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computer program abstracts

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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 interatomic distances in a material. Recent applications have proved the PDF technique to be a powerful local-structure probe of nanostructured materials (Egami & Billinge, 2003; Billinge & Kanatzidis, 2004), in addition to 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 $S(Q)$ 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 software is menu driven and not particularly 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 the program *PDFgetX2*, a user-friendly graphical user interface (GUI) has been built to facilitate user interaction with the data. Standard corrections (Egami & Billinge, 2003) due to background subtraction, sample absorption, polarization and Compton intensities are available. In particular, for the recent RA-PDF development (Chupas *et al.*, 2003), oblique incident-angle correction and the 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* (Proffen & Billinge, 1999; 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* (Jeong *et al.*, 2001) (no longer supported by us), *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*. 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 MByte hard-disk space, while the current *PDFgetX2* distribution requires about 17 MByte.

4. Program specification

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 arising 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 reference guide. Executable and related help files are downloadable from the *PDFgetX2* Web page at http://www.pa.msu.edu/cmp/billinge-group/programs/PDFgetX2/.

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

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