Crystal Structure Determination and Refinement from Serial Precession Electron Diffraction

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The success of precession electron diffraction (PED) in the field of electron crystallography can be measured by how its use has led to major technical breakthroughs for better crystallographic characterizations. For instance, its use on zone-axis electron diffraction patterns for crystal structure determination [1], which later was extended to the initial 3D electron diffraction data acquisition protocol [2], or for 4D-STEM applications such as phase, orientation and strain mapping [3, 4]. This presentation intends to show how PED can also be used as an advantageous tool in a serial crystallography experiment for improved crystal structure analyses.

Serial electron crystallography has gained attention during last years for the structure determination of crystalline compounds that are sensitive to the irradiation of the electron beam [5,6]. By recording a single electron diffraction pattern per crystal, indexing thousands to tens of thousands of such patterns, and merging the reflection intensities of the successfully indexed patterns, one can retrieve crystal structure models with strongly mitigated beam damage contributions [7]. The requisite of a high number of patterns is mandated by the proper sampling of partially integrated reflections as well as the reduction of the dynamical effects through the averaging across the serial dataset, becoming the technique's bottleneck if such acquisition is not done in a fully automated way. The use of precession accomplishes these two points in each pattern, leading to more uniform reflection intensities through the serial dataset and hence reduces the number of crystals to be measured. Furthermore, structure refinements based on the dynamical diffraction theory become possible due to the diffraction volume integration of beam precession, providing a novel approach for more accurate structure models. This presentation will demonstrate the advantage of precession through baryte as a proof-of-concept, and its potential application for metal-organic frameworks and small molecule organics. In this way, SerialPED will be presented as a new technique for reliable and precise crystal structure characterizations.

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