Multiscale Modeling of Block Copolymer Directed Assembly and its Application to Sub-Lithographic Patterning

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Block copolymer lithography (BCL) is gradually emerging as a viable alternative for patterning at sub-lithographic length scales. While considerable progress has been made over the past decade, a number of significant issues must be addressed for BCL to find widespread use in commercial, large-scale processes. Past work has shown that a number of variables can be used to direct the assembly of copolymers on patterned substrates. These include the molecular weight of the polymeric constituents, the composition of the copolymers and their blends, the interactions between different blocks and the substrate, and the commensurability (or lack thereof) between a substrate pattern and the inherent morphology of the copolymer material. Predicting the behavior and structure of thin films on patterned substrates remains a challenge; the morphologies that arise are often very different from those for the corresponding bulk material, reinforcing the fact that the copolymer thin film and substrate must be regarded as a completely new system that can bear little resemblance to the bulk (substrate-free) material.

Over the past decade, our group at the University of Wisconsin has 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 the theoretical and computational approaches that have been developed to arrive at that understanding[1,2], along with their advantages and limitations, and a discussion of the corresponding experimental observations. As shown in this talk, these approaches are truly predictive 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 origin of defects.

Particular emphasis will be placed on the concept of pattern interpolation and sub-lithographic patterning[3,4]. The overall goal is to rely on the spontaneous but controlled assembly of copolymers to arrive at dense patterns with characteristic dimensions in the tens of nanometers, while using sparse patterns defined on larger length scales. This presentation will encompass interpolation in the context of several distinct motifs of interest to the semiconductor industry, where large throughput simulations have enabled a fundamental understanding of interpolation with lines, spots, and squares. A comparison of results for various approaches, including chemical patterning and topographic patterning will also be presented. General correlations and design rules in terms of predicted free energy minima will be discussed for analysis of a number of experimental observations, including some related to pattern quality and process latitude.

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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, in press (2010).