MS24-2-4 Dynamical Diffraction Simulations of Continuous-Rotation Electron Diffraction Data
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Abstract
Structure solution utilizing 3D-ED (three dimensional electron diffraction) has grown in interest since the turn of the 21st century. The interest and accessibility of the technique is due to the increase in computing power, TEM control, detector advances and method developments. However, the R–factor for ED refinements remain far above that of X–ray or neutron diffraction measurements. This is often referred to as the 'R-factor gap'. The cause of this problem is still not completely understood, however the most significant contributing factor is probably multiple scattering, which requires dynamical theory rather than the kinematic models appropriate for other methods such as X-ray diffraction.Here, we use Bloch-wave dynamical electron diffraction simulations using the f elix (Beanland et al., 2019) code to produce large–angle convergent beam electron diffraction (LACBED) patterns that correspond to a continuous rotation electron diffraction (cRED) experiment. In combination with experimental corrections to integrated intensities[1], we find significant reductions in R–factor when comparing experimental data with dynamical intensities rather than kinematical ones.

Fig. 1. Two examples of rocking curves in cRED data taken from a single crystal silicon (110) lamella. Most rocking curves are a simple peak like the $\bar{9}\bar{3}\bar{3}$ reflection in (a). A few rocking curves showed complex (dynamical) structure such as the 311 reflection shown in (b). Corresponding LACBED simulations for a specimen 170nm thick are shown in c) and d), with the nominal beam path marked as a red line and frame numbers marked in yellow. Intensity profiles along the red line give the rocking curves (e) and (f). Applying the angular range of the incident beam as a convolution to the simulation gives simulated rocking curves that are a good match to experiment.

References
Beanland, R., Evans, K., R¨omer, R. A. & Hubert, A. J. M., (2019). Felix bloch wave simulation:Source code. URL: https://github.com/WarwickMicroscopy/Felixx

Fig 1