Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Coarse Grained Monte Carlo Simulations of Solvent Annealed Block Copolymer Thin Films GURDAMAN KHAIRA, SU-MI HUR, JUAN DE PABLO, University of Chicago — Solvent annealing has been shown to provide an effective means for controlling the self assembly of block copolymer thin films. However, the current theoretical understanding of solvent annealing processes is limited. We have developed a particle based coarse-grained model to study the solvent annealing and the effect of process variables on the self assembled structure of block copolymer thin films. For bulk materials, our model is shown to reproduce the phase behavior reported in experiments. In thin films, our approach enables us to mimic the experimental process, while accessing the large length and time scales relevant to applications in directed self assembly. In this presentation, we will discuss the effects of solvent-polymer interactions, solvent vapor pressure and solvent evaporation rate on the morphology of ordered domains.

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Date submitted: 09 Nov 2012 Electronic form version 1.4