Real time data collection in multidimensional diffraction and parameter spaces

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Data from an operando and in situ diffraction experiment provide real time information on material's response to external stimuli (temperature, pressure, stress, electric and magnetic field, photochemical excitations, *etc.*). For kinetic and dynamic structural studies it would be ideal to collect diffraction pattern that encompasses continues volume of 3D reciprocal space of interest while keeping all the relevant external stimuli on the sample with the same timestamp to that of the individual events recorded in detector space. In this presentation, I will discuss the multidimensional approach in both diffraction and parameter spaces with the use of wavelength-resolved Laue technique at the TOPAZ beamline of the ORNL Spallation Neutron Source (SNS).

The SNS TOPAZ is a high-resolution single crystal diffractometer for the study of nuclear and magnetic structures of materials at sub-atomic resolution. The array of the TOPAZ neutron time-of-flight detectors covers a large 3D volumes of Q-space (after unit conversion of each event data from detector *x*, *y* and neutron wavelength λ in diffraction space). The crystal orientation can be optimized with the local CrystalPlan software[1] for highly efficient reciprocal space surveys. Connecting the timestamp of event data with that of external stimuli provides the tools needed to resample the multidimensional dataset. Examples will be presented for temperature slicing [2] and time filtering [3] of event-based single crystal neutron diffraction data. This approach has opened a new avenue to probe structural phase transitions and dynamics in real time. It will not only mimic the pump-probe protocols used in X-ray study, but also extends the measured diffraction and parameter space to multiple dimensions (neutron event data in 3D *Qx*, *Qy*, *Qz* and one or more external stimuli at time stamp *t*). In addition, high-resolution diffraction data measured on TOPAZ can be used to resolve the far-from-equilibrium atomic motions in materials and determine the three-dimensional crystal and molecular structures while they are in metastable or short-lived intermediate states.

Reference

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[3] C. M. Fancher, C. Hoffman, V. Sedov, A. Parizzi, W. Zhou, A. J. Schultz, X. P. Wang, and D. Long, 'Time filtering of event-based neutron data; a pathway to study the dynamic structural responses of materials.' *Manuscript submitted for publication*.