Poster

Analysing the frame scaling and orientation matrix in the presence of appreciable dynamic diffraction effects utilizing simulated 3D ED data.

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With the advent of 3D Electron diffraction (3D ED) data acquisition and processing techniques, electron crystallography has emerged as a powerful technique for accurate structure solutions and refinements at the atomic level [1]. In data processing of 3D ED data, the reflection intensities obtained from each frame must be corrected for experimental effects and one of the methods to achieve this is to have all the frames ideally on the same scale. While processing the Quartz dataset in PETS2[2], we observed an apparent decrease in the frame scales on the frames that contain diffraction patterns close to a low-index zone axis (Fig. 1a). 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. To understand the effect of the dips in the scaling during processing, we used JANA2020 and Dyngo [3] to generate a simulated 3D ED dataset with all frames on the same scale. We then processed this data set in PETS2 as if it were an experimental dataset. The frame scales reproduced the dips observed in the experimental data (Fig.1b), showing clearly that the dips stemmed from the dynamical diffraction effects.

When reprocessing the simulated dataset in PETS2, we refined the orientation matrix with three different algorithms available in PETS2: (1) refine UB + cell, (2) refine cell from d, and (3) refine cell and distortions also to see the effect of the orientation matrix in the dynamical refinement. We then refined the data processed with PETS in Jana again. The idea was that if the processing in pets is error-free, we should obtain a very low R-factor. The refinement indeed yielded quite low R-factors. However, there was a difference in the R-factors depending on the orientation matrix from PETS2 (Table 1), showing that the slight variations in the orientation matrix refinement in PETS2 leads to an increase in R-factors. These increased R-factors could be reduced again by optimizing the frame orientation in JANA2020.

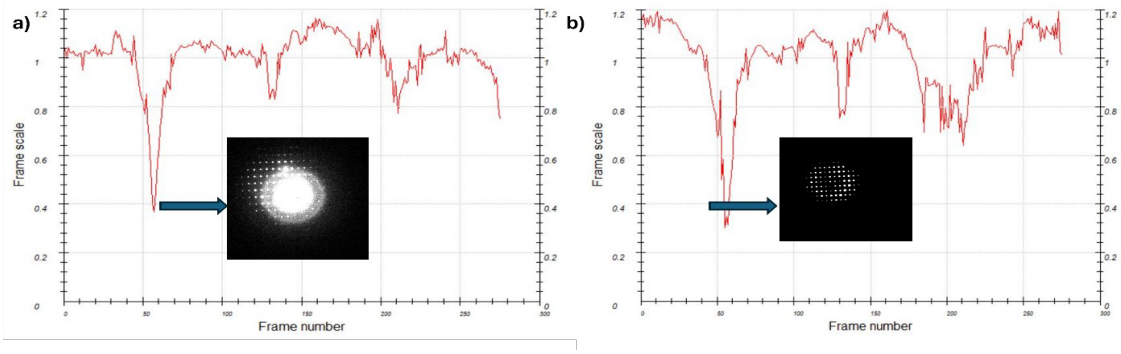

Fig.1 a) Frame scales of Quartz, continuous rotation dataset experimental. b) Frame scales of Quartz, continuous rotation dataset simulated

Table 1: Comparison of dynamical R-factors for simulated Quartz data set(precession), with differences in Orientation Matrix extracted from PETS2.

	Orientation matrix			
	Reference (simulated)	**Refine UB+cell**	**Refine cell from d**	**Refine cell and distortions**
R(all)	0.33	1.11	1.03	0.45
wR(all)	0.29	1.05	0.94	0.35

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This research was funded by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956099 (NanED – Electron Nanocrystallography – H2020-MSCA