



Contribution ID : 52

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Getting better statistics: variable count time data collection with large linear detectors.

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X-ray diffraction data are normally collected with a fixed count time (FCT) per step. With this data, the intensities of the diffraction peaks decrease with increasing angle, primarily due to the effects of atomic scattering factors, Lorentz-polarisation, atomic displacement parameters, and absorption. In diffractometers with point or small linear detectors, these changes can be counteracted by systematically varying the counting time as a function of diffraction angle. This variable-count-time (VCT) approach has been shown to produce data of superior quality for structure determination and refinement, as all peaks have similar intensities, allowing them to contribute equally to the analysis process.

With the advent of large linear detectors, the ability to change the counting time as a function of angle has been removed. A computer program has been written to construct a VCT diffraction pattern by the progressive summation of a series of conventional FCT diffraction patterns. This approach extends the collection of VCT data to large linear detectors, where traditional VCT is impossible. The program can also be used to simulate the construction process as an aid in experimental planning. An example application is given.

Level of Expertise

Experienced Researcher

Presenter Gender

Man

Pronouns

He/Him

Which facility did you use for your research

Australian Synchrotron

Students Only - Are you interested in AINSE student funding

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

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