MS24-1-3 Refinement parameters in dynamical electron diffraction
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Abstract
The structure factor equation elegantly captures the effect of atomic structure on diffracted intensities:
The only parameters are the Miller indices of the diffracted beam g = hkl, the atomic coordinates rj, scattering factor fj, and thermal factor Tj for all N atoms in the unit cell. In X-ray diffraction (XRD), the structure factor Fhkl is chosen to be the point of contact between theory and experiment, taking the diffracted intensity to be given by Ihkl = FhklF*hkl, where F*hkl is the complex conjugate of Fhkl. Other effects such as absorption, extinction, background, mosaicity, scaling, fluctuations in the incident X-ray beam intensity, Lorentz factors and polarisation are taken to be experimental issues, which can be corrected to obtain the 'true' diffracted intensity Ihkl.
In electron diffraction (ED) although the structure factor equation is still important, coupling between different diffracted beams and multiple scattering means that a calculated Ihkl is only approximated by FhklF*hkl, and can be very different when these dynamical diffraction effects are strong. This does not mean that diffracted intensities in ED are fundamentally unreliable – they can be calculated with reasonable accuracy, if the geometry is known to very high precision (<0.5 mrad) at all times (due the exquisite sensitivity of multiple scattering to orientation of the crystal). Furthermore, it is no longer possible to consider scattering effects such as extinction, absorption, background and mosaicity as experimental parameters and they must instead be brought into the calculation of a diffracted intensity.
As a result, the point of contact between experiment and simulation in a dynamical electron diffraction refinement should in principle be rather different to that of X-rays. Here, the experimental corrections in a continuous rotation electron diffraction (cRED) experiment are evaluated for crystals of silicon and tyrosine in comparison with dynamical electron diffraction simulations performed using the Bloch-wave method. (Fig. 1)

Structure Factor Equation

$$F_{hkl} = \sum_{j=1}^{N} f_j(\theta) T_j \exp\left(2\pi i \mathbf{g} \cdot \mathbf{r}_j\right)$$

Fig. 1