Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Progress on a 'spectral filtering' for SCFT algorithms: Removing topological defects in block copolymer simulations SCOTT SIDES, Tech-X Research Corporation, BOBBY SUMPTER, Oak Ridge National Labs — Using block copolymers as mesoscale templates has potential applications for improved photovoltaic devices, fuel-cells and magnetic storage media. For many of these applications the long-range order and orientation of the copolymer phase-separated domains is crucial. Self-consistent field theory (SCFT) for dense polymer melts has been highly successful in describing complex morphologies in block copolymers. Field-theoretic simulations based on SCFT theory are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics. It has been shown that real-space numerical SCFT calculations can describe certain features of topological defects in a bulk copolymer. However, for large SCFT simulations the presence of these topological defects can obscure the identification of the appropriate lowest-energy space group for a complex block copolymer mixture. A 'spectral filtering' algorithm has been shown to help reduce the presence of topological defects in SCFT calculations of block copolymer structure by removing certain frequency components of the chemical potential fields during the simulation. Further progress on this filtering method will be presented and shown to improve the removal of defects in large, 3D-SCFT simulations.

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Date submitted: 03 Dec 2007 Electronic form version 1.4