

KN13

Analyzing single-crystal diffuse scattering

R. Neder

Friedrich-Alexander-Universität Erlangen-Nürnberg - Erlangen (Germany)

Materials with a disordered structure still pose a challenge with respect to an accurate and complete description of their structure. The analysis of just the Bragg reflection intensities will yield a different structural model compared to the analysis of the diffuse scattering. While the former yields a structure projected into a single unit cell, the latter yields an structural model that allows to view the local deviations from the average structure.

In recent years experimental data collection of the diffuse scattering has become much less tedious. Compared to pure Bragg data the challenges imposed are due to the very different local intensity scales of Bragg and diffuse scattering, inversely coupled to very different extend in reciprocal space. New neutron based instruments like Corelli, new low background X-ray detectors and the rise of electron diffraction techniques allow a faster and better data collection strategy.

The data analysis has greatly benefited from the development of the 3D-Delta-PDF technique. This technique yields a much less difficult access to starting models and offers a good complementary approach to quantitative data analysis based on reciprocal space data.

The lecture will review the current experimental and data analysis developments.