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Coarse-grained modeling of polystyrene at different concentrations using the Iterative Boltzmann Inversion technique BESTE BAYRAMOGLU, ROLAND FALLER, UC Davis — We present systematic coarse-graining of several polystyrene models and test their performance under confinement and eventually in brush systems. The structural properties of a dilute polystyrene solution, a polystyrene melt and a confined concentrated polystyrene solution at 450K, 1 bar were investigated in detail by atomistic molecular dynamics simulations of these systems. Coarse-graining of the models was performed by Iterative Boltzmann Inversion Technique (IBI), in which the interaction potentials are optimized against the structure of the corresponding atomistically simulated systems. Radial distribution functions, bond, angle and dihedral angle probability distributions were calculated and compared to characterize the structure of the systems. Good agreement between the simulation results of the coarse-grained and atomistic models was observed.

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