Contribution ID: **20** Type: **Poster**

Machine Learning-Based Crystal Structure Direct Prediction from Neutron Powder Diffraction

Tuesday, 9 April 2024 18:30 (20 minutes)

The neutron powder diffraction data represent a one-dimensional projection of the three-dimensional structural information. Compared to single crystal neutron diffraction, the reduction in data dimension adds complexity to structural determination from neutron powder diffraction data. Structure determination with neutron powder diffraction is predominantly a manual endeavor, requiring intricate, specialized expertise to execute. Considering the powerful data dimension reduction and feature extraction capability of machine learning, a machine learning-based algorithm was developed to predict crystal structure directly from neutron diffraction pattern. Over three hundred thousand crystal structures with different symmetries from the Crystallography Open Database generate the neutron diffraction time-of-flight patterns. The crystal structures were coded to the coulomb matrix by the Ewald sum matrix representation and then composed the training set. The training set was used to train an auto-encoder compressing the coulomb matrix into a latent space. With the assistance of this well-trained auto-encoder, the neutron scattering pattern can be fitted by optimizing the latent space and the coulomb matrix and then the crystal structures can be reconstructed from the latent space. The optimization process is completed by the genetic algorithms.

Primary author: WANG, Hao (China Spallation Neutron Source)

Presenter: WANG, Hao (China Spallation Neutron Source)

Session Classification: Posters

Track Classification: MLC