

Abstract Submitted  
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**Molecular Dynamics of Coarse-grained Ionomers Showing Aggregate Morphology During Deformation** JANANI SAMPATH, LISA M. HALL, The Ohio State University — Ionomers are polymers with a small fraction of charged monomers that have a wide range of applications from dental fixtures and packaging to actuators. We consider dense melts of ionomers and counterions with no solvent. An important aspect of their performance is the aggregation of ions, since ionic aggregates act to hold polymer chains together like temporary cross-links. Because of the size scales involved, it is difficult to obtain a complete 3D microscopic picture of polymer aggregation experimentally; typically the thickness of a sample used in transmission electron microscopy is such that multiple overlapping aggregates appear together. How aggregate structure changes under strain and affects mechanical properties is even less clear. We perform molecular dynamics simulations of ionomers of various architectures, and show aggregate morphology and scattering profiles. We apply uniaxial tensile strain and observe the aggregates align, in qualitative agreement with experimental findings. We also obtain stress-strain curves and will discuss effects of degree of neutralization of the ionomers.

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