Contribution ID: **226** Type: **Oral (Student, Not in Competition) / Orale (Étudiant(e), pas dans la compétition)**

Dynamical self-consistent field theory of phase transition kinetics in AB diblock copolymer melts

Thursday 19 June 2014 10:30 (15 minutes)

We examine the kinetics of phase transitions in AB diblock copolymer melts using a dynamical self-consistent field theory that we recently developed. By applying the variational priniciple to an appropriate dynamical functional integral, which is based on the exact microscopic polymer dynamics, we obtain the self-consistent equations. These equations are then solved through an ensemble of Brownian dynamics simulations of a single chain in a self-consistently determined, dynamical, mean field. We examine the kinetics of transitions between the disordered, lamellar, and cylindrical phases in the diblock copolymer melt. We also test our theory by examining early-stage spinodal decomposition in a binary (A/B) homopolymer blend, and comparing to existing results from the dynamical random-phase approximation, and from single-chain in mean-field simulation. Since our theory is directly connected to the microscopic dynamics, our time scale is directly relatable to the microscopic Rouse time for the chains, and we can follow the dynamics of individual chain conformations as the diblock copolymer microdomains re-arrange during the transition.

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Session Classification: (R1-5) Computational Materials Mini-symposium I - DCMMP-DMBP / Mini-symposium sur les matériaux numériques I - DPMCM-DPMB

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)