Analytics and Autonomy for X-ray Scattering Studies of Soft Nanomaterials

Kevin G. Yager
Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton NY 11973

Self-assembling materials organize into distinct structures owing to thermodynamic energy minimization. Yet the structures observed experimentally frequently depend on kinetic effects and processing history. Block copolymer thin films are one key example of this motif, where the pathway-dependence of ordering can be viewed as a nuisance, or exploited as a tool to enforce a particular kind of desired order. This talk will present x-ray scattering studies of block copolymer self-assembly, emphasizing this non-equilibrium assembly, and will describe the ongoing development of new x-ray scattering methods to enable more efficient study of such systems. In particular, we are developing an autonomous x-ray scattering beamline, which combines deep learning methods for rapid data analysis with general machine-learning methods for automated decision making. This allows rapid exploration of the complex parameter spaces associated with modern materials. Examples of autonomous experiments will be described, including exploration of combinatorial libraries, and realtime control of photo-thermal processing.