

It's PDF, Jim, but not as we know it ...

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Pair Distribution Function (PDF) analysis, a method for obtaining local structural information, is obtained by Fourier transforming "total-scattering" (TS) data, which extends to high Q ($Q=4\pi\sin(2\theta/2)/\lambda$); data must also have a high signal-to-noise ratio (SNR) across the measurement range. For a long-time it was only possible to collect suitable TS-data at neutron and synchrotron sources. Dedicated beamlines have been developed, optimised for collection of TS-data: e.g. XPDF, Diamond[1]; ID15A, ESRF[2]; and P02.1, PETRA III/DESY[3]. Getting access to these facilities remains a challenge, in terms of competition for time and long lead times once beamtime is granted. Lab diffractometers have made major steps forward, with floor-standing systems allowing rapid collection of TS-data to $Q_{\text{Max}}\sim 21\text{\AA}^{-1}$ (using Ag-radiation), with good SNR. Such TS-data produce PDFs with good r -space resolution. Dedicated PDF systems remain out of reach for most research groups and many institutions.

The use of single crystal diffractometers for PDF studies, e.g. the D8 QUEST or D8 VENTURE is reported. These instruments require almost no changes to allow collection of TS-data, since they are often equipped with high-energy X-ray sources. Data processing to convert the 2D TS-data to a PDF is the same as that already used on beamlines.

We also report recent developments in lab XRD diffractometers yielding TS-data suitable for processing to PDFs, PDFs were collected on a D6 PHASER benchtop diffractometer, equipped with a Mo-K α source. Data were collected in capillary-transmission and reflection Bragg-Brentano geometries. All PDF data have been processed using DIFFRAC.EVA[4].

The presentation will show that using modern diffractometers, can significantly ease access to the technique, allowing more researchers to gain insights into the local structure of their samples.

[1] P.A.Chater et al., *Acta Cryst.*, A73, C69

[2] G.B.M.Vaughan *et al.*, *J. Synchrotron Radiat.*, 27, 515

[3] A.-C.Dippel *et al.*, *J. Synchrotron Radiat.*, 22, 675

[4] M.T.Wharmby et al., in preparation.