Detailed Molecular Dynamics Studies of Block Copolymer Directed Self-Assembly: Effect of Guiding Layer Properties on Block Copolymer Directed Self-Assembly

Andrew Peters, Richard A. Lawson, Peter Ludovice Clifford L. Henderson*
School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0100, * Corresponding Author: cliff.henderson@chbe.gatech.edu

Directed self-assembly (DSA) of block copolymers, which relies on the use of surface features to guide the phase separation of the block copolymer into structures with long range order and precise registration, is a very promising technique for producing sub-30 nm pitch regular patterns. These patterns could be used as an enhancement to current lithographic techniques for manufacturing integrated circuit features below the current minimum pitch of ~80nm provided by leading edge 193nm lithography tools. However, roughness and defectivity of the surface guiding patterns produced using optical lithography and their effect on DSA processes, especially at relatively low values of χN (where χ is the Flory-Huggins parameter for the block copolymer and N is the polymer degree of polymerization), is not well understood at this point. Line-edge roughness (LER) and line-width roughness (LWR) could be the limiting factor in DSA lithography, not the absolute resolution limit or even the defectivity. This could be particularly true at χN values near the order-disorder transition (ODT). This paper will seek to answer many of these questions by using highly detailed, large scale molecular dynamics simulations of diblock copolymer DSA. These simulations are based on molecular dynamics of coarse-grained polymer chains simulated using graphics processing units (GPUs) to perform the calculations. It is well known that defects in the guiding pattern are often healed to some extent during DSA processing (Nealey 2008), but to what degree mis-sized or misplaced guiding patterns affect final DSA pattern roughness, especially near the ODT, is unknown and will be discussed in this paper. The effect of topography caused by the underlying guiding patterns is also thought to have an important effect in DSA processes, but again these effects have not been rigorously studied or characterized. Finally, unlike PS-b-PMMA, many of the block copolymer materials being considered for sub-20nm pitch patterning have highly asymmetric cohesive energy densities. While such cohesive energy differences in block copolymers are known to drive asymmetry in properties such as the polymer phase diagram (Bates 1999), the effect of such energetic differences between the blocks has not been rigorously characterized in terms of DSA properties such as pattern LER/LWR. A discussion of early studies of the DSA behavior of such block copolymers with such energetic asymmetry using molecular dynamics simulations will also be provided.

P. Nealey et al. Langmuir, 24, 1284-1295, 2008

F. S. Bates and G. H. Fredrickson, Phys. Today 52_2_, 32 _1999_.