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Modeling Solvent Evaporation from Glass-Forming Polymer Films by MD Simulations JORG BASCHNAGEL, SIMONE PETER, HENDRIK MEYER, Institut Charles Sadron, Strasbourg — By means of molecular-dynamics simulations we study solvent evaporation from glass-forming, free-standing and supported polymer films. Polymers are represented by a commonly employed bead-spring model, solvent molecules are modeled as Lennard-Jones particles, and polymer-solvent interactions are tuned such that good-solvent conditions are realized. We start the simulations from a dense solution with a solvent content of 20% and explore the evaporation process for temperatures T above and below the glass transition temperature $T_{\rm g}$ of the pure polymer film. At all T we observe the formation of a polymer-rich crust at the free surface upon solvent evaporation. For $T > T_{\rm g}$ we can reproduce the simulation results (reduction of film thickness with time, solvent and polymer density profiles, etc.) by a Fickian diffusion model with a constant diffusion coefficient. For $T < T_{\rm g}$ deviations from Fickian diffusion are observed. We suggest that these deviations may be rationalized by a diffusion coefficient of the solvent, which depends on film composition and distance from the free surface. We attempt to compare our results to recent experiments.

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