TECHNICAL REPORT

Inventory of data reduction and analysis software used in high-energy X-ray research at PETRA III (WAXS, SAXS, GIWAXS, GISAXS, PDF)

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“Inventory of data reduction and analysis software used in high-energy X-ray research at PETRA III (WAXS, SAXS, GIWAXS, GISAXS, PDF)”
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Preface

This inventory catalogs the software programs that have proven to be useful to the Swedish research community that conducts research at the PETRA III synchrotron, including the PETRA III Swedish Materials Science beamline.

Based on publications from 2018, the inventory categorizes the various software programs used in research as either data reduction software for 2D area detector X-ray scattering images or data analysis software for WAXS, SAXS, GIWAXS, GISAXS, and PDF.

Each software program has a short description of its functionality, a note of its developer, links to the original publication describing the scientific method that the software is based upon, as well as the site for downloading the software program.

Contents

1. Introduction

For synchrotron X-ray experiments such as wide-angle X-ray scattering (WAXS) and small-angle X-ray scattering (SAXS), the data processing procedure is generally divided into two steps: data reduction and data analysis. Since the X-ray scattering patterns are mostly collected using a two-dimensional detector, data reduction is a routine that integrates the two-dimensional scattering intensity image into a one-dimensional pattern. This one-dimensional pattern is then assessed by data analysis routines to extract structural information about the materials under investigation.

The data reduction and data analysis steps are generally performed using different software routines. A number of data reduction software packages have been developed mainly by the different synchrotron X-ray sources, such as Advanced Photon Source (APS), European Synchrotron Radiation Facility (ESRF) and PETRA III (Positron-Elektron-Tandem-Ring-Anlage).

High sampling rate synchrotron experiments using high-brilliance X-rays collect a large amount of data, which is pushing the development of software for data reduction and analysis. Specifically, online data reduction and analysis in real time become important to adjust the experimental parameters interactively during the measurements.

Since two-dimensional area-detectors are widely used for WAXS (also known as X-ray diffraction, including both powder XRD and single-crystal XRD), SAXS, grazing-incidence WAXS (GIWAXS), GISAXS, etc., the data reduction software needs to be compatible with the different instruments and techniques. The data reduction software has three main functions: detector geometry calibration (calibrate detector orientation and position using calibrants), mask creation (define the image areas of interest for the subsequent integration) and azimuthal integration (the averaging of pixel intensities with the same Q or 2θ value in some chosen angular sector).

A variety of software packages have been developed for data analysis of synchrotron X-ray data on different types of materials using different techniques. The variety and development pace of software and detectors however sometimes causes compatibility problems between the data reduction software and data analysis software because the output file of data reduction works as the input file for data analysis. If you face this issue, consulting the beamline scientists at the specific beamline of the particular radiation source that you have used is always helpful. In some cases however you may need to write your own software routines e.g. develop a data convertor program to solve any compatibility problems.

Since a multitude of software programs have been developed for the various techniques based on high-energy X-rays, it is challenging to include all of them here. Instead, this report aims to collect the most commonly used software at the Swedish Materials Science beamline or by Swedish users at PETRA III.

2. Sources and methods

This inventory is primarily intended to provide a straightforward introduction to the software options that have proven to be of use to the Swedish research community who conduct research at the PETRA III synchrotron, especially the Swedish Material Science beamline.

The method therefore firstly identified relevant information sources, namely publications that cited the use of:

- The PETRA III Swedish materials science beamline (P21.1 and P21.2) in the calendar years 2019[1], 2020, 2021 and the first quarter of 2022
- All other PETRA III beamlines, which had an author affiliated with a Swedish university, in the years 2018, 2019 and 2020.

From DESY's DOOR system, a total of 198 publications were identified as sources of information.

The publications were then assessed to identify:

- The PETRA III beamline, the associated X-ray measurement technique, used in these publications. These are illustrated in Figures 1-4 below.
- The data reduction and data analysis software packages that were used in the research

We then went on to identify:

- The software developer
- The original reference describing the scientific and technical theory and methodology that was used to develop the software
- Official websites where the software is further described and can be downloaded
- Additionally, we determined whether the software was freeware or requires a license[2]

For each of the identified software programs, this information is reported in Sections 3–7. Section 3 catalogues the identified data reduction software programs for 2D area detector X-ray scattering images using WAXS and SAXS instrument configurations. Sections 4–7 catalogue the identified data analysis software programs for 2D area detector X-ray scattering images using WAXS and SAXS instrument configurations, WAXS, SAXS, GISAXS, GIWAXS, and PDF.

[1] The Swedish Materials Science beamline at PETRA III first became operational during 2019.

[2] We use the term freeware to indicate that the software can be used, without incurring a fee, for non-commercial purposes. Many software developers however prohibit using their programs for research that is conducted for commercial purposes. Other developers have therefore produced software programs for commercial research use. Such software mostly incurs a fee as part of the licensing agreements. Nonetheless, even freeware has terms and conditions for its use. It is therefore emphasized that users are responsible for ensuring that their use of a program is compliant with licensing or other terms and conditions that are stipulated by the developer (see also Section 9).

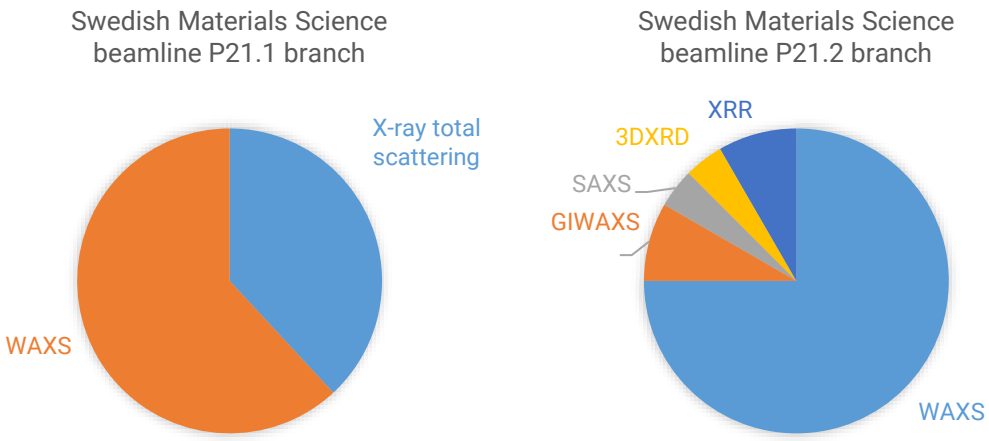

Figure 1. Pie charts of the experimental techniques used in the 47 scientific articles that involved experiments at the two branches of the PETRA III Swedish Materials Science beamline during the period 2019-Q12022.

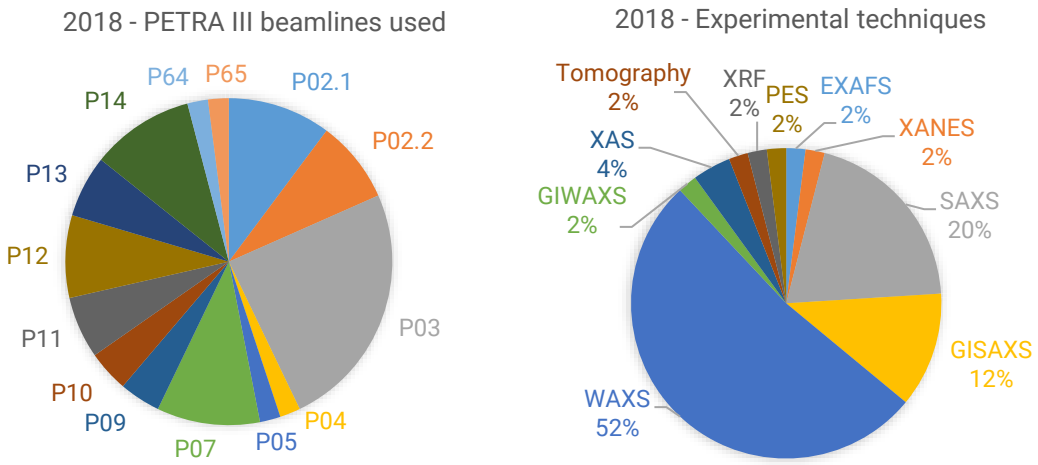

Figure 2. Pie charts of the PETRA III beamlines and experimental techniques that were used in the 60 scientific articles with Swedish (co)authors which were published in 2018.

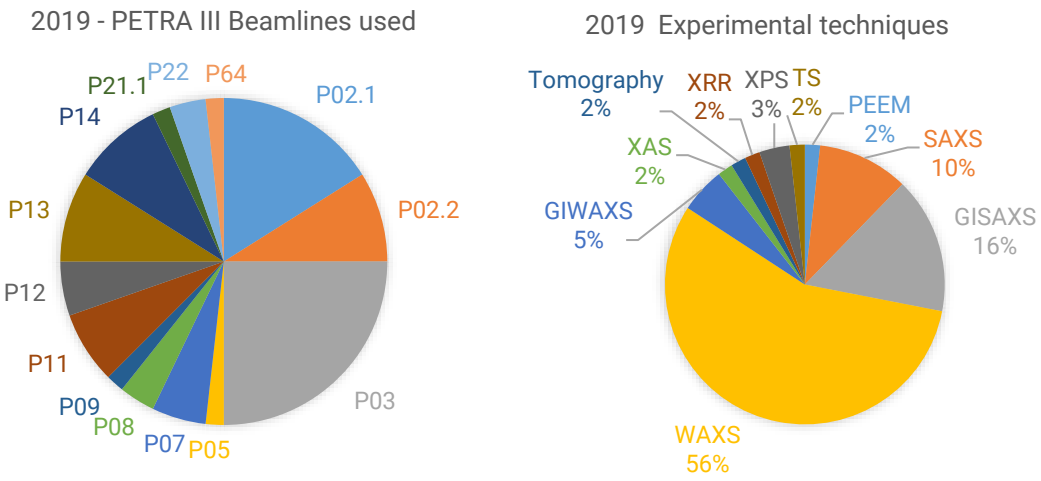

Figure 3. Pie charts of the PETRA III beamlines and experimental techniques that were used in the 60 scientific articles with Swedish (co)authors which were published in 2019.

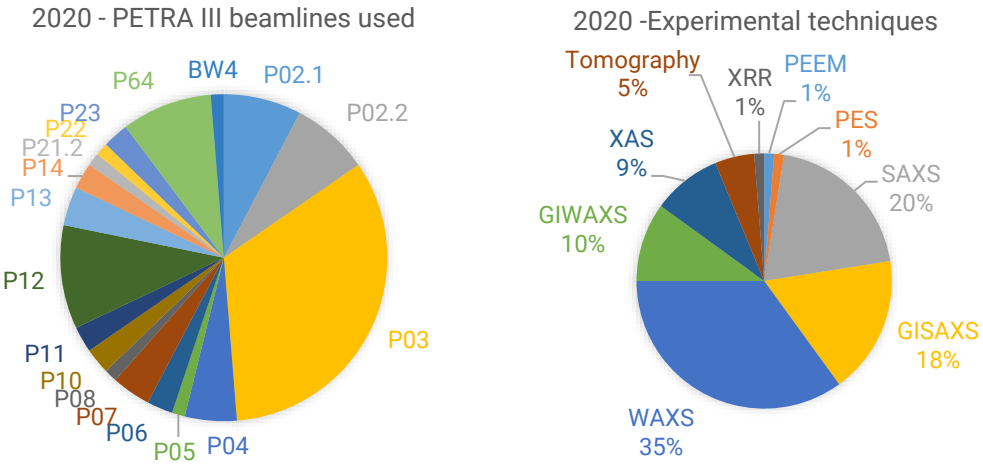

Figure 4. Pie charts of the PETRA III beamlines and experimental techniques that were used in the 88 scientific articles with Swedish (co)authors that were published in 2020.

3. Data reduction software for 2D area detector X-ray scattering images: WAXS and SAXS

The data reduction software programs identified from the sources described in Section 2 are as follows.

Software program	Developer	Freeware or licence	Techniques
Dioptas	APS	Freeware	WAXS
PyFAI	ESRF	Freeware	SAXS, WAXS
DPDAK	PETRA III	Freeware	SAXS, WAXS, GISAXS
Nika	APS	Freeware	SAXS, GISAXS, WAXS, GIWAXS
Datasqueeze	U. Pennsylvania	Freeware	WAXS, SAXS
Fit2D	ESRF	Freeware	WAXS, SAXS

Dioptas

Dioptas is a Python-based program, with a GUI, for fast analysis of powder X-ray diffraction images. Dioptas has capabilities for detector geometry calibration, creating masks, data reduction/integration, pattern overlay, background subtraction and showing phase lines, etc. Dioptas can be used for online data processing and post experiment data analysis for both synchrotron and laboratory-based XRD data. For azimuthal integration, Dioptas uses the python PyFAI library.

Developer: APS

Original ref.: https://doi.org/10.1080/08957959.2015.1059835

Official web & download: http://www.clemensprescher.com/programs/dioptas

https://github.com/Dioptas/Dioptas

PyFAI

PyFAI is a Fast Azimuthal Integration Python library for SAXS and WAXS experiments, with both command line interface and minimalistic graphical user interface (GUI) for detector geometry calibration and azimuthal integration.

Developer: ESRF

Original refs.: https://doi.org/10.1107/S1600576715004306

https://doi.org/10.1088/1742-6596/425/20/202012

Official web & download: https://pyfai.readthedocs.io/en/master/index.html

https://pypi.org/project/pyFAI/

https://github.com/silx-kit/pyFAI

DPDAK

DPDAK is a Python-based GUI-program for fast online data reduction and analysis (including general curve fitting, etc.) of SAXS, WAXS, GISAXS and X-ray fluorescence data. The calibration and integration of SAXS and WAXS data in DPDAK is implemented using the PyFAI library, and the combination of PyFAI library and DPDAK GUI is suggested to replace Fit2D (no longer being developed).

Developer: PETRA III

Original ref.: https://doi.org/10.1107/S1600576714019773

Official web & download: https://confluence.desy.de/display/DPDAK

https://stash.desy.de/projects/DPDAK/repos/dpdak/browse

Nika

Nika is a package of Igor Pro for correction, calibration and reduction of SAXS, as well as GISAXS, WAXS, GIWAXS, SANS data. Combing Nika and Irena packages, one can seamlessly perform data reduction and data analysis of SAS data.

Developer: APS

Original ref.: https://doi.org/10.1107/S0021889812004037

Official web & download: https://usaxs.xray.aps.anl.gov/software/nika

https://github.com/jilavsky/SAXS_IgorCode/wiki

Datasqueeze

Datasqueeze is a program with a GUI for analyzing data from 2D X-ray detectors, with basic functions including image calibration, data reduction, and least-squares fitting. It is particularly useful for analyzing powder diffraction data, diffuse scattering from polymers or liquid crystals, or SAXS from polymers, colloids, gels, or solutions.

Developer: University of Pennsylvania

Original ref.: Heiney PA. Datasqueeze: a software tool for powder and small-angle X-ray diffraction analysis. Comm Powder Diffr Newsletter. 2005;32:9–11

Official web & download:
https://www.physics.upenn.edu/~heiney/datasqueeze/index.html

Fit2D

Fit2D is a program developed for data reduction of powder X-ray diffraction, including capabilities of detector calibration, masking operations, data integration and analysis.

Note that this program has not been developed since 2016.

Developer: ESRF

Original ref.: https://doi.org/10.1080/08957959608201408

Official web & download: https://www.esrf.fr/computing/scientific/FIT2D/

4. Data analysis software for WAXS

The data analysis software programs for WAXS experimental setups are catalogued according to their approach to data analysis. Three approaches were identified:

- Pattern matching/Qualitative phase analysis
- Peak fitting, and
- Rietveld refinement/Quantitative phase analysis

4.1 Pattern matching/Qualitative phase analysis

The data analysis software programs that use pattern matching or qualitative phase analysis approaches are:

Software program	Developer	Freeware or licence
QualX2.0	IC-CNR Bari	Freeware
Match!	Crystal Impact	Licence

QualX2.0

QualX2.0 is a program, written in Fortran and C++, for qualitative analysis of powder diffraction data, i.e. phase identification by querying both PDF (Powder Diffraction File) and COD (Crystallography Open Database) based on a (d-spacing, intensity) search-match approach.

Developer: IC-CNR Bari

Original ref.: https://doi.org/10.1107/S1600576715002319

Official web & download: http://www.ba.ic.cnr.it/softwareic/qualx/

Match!

Match! is software for phase identification of powder diffraction data. It compares the experimental diffraction pattern with reference patterns from a database. Quantitative analysis (Rietveld refinement) can also be performed in Match! using the FullProf program.

Developer: Crystal Impact

Original ref: Not specified by the developer

Official web: http://www.crystalimpact.com/match/

4.2 Peak fitting

The data analysis software programs that use peak fitting analysis approaches are:

Software program	Developer	Freeware or licence
LIPRAS	North Carolina State University	Freeware
Origin	OriginLab	Licence

Single or multiple peak fitting is a relatively simple operation. Therefore, in the publications identified (see Section 2), several authors also used programming tools such as Python or Matlab to perform those fitting procedures, or they writing their own code.

LIPRAS

Lipras has a GUI for using Line-Profile Analysis Software that makes least-squares fits of Bragg peaks in powder diffraction data, with the capability of conducting Bayesian inference on the resulting least-squares results.

Developer: North Carolina State University

Original ref.: https://doi.org/10.13140/RG.2.2.29970.25282/3

Official web & download: https://se.mathworks.com/matlabcentral/fileexchange/62162-line-profile-analysis-software-lipras

Origin

A data graphing and analysis software, with capablities of single and multiple peak fitting.

Developer: OriginLab

Official web: https://www.originlab.com/

4.3 Rietveld refinement/Quantitative phase analysis

The data analysis software programs that use Rietveld refinement or quantitative phase analysis approaches are coupled to the WAXS experimental technique and are as follows:

Software program	Developer	Freeware or licence	Technique
FullProf	ILL	Freeware	Powder XRD
WinCSD	Max-Planck-Institut fur Chemische Physik fester Stoffe	Freeware	Single-crystal XRD, powder XRD
GSAS-II	APS	Freeware	Single-crystal XRD, powder XRD
Maud	Univ. Trento	Freeware	Powder XRD
JANA2006	Institute of Physics, Academy of Sciences of the Czech Republic	Freeware	Single-crystal XRD, powder XRD
TOPAS	Bruker	Licence	Single-crystal XRD, powder XRD
HighScore Plus	PANalytical	Licence	Powder XRD

FullProf

A program mainly developed for Rietveld refinement of neutron diffraction and powder XRD data, allowing batch processing (critical for in-situ measurements), with other capabilities such as pattern matching and crystal structure refinement.

Developer: ILL

Original ref.: https://doi.org/10.1016/0921-4526(93)90108-I

Official web & Download: https://www.ill.eu/sites/fullprof/

WinCSD

A Crystal Structure Determination and crystallographic calculation software using single-crystal XRD, powder XRD and neutron diffraction data.

Developer: Max-Planck-Institut fur Chemische Physik fester Stoffe

Original ref.: https://doi.org/10.1107/S1600576714001058

Official web & Download: http://www.wincsd.eu

GSAS-II

GSAS-II is Python-based General Structure and Analysis System – comprehensive crystallographic package that can be applied to all stages of crystallographic analysis, such as data reduction, structure solution and structure refinement using single-crystal and powder diffraction data from neutron and X-ray sources, with powerful batch processing capabilities.

Developer: APS

Original ref.: https://doi.org/10.1107/S0021889813003531

Official web & Download: https://subversion.xray.aps.anl.gov/trac/pyGSAS

Maud

Maud is a general program for Material Analysis Using Diffraction from neutron and X-ray sources, with the basis on Rietveld refinement, together with other features like data reduction and X-ray fluorescence full pattern fitting. Even if the software allows a whole range of analysis, it is particularly well suited for texture and stress/strain analysis.

Developer: University of Trento

Original ref.: https://doi.org/10.1016/j.nimb.2009.09.053

Official web & Download: http://maud.radiographema.eu/

JANA2006

JANA2006 is a crystallographic program for structure determination of modulated structures (especially), magnetic structures and standard structures using single-crystal or powder diffraction data from X-ray, neutron and electron sources.

Developer: Institute of Physics, Academy of Sciences of the Czech Republic

Original ref.: https://doi-org.focus.lib.kth.se/10.1515/zkri-2014-1737

Official web & Download: http://jana.fzu.cz/

TOPAS

TOPAS is a nonlinear least-squares optimization program written in C++, with functionalities including peak fitting, Rietveld refinement, Pawley and Le Bail refinement, single-crystal refinement, pair distribution function refinement, constant wavelength neutron refinement, TOF refinement, etc.

Developer: Bruker

Original ref.: https://doi.org/10.1107/S1600576718000183

Official web: http://www.topas-academic.net/

https://www.bruker.com/products/x-ray-diffraction-and-elemental-analysis/x-ray-diffraction/xrd-software/topas.html

HighScore Plus

A powder diffraction data analysis software enabling the whole range of crystallographic analyses, including phase identification, Rietveld refinements, Pawley and Le Bail refinement, solving crystal structures, etc.

Developer: PANalytical

Original ref.: https://doi.org/10.1017/S0885715614000840

Official web: https://www.malvernpanalytical.com/en/products/category/software/x-ray-diffraction-software/highscore-with-plus-option

5. Data analysis software for SAXS

The data analysis software programs for SAXS are as follows:

Software program	Developer	Freeware or licence
Irena	APS	Freeware
SASView	—	Freeware
McSAS	—	Freeware
ATSAS	EMBL	Freeware

Irena

An Igor Pro-based tool suite for analysis of small-angle scattering using X-rays and neutrons. It includes a wide range of models with size distributions of various particle shapes.

Developer: APS

Original ref.: https://doi.org/10.1107/S0021889809002222

Official web & download: https://usaxs.xray.aps.anl.gov/software/irena

SASView

A software package for small-angle scattering analysis. It allows least-square fitting of various models with different shapes, size distributions, structure factors, etc.

Developer: See the official website

Official web & download: https://www.sasview.org/

McSAS

A software based on Monte Carlo algorithm to fit the distribution of particles (different shapes available) to the experimental data.

Developer: Two reference groups described in the original reference

Original ref.: http://dx.doi.org/10.1107/S1600576715007347

Official web & download: https://bitbucket.org/pkwasniew/mcsas/src/master/

ATSAS

A program suit for the processing, modelling, analysis and visualization of SAS data from biological macromolecules.

Developer: EMBL

Original ref.: https://doi.org/10.1107/S1600576720013412

Official web & download: https://www.embl-hamburg.de/biosaxs/software.html

6. Data analysis software for GISAXS and GIWAXS

The data analysis software programs for GISAXS and GIWAXS are as follows:

Software program	Developer	Freeware or licence
GIXSGUI	APS	Freeware
IsGISAXS	Institut des NanoSciences de Paris	Freeware
FitGISAXS	Institut d'P, CNRS	Freeware
BornAgain	Scientific Computing Group at MLZ Garching	Freeware
NANOCELL	Hillhouse Research Group	Freeware
HipGISAXS	Hillhouse Research Group	Freeware
SimDiffraction	Norwegian University of Science and Technology	Freeware
Diffraction Pattern Calculator (DPC)	Princeton University	Freeware

GIXSGUI

A Matlab-based package for visualization and processing of GIXS data from nanostructures/nanocomposites in thin-foils and at surface, with capabilities of data reduction, 3D nanostructure indexing, etc.

Developer: APS

Original ref.: https://doi.org/10.1107/S1600576715004434

Official web & download: https://www.aps.anl.gov/Sector-8/8-ID/Operations-and-Schedules/Useful-Links/Sector-8-GIXSGUI

IsGISAXS

A Fortran program for shape and correlation analysis of islands supported on a substrate, including two working modes – a simulation mode and a data analysis mode.

Developer: Institut des NanoSciences de Paris

Original ref.: https://doi.org/10.1107/S0021889802006088

Official web & download: https://www.insp.upmc.fr/oxydes/IsGISAXS/isgisaxs.htm

FitGISAXS

An IgorPro-based software package for modelling and analysis of GISAXS data for supported or buried scatterers in two or three dimensions, as well as interface roughness correlation.

Developer: Institut P', CNRS

Original ref.: https://doi.org/10.1107/S0021889810020352

Official web & download: https://pprime.fr/?q=fr%2Fnanoparticules-nanostructures

BornAgain

A software for simulating and fitting of GISAXS and GISANS data. It supports polarized GISAXS and GISANS.

Developer: Scientific Computing Group at MLZ Garching

Original ref.: https://doi.org/10.1107/S1600576719016789

Official web & download: https://www.bornagainproject.org

NANOCELL

A software for simulating the Bragg diffraction peaks from nanostructured thin foils using GISAXS and SAXS.

Developer: Hillhouse Research Group

Original ref.: https://doi.org/10.1021/jp0566008

Official web & download: https://sites.google.com/uw.edu/hillhouse/home

HipGISAXS

A fast GISAXS data simulation code using parallelized high-performance computing, such as clusters and supercomputers.

Developer: Lawrence Berkeley National Laboratory

Original ref.: https://doi.org/10.1107/S0021889813025843

Official web & download: https://hipgisaxs.github.io/

SimDiffraction

A program for GIWAXS analysis of textured films.

Developer: Norwegian University of Science and Technology

Original ref.: https://doi.org/10.1107/S0021889808001064

Download: Contacting https://www.ntnu.edu/employees/dag.breiby

Diffraction Pattern Calculator (DPC)

A Matlab GUI toolkit for identification of unit cell lattice parameters from GIWAXS data.

Developer: Princeton University

Original ref.: https://doi.org/10.1107/S1600576714022006

Official web & download: https://loogroup.princeton.edu/research/software

7. Data analysis software for PDF

Software program	Developer	Freeware or licence
PDFgetX2	Michigan State University	Freeware
PDFgetX3	Columbia University	Freeware
XPDFsuite	Columbia University	Licence

PDFgetX2

A GUI for obtaining atomic pair distribution function from powder XRD data.

Developer: Michigan State University

Original ref.: https://doi.org/10.1107/S0021889804011744

Official web & download: https://web.pa.msu.edu/cmp/billinge-group/programs/PDFgetX2/

PDFgetX3

A Python-based rapid and highly automated program for obtaining atomic pair distribution function from powder XRD data.

Developer: Columbia University

Original ref.: https://doi.org/10.1107/S0021889813005190

Official web & download: https://www.diffpy.org/products/pdfgetx.html

XPDFsuite

A complete software solution for high throughput pair distribution function transformation, visualization and analysis, including SrXplanar to process 2D diffraction image, PDFgetX3 to transform PDF, and PDFgui to build and fit the structure model.

Developer: Columbia University

Original ref.: https://arxiv.org/abs/1402.3163

Official web: https://www.diffpy.org/products/xPDFsuite

8. Useful links

- International Union of Crystallography (IUCr) crystallographic software list: https://www.iucr.org/resources/other-directories/software
- Catalog of data analysis software at the Advanced Photo Source (APS): https://www.aps.anl.gov/Science/Scientific-Software
- GISAXS Community Website/software: http://gisaxs.com/index.php/Software
- SAS Portal/software: http://smallangle.org/content/Software

9. Disclaimer

All software is subject to terms and conditions governing the right-to-use. These are specified by the developer. It is the responsibility of the user to ensure that their use of software programs is compliant with such terms.

10. Acknowledgements

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11. About CeXS

The Center for X-rays in Swedish Materials Science (CeXS) was formed in 2019 by KTH Royal Institute of Technology in partnership with Linköping University. CeXS roles include governance of the PETRA III Swedish Materials Science beamline and monitoring Swedish priviledged access to PETRA III beamlines. In 2022, Uppsala University became an affiliate to CeXS.

Read more about CeXS activities on cexs.kth.se.

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