MS16-2-1 Seed-skewness algorithm paired with instrument model refinement for signal detection in time-resolved Laue photocrystallography
#MS16-2-1

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Abstract
An efficient 1-dimensional seed-skewness (SS) algorithm adapted for X-ray diffraction signal detection along with signal integration procedure is presented. The method performs well for both the standard single-crystal X-ray diffraction data, as well as for time-resolved (TR) Laue photocrystallographic data collected at the Advanced Photon Source and European Synchrotron Radiation Facility. It enables efficient separation of signal from the background in single 1-dimentional data vectors, it is capable of determining small changes of reflection shapes and intensities resulting from exposure of the sample to laser light, and it is especially attractive for extracting relatively weak reflections from the background. The last is possible through the adjustment of “trust level” and “signal level” parameters in the algorithm.Performance of the algorithm is compared with the already reported Kruskal-Wallis test method[1]. Both methods perform competitively in terms of speed and determining the intensity of strong reflections, while the parameterization of the SS method allows for more efficient tuning of the algorithm to improve its sensitivity towards weak reflections.Furthermore, a novel instrument model refinement approach which allows to obtain precise detection parameters, such as detector distance and X-ray beam centre is presented. It is shown that relatively small adjustments in these parameters can significantly improve orientation-matrix matching procedures used during TR Laue data processing.Finally, a series of TR Laue experiments was carried out on selected model small molecule complexes, and the resulting data was processed with the use of the novel algorithm. The obtained results are presented and discussed.

References
[1] J. A. Kalinowski, et al., J. Synchrotron Rad. 2012, 19, 637.