Poster Presentation

RigakuIntegrate : A New Single Crystal Integration Program

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RigakuIntegrate is a new single crystal integration program designed to increase integration accuracy by optimizing the reflection domain to exclude all but relevant elastic scattering. Instead of integrating over a shoebox domain, RigakuIntegrate sums over a tailored detector region that incorporates the known diffraction physics of each reflection as it passes through the Ewald sphere, combined with the known properties of the area detector. The reciprocal space reflections are modelled by ellipsoids that account for the crystal radius, beam crossfire, mosaicity, and wavelength dispersion. In case of laboratory sources separate ellipsoids are assigned to each of the $K\alpha1$ and $K\alpha2$ components. The passage of the reflection through the diffraction condition is modeled by the intersection of the ellipsoid(s) with the Ewald sphere, resulting in a set of ellipses. This set of intersection ellipses is then projected onto the detector plane along the scattered ray direction. Interaction with the detector sensor is modeled by appropriate convolution, resulting in reflection-specific integration domains over the surface of the detector. Results from crystals ranging in quality from exquisite (a charge density analysis of oxalic acid at 100K using a RAPID IP detector) to marginal (a highly mosaic and split crystal that refines to R1(all data) = 2.6% using a Pilatus detector) will be presented.

Keywords: integration program, single crystal diffraction, area detector