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**Coarse-Graining Polymer Field Theory for Fast and Accurate Simulations of Directed Self-Assembly**[1] JIMMY LIU, KRIS DELANEY, GLENN FREDRICKSON, University of California Santa Barbara — To design effective manufacturing processes using polymer directed self-assembly (DSA), the semiconductor industry benefits greatly from having a complete picture of stable and defective polymer configurations. Field-theoretic simulations are an effective way to study these configurations and predict defect populations.

Self-consistent field theory (SCFT) is a particularly successful theory for studies of DSA. Although other models exist that are faster to simulate, these models are phenomenological or derived through asymptotic approximations, often leading to a loss of accuracy relative to SCFT.

In this study, we employ our recently-developed method to produce an accurate coarse-grained field theory for diblock copolymers. The method uses a force- and stress-matching strategy to map output from SCFT simulations into parameters for an optimized phase field model. This optimized phase field model is just as fast as existing phenomenological phase field models, but makes more accurate predictions of polymer self-assembly, both in bulk and in confined systems. We study the performance of this model under various conditions, including its predictions of domain spacing, morphology and defect formation energies.

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