Graphoeptiaxy directed self-assembly of lamellar phase symmetric block copolymers in the presence of two dimensional template patterns

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The formation of line-space patterns by directed self-assembly (DSA) of block copolymers (BCPs) is a well-known process. In graphoepitaxy DSA, a topographic relief or template is created on a chemically neutral surface. Confinement of the BCP between the sidewalls of the template provides an ordering force that drives the pattern into registry with the surface topography. The gap between two template lines required to form a given number of self assembled polymer phases in a symmetric lamellar phase BCP can be calculated using a simple analytic model of the free energy per copolymer chain[1]. Results of this model are plotted in Fig. 1(a). Applying a threshold function to this data gives approximate ranges for favorable gap spacing (Fig. 1(b)). Test patterns based on this understanding were fabricated using electron beam lithography (EBL) to pattern hydrogen silsesquioxane (HSQ) resist on a neutral polymer surface. DSA was performed using a polystyrene-poly(methyl methacrylate) (PS-PMMA) BCP. The PMMA phase was removed from the self-assembled pattern by selective reactive ion etching (RIE) and the patterns were imaged in an SEM. The results of this study are shown in Fig. 1(c). The data shows good agreement with the model.

Circuit patterning using graphoepitaxy DSA may benefit from a localized change in the number of self assembled lines occasioned by a modulation in the template gap spacing. This modulation would create 2D template geometries that have not been previously studied. Using the fabrication process described above, we created test patterns to intentionally abruptly modulate the gap spacing Fig. 2(a). The experimental results are shown in Fig. 2(b) and reveal that the modulation in the number of self-assembled lines is absorbed almost entirely by the truncation of a PS and PMMA phase. Moreover, this transition occurs rapidly and with minimal distortion to either phase.

An abrupt change in geometry may be unrealistic for templates patterned by 193nm immersion (193i) lithography where corner rounding is a known limitation. To investigate the impact of template corner rounding on DSA we performed a printing simulation of the target pattern assuming a 193i imaging process (Fig. 3(a)). The results of the simulation were printed with EBL and DSA was performed as described above (Fig. 3(b)). A clear modulation in the number of lines occurs in spite of the more gradual transition. However, the distance over which the modulation occurs is increased. Furthermore, both the PS and PMMA phases show significant distortion in the transition region. The experimentally observed results agree well with 3D Monte Carlo simulations of DSA in similar template geometries and indicate that the resulting behavior is required to reach thermodynamic equilibrium (shown in Fig. 4). These results demonstrate that corner rounding is a critical parameter in the design of DSA template patterns. The impact of this effect on circuit patterning with DSA will be discussed in more detail along with additional experimental and simulation results.

[1] F.S. Bates and G.H. Fredrickson, Physics Today, Feb 1999 p 32-38

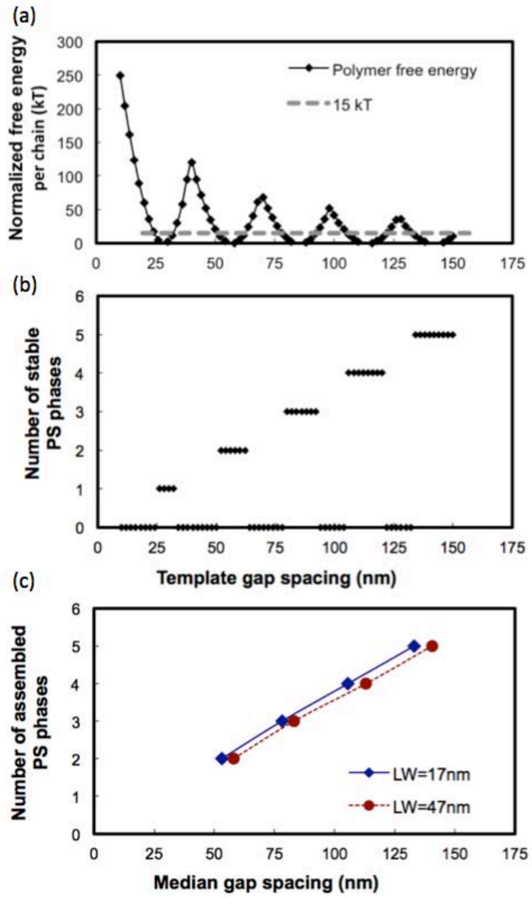

Figure 1: (a) Free energy of a PS-b-PMMA BCP with a natural length, L_o, of 29nm confined within a gap of varying size using the model discussed in reference 1. The data is normalized by kT (b) Thresholding of gap sizes within a 15 kT range plotted as a function of the number of self assembled PS phases which can be formed in that gap (c) Experimentally determined median gap spacing for DSA of 2 to 5 lines as a function of template line width (LW). The median gap spacing for DSA was determined by taking the median of the range over which the desired number of PS phases were formed. The dependence on LW is a consequence of the interaction between the BCP and the template feature.

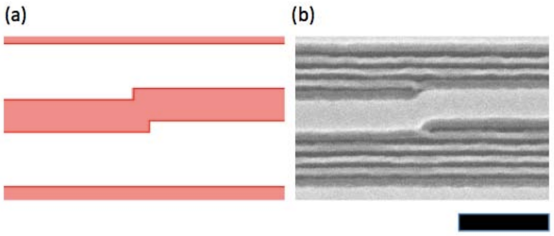

Figure 2: (a) Template designed to produce an abrupt transition between two different numbers of PS phases. Top: 3 to 2. Bottom: 3 to 4. (b) SEM image after DSA and removal of the PMMA phase with selective RIE. The scale bar corresponds to 200 nm.

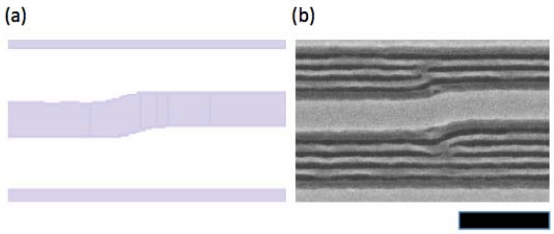

Figure 3: (a) Template derived from 193i printing simulation of the template shown in figure 2(a). (b) SEM image after DSA and removal of the PMMA phase with selective RIE. The scale bar corresponds to 200 nm.

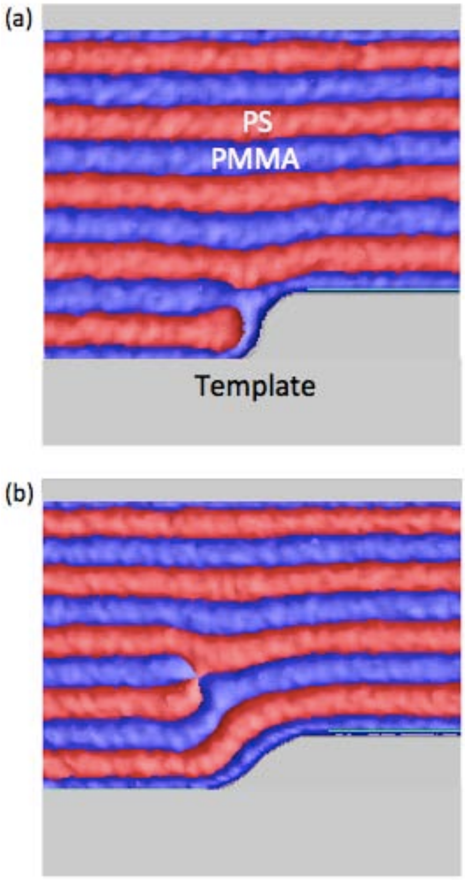

Figure 4: Monte Carlo simulation of a transition between self-assembled complete PS lines in a PS-PMMA BCP with L_o = 29nm. The simulation results agree well with the SEM images. In particular, the simulation captures the observed sensitivity to corner rounding. When the transition is abrupt (a), the modulation in number of lines occurs primarily from a truncation of a PS and PMMA phase, minimizing distortion in the phases outside the transition region. In contrast, the more gradual transition in the template (b) causes the modulation to take place over a larger distance. Moreover, there is significant distortion in the PS and PMMA phases closest to the template.