Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Accelerating the search for globally stable block polymer microphases using genetic algorithms[1] CAROL TSAI, KRIS DELANEY, GLENN FREDRICKSON, UC Santa Barbara — The diverse array of block copolymer (BCP) applications is possible because in the melt state, various morphologies that are periodic structures on the nanoscale emerge depending on the particular composition and architecture of the BCPs used. However, knowing which compositional parameters to use to obtain materials with desired properties is a Herculean task: there is an enormous parameter space to search. Furthermore, the problem is exacerbated by the fact that even at a fixed set of compositional parameters, it is difficult to determine the globally stable morphology and low-lying metastable states that will emerge, as complications arise from a rough free-energy landscape: a self-consistent field search may become trapped in high-energy metastable states, resulting in long and computationally expensive searches. We show that genetic algorithms, which are a biologically-inspired global search heuristic, may be a promising way to ameliorate this problem when used in conjunction with local optimizations performed by SCFT.

[1]NSF-GRFP, NSF DEMREF DMR-1332842, UCSB CNSI CSC

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Date submitted: 08 Nov 2014 Electronic form version 1.4