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PDFgetX2: a GUI driven program to obtain the pair distribution function from X-ray powder diffraction data

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1. The crystallographic problem

The pair distribution function (PDF) reveals directly in real space the inter-atomic distances in a material. Recent applications have proved the PDF technique as a powerful local structural probe of nanostructured materials (Egami & Billinge, 2003; Billinge & Kanatzidis, 2004), as well as its traditional use to study liquids and glasses (Furukawa, 1962; Wright, 1998). The experimental PDF is obtained by a sine Fourier transformation of the total-scattering structure function $S(Q)$, where Q is the magnitude of the scattering vector. To obtain the $S(Q)$ from raw scattering intensities many corrections have to be made to account for various instrument and sample effects. Adding to this complexity, most existing X-ray data PDF analysis softwares are menu driven and less user-friendly. Reproducing an earlier data analysis has been difficult because data processing parameters are usually kept in the notebook other than with the data. Cross-platform compatibility has also been an issue.

2. Method of solution

In program PDFgetX2, a user-friendly graphical user interface (GUI) has been built to facilitate user interactions with data. Standard corrections (Egami & Billinge, 2003) due to background subtraction, sample absorption, polarization, Compton intensities are available. Particularly, for the recent RA-PDF development (Chupas *et al.*, 2003), oblique incident angle correction and and empirical energy dependence of the detection efficiency are also implemented. Standard uncertainties due to finite counting statistics are estimated and propagated in all steps. The final $S(Q)$ and $G(r)$ data files are multiple-column ASCII files with the processing parameters in the header. The $S(Q)$ data also contain the Faber-Ziman coefficients for all partial structure factors as additional columns. The $G(r)$ file format is compatible with the PDF modeling programs PDFFIT and DISCUS (Th. Proffen & Billinge, 1999; Th. Proffen & Neder, 1997). The interactive data language (IDL[1]) is chosen as the software environment, ensuring cross-platform compatibility. In comparison with our menu driven program PDFgetX (I.-K. Jeong *et al.*, 2001) (no longer supported by us), the PDFgetX2 offers numerous new features and expanded capabilities.

3. Software and hardware environment

The commercial IDL licensed distribution (version 6.0 or higher), or the freely downloadable IDL Virtual Machine (IDL^{VM}), is the only prerequisite to run PDFgetX2. The IDL^{VM} is available from the download section of the IDL website http://www.rsinc.com/download/. Platforms supported by IDL include Linux/UNIX, WINDOWS, and MACINTOSH. No specific hardware is used by PDFgetX2. Installation of IDL may use up to 200 MB hard disk space, while the current PDFgetX2 distribution takes about 17 MB disk space.

4. Program specification

Program PDFgetX2 should run in the same way on all supported platforms as the same source is used. The look and feel of the GUI may vary slightly. The program offers flexible choices of data corrections. Essentially all processing parameters are accessible from the GUI. Most intermediate data during correction steps can be directly visualized for quick problem diagnosis. The $S(Q)$ and $G(r)$ data are automatically saved by default.

5. Documentation and Availability

A short tutorial with example data sets can be found in the PDFgetX2 manual that is distributed with the main program, which also includes a complete reference guide. Program executable and related help files are downloadable from PDFgetX2 web page at http://www.pa.msu.edu/cmp/billinge-group/programs/PDFgetX2/.

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References

Billinge, S. J. L. & Kanatzidis, M. G. (2004). *Chem. Commun.* pp. 749–760.

Chupas, P. J., Qiu, X., Hanson, J. C., Lee, P. L., Grey, C. P. & Billinge, S. J. L. (2003). *J. Appl. Crystallogr.* **36**, 1342–1347.

Egami, T. & Billinge, S. J. L. (2003). *Underneath the Bragg Peaks: Structural analysis of complex materials*. Oxford, England: Pergamon Press, Elsevier.

Furukawa, K. (1962). *Rep. Prog. Phys.* **25**(1), 395–440.

I.-K. Jeong, Thompson, J., Turner, A. M. P. & Billinge, S. J. L. (2001). *J. Appl. Crystallogr.* **34**, 536.

Th. Proffen & Billinge, S. J. L. (1999). *J. Appl. Crystallogr.* **32**, 572–575.

Th. Proffen & Neder, R. B. (1997). *J. Appl. Crystallogr.* **30**, 171–175.

Wright, A. (1998). *Glass Physics and Chemistry*, **24**, 148–179.

[1] IDL is a registered trademark of Research Systems, Inc. for their Interactive Data Language software

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