Time-Resolved Structural Studies: Strategies for Rapidly Imaging and Analyzing Large Data Sets

Matthew J Kramer
Ames Laboratory and the Department of Material Sciences and Engineering
Ames, IA 50011

Recent advances in neutron and synchrotron X-ray sources have greatly increased the available flux to the samples, decreasing counting times necessary for reliable statistics while improvements in detectors efficiencies have further reduced data collection times. Third generation synchrotrons now have sufficient flux at high energies (> 40 keV), i.e., high energy X-ray diffraction (HEXRD), so that transmission experiments, similar to those at neutron facilities, can be performed. These high flux sources, in conjunction with an area detector, have reduced data collection times to a few minutes to even a few seconds or less. This allows for obtaining hundreds of diffraction patterns in a few hours or less. The underlying rational for obtaining such rapid data is to analyze the underlying atomic structural changes which may occur during solid state phase changes in the same time frame as traditional thermal analysis is preformed. Now even non-crystalline systems can be quantitatively analyzed; such as solidification or melting. Processing such large data sets can be challenge. I will present a 3D plotting program designed to be used in conjunction with large diffraction data sets to rapidly interrogate large data bases (up to 1000 scans). Differentiating the data with respect to the process variable provides a rapid means of analyzing for structural changes at phase transformations. A series of case studies involving displacive and reconstructive phase transitions and an example of melting and solidification will be presented.