

## GSAS-II for High Pressure Diffraction

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Abstract:

The GSAS-II package is a modern, comprehensive and extensible package for analysis of all types of diffraction data on multiple scales: crystallography (including 3+1 superspace modulated structures), small-angle scattering and Rietveld refinement; with single-crystal or powder diffraction measurements; with x-rays or neutron probes, where the latter may be at constant-wavelength or time-of-flight. For crystallographic analysis, structural models can be fit to many datasets of any type in combination. GSAS-II also provides a novel capability to fit a parametric series of datasets. GSAS-II can be run on Windows, Linux and Mac computers with Intel-compatible processors. All GSAS-II functionality can be accessed through a graphic user interface; selected functionality can be accessed via a Python-based applications interface. For this presentation, a brief introduction will be made about GSAS-II and then topics of greatest interest to the high-pressure community will be covered, as time allows: 2-D image calibration, masking and integration; writing importers for new data formats; automating image processing and refinements; simplifying model complexity through constraints, restraints and rigid bodies.