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Role of Ionic Clusters in Dynamics of Ionomer Melts: From Atomistic to Coarse Grained Simulations[1]

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Ionomers, polymers decorated with ionizable groups, have found application in numerous technologies where ionic transport is required. The ionic groups associate into random clusters resulting in substantial effect on structure, dynamics and transport of these materials. The effects of topology, size and dynamics of these aggregates however remain an open question. Here we probe cluster formation correlated with polymer dynamics through a model system of randomly sulfonated polystyrene (SPS) melts with molecular dynamics (MD) simulations over a broad time and length scales ranging from that within the ionic clusters through polymer segmental dynamics to the motion of the entire molecules. The cluster evolution was probed by fully atomistic studies. We find ladder-like aggregates that transform to globule-like with increasing the dielectric constant of media for sodium neutralized SPS. With increasing dielectric constant, the size of the aggregates decrease and their number increases. Concurrently, the mobility of the polymer increases. The counterion radius and valency affect both morphology and dynamics as is evident in the calculated static and dynamic structure factors. It is further manifested in the results of viscosity obtained through non-equilibrium molecular dynamics technique. Finally, to access larger length scales a three bead coarse-grained model to describe sulfonated styrene that we have developed will be discussed in view of the outstanding challenges in ionic polymers.

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