Software tools for neutron wavelength-resolved Laue diffraction in multi-dimensional diffraction and parameter spaces

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Developments of area detector technologies and processing software have been continuously evolving and are now enabling routine collection of single crystal data that can be transformed into volumes of diffraction space. In practice, single crystal diffraction data are collected in three modes with X-ray or neutron radiation: as monochromatic 2D diffraction slices, polychromatic 2D diffraction (Laue) images or wavelength resolved (3D Laue) diffraction volumes, where the first and last can be used to reconstruct a complete 3D volume of reciprocal space. Hitherto, high resolution wavelength resolved Laue diffraction volumes are currently only routinely collected at accelerator-based spallation neutron facilities; here the spread of neutron kinetic energy is separated into a wavelength distribution by relating neutron travel time (TOF) from source to sample to its wavelength λ via the de Broglie equation. Wavelength-resolved Laue method extends the diffraction pattern from the 2D detector space (x, y) to a 3D volume in (x, y, λ) with the third dimension along the neutron TOF direction for each sample orientation. As an instrument with full 4 pi coverage does not exist, multiple orientations are taken and combined according to detector coverage and crystal symmetry to build a continuous, spherical diffraction volume in reciprocal space.

This presentation will showcase the software tools developed for TOPAZ beamline at the ORNL Spallation Neutron Source (SNS). TOPAZ is a high-resolution single crystal diffractometer that uses an array of area detectors with fast detection time (< 1 µsec) for neutron wavelength-resolved Laue diffraction. TOPAZ data are recorded and stored in neutron event mode, tracking the relevant metadata, and timestamps for individual neutron events. Event-based data collection enables the study of the material response to external stimuli, effectively expanding the measurement capability beyond three dimensions into multidimensional parameter spaces (Temperature, Electric field, etc.) in unprecedented detail.