Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Effect of Aggregation on the Mechanical Properties of Ionomers from MD Simulations[1] JANANI SAMPATH, LISA M. HALL, The Ohio State University-Columbus — Ionomers are polymers with a small fraction of charged monomers; these bound ions, along with free counterions, tend to aggregate together strongly in the absence of solvent. Ionic aggregates can act like temporary cross-links, giving rise to interesting mechanical properties. We perform coarse-grained molecular dynamics simulations of ionomers with various spacings of charges along the chain, representing experimental precisely spaced, neutralized poly(ethylene-co-acrylic acid) materials. We calculate aggregate morphology, dynamics, and scattering profiles and study the systems during uniaxial tensile strain to understand how aggregate structure changes under deformation and affects mechanical properties. Anisotropic structure factors (parallel and perpendicular to the direction of pull) and visualization shows that the aggregates align, in qualitative agreement with experimental findings. Stress-strain curves at different strain rates are also obtained. A modification of the model to account for unneutralized acid groups by adjusting their Lennard-Jones interaction strengths with each other and with ionic groups will also be discussed.

[1]This material is based upon work supported by the National Science Foundation under Grant 1463103

Janani Sampath
The Ohio State University-Columbus

Date submitted: 06 Nov 2015 Electronic form version 1.4