Surface Affinity Effects On Confined Thin Film Block Copolymers Using Self Consistent Field Theory Modeling

ADAM HANNON, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Institute of Technology — Self consistent field theory (SCFT) applied to inhomogeneous thin film block copolymer systems allows for the exploration of a wide array of potential equilibrium ordered morphologies at the nanoscale through varying parameters such as $\chi$, the segmental Flory-Huggins parameter, $N$, the polymer degree of polymerization, and $f$, the volume fraction of the minority polymer component. In addition, boundary conditions of the chemical potential fields in the field theory can be specified to model surface features such as polymer brush layers and topological templating features from lithography that enrich the possible morphologies observed [Macromolecules 2010, 43, 8290–8295]. In this presentation, we show how the orientation and surface morphology of diblock copolymers with large $\chi N$ varies with surface affinity, surface shape, and $f$ for confined thin film systems. Surfaces neutral to both polymer species are examined, as well as surfaces preferential to both the minority and majority polymer components with fine variances in the magnitude of the surface affinity. Commensurability of the ordered structures is examined as well by varying simulation cell size. The results of the study will be applied to the generation of complex features for nanolithography applications.