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Coherent X-ray diffraction with a convergent beam

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With the development of improved multilayer Laue lenses (MLLs) [1] and sensitive wavefront diagnostics [2,3], it is now possible to focus X-ray beams at synchrotron radiation facilities and X-ray free-electron lasers to spot sizes of 5 nm or less. These are diffractive optics made by layer deposition, in which the layer period varies inversely with distance from the optical axis and the layers are wedged [4] to ensure that the tilt of the layers satisfies the Bragg condition. In this way, an MLL is the physical embodiment of the Ewald sphere. The convergence angle of these lenses can exceed 0.03 rad for a wavelength of 0.7 nm (17 keV) This convergence is often greater than the angular separation of Bragg peaks in a macromolecular crystal, which is equivalent to saying that the focal spot is smaller than the unit cell of the crystal. This creates several interesting opportunities for the study of the structure of macromolecular crystals. When the crystal is placed in the focus, Bragg peaks may overlap and interfere [6], but extremely short exposure times are required to avoid radiation damage, requiring snapshot diffraction using XFEL pulses. Indexing and classification algorithms could then be used to generate a ptychographic dataset [7] that is a function of crystal orientation and the location of the focus relative to the unit cell. Damage can also be avoided by placing the crystal in the beam diverging from the focus, allowing topographic imaging of the crystals and Bragg lines that give fully-integrated reflections. This approach also has benefits for crystals with unit cell dimensions that are smaller than the focus size. It enables a simplified approach for multi-Bragg ptychography and the characterisation of strain and defects at high resolution. Experimental results and analysis of convergent-beam diffraction from protein and inorganic crystals will be presented.

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