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Evaporation and interdiffusion of solvent in polymer films MESFIN TSIGE, Southern Illinois University Carbondale, GARY S. GREST, Sandia National Laboratories — Solvent evaporation from homopolymer and heteropolymer films along with the interdiffusion of solvent into these films is studied using large scale molecular dynamics and grand canonical Monte Carlo simulations. As the solvent evaporates, a sharp increase in polymer density at the film/vapor interface is observed. The rate of solvent evaporation, for both homopolymer and heteropolymer films is found to decrease exponentially with time. For multiblock films the resulting domain structure is found to be strongly affected by the relative stiffness of the two blocks. In the interdiffusion study, the shape of the solvent concentration profile and the weight gain by the film can be related to the diffusivity. For homopolymer films, although the diffusivity is found to be strongly concentration dependent especially as one approaches the glass transition temperature of the polymer, the weight gain scales as $t^{1/2}$ for all cases studied, which is expected for Fickian diffusion. For a multiblock copolymer film in which the stiffer block is below the glass transition temperature is also studied, even though the solvent swells only the softer block of the copolymer, the weight gain by the film remains Fickian.

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