Free Energy and Frequency of Defects in Chemoepitaxial Block Copolymer Directed Self-Assembly: Effect of Pattern Density Multiplication Factor, Defect Size, and Defect Position

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ABSTRACT

Block copolymers (BCPs) can microphase separate to form periodic structures with nanoscale domain sizes. This inherent ability to naturally form large arrays of uniformly sized nanoscale features can be harnessed for deterministic nanopatterning by aligning and registering such block copolymer patterns using lithographically patterned underlayers that guide the self-assembly process. This type of process is commonly referred to as directed self-assembly (DSA). For example, optical lithography can be used to make guiding underlayers that use chemoepitaxy to attract one of the polymer blocks preferentially to "pinning" features on the surface that provide long range order in the block copolymer features and reduce the number of defects. By making an underlayer pattern with a repeat distance in the "pinning features" that is an integer multiple of the natural repeat distance of the BCP microphase separated features, pattern density multiplication of the original lithographically defined pinning features can be achieved. Increasing the level of density multiplication requires less optical lithographic effort due to the more relaxed pitches of the pinning features and potentially larger feature size. However, higher density multiplication also provides less guidance to the BCP film which will naturally increase the frequency of defects in the patterned features. In this work, we use a coarse-grained molecular dynamics model coupled with thermodynamic integration to calculate the relative free energy of defect-free states and a variety of dislocation pair defects as the pattern density multiplication is increased in chemoepitaxial DSA. It is expected that as the density multiplication increases, the relative free energy of these defects will decrease and thus the frequency of defects will become larger. Additionally, the relative free energy will be calculated for varying dislocation pair sizes and positions over the patterned underlayer to determine in what type and position of such defects are most stable. The defect scaling rules obtained from this work can be used in conjunction with experimental defect benchmarking data to estimate the expected defect frequency for DSA patterning processes.

Keywords: directed self-assembly, block copolymer, multiplication density, defects, dislocation pair