**Oral presentation**

# Including mosaicity effects in the dynamical refinement against 3D ED data

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Crystal structure determination from 3D electron diffraction (3D ED) data must deal with the dynamical diffraction effects present whenever electrons interact with a crystal. Although it is possible to perform structure refinement without taking the dynamical diffraction theory into account (a procedure called kinematical refinement), the best results are obtained when the dynamical diffraction theory is used (dynamical refinement) [1,2].

The implementation of dynamical refinement described in [1] and used in all dynamical refinements so far assumes the crystal is perfect. The imperfections in real crystals lead to the deviation of the diffracted intensities from the perfect model and, thus, to difficulties in getting good fits with dynamical refinement.

To address this problem, a model for the dynamical calculation of diffracted intensities was developed that takes crystal imperfections into account. Describing the imperfections exactly is impossible in practice. Therefore, an approximate approach was developed based on the model of a mosaic crystal: an assembly of small ideal crystals which are mutually rotated and shifted.

The model includes two types of mosaicity (Fig. 1). One assumes that the mosaic blocks are so large that they span the whole crystal thickness. This is a good model, e.g., for a bent crystal. The intensities diffracted from several blocks are summed incoherently, and this type of mosaicity is, therefore, denoted *incoherent mosaicity*. The second mosaicity type describes the case when the mosaic blocks are stacked on top of each other when viewed along the beam. This model is called *coherent mosaicity* and is more appropriate for describing, e.g., dislocations and other microscopic defects. Both models were implemented in the computer program Dyngo, which performs dynamical calculations within the crystallographic computing system Jana2020 [3]. The main parameters of both types of mosaicity are the standard deviations of the orientation of the mosaic blocks from the average.

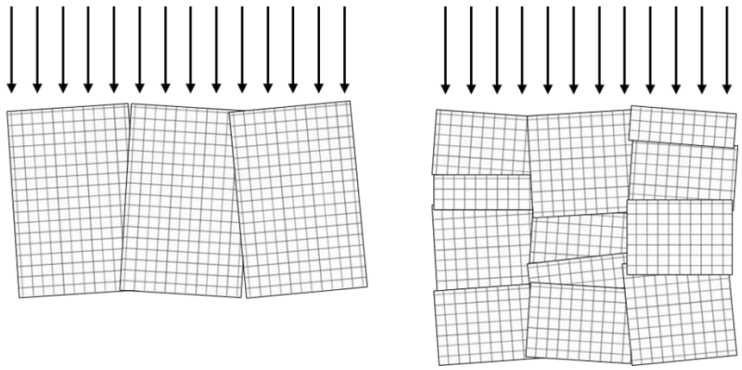

**Figure 1**. Incoherent (left) and coherent (right) mosaicity model.

The model was tested on the mineral epidote and amino acid L-alanine. Including the mosaicity in the refinement significantly improved the fit in both cases. For epidote, the R1(obs) value decreased from 10.80% to 6.94%. For L-alanine, R1(obs) decreased from 10.24% to 6.71%. In epidote, the dominant mosaicity effect was found to be the coherent mosaicity, while for L-alanine, the more important mosaicity type was the incoherent mosaicity.

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