Poster

Challenging shortcomings in the field of 3D ED: a new cross-platform solution for various experimental set-ups

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Structure models are crucial for the deeper understanding of properties of all sorts of crystalline materials and are usually derived by X-ray diffraction (XRD) methods. Due to the limits of single-crystal XRD experiments however, it becomes increasingly difficult to analyse crystals below the submicrometric border. On the other side, electron diffraction (ED) can be performed on much smaller particles, allowing us to take a dive into the nanoworld and investigate crystals too complicated or even impossible to grow beyond the nanometer scale. With the help of 3D ED protocols it became possible over the last two decades to collect and process a multitude of ED patterns, scanning most of the reciprocal space and allowing single-crystal structure analysis and refinement solely based on ED data [1].

Here we present the python-based program *eHermelin* enabling the collection of stationary and continuous 3D ED data, running in principle on many different camera and transmission electron microscope setups and thus making 3D ED available for a broader scientific community (see Fig. 1). The challenges arising from the long read-out times of CCD cameras are intercepted by introducing new data collection protocols, offering the possibility of stepwise-continuous and integrated beam tilting, benefiting the user from much better data quality compared to stationary data. Further, the combination of automatic crystal tracking routines with our acquisition protocols allows position controlled and fast low-dose experiments, studying even beam-sensitive materials.



Figure 1. Tackling several set-up challenges in the realisation of 3D ED experiments, our program *eHermelin* opens up a way for a broader scientific community.

 Mauro Gemmi, Enrico Mugnaioli, Tatiana E. Gorelik, Ute Kolb, Lukas Palatinus, Philippe Boullay, Sven Hovmöller and Jan Pieter Abrahams (2019). ACS Central Science 5(8), 1315-1329.