Contribution ID: **22** Type: **not specified**

X-ray Powder Diffraction Facilities Available at the Advanced Photon Source

Tuesday 8 May 2018 09:10 (15 minutes)

The facilities at the APS for powder diffraction includes the very high resolution 12-crystal analyzer/detector diffractometer (11-BM-B) which operates at medium energy (20-33keV) and a high throughput 2D imaging detector instrument (17-BM-B) that operates also at somewhat higher energy (27-51keV). Canonical measurement times on 11-BM are circa 1 hour/scan, while 17-BM can collect a dataset in seconds. The APS also has other diffraction beamlines optimized for PDF measurements, surface scattering, small-angle scattering and engineering studies. 11-BM operates ˜50% of the time via a mail-in system that allows rapid turnaround (2-6 weeks) producing data often suitable for structure solution and Rietveld refinement for complex materials, with the balance used for on-site users. The 17-BM instrument, coupled with Argonne's data processing/analysis software (GSAS-II) allows tracking of experiments in real time with both powder patterns and pair distribution function (PDF) data produced from image integrations done as in situ experimental or operando conditions (temperature, gas atmosphere, humidity, etc.) are varied. The GSAS-II software package is a fully developed, open source, crystallographic data analysis system written almost entirely in Python. For powder diffraction, it encompasses the entire data analysis process beginning with 2D image integration, peak selection, fitting and indexing, followed by intensity extraction, structure solution and ultimately Rietveld refinement, all driven by an intuitive graphical interface. Significant functionality of GSAS-II also can be scripted to allow it to be integrated into workflows or other software. This talk will cover these capabilities with some examples.

Primary authors: Dr TOBY, Brian (Advanced Photon Source); Prof. VON DREELE, Robert (Advanced Photon Source)

Presenters: Dr TOBY, Brian (Advanced Photon Source); Prof. VON DREELE, Robert (Advanced Photon Source)

Session Classification: Beamline Overview

Track Classification: Tuesday, May 8th Morning (Day 2 Workshop)