Probing material reactivity using X-ray pair distribution function methods

Karena W. Chapman

X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, Il 60439, USA.

Understanding how advanced functional materials react and transform, at an atomic scale, is a characterization challenge with many diverse phenomena possible; components with varying particle size, morphology, and microstructure can evolve from multi-atom clusters to multi-million atom crystals. The pair distribution function (PDF) method shows great promise for providing quantitative insight such reactions. Recent advances in experimental methods, have improved the efficiency of X-ray PDF measurements, to allow time-resolved experiments with sufficient resolution to study reactions in solid materials. The PDF analysis probes the complete reaction from clusters to bulk, amorphous or crystalline, liquid or solid. This is in contrast to Bragg crystallographic analysis which is “blind” to the clusters which nucleate before growing into long-range ordered materials. The structural insights from the PDF data are obtained in parallel with phase concentration to allow different components to be distinguished and a robust quantitative analysis.