Oral presentation

The influence of multiple scattering, absolute structure, absorption and bonding on 3D-ED data

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Scattering mechanisms that are specific to electron diffraction (ED) have a noticeable effect on measured intensities, with no counterpart in other diffraction measurements such as X-ray and neutron diffraction where single scattering dominates. While this brings the opportunity to access information that is otherwise difficult to obtain, it also adds to the complexity of the analysis that is required for ED data.

In three-dimensional (3D) ED, where large numbers of diffracted intensities are collected from one or more crystals (for example during continuous rotation of the crystal) these effects change the statistical distribution of intensities, producing both increases and decreases for individual reflexions in comparison with the kinematic scattering model. For example, as noted by Palatinus[1], multiple scattering tends to reduce the intensities of strong reflexions and boost those of weak reflexions. Here, we are interested to discover whether absolute structure in acentric crystals, 'absorption' of electrons through thermal diffuse scattering (TDS) into a continuous background, and charge transfer between atoms also affect 3D ED data in characteristic ways. This is investigated using Bloch-wave simulations for materials of different symmetries and ranges of atomic number, using an absorptive potential to model TDS and a kappa model of changes in atomic radius due to charge transfer. We find that their influence is both significant and strongly coupled to the orientation of the crystal, emphasising the need to precisely establish the geometry of an electron diffraction experiment to obtain reliable results.

[1] Palatinus, L., Petricek, V. & Correa, C. A. (2015). *Acta. Cryst. A***71**, 235.