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Gibbs Ensemble Simulations of the Solvent Swelling of Polymer Films THOMAS GARTNER, THOMAS EPPS, III, ARTHI JAYARAMAN, University of Delaware — Solvent vapor annealing (SVA) is a useful technique to tune the morphology of block polymer, polymer blend, and polymer nanocomposite films. Despite SVA's utility, standardized SVA protocols have not been established, partly due to a lack of fundamental knowledge regarding the interplay between the polymer(s), solvent, substrate, and free-surface during solvent annealing and evaporation. An understanding of how to tune polymer film properties in a controllable manner through SVA processes is needed. Herein, the thermodynamic implications of the presence of solvent in the swollen polymer film is explored through two alternative Gibbs ensemble simulation methods that we have developed and extended: Gibbs ensemble molecular dynamics (GEMD) and hybrid Monte Carlo (MC)/molecular dynamics (MD). In this poster, we will describe these simulation methods and demonstrate their application to polystyrene films swollen by toluene and n-hexane. Polymer film swelling experiments, Gibbs ensemble molecular simulations, and polymer reference interaction site model (PRISM) theory are combined to calculate an effective Flory-Huggins χ (χ_{eff}) for polymer-solvent mixtures. The effects of solvent chemistry, solvent content, polymer molecular weight, and polymer architecture on χ_{eff} are examined, providing a platform to control and understand the thermodynamics of polymer film swelling.

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