Analysing the frame scaling in the presence of appreciable dynamical diffraction effects of 3D ED data.

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With the advent of 3D Electron diffraction(3D ED) data acquisition and processing techniques, electron crystallography has garnered significant interest over the last few years for accurate structure solutions and refinements [1]. In data processing of 3D ED data, the reflection intensities obtained from each frame must be corrected for experimental effects such as absorption, changes in sample illumination, and to some extent radiation damage. One of the methods to achieve this is to have all the frames ideally on the same scale [2]. We analyzed the problem of frame scaling during the 3D ED data processing using the software PETS2 [3]. The scaling in PETS2 is done by least-squares minimization of the difference between measured and fitted intensity profiles. Following the formalism of Hamilton et al [4], a scale is determined for each frame and the individual reflections in the frames are corrected by dividing the measured intensity by its frame scale. During this scaling procedure, an apparent decrease in the frame scales is observed on the frames that contain diffraction patterns close to a low-index zone axis. This decrease is not related to an actual weakening of the diffraction signal; therefore, it is clearly an artifact coming from the special crystal orientation. We decided to investigate the origin of this effect to obtain proper frame scales.

We observed a significant difference between the measured and fitted reflection profiles close to the zone axis for strong reflections at low diffraction angles. (Figure 1). On the zone axis, the observed intensity drops below the expectation. This effect is not observed in the profiles of weaker reflections. This observation indicates that the reason for the mismatch is strong dynamical diffraction effects affecting strong reflections at the zone axis. Even though the number of affected reflections is small, they are strong outliers and significantly affect the overall scale. When these outliers are removed, the scaling of the zone-axis frames can be improved, and the drop in the scales is eliminated.

Fig1.a) A plot of frame scales of sample data collected with precession electron diffraction and processed in PETS2. The crystal passes through a zone axis around frame 43; b) Observed (blue circles) and fitted (orange diamonds) reflection profile of the reflection 420 as a function of the frame number.


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