Center for Accelerating Materials Modeling from Spallation Neutron Source Data

Thomas Proffen, Jose Borreguero Calvo, Stuart Campbell, Vickie Lynch, Andrei Savici1, Monojoy Goswami2, Galen Shipman2, Bobby Sumpter, Olivier Delaire, Jiawang Hong, Jennifer Niedziela

Neutron scattering enables simultaneous measurement of structural and dynamic properties of materials from the atomic scale (0.1 nm, 0.1ps) to the mesoscale (1um, 1us). These ranges are remarkably complementary to current capabilities of computational modeling and the simplicity of the scattering cross section allows the prediction of neutron scattering data relatively straightforwardly from atomic trajectories in a computer model. As such, our goal is to accelerate the rate of scientific discovery through the integration of materials modeling and simulation into all aspects of the neutron scattering experimental chain. This enables refinement of model parameters such as force fields and allows researchers to compare model and experimental results in near real time. These advances will facilitate our ability to perform validated materials modeling to achieve capabilities for materials by design. Our science focus is to understand the mesoscopic dynamics and transport in crystalline and non-crystalline materials that underpin diffusive phenomena of single particle properties such as mass, proton, and ion transport that are facilitated by collective motions.