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Solvent-Assisted Self-Assembly of Block Copolymer Films: A Simulation Approach SU-MI HUR, GURDAMAN S. KHAIRA, PAUL NEALEY, Institute for Molecular Engineering, University of Chicago, MARCUS MÜLLER, Institut für Theoretische Physik Georg-August Universität, JUAN J. DE PABLO, Institute for Molecular Engineering, University of Chicago — Solvent annealing has been shown to provide an effective means for controlling the self assembly in block copolymer films; it also provides opportunities to create structures that cannot be achieved by thermal annealing. The intrinsic non-equilibrium nature of these processes presents challenges to their theoretical understanding. We have developed an efficient simulation tool for modeling the solvent annealing of block copolymer films that enables study of the evolution of microstructure and the transformations between various microphases in response to film swelling and solvent evaporation. We study the effect of process and thermodynamical variables such as solvent pressure, molecular weight and segregation force, on the self assembled structure of block copolymer thin films. And we identify conditions that lead to a defect-free copolymer morphology. We also discuss the effects of relative time scales of solvent evaporation, diffusion of solvent and of polymer chains on the self-assembly of block copolymer thin films.

Su-Mi Hur
Institute for Molecular Engineering, University of Chicago

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