

# Machine Learning Assisted Automation of Single Crystal Neutron Diffraction

Yiqing Hao<sup>1</sup>, Erxi Feng<sup>1</sup>, Dan Lu<sup>1</sup>, Leah Zimmer<sup>1</sup>, Zachary Morgan<sup>1</sup>, Bryan C. Chakoumakos<sup>1</sup>, Guannan Zhang<sup>1</sup>, Huibo Cao<sup>1</sup>

<sup>1</sup>Oak Ridge National Laboratory

haoy@ornl.gov

Neutron scattering is a versatile and powerful technique widely used in materials science to gain insights into materials' properties and uncover new materials. However, this method is often expensive and time-consuming, requiring advanced detector technology and complex data reduction and analysis procedures. Machine learning (ML) has opened new avenues for neutron diffraction data reduction and experiment operation. In this regard, an ML-assisted data reduction and analysis method has been proposed and utilized at HB-3A DEMAND at HFIR, ORNL. The method is designed to recognize Bragg peaks with high precision and identify the corresponding regions of interest. Once the peaks are recognized, the method can automatically align a measured crystal and optimize the data collection using user-provided information and uncertainty quantification values of the detected peaks. The proposed method has been shown to perform exceptionally well in various complex sample environments, enabling automated single-crystal neutron diffraction. This method's success can dramatically accelerate the discovery of new materials with unique properties. The ability to automate the data collection process will also free up valuable time for researchers to focus on other aspects of their research, leading to more efficient and productive experiments.

The research at Oak Ridge National Laboratory (ORNL) was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Advanced Scientific Computing Research under the contract ERKJ387, and Office of Basic Energy Sciences, Early Career Research Program Award KC0402020, under Contract DE-AC05-00OR22725. This research used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by ORNL.

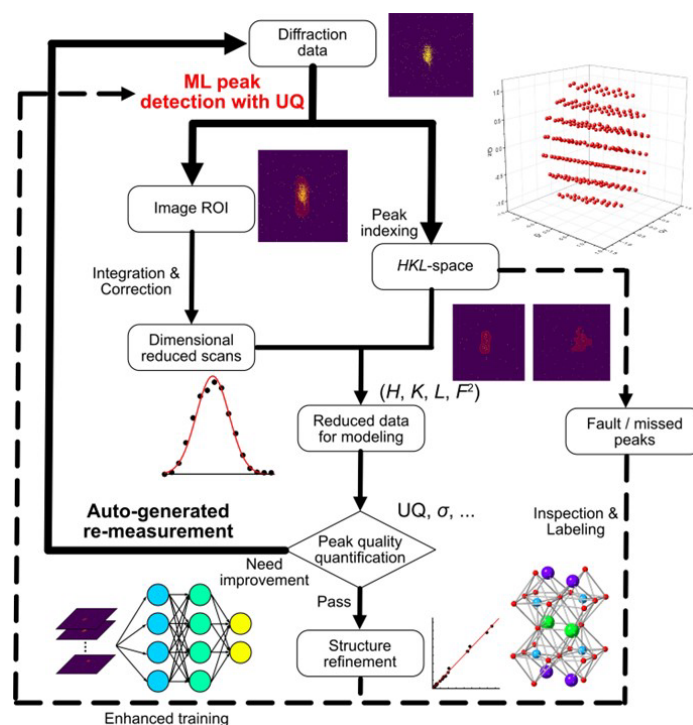


Figure 1