

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Architecture phase diagram for branched block copolymers:

SCOTT SIDES, Tech-X Corporation, BOBBY SUMPTER, Oak Ridge National Labs, TECH-X/ORNL COLLABORATION — Self-consistent field theory (SCFT) for dense polymer melts has been highly successful in describing complex morphologies in block copolymers. Field-theoretic simulations such as these are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics, while still incorporating more realistic polymer models than many macroscopic, continuum simulations. Using block copolymers as mesoscale templates has potential applications for improved photovoltaic devices and fuel-cells. Many of these applications require control over the domain size of the phase-separated regions. One possible method is changing the architecture of branched copolymers. In this talk I will outline the SCFT method, discuss some efficient methods of numerically solving the SCFT equations and present results for modeling PI-PS block copolymers. The results will be compared to experimental data examining the influence (structure and mechanical properties) of adding more branches of PS along a PI backbone. These copolymer configurations include one PS branch at each graft point on PI, 2 PS's, and up to 4 PS's branches with varying number of branch points on the PI backbone.

Scott Sides
Tech-X Corporation

Date submitted: 20 Nov 2006

Electronic form version 1.4