

Seed-skewness algorithm for x-ray diffraction signal detection in the time-resolved synchrotron Laue photocrystallography

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Efficient 1-dimensional seed-skewness algorithm adapted for X-ray diffraction signal detection together with signal integration procedure are presented. The method was shown to work well for both the standard single-crystal X-ray diffraction data, as well as, for more specific photocrystallographic time-resolved Laue data collected at Advanced Photon Source and European Synchrotron Radiation Facility. It enables reasonable separation of signal from the background in single 1-dimensional data vectors, it is capable of determining small changes of reflection shapes and intensities resulting from exposure of the sample to laser light, and allows for extracting relatively weak reflections from the background. The last is possible through adjusting of “trust level” and “signal level” parameters in the algorithm. Otherwise, the procedure is objective and does rely only on skewness computation and its subsequent minimization, which enable the best possible background estimation. The intensities of strong reflections are determined comparably as via the Kruskal-Wallis test method, whereas weak reflections are more sensitive to the algorithm setting parameters. In turn, both methods estimate the background level equally-well.

Keywords: seed skewness; signal detection; integration; laue crystallography

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