Exploring Novel Block Copolymer Microstructures via Reciprocal-Space Niching Genetic Algorithms and Self-Consistent Field Theory

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Abstract body:

Block copolymer self-assembly provides a versatile platform for designing and fabricating nanostructures across a wide range of applications. A primary theoretical tool for investigating this process is the self-consistent field theory (SCFT), a well-established framework that enables the systematic identification of thermodynamically stable self-assembled states. However, exploring the most stable self-assembled microstructure in a given parameter space is known to be a challenging task in SCFT [1] since the free energy landscape encapsulates multiple local metastable states, trapping the optimization process. Owing to this limitation, conventional SCFT studies often rely on prior experimental knowledge to construct candidate libraries for free-energy comparison, limiting their ability to discover novel phases [2]. In this contribution, we develop a reciprocal-space niching genetic algorithm (RPGA) coupled with SCFT to automatically search for a global stable structure from a random state without any prior knowledge. The algorithm is designed by taking the reciprocal-space representation of periodic material as its "composite" gene for selection, crossover, and mutation to find out potential candidates. Furthermore, we equip the RPGA with the lattice island model, one of the ideas from the niching method with the lattice system, to mitigate the sensitivity of cell shape issues in SCFT. All simulations are parallelized by an in-house multi-GPU platform to accelerate large cell 3D simulations. We validate our algorithm by comparing the assemblies of conformationally symmetric as well as asymmetric diblock copolymer systems in various sets of parameter space. It can be shown that our RPGA+SCFT algorithm can explore classical and complex network phases, such as gyroid or Fddd, and exceptionally stable Frank-Kasper A15 phase within 20 iterations with a reasonable population size. In addition, the approach can unify some of the hyperparameter settings for different sets of parameter space, reducing the need for case-by-case tuning. We anticipate that this framework can be extended to more intricate block copolymer architectures, thereby accelerating the discovery of novel stable phases through high-performance computation.

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Publications Reference

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[2] A. Arora, J. Qin, D.C. Morse, K.T. Delaney, G.H. Fredrickson, F.S. Bates, K.D. Dorfman, Broadly Accessible Self-Consistent Field Theory for Block Polymer Materials Discovery, Macromolecules, 49 (2016) 4675-4690.