

AUTOMATED PROCESSING OF 2D POWDER DIFFRACTION DATA

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We present a software developed for automated processing of 2D powder diffraction datasets as for instance acquired with an image plate setup. For structural analysis, such 2D data usually is integrated to 2ϑ -scan powder diffraction patterns. Our software is capable to automate such integrations including a geometry correction and automated masking of intensities pixels not resulting from the powder sample (beam stop shadow, single crystal spots etc.). For the geometry correction, parameters obtained by the software Fit2D are used. Automated masking is achieved by an analysis of the Poisson distributed intensities of a ring of constant 2ϑ during which all pixels with intensities outside $n\cdot\sigma$ from the mean intensity are excluded. Especially single crystal spots, for instance resulting from diamonds of a diamond anvil cell as used for high-pressure investigations, are readily detected during this procedure. Such single crystal spots would otherwise yield peaks in the integrated datasets and aggravate data analysis. The intensity uncertainty s_I assigned to each $2J$ -bin is assumed to be given by the uncertainty of a Poisson-distributed quantity

$$s_I = \sqrt{\bar{I}/N}$$

where \bar{I} is the mean intensity on the ring of constant $2J$ used for the integration and N is the number of pixels contributing to this $2J$ -bin. Therefore, the decrease of reflection intensity with increasing $2J$ is partly balanced by a decrease in intensity uncertainty due to a larger number of contributing pixels on the rings of increasing radius. The integrated datasets may be directly output to files readable by the Rietveld packages GSAS or FullProf.

Furthermore, our software is capable to produce pole density figures from 2D datasets. For quantitative texture analysis with an image plate setup, diffraction patterns of various sample orientations are measured. The, due to texture, inhomogeneous intensity distributions on the Debye-Scherrer rings are corrected for background and absorption and converted to pole density figures. Naturally, such pole density figures obtained in transmission geometry are incomplete. With a statistical approach, the orientation distribution of the crystals in the sample can be reconstructed from such incomplete pole density figures.