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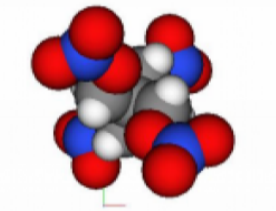
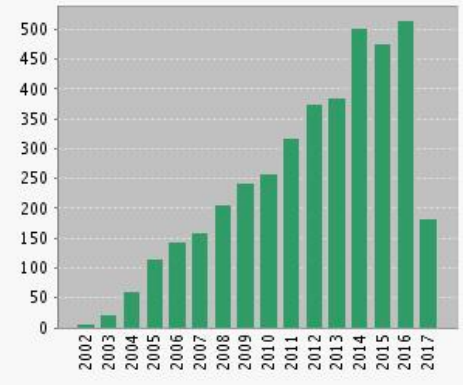
GSAS-II: WHAT DOES IT DO? WHAT IS NEW? WHAT IS COMING AND WHAT IS NOT.

GSAS-2



ROBERT B. VON DREELE BRIAN H. TOBY

FOR DIFFRACTION ANALYSIS, GSAS & EXPGUI ARE WIDELY USED



EXPGUI citations/year; Web of Science

- **Need a new code, GSAS & EXPGUI**
  - **are hard to maintain**
  - **Impossible to expand**

Wide Range of Fields

Web of Science Category	% of total
CHEMISTRY PHYSICAL	31.6
MATERIALS SCIENCE MULTIDISCIPLINARY	30.4
PHYSICS CONDENSED MATTER	15.7
CHEMISTRY INORGANIC NUCLEAR	14.2
CHEMISTRY MULTIDISCIPLINARY	12.1
PHYSICS APPLIED	8.6
NANOSCIENCE NANOTECHNOLOGY	7.7
CRYSTALLOGRAPHY	6.6
MINERALOGY	6.4
METALLURGY METALLURGICAL ENGINEERING	4.9
ELECTROCHEMISTRY	4.9
GEOCHEMISTRY GEOPHYSICS	4.7
ENERGY FUELS	4.5
MATERIALS SCIENCE CERAMICS	4.0
CHEMISTRY APPLIED	2.3
PHYSICS ATOMIC MOLECULAR CHEMICAL	2.0
PHYSICS MULTIDISCIPLINARY	2.0

Highly utilized in DOE/SUF

Argonne	DE-AC02-06CH11357	11.1%
Brookhaven	DE-AC02-98CH10886	3.5%
Lawrence Berkeley	DE-AC02-05CH11231	1.6%
HPCAT/DOE-NNSA	DE-NA0001974	1.5%
GSECARS/DOE-Geo	DE-AC52-06NA25396	1.4%
HPCAT/DOE-BES	DE-FG02-99ER45775	1.4%
National Basic Research Program of China	2011CB808200	1.3%

20%

GSAS-II: A MODERN ANALYSIS PACKAGE FOR ALL ASPECTS OF CRYSTALLOGRAPHY

GSAS-II is intended to replace GSAS & EXPGUI with a new, modern, extensible, and *open-source* crystallographic analysis

- Support all aspects of diffraction data analysis (from raw data to publication), including capabilities not in GSAS/EXPGUI
- Facile processing of large numbers of similar datasets
- Written with modern code (Python)
- Incorporates extensive visualization
- Use parameters that "make sense"
- Designed around GUI
- Design goal: Novice friendly, but expert efficient

GSAS-II reads powder diffraction images from all appropriate APS beamlines, as well as the Curiosity Rover on Mars!

B.H. Toby and R.B. Von Dreele, "GSAS-II: The Genesis of a Modern Open-Source All-Purpose Crystallography Software Package". *Journal of Applied Crystallography*. **46**: p. 544-9 **(2013)**.

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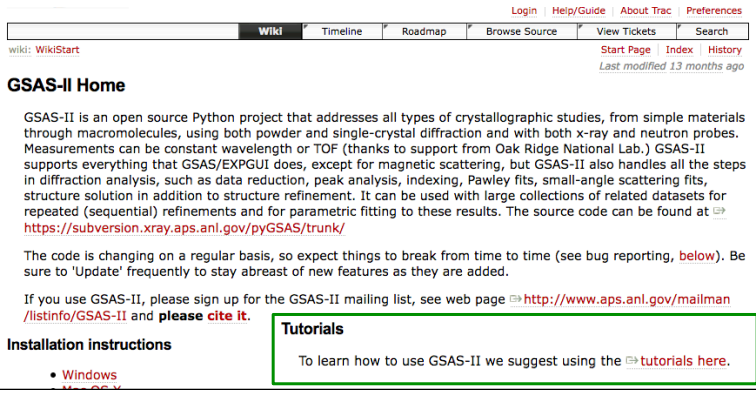
FOR MORE INFO

See GSAS-II "home page" https://subversion.xray.aps.anl.gov/trac/pyGSAS. Includes

- Installation instructions
- Tutorials
- Developer notes (~200 pages)
- Mailing list
- Project tracking info (N.B. not all tools are in use)



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Last modified 13 months ago

GSAS-II Home

GSAS-II is an open source Python project that addresses all types of crystallographic studies, from simple materials through macromolecules, using both powder and single-crystal diffraction and with both x-ray and neutron probes. Measurements can be constant wavelength or TOF (thanks to support from Oak Ridge National Lab.) GSAS-II supports everything that GSAS/EXPGUI does, except for magnetic scattering, but GSAS-II also handles all the steps in diffraction analysis, such as data reduction, peak analysis, indexing, Pawley fits, small-angle scattering fits, structure solution in addition to structure refinement. It can be used with large collections of related datasets for repeated (sequential) refinements and for parametric fitting to these results. The source code can be found at https://subversion.xray.aps.anl.gov/pyGSAS/trunk/

The code is changing on a regular basis, so expect things to break from time to time (see bug reporting, below). Be sure to 'Update' frequently to stay abreast of new features as they are added.

If you use GSAS-II, please sign up for the GSAS-II mailing list, see web page http://www.aps.anl.gov/mailman/listinfo/GSAS-II and **please cite it**.

Installation instructions

- Windows

Tutorials

To learn how to use GSAS-II we suggest using the tutorials here.

WHAT DOES GSAS-II DO?

- Calibrate and integrate area detector data
- Crystallographic fitting of single crystal and powder data (lab, synchrotron, TOF and CW neutron)
  - Allows any number of data sets and phases
- Powder data:
  - Fit arbitrary peaks
  - Autoindexing
  - Structure solution (charge flipping & Monte Carlo)
  - Stacking fault simulations
  - Size/μStrain fitting (optionally anisotropic w/visualization)
- Sequential fitting (fit a single model to 10^n data sets)
  - Parametric fitting
- Applied stress fitting (from raw images)

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WHATS NEW?

- Stacking fault simulations
- Single crystal twinning
- 3+1 supersymmetry: fits for incommensurate modulated structures
- PDF determination from powder data
- Streamed automated integration and PDF computation
- Commensurate neutron magnetic scattering (color space groups)
- Heterogeneous sequential fits
- Simplified installation process
- Absolute detector calibration from series of images with known relative placement
- Small angle scattering (x-rays, CW?)

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WHAT IS BEING WORKED ON

- Bug fixes (always!)
- Scripting capability (API) for GSAS-II; implemented on as as-needed basis (starting with 11-BM calibration)
- Reflectometry fitting
- Generation of CW instrumental parameters from fundamental parameters
- Refinement of stacking fault parameters

THINGS WE PLAN TO WORK ON

- Technical manual (Book: the math behind GSAS-II)
- Sequential fits with groups of histograms/refinement
- Sequential fit restraints
- Testing (& fixes) for wxPython 4.0 and Python 3.x
- More tutorials
- Override size/placement of windows via config. options

Maybe:

- Multiple core implementation
- Combined PDF/Rietveld fitting
- Maximum Entropy Fourier maps

DESIRED, BUT NOT WITHIN (NON-) FUNDING SCOPE

Need a long-range plan that brings new "talent" into computational crystallography

- Incommensurate magnetic scattering
- Generation of special site constraints for supersymmetry groups
- Fundamental parameters-generated peak profiles
- Full API implementation

TOPICS FOR FUTURE MEETINGS

(updated with meeting comments)

- June 12: Reflectometry fitting in GSAS-II
- July 10: Sequential/Parametric fitting
- August 14: Metadata handling (image import) – is day before DOE review a problem?
- September 11:

USER FEEDBACK

(from comments at meeting)

Other development topics:

- GISAXS modeling? Start with side discussion with Joe Strzalka
- Expand multi-image secondary fit for more versatile fitting: side discussion with Steven Weigand
- How to handle spatial aberrations in area detectors? (Sector 1 need)

Other discussion topics

- How to encourage code sharing (importers, etc.)
- Search-Match inside GSAS-II?