Increasing the Precision of Quantitative CBED Structure Factor Measurements

Philip Nakashima, *School of Physics and Materials Engineering, Monash University, Victoria 3800, Australia.* E-mail: Philip.Nakashima@spme.monash.edu.au

A new method of eliminating residual geometric distortions in convergent beam electron diffraction (CBED) patterns has been developed. It is integrated into quantitative CBED (QCBED) pattern-matching refinements of structure factors and significantly reduces uncertainties in experimental charge density measurements.

At present, a three- to fourfold improvement in structure factor measurement precision is reported in the case of corundum, over more conventional geometric distortion corrections employed in QCBED. This has resulted in a spread of multiple measurements of the same structure factor that is much smaller than the difference between different theoretical charge density models (density functional theory (DFT) and periodic Hartree-Fock (PHF) calculations) [1].

This new QCBED form shows heightened sensitivity to uncertainties in atomic coordinates, unit cell and atomic displacement parameters (ADPs). This is shown by introducing changes to these parameters and comparing resultant distributions of structure factor measurements using the new technique and parallel cycles of the more conventional form of QCBED (acting as a control).

Significant improvements to the precision of structure factor measurements at the higher order end of the QCBED range implies that merging QCBED and X-ray structure factor measurements will result in more reliable scale factor determinations for the latter and therefore, more accurate experimental charge density maps.

[1] Nakashima P.N.H., *J. Appl. Cryst.*, 2005, *in press*.

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