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Inverse design of bulk morphologies in block copolymers using particle swarm optimization MIHIR KHADILKAR, KRIS DELANEY, GLENN FREDRICKSON, UC Santa Barbara — Multiblock polymers are a versatile platform for creating a large range of nanostructured materials with novel morphologies and properties. However, achieving desired structures or property combinations is difficult due to a vast design space comprised of parameters including monomer species, block sequence, block molecular weights and dispersity, copolymer architecture, and binary interaction parameters. Navigating through such vast design spaces to achieve an optimal formulation for a target structure or property set requires an efficient global optimization tool wrapped around a forward simulation technique such as self-consistent field theory (SCFT). We report on such an inverse design strategy utilizing particle swarm optimization (PSO) as the global optimizer and SCFT as the forward prediction engine. To avoid metastable states in forward prediction, we utilize pseudo-spectral variable cell SCFT initiated from a library of defect free seeds of known block copolymer morphologies. We demonstrate that our approach allows for robust identification of block copolymers and copolymer alloys that self-assemble into a targeted structure, optimizing parameters such as block fractions, blend fractions, and Flory chi parameters.

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