Directed Self-Assembly of Cylinder-Forming Block Copolymers Using Pillar Topographic Patterns

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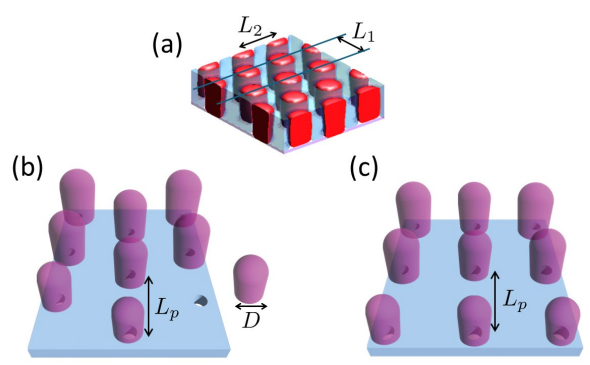
Abstract

We study the directed self-assembly of cylinder-forming block copolymers (BCPs) guided by pillar patterns using density functional theory. By varying the pitch and diameter of hexagonally and tetragonally arranged pillars, we analyze the replication behavior of BCP cylinders. Structure maps reveal conditions for triple, quadruple, or double replications. These insights support contact hole multiplication strategies in semiconductor patterning.

Introduction



- Directed self-assembly (DSA) enables nanoscale patterning via block copolymers (BCPs).
- Contact hole multiplication is achieved using grapho-epitaxial DSA with pillar arrays.
- Pattern outcome depends on BCP geometry and pillar pattern design.
- This study maps how pillar geometry affects pattern replication efficiency.

Simulation Methods

- BCP self-assembly was simulated using mesoscale density functional theory based on a Landau–Ginzburg free energy functional of the order parameter $\psi(\mathbf{r}) = \phi(\mathbf{r}) - f$ (local deviation of A-monomer fraction $\phi(\mathbf{r})$ from its average value f at the position $\mathbf{r}$):

$$F(\Psi) = \int d\mathbf{r}\left[-\frac{\tau}{2}\Psi^2(\mathbf{r}) + \frac{\mu}{3!}\Psi^3(\mathbf{r}) + \frac{\lambda}{4!}\Psi^4(\mathbf{r}) + \frac{d}{2}\left\{\nabla\Psi(\mathbf{r})\right\}^2\right]$$

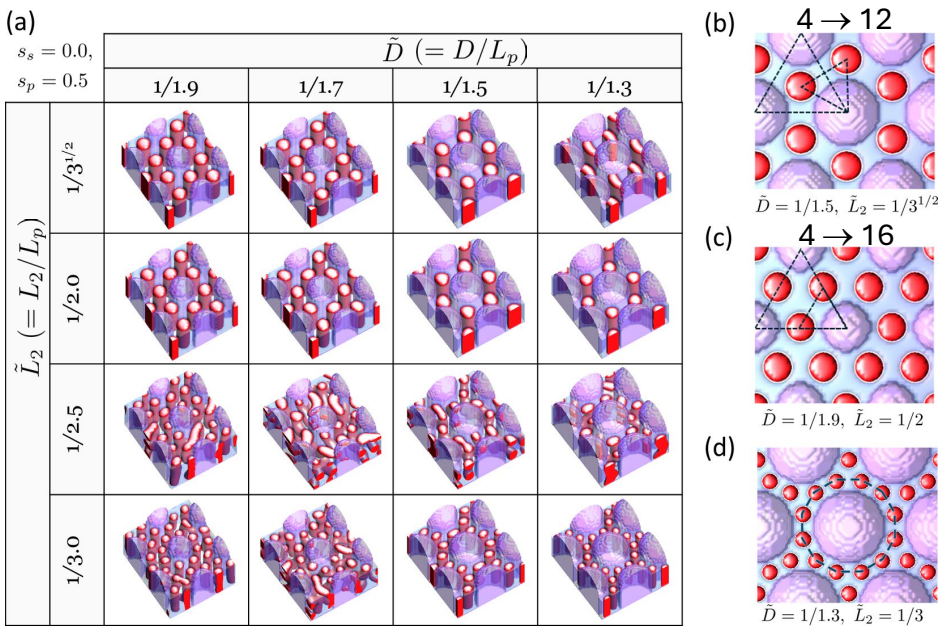
- The modified diffusion equation governing the dynamics of $\Psi(\mathbf{r})$ is given as

$$\frac{\partial\Psi(\mathbf{r})}{\partial t} = M\nabla^2\frac{\partial(F + F_{surf})}{\partial\Psi(\mathbf{r})} + \xi(\mathbf{r})$$

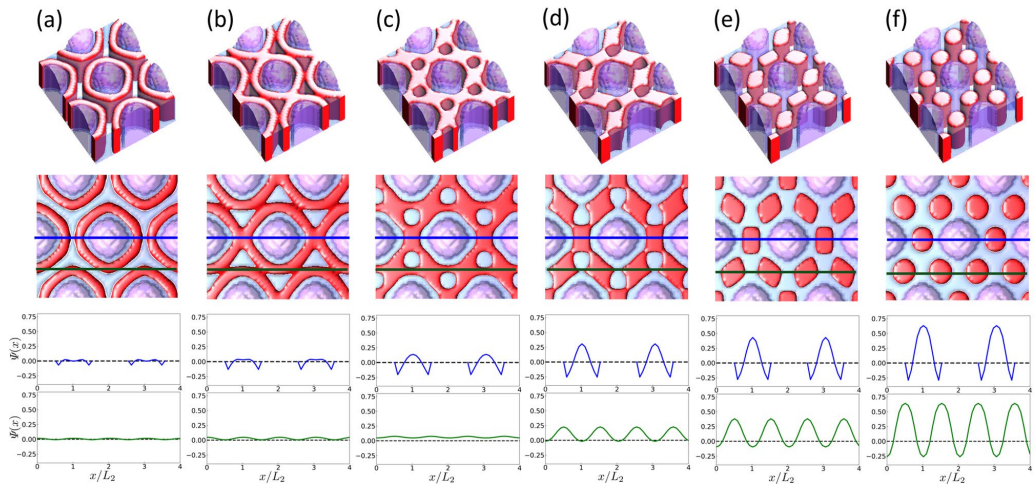
- Key physical parameters: f = 0.3 (BCP composition); χN= 18 (degree of incompatibility via τ); s_t = 0 neutral top(t) surface via F_{surf}); $s_p > 0$, $s_s \geq 0$ (selective pillar(p) and substrate (s) via F_{surf})
- Pillar geometry: Pillar arranged in hexagonal or tetragonal array.
- Periodic boundary conditions in x, y; reflective in z .

Results

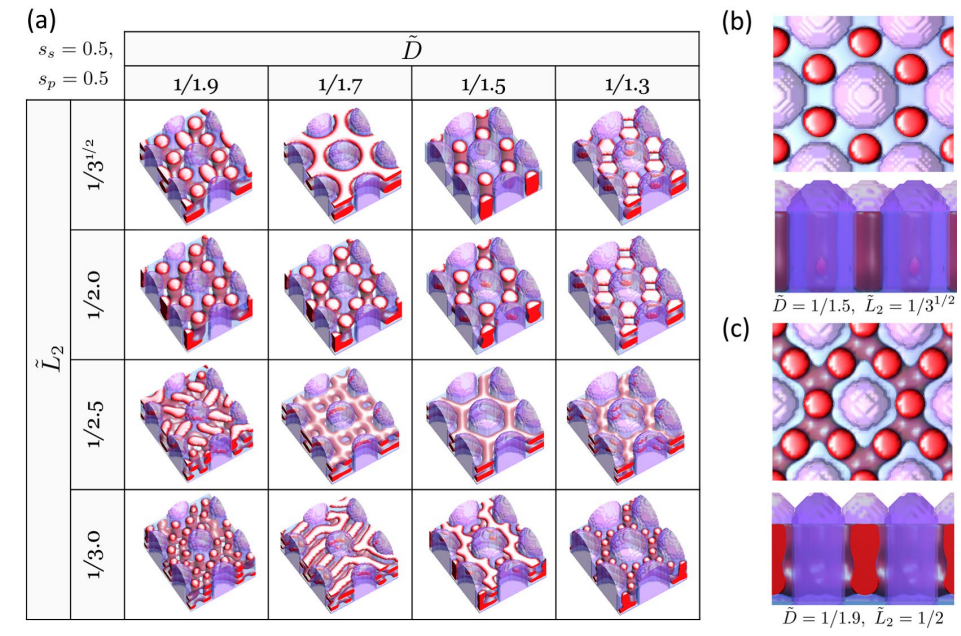
- Replication Behavior of Cylinder-Forming BCPs under Hexagonal Pillar Arrays (**hexagonal** array; neutral substrate; B-selective pillar)



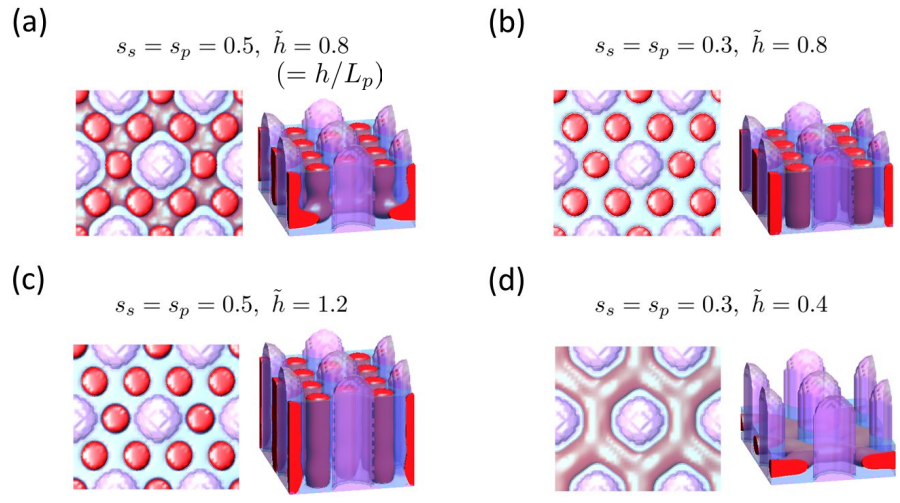
- Formation Pathway of DSA Structures over Time (**hexagonal** array; neutral substrate; B-selective pillar)



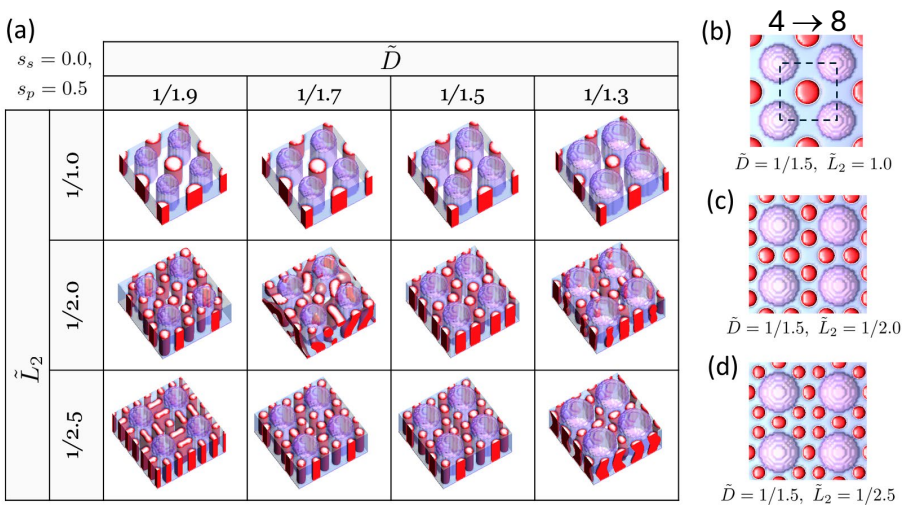
- DSA Structure Map with Pillar and Substrate Selectivity (**hexagonal** array; B-selective substrate; B-selective pillar)



- Effect of Surface Selectivity and Film Thickness on DSA (**hexagonal** array; B-selective substrate; B-selective pillar)



- DSA Structure Map under Tetragonal Pillar Arrays (**tetragonal** array; neutral substrate; B-selective pillar)



Conclusions

- We investigated the directed self-assembly of cylinder-forming BCPs guided by pillar arrays using mesoscale density functional theory.
- Under hexagonally arranged pillars, we achieved threefold, fourfold, and sevenfold replication of contact holes, depending on pillar pitch and diameter. In contrast, tetragonal arrays supported only twofold replication due to symmetry constraints.
- These results agree with experimental trends and offer a theoretical framework for designing DSA systems for contact hole multiplication in advanced lithography.

Acknowledgments

This work was supported by Samsung Electronics.