4CF12-2012-020024

Abstract for an Invited Paper
for the 4CF12 Meeting of
the American Physical Society

Accelerating Nanoscale Research with Neutron Total Scattering: Linking Structure and Function in Finite Materials

KATHARINE PAGE, Los Alamos National Laboratory

h $-abstract-$\pard In contrast to bulk materials, nanomaterials and nanoparticles, comprised of a few hundred to tens of thousands of atoms, require every atom's position to be located in order to understand their structure-property relationships. New behavior can arise with a constricted, expanded, or distorted lattice, variation in surface termination structure, ligand capping or stabilization, or with the increasingly diverse set of shapes and architectures appearing in nanoscience literature today: tubes, pyramids, stars, core-shell and matrix-confined particles, multilayer films, etc. Pair distribution function (PDF) analysis, based on spallation neutron or synchrotron x-ray total scattering data, has emerged as a very promising characterization method for nanomaterials in recent years. Total scattering methods provide information about every pair of atoms probed in a diffraction experiment and thus contain an unexploited wealth of information for finite systems. In this contribution we will present our work establishing the influence of particle size and shape on the nature and correlation of local atomic dipoles in finite ferroelectric systems. We also review current data-driven modeling capabilities and outline the need for evolution of robust computational tools to follow other complex nanoscale phenomena with scattering data. \pard-/abstract-\