Machine learning assisted reverse Monte Carlo modeling for neutron total scattering data

Y. P. Zhang¹, P. Cuillier², M. G. Tucker¹

¹Neutron Scattering Division, Oak Ridge National Laboratory, 1 Bethel Valley Rd. Tn, 37830. ²Materials Science and Engineering, Ohio State University, 122 Hitchcock Hall, 2070 Neil Avenue, Columbus, OH 43210.

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In the area of atomic-level structure modelling, there are two well-known parallel problems. The theory driven modelling usually cannot fully account for the disorder of practical system and therefore may fail to reproduce the complete picture of structure model as observed experimentally. The data driven approach tries to derive the structural model from the experimental data in a reverse manner (i.e., data to model) and therefore naturally is able to catch features observed experimentally. But quite often it lacks the accurate coverage of energetic landscape from the theoretical perspective. In this contribution, we aim at bringing in a novel approach combining the theoretical and experimental considerations. To realize this, the LAMMPS module for energy calculation is implemented into the reverse Monte Carlo routine (here, the RMCPProfile package was used) for modelling total scattering data. Through such a combined approach, atomic positions would be adjusted according to the agreement with experimental scattering data and the energy landscape simultaneously. Specifically concerning the energy calculation, the Gaussian processing-based machine learning routine for potential field construction is employed here. Such an approach, at the same time providing density functional theory level of accuracy, guarantees a reasonably short computational time which is required for the metropolis algorithm for structure modelling. The LAMMPS implemented RMCPProfile package for conducting the combined modelling is generally applicable to utilize neutron and X-ray total scattering data, X-ray absorption spectroscopy data, electron scattering data, etc. for structure modelling to provide insights into structure-property link of general condensed matter systems.

Figure 1. RMC+LAMMPS for driving atomic configuration.