A Molecular View of Block Copolymer Directed Assembly and its Application to Sub-Lithographic Patterning

J.J. de Pablo and P.F. Nealey
Department of Chemical and Biological Engineering
University of Wisconsin - Madison
1415 Engineering Drive, Madison, WI 53706

Directed copolymer assembly (DCA) has emerged as a promising alternative for patterning at sub-lithographic length scales. Much progress has been made over the past decade, but a number of significant challenges remain. At the University of Wisconsin – Madison we have adopted a truly concerted experimental and computational approach aimed at gaining a fundamental understanding of directed copolymer assembly on nanopatterned substrates. This presentation will provide an overview of recent theoretical and computational approaches that have enabled the use of models and simulations as true design tools[1,2,3,4], along with their advantages and limitations, and a discussion of some emerging predictions and the corresponding experimental observations. As shown in this talk, these approaches can predict thermodynamic and dynamic properties, and rely only on knowledge of composition and molecular architecture of all components. They serve to predict different morphologies, the boundaries between them and, when imperfect states arise, they help determine the free energy (and corresponding probability) of defects. They also serve to evaluate the merits of different patterning strategies, such as chemical epitaxy or graphoepitaxy[5], or to interpret the results of experiments, particularly when new structures are discovered[6]. More recently, simulations have allowed us to determine the dynamic pathways by which equilibrium and non-equilibrium morphologies arise in directed self assembly, both during standard spin-coating applications and during solvent annealing processes. The latter development is allowing us to develop a series of new patterning strategies that could expand considerably the palette of available morphologies for device fabrication.

---

1 F.A. Detcheverry et al., Soft Matter, 5, 4858-4865 (2009).
2 F.A. Detcheverry et al., Physical Review Letters, 102, Article Number 197801 (2009).
3 R. Ruiz et al., Science, 321, 936-939 (2008).
4 F.A. Detcheverry et al., Macromolecules, 43, 3446-3454 (2010).
5 F.A. Detcheverry et al., Macromolecules, 43, 6495-6504 (2010).
6 S. Ji et al., Advanced Materials, 23, 3692 (2011).