Methods and Tutorials – Powder Diffraction

Rietveld analysis

- Background material

McCusker L. B., Von Dreele R. B., Cox D. E., Louërd D. and Scardi P., "Rietveld refinement guidelines", *Journal of Applied Crystallography*, **32**, 1, 36-50 (1999).

Dinnebier R.E., Leineweber A., Evans J. S. O., "Rietveld Refinement: Practical Powder Diffraction Analysis using TOPAS" De Gruyter (2019).

Toby B. H., "R factors in Rietveld analysis: How good is good enough?", *Powder Diffraction*, **21**, 1, 67-70 (2006).

- Tutorials and Manuals:

Data reduction
Data Reduction (POWGEN data)
Accessing autoreduced data and combining data (HB-2A data)
(OLD WAY NO LONGER SUPPORTED: Data reduction instructions)
Instruction videos for Powder data reduction. (HB-2C data)
Manuals for Powder data reduction. (HB-2C data)

Data Analysis
Modern Methods in Rietveld Refinement and Structural Analysis School (Exercises on refining X-ray and neutron data): https://sites.google.com/a/stonybrook.edu/mmrrsa-portal/past
TOPAS http://community.dur.ac.uk/john.evans/ta_tutorials/TA-Tutorials.html John Evans' Topas tutorial webpage

(POWGEN data)

Mantid Mantid Tutorial - Finding Structural Change from Event Data Peter Peterson
FullProf Fullprof refinement example
GSAS & EXPGUI GSAS/EXPGUI refinement example
GSAS-II GSAS-II joint X-ray/neutron refinement using 11BM and POWGEN data
TOPAS TOPAS refinement example

(NOMAD data)

FullProf Fitting-Data-in-Fullprof
GSAS & EXPGUI Fitting-Data-in-GSAS
GSAS-II Fitting-Data-GSAS-II
TOPAS Fitting-Data-in-TOPAS
JANA2006 Fitting-Data-in-JANA2006-Bank4 Fitting Data-in-Jana2006-Fourbanks

(HB-2A data)

FullProf Rietveld Refinement of HB-2A Data Using FullProf Software

- Software

TOPAS http://www.topas-academic.net/

TOPAS-Academic is a Windows based general non-linear least squares system driven by a scripting language. A Rietveld program for laboratory x-ray diffraction, synchrotron, single crystal, and neutron fixed wavelength and TOF data.

GSAS II https://subversion.xray.aps.anl.gov/trac/pyGSAS

Python project for determination of crystal structures using both powder and single-crystal diffraction with extensive visualization capabilities.

FullProf https://www.ill.eu/sites/fullprof/

Crystallographic programs *mainly* developed for Rietveld analysis of neutron (constant wavelength, time of flight, nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle 2theta.

JANA http://jana.fzu.cz/

Crystallographic Computing System for Standard and Modulated Structures.

Structure solution and refinement of powder and crystal / magnetic structures (CW and TOF neutron).

GSAS & EXPGUI https://www.ncnr.nist.gov/xtal/software/downloads.html

Software package to fit structural models to x-ray and neutron diffraction data. It can be used with both single-crystal and powder diffraction data (Rietveld analysis). EXPGUI is a Graphical user interface to GSAS.

Notes - FullProf and GSAS & GSAS-II are Rietveld refinement packages for determination of nuclear and magnetic structures as well as other kind of materials.

Total scattering analysis

- Background material:

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

Neder R., Proffen T., "Diffuse Scattering and Defect Structure Simulation", Oxford University Press, 2008 (book).

Billinge S. J. L., Levin I., "The Problem with Determining Atomic Structure at the Nanoscale", *Science*, **361**, 561-565 (2007).

Billinge S. J. L., "The rise of the X-ray atomic pair distribution function method: A series of fortunate events", *Philosophical Transactions of the Royal Society A Mathematical, Physical and engineering sciences*, **377**, 2147, (2019).

Tucker M. G., Keen D. A., Dove M. T., Goodwin A. L., Hui Q., "RMCProfile: reverse Monte Carlo for polycrystalline materials", *Journal of Physics: Condensed Matter*, **19**, 33, 335218 (2007).

Keen D. A., Goodwin A. L., "The crystallography of correlated disorder", *Nature*, **521**, 303–309 (2015).

Keen D. A., "Total scattering and the pair distribution function in crystallography", *Crystallography Reviews*, **26**, 3, 141–199 (2020).

Keen D. A., "A comparison of various commonly used correlation functions for describing total scattering", *Journal of Applied Crystallography*, **34**, 2, 172–177 (2001).

Peterson P. F., Olds D., McDonnell M. T., Page K., "Illustrated formalisms for total scattering data: a guide for new practitioners", *Journal of Applied Crystallography*, **54**, 1, 317–332 (2021).

Playford H. Y., Owen L. R., Levin I., Tucker M. G., "New insights into complex materials using Reverse Monte Carlo modeling", *Annual Review of Materials Research*, **44**, 429-449 (2014).

Petkov V., "Nanostructure by high-energy X-ray diffraction", *Materials Today*, **11**, 11, 28–38 (2008).

Proffen T., "Analysis of disordered materials using total scattering and the atomic pair distribution function", *Reviews in Mineralogy and Geochemistry*, **63**, 255–274 (2006).

Proffen T., Billinge S. J. L., Egami T., Louca D., "Structural analysis of complex materials using the atomic pair distribution function - A practical guide", *Zeitschrift fur Kristallographie*, **218**, 2, 132–143 (2003).

Olds D., Saunders C. N., Peters M., Proffen T., Neuefeind J. N., Page K., "Precise implications of real-space PDF modeling from effects intrinsic to modern time of flight neutron diffractometers", *Acta Crystallographica Section A*, **74**, 293-307 (2018).

Olds D., Wang H. W., Page K., "DShaper: An approach for handling missing low-Q data in pair distribution function analysis of nanostructured systems", *Journal of Applied Crystallography*, **48**, 1651–1659 (2015).

- Tutorials and Manuals:

  Fourier Information (NOMAD data)

  Data Reduction

  (NOMAD data)

  Addie How to Post Process Data with Addie

  Addie How to View Bragg Patterns with Addie

  Addie How to View and Analyze Total Scattering Patterns with ADDIE

  Data Reduction Manuals (NOMAD data)

  Data Reduction (POWGEN data)

  Data Analysis

  TOPAS PDF Fitting of SnO_2 and SnO_2/MoO_3 mixture John Evans' Topas tutorial webpage

  PDFgui Fitting-Data-in-PDFgui (NOMAD data)

  2019 PDFgui tutorials here

  DiffPy Fitting-Data-in-DiffPy-CMI (NOMAD data)

  ADD2019 DiffPy-CMI workshop materials: *https://github.com/diffpy/add2019-diffpy-cmi*

  RMCProfile: (http://www.rmcprofile.org/Tutorial)

- Software

PDFgui https://www.diffpy.org/products/pdfgui.html

Small box modeling

PDFgui is a convenient and easy to use graphical front end for the PDFfit2 refinement program. It is capable of full-profile fitting of the atomic pair distribution function (PDF) derived from x-ray or neutron diffraction data. It comes with built in graphical and structure visualization capabilities.

Topas Academic http://www.topas-academic.net/

RMCProfile www.rmcprofile.org

Big box modeling

Reverse Monte Carlo (RMC) for crystalline and disordered materials. This version of RMC can determine the local structure of crystalline materials while still being capable of analyzing disordered systems.

DISCUS/DIFFEV https://github.com/tproffen/DiffuseCode/releases

Multi-level/ Complex Modeling

http://tproffen.github.io/DiffuseCode/

Addie https://github.com/neutrons/addie

ADDIE stands for **AD**vandced **DI**ffraction **E**nvironment, a data reduction application for total scattering powder diffraction data.

Diffpy http://www.diffpy.org/

DiffPy - Atomic Structure Analysis in Python

Free and open-source software project to provide python software for diffraction analysis and the study of the atomic structure of materials.

fullRMC https://bachiraoun.github.io/fullrmc/

fullrmc which stands for FUndamental Library Language for Reverse Monte Carlo is different than traditional RMC but a stochastic modelling method to solve an inverse problem whereby an atomic/molecular model is adjusted until its atoms position have the greatest consistency with a set of experimental data.

DISSOLVE https://github.com/disorderedmaterials/dissolve
A simulation tool for the interrogation of neutron scattering data, typically total neutron scattering data. It builds on the techniques established in the Empirical Potential Structure Refinement (EPSR) method by Soper.