

Oral Contributions

[MS11 - 04] Cracked Crystals: an Integration Challenge.

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Keywords: intensity integration; mosaic model;
assessment of results

A plate-shaped crystal of a niobium alkoxide was cracked into two fragments, related by a 1.7 ° rotation about an arbitrary axis. Different approaches to integrate the intensity data were investigated and the results are presented and discussed here.

- Box integration with Eval14 [1] using a single orientation matrix and relatively large isotropic mosaic model.
- Profile fitting with the Saint program [2] based on a single orientation matrix.
- Profile prediction as implemented in Eval15 [3]. Two orientation matrices are used, resulting in an HKLF5 type of reflection file for a “twin” refinement in SHELXL [4].
- Profile prediction with Eval15 using a single orientation matrix and an advanced mosaic model with two maxima for the individual fragments.

The last methods gives the best results as can be seen in the R-values and the residual densities.

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