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Synchrotron powder diffraction simplified; management of an APS mail-in program

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Synchrotrons have revolutionized powder diffraction. They enable rapid collection of data with tremendous angular resolution and exceptional statistics. High resolution powder diffraction beamlines employing multiple single crystal analyzer detectors routinely reveal subtle crystallographic distortions undetectable on other powder instruments, and are an important tool at most modern synchrotrons for structural studies of a diverse range of materials. Beamline 11-BM at the Advanced Photon Source (APS) is a dedicated high resolution (ΔQ/Q ~2×10-4) powder diffraction instrument which uses vertical and horizontal beam focusing capabilities and a counting system consisting of twelve perfect crystal analyzers paired with scintillator detectors. This APS beamline supports both traditional on-site experiments and a highly successfully rapid access mail-in program mode. This mail-in program has greatly simplified access for a growing user community (> 250 in 2013) to world-class synchrotron quality powder data for their research and resulting publications (> 100 11-BM citations in 2013). The presentation will provide an overview of 11-BM's unique mail-in program. It will be presented both from the view of an external remote user, and will also highlight the numerous alignment, calibration, correction and merging software routines needed to efficiently and accurately reduce the numerous multi-bank detector datasets associated with a high throughput user program. An integrated web interface has been developed to serve as a user-friendly relational database interface for tracking of samples and datasets throughout all stages of the measurements; from the initial user request to sample disposal. The database and software tools critical for this high-throughput synchrotron powder diffraction program will be discussed in detail. More information about the 11-BM and its mail-in program can be found on the beamline webpage: http://11bm.xray.aps.anl.gov

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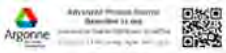

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