The Moving Diffraction Beam Problem on The Dual Imaging and Diffraction Beamline (DIAD)

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DIAD is a synchrotron beamline currently under construction at the Diamond Light Source (DLS). The beamline has been designed to enable combined diffraction and full field tomography experiments for in-situ processing, with switching between the two techniques at frequencies up to 10 Hz.

In order to allow diffraction and tomography in the same laboratory coordinate space at the sample position, DIAD uses some non-standard approaches to conducting diffraction experiments where the diffraction beam scans the sample and the detector remains stationary. This project aims to deliver two important requirements for DIAD to operate: the first is a reliable numerical approach for the processing of data in this unique scanning mode, the second is an accurate quantification of uncertainties that propagate through the diffraction data reduction method. Initial testing has verified an approach we now wish to formally follow.

Our approach to the numerical correction is to use the NeXus standard file tree (Konnecke, 2015) to track motor positions for the focusing Kirkpatrick-Baez (KB) mirrors (which defines the position of the focal spot on the sample) relative to a central (0,0) position on the sample. Following the calibration for the central position we then use the transformation tree to create a new set of detector pixel q-space values for every measurement point (representing a view of moving the world around the detector). This approach is computationally simple and is readily implemented within existing data analysis frameworks such as the DAWN data processing pipeline(Basham, 2015).

In this poster the preliminary results from the verification studies of our reduction method will be presented alongside results obtained from experiments. We have applied our method to several simulated diffraction patterns in DAWN to investigate the suitability of the proposed reduction. With these simulated data the initial calibration is near certain and movements of arbitrarily large distances can be corrected using our method. A more realistic 'real-life' scenario arises when the central calibration has a higher degree of uncertainty. In this case the distance over which the proposed correction solution is valid will be smaller. To investigate the useful bounds for our method a more representative simulation of diffraction patterns typical for DIAD were required. For this reason, in conjunction with the simulated results data reductions of real diffraction data for a moving source has been conducted on datasets collected on the I24 and B16 beamlines at DLS. On I24 a cerium oxide powder standard was measured and the detector was positioned perpendicular to the incident beam direction. From these data our approach has shown to be an effective way of correcting data at a detector at a swing angle of 0° with the source step scanning in 20 µm and 200 µm steps up to a distance of 1 mm in the vertical direction from the central calibration point. The set-up of I24 ensured that these data represented an optimal calibration set-up with six full rings of the powder standard being suitable for automated fitting. DIAD will be aiming to measure data at high tilt angles and this represents a less optimal position for calibration. A second experiment has been carried out on the B16 beamline at DLS where the detector was positioned at two positions (detector swing set to ~0° and ~45°). Measurements were conducted on a flat plate of silicon powder (NIST SRM 640d). During this experiment 200 µm step movements in both horizontal and vertical axes were used.

From this work it is expected that once the key geometrical and sample related parameters affecting the accuracy of the central diffraction location have been quantified, future users of DIAD will be more informed about the typical accuracy of the non-standard diffraction data collection strategy. Alongside this, advice on suitable sample geometries can also be provided to users.

References

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Konnecke, M. A. (2015). The NeXus data format. *J. Appl. Cryst., 48*, 301-305. doi:10.1107/S1600576714027575