Contribution ID: **102** Type: **Poster Only**

Commissioning on-the-fly, autonomous neutron diffraction experiments for exploring spin flop transitions for ☒-Fe2O3

The Experimental Steering for Powder Diffraction (ESPD) project aims to help develop and commission automation and steering neutron powder diffraction experiments. Recently, successful experiments on the Nanoscale-Ordered Materials Diffractometer (NOMAD) at the Spallation Neutron Source (SNS) were conducted for the ESPD project and results will be presented. Specifically, iron(III) oxide / hematite (☒-Fe2O3) bulk and nanoparticles were measured using NOMAD's cryostream for autonomous navigation of temperature measurements via machine learning (ML) to commission experiment steering capabilities. Two methods were used for the ML decision making for new temperatures: a Bayesian optimization method and a physics-informed method called ANDiE (Autonomous Neutron Diffraction Explorer) developed previously by a team from National Institute of Standards and Technology (NIST). The experiment used the Morin temperature / spin flop transition of ☒-Fe2O3 to autonomously explore using both methods. The ML methods were developed and deployed via the Distributed Interconnected Science Ecosystem INTERSECT) for Active Learning (DIAL) project. The Data Acquisition Group's External Instrument Control (EIC) software was used to securely "talk"to the NOMAD EPICS system to change the temperature of the cryostream and used a combination of INTERSECT ad DIAL services to steer the NOMAD instrument. The data was streamed to a separate instance of INTERSECT running in the National Science Data Fabric for visualization of progress of the experiment. This work provides a foundation to drive progress towards both large-scale compute resources being used to guide experiments at SNS and HFIR as well as promote and mature this capability for the General User Program instead of as one-off, proof-of-concept experiments. The future scientific impact from this study will be significant reduction in experimental time required for neutron diffraction experiments and better exploration of parameter space with the constraint of finite beamtime for Users.

Topical Area

AI and data science

Author: MCDONNELL, Marshall (Oak Ridge National Laboratory)

Co-authors: Mrs MALVIYA-THAKUR, Addi (Oak Ridge National Laboratory); GOOCH, Amy; AYRES, Andrew (Oak Ridge National Laboratory); SHRIVASTAVA, Ankit (Oak Ridge National Laboratory); MCDANNALD, Austin (National Institute of Standards and Technology); VACALIUC, Bogdan (Spallation Neutron Source); VAN AUKEN, Emily (Oak Ridge National Laboratory); KUSNE, Gilad (National Institute of Standards and Technology); SCORZELLI, Giorgio (University of Utah); WATSON, Greg (Oak Ridge National Laboratory); CAGE, Gregory (Oak Ridge National Laboratory); MARQUEZ, Jack (University of Tennessee); LIU, Jue (Oak Ridge National Lab); GOFRON, Kaz; NG, Kin Hong (University of Tennessee); Mr DRANE, Lance (Oak Ridge National Laboratory); DAEMEN, Luke (Oak Ridge National Laboratory); DOUCET, Mathieu (ORNL); TUCKER, Matthew; TAUFER, Michela (University of Tennessee Knoxville); LAIU, Paul (Oak Ridge National Laboratory); GREGORY, Ray (Oak Ridge National Laboratory); DEWITT, Stephen (Oak Ridge National Laboratory); PASCUCCI, Valerio (University of Utah); RATCLIFF, William (NIST); Dr ZHANG, Yuanpeng (ORNL); THURMAN, Zach (Oak Ridge National

Laboratory)

Presenter: MCDONNELL, Marshall (Oak Ridge National Laboratory)