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Finding Optimal Templates for the Directed Self-Assembly of Thin Film Block Copolymers with Inverse Self-Consistent Field Theory Simulations ADAM HANNON, YI DING, WUBIN BAI, CAROLINE ROSS, ALFREDO ALEXANDER-KATZ, Massachusetts Inst of Tech-MIT — Achieving sub-10 nm patterns with non-periodic features is a key goal in the development of next generation integrated circuits devices. One route to create such features at this length scale is the directed self-assembly of thin film block copolymers (BCPs). Inverse design methods are becoming a key part in developing templates needed for given target patterns where the required template is both non-intuitive and requires optimization. Here we use a self-consistent field theory based inverse design algorithm to find template solutions for target structures. Recent studies have revealed a wide parameter space with multiple solutions for given target structures. Using fidelity and topology functions, we characterize how well different template solutions yield given target structures and refine these solutions beyond simply being free energy minimum solutions. Experiments using polystyrene-*b*-polydimethylsiloxane BCPs templated by hydrogen silsesquioxane posts are used for verifying and refining the simulation results. Results show that key factors influencing the fidelity and topology of the samples include the effective volume fraction of the solvent annealed system, size of the posts, and areal post density. Optimization of these parameters achieves refined template solutions with better reproducibility and lower defectivity both computationally and experimentally.

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