Advanced Total Scattering Analysis of Disordered and Nano-Crystalline Materials

Th. Proffen
Neutron Data Analysis and Visualization Division, Neutron Sciences
Oak Ridge National Laboratory

As new materials with new properties are discovered, their structural complexity many times increases as well challenging traditional structural characterization techniques with extended defects, co-existence of crystalline and amorphous phases or their nano-crystalline nature. Over the past decade, total scattering analysis and advanced materials modeling have taken advantage of improvements in scattering instrumentation, computing power and emerging user friendly software and allowed scientists to tackle more and more complex structural materials.

This presentation will provide an overview of total scattering modeling techniques from simple small-box modeling of a structure as a function of length scale, to large-box modeling using the Reverse Monte Carlo (RMC) technique to advanced refinements of complex structural models and nano-particles.