Oral Contributions

[MS43] "How to" session

Co-Chairs: Céline Mariette (FR), Hans-Beat Burgi (CH)

[MS43-01] 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. Pro¬vided that high quality crystals, modern diffrac¬tometers 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 scat¬tering. 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 diver¬gency and monochromaticity, crystal orientation relative to the oscillation axis etc. may, however, heavily bias the observed profiles and thus the re¬sults 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 reflec¬tions. (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 there¬fore 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 sig¬nal of interest. In this contribution we will demon¬strate 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 struc¬tural results obtained from the diffuse scattering.

Keywords: diffuse scattering, data reduction, data collection