Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Atomistic molecular dynamics simulations of model ionomers
DAN BOLINTINEANU, MARK STEVENS, AMALIE FIRSCHKNECHT, Sandia National Laboratories — Ionomers are polymers that contain a small fraction of ionic groups. Due to their unique electrical properties, ionomers are being investigated as potential solid electrolytes in mobile battery applications. However, a lack of fundamental understanding of the relationship between ionomer chemistry, morphology and ion transport have hindered such efforts. To this end, we report atomistic molecular dynamics (MD) simulations of a model ionomer (polyethylene-co-acrylic acid) neutralized with different ions at various neutralization levels. The structure factor computed from the simulations is in good agreement with experimental X-ray scattering data, which provides strong validation of the simulation methods. Our simulations provide additional insight into the shape and size distribution of ionic clusters; in particular, we observe large networks of string-like clusters, and report quantitative features of these structures as a function of ionic group spacing in the polymer backbone, counterion type and neutralization level. We also investigate several features of ion transport in these systems. Since ion diffusion is slow relative to the time scales accessible to our simulations, we limit discussion to local, qualitative features of the ion transport mechanism.

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Date submitted: 21 Nov 2011 Electronic form version 1.4