Abstract Submitted for the MAR12 Meeting of The American Physical Society

Morphology of ABC linear triblock polymer melts: selfconsistent-field theoretic simulation approach<sup>1</sup> MOUGE MOHAGHEGHI, BAMIN KHOMAMI, Dept. of Chemical and Biomolecular Eng., University of Tennessee, Knoxville, TN — It is well known that block copolymer morphologies resulting from microphase separation finds wide spread use in many applications, including nanolithographic templates, membranes, and electronic arrays. In this study, we have performed self-consistent field theoretic based simulations to examine the plethora of self-assembled morphologies obtained in symmetric linear ABC Tri-block polymer melts in bulk and confined films. Specifically in bulk systems, the conditions leading to lamellae, tetragonal cylinders, sphere, perforated lamellae, and network morphologies have been elucidated at various volume fractions of middle (B) block. In general, the predicted morphologies are in good agreement with the limited number of published experimental studies. The effect of confinement on the microphase separation is also studied by performing simulations of two neutral parallel walls. Overall, we observe lamellar and cylindrical domains that are oriented parallel to the walls; however, lamellar domains could become perpendicular to the neutral walls when the natural period of lamellae is incommensurate with the film thickness. Our calculations form the basis for understanding the stability of parallel and perpendicular orientations in thin films of ABC tri-block polymeric systems.

<sup>1</sup>This work is supported by NSF through funding grant EPS-1004083.

Mouge Mohagheghi Dept. of Chemical and Biomolecular Eng., University of Tennessee, Knoxville, TN

Date submitted: 15 Nov 2011

Electronic form version 1.4