

# Integrated analysis for both diffuse and Bragg single crystal neutron scattering

Zachary Morgan<sup>1</sup>, Feng Ye<sup>2</sup>

<sup>1</sup>Oak Ridge National Laboratory<sup>2</sup>N/A

*morganzj@ornl.gov*

Mapping large volumes of reciprocal space with position sensitive detectors for single crystal diffuse scattering analysis requires the collection of data over many sample orientations require a well-calibrated instrument. Improvements in instrument calibration including the He3-tube banks and sample position for the time-of-flight Laue spectrometer CORELLI at the Spallation Neutron Source make this task possible. These large volumes are more easily reduced into data for analysis using 3D-delta PDF or Monte Carlo methods for magnetic and structural disorder investigations. Recent developments in Monte Carlo tools will be discussed showcasing data from the beamline. As calibration and diffuse scattering tools continue to improve, the demand for integrating Bragg intensities for structure refinement from these experiments is growing. A new approach to obtain the intensities from nuclear and satellite reflections that utilizes ellipsoidal envelopes will be discussed. This includes the appropriate handling of wavelength-dependent corrections. The result of which is a developing and integrated approach for analyzing diffuse and Bragg neutron scattering from single crystals. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.