Study of Block Copolymer Lithography using SCFT: New Patterns and Methodology

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Annual Meeting
Monday, February 2, 2009

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Outline

- Motivation & Block Copolymer Lithography
- Numerical Method
- AB + B’C (+ Confinement)
- AB+ A + Confinement
- Mixed Polymer Brushes + Confinement
Lithography

- Optical printing of complex circuit diagrams into pattern on the wafer (through mask onto photo-resist)

- Complicated, expensive, and critical process of modern integrated circuit (IC) manufacturing

- Scaling is limited by wavelength of light (\( > 22\text{nm} \))

- Equipment cost exponentially increases as reducing the dimension.

New families of imaging materials and novel approaches

Aurangzeb Khan, Lecture note of VLSI Design system
Block Copolymer Lithography

- Promising high resolution lithographic tool
- Microscopic phase separation in the scale of $O(10\, nm)$
- Various types of geometries in block copolymer thin film

- Parallel lamellar
- Perpendicular lamellar
- Parallel cylinder
- Perpendicular cylinder
- Sphere

Control of Microdomain Ordering

- High resolution - demand for smaller device structures
- Placement accuracy
- Reduction of defects density - yield loss
- Throughput - manufacturing cost
- Some applications require long-range perfect ordering.

Mechanical flow field
Electrical field
Temperature gradient
Chemically patterned substrate
Topographically patterned substrate

“Graphoepitaxy”
:Topographically Patterned Substrate

- **Bottom-up** self-assembly of block copolymers on 10 nm scales
- **Top-down** conventional lithography in generating micron-scale wells
- Lateral confinement can promote defect-free self-assembled block copolymer features.


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SCFT Algorithm

Start:
Generate Random Initial Field Configurations \( w(x,0) \)

Solve Modified Diffusion Equation for chain propagator \( q(x, s ; [w]) \)

Solve the Single Chain Partition Function \( Q \)

Calculate the densities

Update the field \( w(x,t) \)

Convergence Criterion is Satisfied?

\[ \left| \frac{\delta H[w]}{\delta w} \right| \ll 1 \]

END

Y

N
How to Implement Confinement Wall

- Predetermined wall density function
  \[ \rho_w(x) \]
- Four-fold modulated tanh function
- Local incompressibility
  \[ \rho_A(x) + \rho_B(x) + \rho_w(x) = \rho_0 \]
- Include contact interaction between the wall and A- and B- segments: possible to implement A- or B-wetting wall
  \[ H_I \sim \chi_{wA} \rho_w(x) \hat{\rho}_A(x) + \chi_{wB} \rho_w(x) \hat{\rho}_B(x) \]
Alternative Approach to Square Confinement

- Masking method:
  - Periodic B.C with plane wave basis
  - Adaptable to non-symmetric well geometries
  - Slow convergence
  - Wasted computation in the masked area

- Alternative approach using sine wave basis function
  - Use the actual cell
  - Dirichlet boundary condition at the edges
  - Sine wave basis
  - Sine FFT, rather than the complex FFT
  - No wasted computations in the masked areas
  - Faster convergence in the field update scheme
Overview

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AB + B’C

Square array: canonical structure defined by Semiconductor Industry Association (SIA)

ABC triblock copolymer

Binary blend of AB and B'C diblock copolymers in which the B and B' blocks have attractive supramolecular interactions

When do we observe square lattice?

→ SCFT simulations of the system varying $\chi_{BB}N$, $\chi_{AC}N$ and $\chi N(\ A/B(B'),\ C/B(B'))$


Effect of repulsive interaction between A and C, $\chi_{AC}N$

Fixing $\chi_{BB'}N = -7.468$, $\chi_N = 18.875$, $f_{B/B'} = 0.7$

Increasing repulsive interaction between the minor blocks A and C, $\chi_{AC}N$

<table>
<thead>
<tr>
<th>5</th>
<th>10</th>
<th>15</th>
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<th>25</th>
<th>30</th>
<th>35</th>
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<tr>
<td>A+C</td>
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A and C are micible.

A and C segregate into the core and shell of the cylinders in order to reduce A/C contacts.

Disordered

Free energy cost of A/C contacts are larger than for the A/B(B') and C/B(B').

Cylinders composed solely of either the A or C component.
Phase Diagram of AB+B’C

Fixing $\chi_{BB’N} = -7.468$

Increasing repulsive interaction between the minor blocks A and C, $\chi_{ACN}$

5 10 15 20 25 30 35 40

Representative density profiles of A and C

Increasing repulsive interaction between other blocks, $\chi^N$
AB+B’C in a square well

- Square lateral confinement controls and improves defect-free tetragonal ordering
- $\chi_{BB'}N = -3.468,$
- $\chi_{AC}N = 55.5$
- $\chi N = 13.875 \text{ (A/B(B') and C/B(B'))}$
- C attractive and A repulsive square wall
- Side length, $L = 84R_g \sim 1 \mu m$

Evolution of A segment concentration
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AB + Square well

Representative density profiles of A segment

χN = 13.75  15.75  17

Tetragonal ordering is induced by the square lateral confinement during annealing stage.

Lattice subsequently twists into hexagonal ordering in order to reduce the stress in the interstitial sites.

\[ f_A = 0.7 \]

A-attractive square well

\[ L = 14 \, R_g \]
AB + A + Square well

Total A-segment density profiles

\[ f_A = 0.7 \]
\[ L = 23 \, R_g \]
B wetting wall
\[ \alpha = 1.75 \, \left( \frac{N_{Ah}}{N} \right) \]
\[ V_{Ah} = 0.23 \]

A homopolymer segment concentration

\[ \alpha = \frac{N_{Ah}}{N} \]
Phase Diagrams

\[ f_A = 0.7, \quad \text{A attractive wall condition} \]
\[ \text{fixed } \alpha = 2.1 \ (N_{Ah}/N) \]
Robustness on Line Edge Roughness

Order parameter

\[
\Psi = \sum_i^N (\phi_B(i) - \phi_{B,ref}(i))^2 = \begin{cases} 
\ll 1, & \text{Tetragonal Ordering} \\
\gg 1, & \text{Defective}
\end{cases}
\]

Present system
Reference system (Tetragonal Ordering)

Perturbation on the wall

\[
A \cdot \cos\left[2\pi\left(x - \Delta\right)/(\lambda L)\right]
\]
Robustness on Line Edge Roughness

- Perturbation on the wall: $\Delta = 0$, 0.5, 1 (R_g)

Tetragonal Ordering
Defective

$L = 16$ (R_g)
AB + A + 60° Bends

\[ f_A = 0.5, \quad L = 18 \ R_g \]

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Mixed Polymer Brushes

- Collaboration with Sandia National Lab.
- Predict phase-separated morphologies and mechanisms
- Understand how the system parameters affect the feasibility of targeted pattern.

Project Proposal of Sandia National Lab.
Laterally Confined Polymer Brush

- Simulation domain: mixed polymer brushes region only
- Prefixed narrow pure polymer brush wall in lateral direction
- Virtual wall in z-direction, including substrate and surface interaction
- Sine basis simulation
- Delta function initial condition of propagator at the grafting point at $z = dz \rightarrow$ one step analytic extension
- Non-uniform grafting density over the substrate due to lateral wall
Surface Interaction

\[ f_A = 0.5 \]
\[ \chi_{AB} N = 12 \]

Increasing surface attraction, \( \chi_{w(top)} N \)

Doubling grafting density
Lateral Confinement

\[ f_A = 0.5 \]
\[ \chi_{AB} N = 12 \]

Increase \( N_B \) (=1.5 \( N_A \))

Turn on the B-attractive wall on the side,
\[ \chi_W N = -12 \]

Turn on the B-attractive wall on the side
Ripple Phase in 3D

Laterally confined by pure brush region

Evolution of Long-ranged Defect-free Structure

Pattern size

\[ \sim 56 \, R_g \]

Evolution and self-healing of long-ranged ordering
Conclusions

- Phase diagram of AB+B’C helps us understand to important parameters in designing systems which will produce a square lattice.

- Confinement helps AB+B’C in generating and controlling square ordering.

- AB + A + confinement can generate square lattice and non-regular structures.

- Mixed brushes phase separation can be controlled using a new graphoepitaxy-type technique.