

## Microsymposium

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*3D- $\Delta$ PDF: a routine method for analyzing diffuse scattering from single crystals.*

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With the recent advances in x-ray area detectors, high quality diffuse scattering became readily available. This allows to investigate local order in single crystals and provides invaluable information about real structures of disordered crystals, e.g. stacking probabilities, or structural dynamics. Recently, a new method called Three Dimensional Difference Pair Distribution Function (3D- $\Delta$ PDF) analysis was introduced [1]. It provides direct access to the short range order correlations and allows to investigate the diffuse scattering of both static and dynamic origin in a unified fashion. The method is similar to the powder PDF, but availability of three dimensional diffraction data provides several key differences. Firstly, it allows elimination of Bragg peaks and refinement of diffuse scattering alone which conveniently separates the investigation of average structure from investigation of ordering. Secondly, due to reduced overlap of PDF signals, the correlation coefficients at very long interatomic vectors become accessible. The 3D- $\Delta$ PDF analysis can be performed in the newly developed program Yell [2]. The program supports all types of correlations and contains a fast FFT-based method for diffuse scattering calculation, and the constraints of arbitrary arithmetic expressions.

[1] T. Weber, A. Simonov, *Zeitschrift für Kristallographie*, 2012, 227(5), 238-247., [2] Simonov A., Weber T. Yell <https://github.com/YellProgram/Yell/>

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