

SAXS electron density mapping

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Small angle scattering (SAS) has been the first-choice technique in the structure determination of polymers that possess ordered structures in nanoscale. For instance, physics of block copolymers has been developed based on the phase diagram and lattice constants determined mainly by SAS. Lattice constants measured from a series of samples allowed researchers to come up with a theoretical model that predicts chain conformation of each block. Further analyses such as determining density distribution in the unit cell have been of interest but limited because of the phase problem and also because majority of SAS data are essentially powder diffraction patterns. Often the phase problem has been resolved by preparing better ordered samples such as thin films on substrates, where the substrates can serve as a reference for solving the phase problem. While limited, there have been attempts to calculate real space density distribution of the unit cell from SAXS, too.

In this talk, I will present research projects that required analysis of diffraction peaks measured in small angle x-ray scattering (SAXS). First, a gyroid morphology of a block copolymer blend was revealed to have core-shell configuration. Various unit cell density maps were constructed in the real space and calculated patterns were compared to measured data. Second, charge flipping algorithm was applied to SAXS data analysis, providing a real space density map directly from SAXS data.