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Optimizing the Combination of Solvent Annealing and Directed Self-Assembly in Thin Film Block Copolymer Systems Using Self-Consistent Field Theory ADAM HANNON, KEVIN GOTRIK, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Institute of Technology — We show how self-consistent field theory simulations can be used to optimize the combination of solvent annealing and directed self-assembly using topographical and chemical templating in order to achieve an ultimate goal of arbitrary pattern generation in thin film block copolymer systems. The simulations use a combination of field boundary conditions to model topographical features such as posts and chemically distinct surfaces along with a variety of compositions to model a range of solvent, homopolymer, and block copolymer multi-component blends [Macromolecules 2010, 43, 8290–8295]. Computational results are compared with experimental systems that use polydimethylsiloxane, polystyrene, and polyferrocenylsilane polymers, heptane, toluene, and chloroform solvents, and electron beam lithography created hydrogen silsesquioxane posts. By varying the different polymers used and thus their χ interaction parameters, the relative fractions of solvent and different polymer blocks, and surface feature affinity and shape, the optimal requirements to create arbitrary complex features for nanolithography applications will be demonstrated.

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