Reciprocal Space Reconstruction from 2D Detector Data

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The combination of area detectors with synchrotron radiation sources or even standard laboratory sources is well suited for studies of disordered crystals showing weak satellite reflections or broad diffuse scattering phenomena. However, processing and visualisation of the experimental data requires advanced features covering non-integer indexed positions in reciprocal space (modulated structures, twinning) as well as a complete pixel-wise data processing to remap the irregular spaced experimental data to a regular grid. Moreover, synchrotron data usually need special post data collection processing features, eg. rescaling, background corrections.

Apart from tools for the latter processing features special emphasis was paid on the further software development for reciprocal space reconstruction. Since available programs (Estermann, 2001) strongly depend on dedicated experimental setups (rotation method), support for a four-circle diffractometer geometry (Eulerian, Kappa) has been implemented. Special versions are tailored to laboratory setups (Bruker-Nonius/Smart/Apex2, Bruker-Nonius/KappaCCD) with fixed geometry whereas other versions aim for typical synchrotron hard- and software setups (MarCCD/XDS) (Kabsch, 1999). Despite earlier versions for the latter combination, the programs now allow to define arbitrary diffractometer geometries and different raw data formats. All reconstruction programs include advanced pixel-wise corrections (polarisation, scaling, background, phosphor incidence).

Since the pixel-wise remapping of larger reciprocal volumes may result in huge temporary data sets (binary), new features include an optional binning to a regular grid with an automatic reciprocal axes rescaling and the definition of up to 25 arbitrary reciprocal planes of interest. The latter data are saved in text format to provide an interface to common plot programs (eg. Kuplot, Origin). All programs are mainly command line driven in order to allow for simple generation of automated scripts and cross-network use (Windows, Linux). A graphical user interface is currently under development.

The software tools were successfully applied in studies of diffuse scattering in REE-doped Ge-mullites, high/low-temperature and high-pressure experiments on relaxor ferroelectrics as well as tungstate-based laser host materials.

References

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