Poster Presentation

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Accurate structure refinement from 3D electron diffraction data

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Structure determination from electron diffraction data has seen an enormous progress over the past few years. At present, complex structures with hundreds of atoms in the unit cell can be solved from electron diffraction using the concept of electron diffraction tomography (EDT), possibly combined with precession electron diffraction (PED) [1]. Unfortunately, the initial model is typically optimized using the kinematical approximation to calculate model diffracted intensities. This approximation is quite inaccurate for electron diffraction and leads to high figures of merit and inaccurate results with unrealistically low standard uncertainties. The obvious remedy to the problem is the use of dynamical diffraction theory to calculate the model intensities in structure refinement. This technique has been known and used before, but it has not become very popular, because good fits could be obtained only for sufficiently perfect and sufficiently thin crystals. It has been shown recently on several zone-axis patterns [2] that the quality of the refinement can be improved by using precession electron diffraction. In the present contribution we demonstrate that the same approach can be successfully used to refine crystal structures against non-oriented patterns acquired by EDT combined with PED (PEDT in short). Because the PEDT technique provides three-dimensional diffraction information, it can be used for a complete structure refinement. Several test examples demonstrate that the dynamical structure refinement yields better figures of merit and more accurate results than the refinement using kinematical approximation.

[1] *U. Kolb, T. Gorelik, E. Mugnaioli, MRS Proceedings, 2008, 1184, 1184-GG01-05,* ***[2]*** *L. Palatinus, D. Jacob, P. Cuvillier, et al., Acta Cryst. A, 69, 171–188*

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