Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Characterization of diblock copolymer lamellar structure from neutron scattering measurements and molecular dynamics simulations CHEOL JEONG, JENNY KIM, SANGCHEOL KIM, NIST - Natl Inst of Stds & Tech, TSUNG-HAN TSAI, E. BRIAN COUGHLIN, University of Massachusetts Amherst, CHRISTOPHER SOLES, NIST - Natl Inst of Stds & Tech — The Nanoscale structure of block copolymers (BCP) with lamellar morphology plays an important role in transport properties for fuel cell and battery application. We develop a paracrystalline model to interpret small angle neutron scattering (SANS) and X-ray scattering (SAXS) data of hydrated amphiphilic BCP lamellar phase in order to elucidate water distribution as well as hydrophilic and hydrophobic domain spacing. We assume Gamma distribution for the fluctuation of lamellar thickness instead of Gaussian. It is observed that BCP can deswell upon hydration along lamellar normal direction due to chain collapse of hydrophobic domain overcoming expansion of hydrophilic domain, which has been compared with coarse-grained molecular dynamics simulation (CGMD). CGMD results show that the variation of interfacial area per chain is strongly correlated to the conformation of hydrophobic chains, domain spacing and water distribution in the hydrophilic domain, compatible with the observation from SANS and SAXS.

Cheol Jeong
NIST - Natl Inst of Stds & Tech

Date submitted: 14 Nov 2014 Electronic form version 1.4