Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Unit cell relaxation with the SCFT of block copolymers ERIC COCHRAN, University of California, Santa Barbara, SCOTT SIDES, University of California, Santa Barbara, DAVE MORSE, University of Minnesota, Twin Cities, GLENN FREDRICKSON, University of California, Santa Barbara — We employ the pseudo-spectral implementation of the self-consistent field theory (SCFT) of linear block copolymer melts to model their equilibrium phase behavior. Here we focus on *unit cell* calculations in which saddle-point configurations are determined iteratively through the simultaneous relaxation of the potential fields and the shape of the simulation volume, which is a parallelepiped of arbitrary dimension. The former is accomplished through either an explicit Euler or semi-implicit Seidel type relaxation of the potential fields. Relaxational cell shape dynamics are dictated by the deviatoric stress tensor, which we compute according to the Parrinello-Rahman-Ray technique recently adapted to SCFT by Barrat and coworkers. Defect-free structures may be obtained by using an initial configuration that is constrained to a particular crystallographic symmetry.

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Date submitted: 30 Nov 2004 Electronic form version 1.4