

## **New Developments in PDF Software: Automatic Processing and Complex Modelling**

Philip A. Chater\*, Dean S. Keeble, Michael T. Wharmby, Timothy C. Spain, Jacob Filik and Heribert Wilhelm  
Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 0DE, U.K.

XPDF is the new, independent side-station to the Extreme Conditions beamline I15 at Diamond Light Source. It is committed to the fast and reliable production of pair distribution function (PDF) data. Integrated data collection and analysis software has been developed which will perform automatic data processing to deliver real-time Bragg, total scattering and PDF data. 2-D scattering data from an area detector can be corrected, integrated to 1-D and processed to X-ray PDFs, all from within a single interface. The first half of this presentation will introduce this new PDF processing software, which is freely available in the DAWN software package [1].

The high throughput capabilities offered by beamlines such as XPDF means that new modelling tools are required to rapidly analyse the PDF data generated. There is also a drive towards investigating increasingly complicated systems with the PDF method. The second half of this presentation will illustrate some of the new PDF analysis methods available within the computer program TOPAS [2]. XPDF data will be used to demonstrate the speed and flexibility of TOPAS, using a variety of examples such as small-molecule rigid-body refinements and nano-structured multi-component systems.

[1] M. Basham, J. Filik, M. T. Wharmby, P. C. Y. Chang, B. El Kassaby, M. Gerring, J. Aishima, K. Levik, B. C. A. Pulford, I. Sikharulidze, D. Sneddon, M. Webber, S. S. Dhesi, F. Maccherozzi, O. Svensson, S. Brockhauser, G. Naray and A. W. Ashton, *J. Synchrotron Rad.* (2015) **22**, 853.

[2] A. A. Coelho, P. A. Chater and A. Kern, *J. Appl. Cryst.* (2015) **48**, 869.