<u>Complex self-assembled patterns from</u> <u>a square grid template with restricted geometry</u>

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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, sub-20-nm bends or meander structures were achieved based on topographic templates using 45.5kg/mol polystyrene polydimethylsiloxane (PS-PDMS) block copolymer¹, but formation of arbitrary patterns required a complicated template geometry.

Here, we demonstrate complex pattern fabrication using a topographic template consisting of a square lattice with a restricted set of geometrical features. This considerably simplifies the template design, and allows block copolymer patterns from all possible template arrangements to be studied.

We used a sparse array of double-dot posts distributed among a dense array of single-dot posts. The pitch of the single-dot post array was varied from 30 nm to 83 nm. As shown in figure 1(a,b), one out of every nine single-dot post was substituted with double-dot posts, which were aligned parallel to the x-axis or y-axis. The surface of the template and substrate was coated by 5kg/mol hydroxyl-terminated PDMS homopolymer and annealed with 45.5kg/mol PS-b-PDMS block copolymer solution. As shown in figure 1(c,d), PDMS cylinders made 90-degree bends when they were templated by a single-dot post array with a period of 35 nm, which is commensurate with the equilibrium period of 45.5 kg/mol PS-b-PDMS. When annealed with this template array, a PDMS cylinder assembled above a double-dot post was oriented parallel to the double-dot post. However, the orientation of a PDMS cylinder assembled above a single-dot post depended on the orientations of four surrounding double-dot posts. Among 16 possible arrangements of double-dot posts which can be generated from 4 doubledot posts $(2^4=16)$, an arrangement with four parallel double-dot posts resulted in parallel PDMS cylinders and an arrangement with one orthogonal double-dot post resulted in a bent PDMS cylinder, as shown in figure 2(b,c).

To verify these observations, so as to gain insight into template design rules for achieving a given target pattern, we generated templates whose doubledot posts were randomly oriented and predicted the final pattern using the above observations. In figure 3(b), green, yellow, and blue lines are predicted PDMS cylinders based on the results in figure 2. Green lines were drawn based on figure 2(c), and then blue lines were drawn based on figure 2(b). Finally, yellow lines were drawn where double-dot posts were linearly aligned. As a result, the final pattern was successfully predicted with three defects, which gives the defect density 0.0093.

¹ J. K. W. Yang, et al., Nature Nanotech., **5**, 256 (2010).



Figure 1. (a) A sparse array of double-dot posts distributed among a dense array of single-dot posts. Each unit cell (defined by blue dotted lines) is composed of eight single-dot posts and one double-dot post. (b) SEM image of templates fabricated by electron-beam lithography. (c~d) SEM images of PDMS cylinders templated by a square array of single-dot posts with a period of (c) 35 nm (d) 41 nm



Figure 2. (a) SEM image of self-assembled PDMS cylinders templated by a square array of single-dot posts and a sparse array of double-dot posts. Red dots are double-dot posts. Yellow box: an arrangement with four parallel double-dot posts, red box: an arrangement with one orthogonal double-dot post. (b~c) PDMS cylinders (red lines) templated by surrounding four double-dot posts. (b) four parallel double-dot posts (c) three parallel double-dot posts and one orthogonal double-dot post



Figure 3. (a) A square array whose double-dot posts were randomly aligned. (b) Predicted final pattern based on the experimental observations. Green lines: PDMS cylinders templated by double-dot posts of an arrangement with one orthogonal double-dot (figure 2c). Yellow lines: PDMS cylinders templated by double-dot posts. Blue lines: PDMS cylinders between parallel PDMS cylinders (figure 2b) (c) SEM image of PDMS cylinders resulted from the given template. Among 648 possible links between pairs of posts, defects were formed with 6 pairs, which gives the defect rate 0.0093. Red circle: defect