

W0343

New Algorithms for Single Crystal Photometry. M.R. Pressprich, Avid Programming, Oregon, WI 53575 USA.

A new program has been developed for integrating single crystal reflection data collected with area detectors. A particular goal is accommodating marginal protein crystals.

The least squares positioning model fits the following geometrical degrees of freedom using analytical derivatives:

- Orientation of the crystal relative to the goniometer mounting bracket.
- Rotational misorientation of the detector relative to the incident beam.
- Rotational misorientation of the scan axis relative to the incident beam.
- Translational misalignment of the crystal, scan axis and detector.
- Unit cell angles and dimensions.

For a single domain crystal the model includes 19 refinable degrees of freedom. Parameters are coupled for refinement of twinned or split crystals.

The image background analysis applies Kalman filtering to separate signal from noise. Predicted background estimates are derived by in-plane Fourier analysis and corrections are made by statistically robust frame-to-frame updating of pixels beyond reflection domains.

Reflection intensities are determined from profile fitting and synthetic aperture (simple summation) photometry. Profile fitting implies that the reflection intensity is determined by adjusting a model profile to best fit the observed reflection shape after background subtraction, and is preferred for weak reflections in the presence of significant background. Synthetic aperture photometry involves summing the background corrected pixels lying within a model profile perimeter, and is generally favored for intense reflections. The extent of the reflection (its support) is determined from the beam spectrum and cross fire, the crystal size, and the detector point spread function.

This research was partially supported by Bruker AXS.