MS96.O04

Nanostructure studies using complex modeling method

P. Juhas[1], M. McKerns[1], S. Billinge[2]

[1]Brookhaven National Laboratory, CMPMSD, Upton, NY, USA, [2]Columbia University, APAM, New York, NY, USA

Accurate characterization of nanostructures is an open difficult problem. Nanoparticle sizes are too small to form a sizable periodic order in atom positions that would give rise to resolved Bragg peaks. A significant number of atoms lie at the surface where their positions can relax and distort. Experimental data from nanoparticles are thus in general more noisy and less signal-rich than from crystals, but their structures have less symmetry and require more variables for their characterization. To overcome these difficulties, we have developed Complex Modeling (CM) approach, which combines multiple experimental and theoretical probes in a common structure optimization routine. The Complex Modeling method is based on the DiffPy software library of forward calculators for pair distribution function, bond valence sums, hard-sphere atom overlaps and third-party routines for small angle scattering simulations and structure restraints for bond lengths and bond angles. The top-level SrFit framework allows flexible setup of optimization schemes by tying available experimental inputs and theoretical and chemical constraints or restraints on the structure. The presentation will provide several examples of Complex Modeling studies of concrete nanostructure systems, such as determination of atomic structure and shape of CdSe quantum dots from PDF and SAXS, structure determination of Au nanoparticle from PDF data and surface optimization, and determination of molecule packing in organic crystals from PDF and chemical constraints.

Keywords: complex modeling, PDF, SAXS