Automated x-ray PDF analysis and ML modeling*

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Abstract

On-the-fly x-ray data analysis of Pair Distribution Function (PDF) measurements is a powerful tool in guiding synchrotron x-ray experiments on disordered materials. For the high energy x-ray beamline 6-ID-D this has been implemented using a combination of Globus and GSAS-II within the Parsl/Balsm Infrastructure. A GSAS-II project file is created at the beginning of the experiment and used as a template for subsequent measurements. Scattering patterns from a large area detector are stored by Globus and analyzed using GSAS-II within a few seconds of data acquisition. The results can be viewed using a web browser. Stringent consistency checks still need to be implemented to ensure the users are aware of data quality and the level of accuracy.

For carefully analyzed, high quality x-ray PDF data that meets the consistency checks, the structural interpretation has been achieved through the development of machine learned interatomic potentials. The underlying principle is simple; if thousands of ab initio molecular dynamics simulations are performed and compared to the diffraction data, the best can be trained to fit the measured x-ray PDF within a specified threshold. Here, an active learning algorithm is used to test and train the simulation models, and a Gaussian Approximation Potential iteratively developed, such that classical molecular dynamics simulations can be performed on a larger number of atoms with near ab initio accuracy. The larger box size model is better able to predict the thermodynamic properties of the material. So far this has been implemented for multiple phases of a refractory oxide, as well as molten salt systems.

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