PDF Analysis of Crystalline and Amorphous Materials on a Home Laboratory Diffractometer

Joseph Ferrara[1], Pierre Le Maguerès[1], Christian Schürmann[2], Mathias Meyer[3], Jakub Wojciechowski[2], Simon Bates[1]

[1]Rigaku Americas Corp, The Woodlands, United States of America;
[2]Rigaku Europe SE, Frankfurt, Germany;
[3]Rigaku Polska Sp. z o. o, Wrocław, Poland;

joseph.ferrara@rigaku.com

There is no question that atomic pair distribution function analysis has had a profound impact on the analysis of crystalline and amorphous materials[1]. As a complement to the use of synchrotron sources for collecting PDF data, we have explored the use of home laboratory-based single crystal diffractometers to analyze both crystalline and amorphous materials. In order to generate the most useful reduced radial distribution functions, G(r), we have found it necessary to modify existing code in CrysAlis^{Pro}[2] and develop new code to generate G(r) data for refinement in PDFgui[3]. In this presentation we will explore the collection and analysis of total scattering data on both crystalline and amorphous materials with wavelengths readily available to home laboratory systems.

[1] Underneath the Bragg Peaks: Structural Analysis of Complex Materials, T. Egami and S. J. L. Billinge, Elsevier, Amsterdam, 2012, ISBN: 978-0-08-097133-9.

[2] Rigaku Oxford Diffraction, (2021), CrysAlisPro Software system, version 1.171.41.64, Rigaku Corporation, Wrocław, Poland.

[3] C. L. Farrow, P. Juhás, J. W. Liu, D. Bryndin, E. S. Božin, J. Bloch, Th. Proffen and S. J. L. Billinge, PDFfit2 and PDFgui: computer programs for studying nanostructure in crystals, J. Phys.: Condens. Matter, 19, 335219 (2007)

Keywords: PDF, total scattering