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Cluster Morphology in Lightly Sulfonated Polystyrene[1] ANUPRIYA AGRAWAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Aggregation of ionic groups into clusters in ionomers renders their unique properties that drive the use in energy applications. The ionic clusters however have a dramatic impact on the rheology of this polymer. Even small fractions of ionic groups (less than 5%), constrain their dynamics, making them difficult to process. Using molecular dynamics simulations, we show that in lightly sulfonated polystyrene melts, the ionic groups aggregate into ladder type clusters. These ladder morphologies prevail for a broad temperature range and degree of sulfonation, although with some variation due to steric effects of the chain. Reducing the electrostatic strength by tuning the dielectric constant changes the cluster morphology from ladder to spherical, which in turn, greatly increases the diffusion of the polymer. The effect of changing the electrostatic strength is comparable to the effect of addition of diluents to this melts. Enhancing the electrostatic screening results in breaking the clusters, whereas increasing temperature within the measured range, results in faster diffusion of the entire polymers while the clusters remain intact.

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