

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Field-theoretic Monte Carlo simulations of a diblock copolymer melt BART VORSELAARS, University of Waterloo, PAWEL STASIAK, University of Reading, MARK MATSEN, University of Waterloo — Using field-theoretic Monte Carlo simulations (MC-FTS) we report on a melt of diblock copolymers. Our focus is on the region near the transition between the disordered and lamellar phase. The MC-FTS method in use [1] makes it possible to study systems with a vast number of chains beyond that what is attainable by classical molecular dynamics simulations, and without compromising on neglecting compositional fluctuations, as is the case with self-consistent mean field theory. The assumption that the fluctuations in the incompressibility field are of a Gaussian nature allows one to use standard MC techniques. We compare the simulation results with predictions from theories that include fluctuations, such as a theory developed by Fredrickson and Helfand (FH) and the recently published renormalized one-loop calculations. Once the incorporation of the ultra-violet divergence is taken care of in an accurate way, the simulation results can be nicely mapped onto the theoretical predictions near the transition region, even for moderate simulation resolutions. [1]: Stasiak and Matsen, *Macromolecules* **46**, 8037 (2013)

Bart Vorselaars
University of Waterloo

Date submitted: 14 Nov 2014

Electronic form version 1.4