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Multiscale modeling of polystyrene dynamics in different environments ROLAND FALLER, QI SUN, FLORENCE PON, UC Davis — Polystyrene is a very abundant and industrially important polymer. We are modeling its dynamical behavior on multiple length scales and different environments. We start with pure PS where we develop a mesoscale polystyrene model based on atomistic simulations. . The non-bonded effective potential is optimized against the atomistic simulation until the radial distribution function generated from the mesoscale model is consistent with the atomistic simulation. The mesoscale model allows understanding the polymer dynamics of long chains in reasonable computer time. The dynamics of polystyrene melts are investigated at various chain lengths ranging from 15 to 240 monomers and the crossover to entangled dynamics is observed. As computer simulations cannot only address average properties of the system under study but also the distribution over any observable of interest we are study mixtures of polystyrene and polyisoprene by atomistic molecular dynamics and calculate correlation times for all segments in the system. We then identify fast and slow segments and can correlate the segment speed with the local neighborhood and obtain that fast segments have a surplus of the faster component in their neighborhood and vice versa. A coarse grained mixture model will be presented as well.

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