-scale structural or dynamics studies for both material and life sciences.

References

[1] Bajt, S. *et al.* X-ray focusing with efficient high-NA multilayer Laue lenses. *Light Sci. Appl.* **7**, 17162–17162 (2018).