Rule-Based Directed Self-Assembly of Circuit-Like Block-Copolymer Patterns

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Topographic templates can be used for guiding the self-assembly of block copolymers to produce complex nanoscale patterns. In our previous work, regular patterns were achieved by using a polystyrene-*b*-polydimethylsiloxane (PS-*b*-PDMS) block copolymer and topographic templates[1]. However, more complex block-copolymer patterns required similarly complex templates. As a result, a complex circuit-layout pattern over a large area can only be achieved using a template with many different and non-periodic features.

Here, we describe an approach to this problem that uses a topographic template consisting of a square lattice of posts with a restricted set of post motifs. Since a finite number of post motifs are considered, block-copolymer patterns from all possible square geometry templates with these post motifs can be studied.

We used a sparse array of double posts distributed among a dense array of single posts. As shown in Figure 1(a), one out of every nine single posts was replaced with a double post. When this template was used to guide a 45.5 kg/mol PS-*b*-PDMS block copolymer with 32 vol% PDMS, the PDMS cylinders that assembled over double posts were aligned parallel to the double post direction. However, the orientation of the PDMS cylinders assembled over single posts depended on the orientations of the neighboring four double posts. We first studied PDMS cylinders surrounded by two double posts. As shown in Figure 1(c), a termination or bend was formed depending on the orientations of the surrounding two double posts. By applying these observations, we predicted the possible block-copolymer patterns surrounded by four double posts (colored regions in Figure 1b). Each double post can be aligned along one of the two directions with 16 (2^4) combinations of the orientations of the four double posts. These 16 combinations can be grouped into four nonequivalent arrangements. On each arrangement, various block copolymer patterns were observed. Figure 1(d-g) show the most frequently observed patterns of the four arrangements. For a Y^4, X^2Y^2, and XY^3 post arrangement, the most frequently observed patterns matched the predicted patterns and the reproducibility were 100%, 64%, and 60% respectively. For an YXYX arrangement, the predicted pattern was not observed. Figure 2 shows five patterns including one matched pattern and four unmatched patterns observed on the X^2Y^2 arrangement. When the free energy of these five patterns were calculated by using a SCFT simulation, the pattern observed with a lower count had a higher energy than the pattern found most often.

To demonstrate that patterns needed for components of integrated circuits (IC) can be fabricated based on our rules, we fabricated an array of bends, one of the essential components of an IC layout. Figure 3(a) shows a proposed template layout to achieve an array of bends. As shown in Figure 3(b), the array of bend was successfully fabricated in accordance with predictions.

[1] J. K. W. Yang, et al., *Nat. Nanotechnol.*, **5**, 256 (2010).

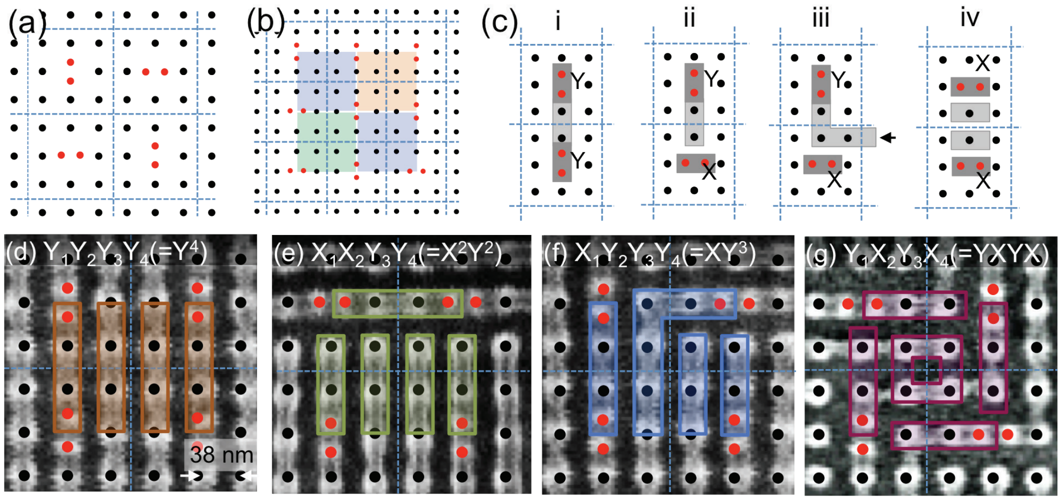

Figure 1. (a) Template used in this study. Black dots: single posts. Red dots: double posts. Blue dotted lines were drawn to clearly show that one out of every nine single posts was replaced with a double post. (b) Schematic diagram showing how a large-area-template can be regarded as a checkerboard of colored regions (unit cells) surrounded by four double posts. (c) Schematic diagrams showing the PDMS patterns on single posts surrounded by two double posts. Dark-gray rectangles: PDMS cylinders assembled on double posts. Light-gray rectangles: PDMS cylinders assembled on single posts. In (iii), an arrow represents a PDMS cylinder comes from a neighboring post. (d-g) SEM images of the most frequently observed patterns formed on the four arrangements. Colored rectangles: predicted PDMS patterns of each arrangement. Different colors were used to distinguish the predicted patterns of different arrangements. We used a notation $X_1X_2Y_3Y_4$, in which 1st, 2nd, 3rd, and 4th letter represent the orientation of the double post in the upper right, upper left, lower left, and lower right quadrant respectively. Y^4 in the parenthesis means that all four double posts were aligned parallel to the *y*-axis.

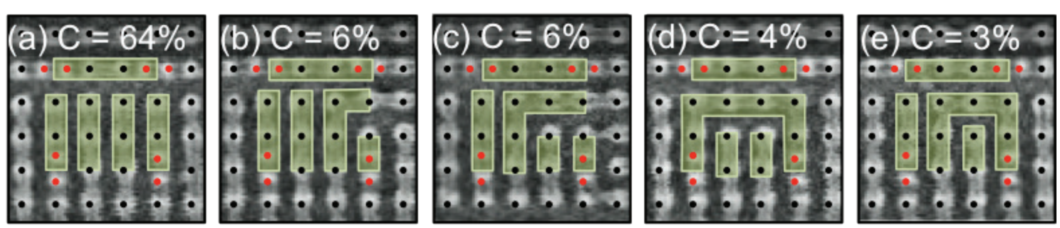

Figure 2. (a-e) SEM images of five patterns including one matched pattern (a) and four unmatched patterns (b-e) formed on the X^2Y^2 arrangement and their counts (C). The periodicity of the template (black dots) was 39 nm.

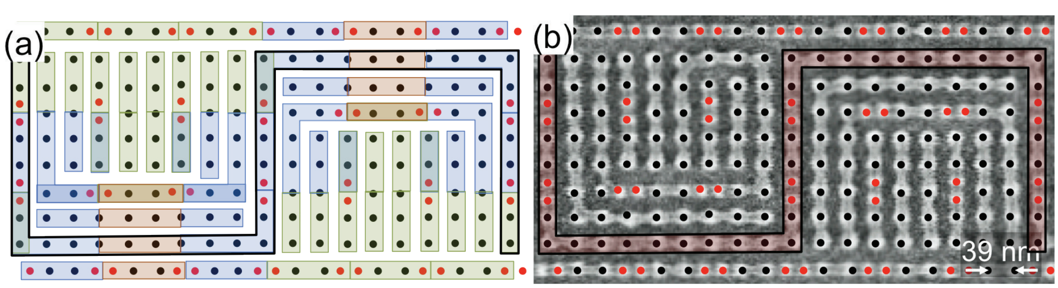

Figure 3. Examples of complex target pattern fabrication. (a) Template layout to fabricate an array of bends. Each color represents the pattern templated by each arrangement. (b) SEM image of the PDMS patterns formed by the template in (a).