Poster Presentations

[MS43-P01] Measurement and Reduction of Diffuse Scattering Data.

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Accurate measurement of Bragg intensities has become almost as simple as pushing a button. Provided that high quality crystals, modern diffractometers and state-of-the-art software are available the accuracy of a Bragg dataset rarely depends on a specific choice of experimental parameters. The opposite is true for measurements of diffuse scattering. Several factors complicate collection of high quality diffuse data sets. (i) The profiles of diffuse scattering data carry much more information about the real structure than the integral diffuse intensity. Experimental factors like scan mode, beam divergency and monochromaticity, crystal orientation relative to the oscillation axis etc. may, however, heavily bias the observed profiles and thus the results obtained from a diffuse scattering analysis. (ii) It is much more complicated to cleanly separate a broad diffuse signal from a broad background as opposed to the extraction of sharp Bragg reflections. (iii) Frequently, diffuse scattering maxima are beneath strong Bragg peaks what also complicates the separation of Bragg and diffuse scattering. (iv) Diffuse scattering is locally very weak and therefore very sensitive to any kind of systematic or statistical errors. (v) Bragg reflections are often heavily overexposed when weak diffuse scattering are measured with a high precision. Many detector types exhibit strong artefacts in such cases (e.g. 'bleeding') that may strongly overlap with the signal of interest. In this contribution we will demonstrate how such problems may be overcome with experimental or numerical, i.e. post-measurement, methods. We will also discuss the impact of not properly corrected experimental data on the structural results obtained from the diffuse scattering.

Keywords: diffuse scattering, data reduction, data collection