Contribution ID: **2582** Contribution code: **THPM117** Type: **Poster Presentation**

Interactive automated Bragg peak identification with 3D neutron scattering data

Thursday, 11 May 2023 16:30 (2 hours)

Neutron scattering experiments have undergone significant technological development through large area detectors with concurrent enhancements in neutron transport and electronic functionality. Data collected for neutron events include detector pixel location in 3D, time and associated metadata, such as, sample orientation, neutron wavelength, and environmental conditions. RadiaSoft and Oak Ridge National Laboratory personnel are considering single-crystal diffraction data from the TOPAZ instrument. We are leveraging a new method for rapid, interactive analysis of neutron data using NVIDIA's IndeX 3D volumetric visualization framework. We have implemented machine learning techniques to automatically identify Bragg peaks and separate them from diffuse backgrounds and analyze the crystalline lattice parameters for further analysis. The implementation of automatic peak identification into IndeX allows scientists to visualize and analyze data in real-time. Our methods include a robust comparison with current analysis techniques which show improvement in a variety of aspects. These improvements will be incorporated into IndeX for visualization to allow scientists an interactive tool for crystal analysis.

Funding Agency

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0021551.

Footnotes

I have read and accept the Privacy Policy Statement

Yes

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Session Classification: Thursday Poster Session

Track Classification: MC8: Applications of Accelerators, Technology Transfer and Industrial Relations and Outreach: MC8.U05: Other Applications