Block Copolymer Directed Self-Assembly Defect Modes Induced by Localized Errors in Chemoepitaxial Guiding Underlayers: A Molecular Simulation Study

As the semiconductor manufacturing industry continues to seek high throughput methods for fabricating devices with sub 10-nm feature sizes, the directed self-assembly (DSA) of block copolymers (BCPs) has been presented as an intriguing and economical alternative to optical lithography. DSA of BCPs guides the microphase separation of the polymer blocks into various highly-ordered morphologies at nanometer length scales with the promise of being more cost effective than alternatives such as multi-patterning or EUV lithography. One potential drawback to BCP DSA is the defectivity inherent at some level in such thermodynamically driven processes due to entropic effects.[1,2] The number of defects in such DSA processes is reduced by using strong physical or chemical guidance of the ordering and placement of the BCP domains on a patterned underlayer. For example, chemoepitaxial processes use a chemically neutral underlayer that is patterned with periodic chemically preferential regions which attract one of the polymer blocks. This modification of the energetic landscape of the self-assembly process can transform what would be a defective fingerprint in a lamellae-forming BCP into a well-ordered line-space type pattern.[3,4] Recent experimental studies have shown that while both chemoepitaxial and graphoepitaxial methods can significantly reduce the number of defects observed in such DSA processes, there are still higher levels of defects than desired, and a limited set of particular defect modes seem to be most prevalent (e.g. bridge defects are one of the most common). Understanding the origins of these defects will be crucial to finally reducing defect levels in DSA processes to values acceptable for high volume manufacturing (HVM).

As mentioned earlier, micro-bridging between lamellar domains near the substrate has become one of the most frequently observed modes of defectivity in experimental DSA process flow testing.[5,6] In such cases, the origins of these defects are still unknown, though there have been speculations regarding the root causes. For example, Sato and coworkers suggested that micro-bridging they observed in a SMART™ type flow with PS-b-PMMA copolymer was induced by hydrophilic pinholes in the underlayer caused by imperfect wetting during the grafting of the neutral brush layer.[7,8] In order to probe possible causes for such DSA BCP defects and to gain a better understanding of the influence of elements of the DSA process (e.g. defects in the guiding underlayer) on the creation of defects in the self-assembled BCP film, coarse-grained molecular dynamics simulations have been utilized in this work to explore the impact of a range of underlayer defects on final DSA BCP pattern defectivity. For example, as shown in Fig. 1, coarse-grained molecular dynamics simulations of BCP annealing have been used to determine the relationship between the types of observed DSA defects and the corresponding radius of localized point defects on an otherwise perfectly patterned chemoepitaxial guiding underlayer. As an example of the results of these simulations, Fig. 2 displays the final position data for BCP films atop defective underlayers with a circular defect radius of $0.05 \cdot L_0$ (a) and $0.50 \cdot L_0$ (b), where L_0 is the pitch of the BCP film. Observing film morphology through annealing time in these simulations shows that in all cases, initially dislocation defects (see Fig. 2b) are created in the vicinity of the underlayer defect. In many cases, as annealing continues, these dislocations appear to anneal to a local perturbation and placement error of the lamellae with respect to the guiding stripes in the underlayer as shown in Fig. 2a. In this work, factors such as defect position, defect shape, and defect density in the underlayer will be probed to begin building an understanding of the likely origins of common DSA defects.

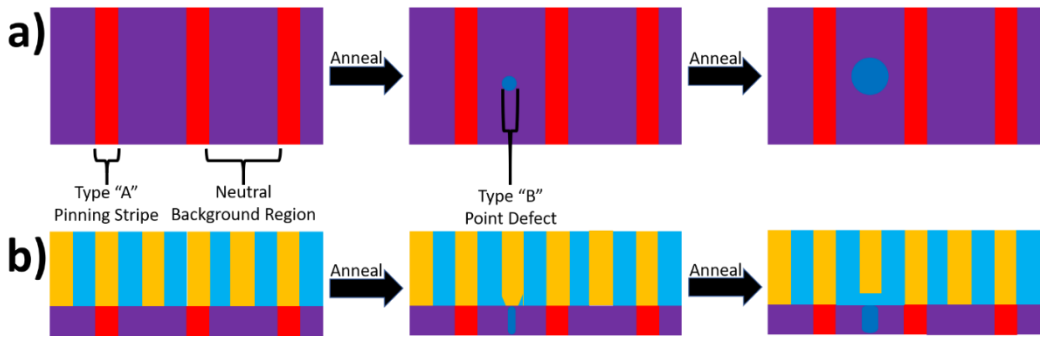

Figure 1. Type "B" point defect of varying radius within the neutral background region of a chemoepitaxial underlayer. A top-down view of the underlayer is shown in (a) as well as a cross-section of the BCP and underlayer in (b).

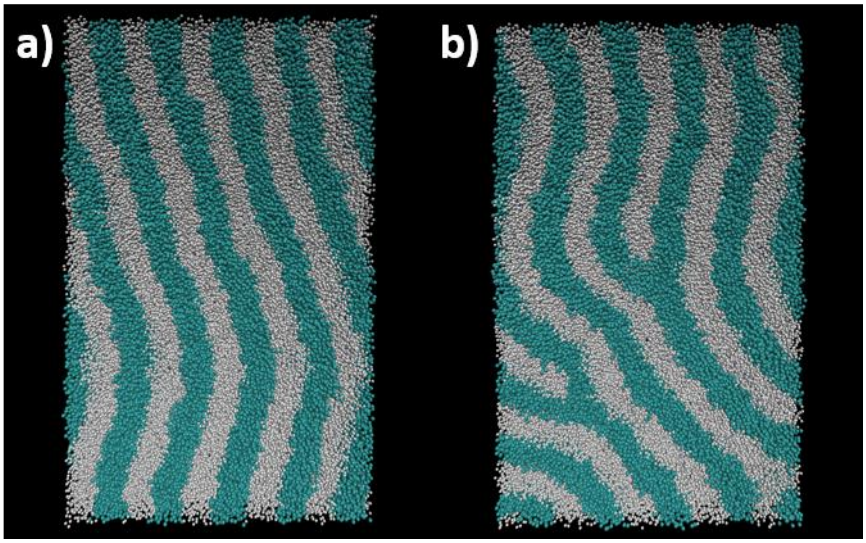

Figure 2. Simulation results of a thin-film BCP annealed for 3 μs atop a defective underlayer with a circular defect radius of 0.05·L0 (a) and 0.50·L0 (b). Although a defect of any radius initially propagates throughout the BCP, smaller defects annihilate much more quickly than larger defects.

References

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