A simulation analysis on defect annihilation in directed self-assembly lithography

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Original simple HP 15nm L/S patterning process using PS-\textit{b}-PMMA

PS short defect
8 chips (9%)

Dislocation defect
6 chips (7%)

OK chip
71 chips (84%)

Table: Average CD, LWR, LER

<table>
<thead>
<tr>
<th>Metric</th>
<th>Average (3(\sigma))</th>
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<tbody>
<tr>
<td>CD (nm)</td>
<td>16.9 (4.6)</td>
</tr>
<tr>
<td>LWR (nm)</td>
<td>4.8 (1.3)</td>
</tr>
<tr>
<td>LER (nm)</td>
<td>3.7 (1.5)</td>
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85 chips / wafer

PS short and dislocation defects are observed at the wafer center and edge after SOG etch.

Y. Seino et al., MNE 2014
Outline

- Grid defects
  - Experimental behavior
  - Simulation results acquired using self-consistent field theory (SCFT)
  - Simulation results acquired using dissipative particle dynamics (DPD)

- Dislocation defects

- Summary
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Characteristic DSA Defect (Grid defect)

* SOG: Spin On Glass, SOC: Spin On Carbon

Although most of these grid defects disappeared after SOG full etching, they could result in the degradation of etching process margin, and therefore, in line edge roughness and open/short defects.
• Grid defects can be decreased with optimum neutral layer and sufficient phase separation annealing.
• The subtle adjustment of the neutral layer toward a more neutral condition results in the decrease of the grid defects.
Simulation model

- SCF simulation, masking method
- BCP: \( \chi_N = 20, L_0 = 30 \text{ nm} \) (PS-\( b \)-PMMA)
- top: neutral (\( \chi_{PMMA-top} = 2, \chi_{PS-top} = 2 \))
- pinning: PMMA attractive (\( \chi_{PMMA-PIN} = 1, \chi_{PS-PIN} = 2 \))
- bottom: PMMA attractive (\( \chi_{PMMA-BTM} = 1.3, \chi_{PS-BTM} = 2 \))

- film thickness=1.5\( L_0 \)
- pinning height=0.68\( L_0 \)
- pinning width=0.5\( L_0 \)
- pinning period=3\( L_0 \)
3 stable/metastable morphologies including grid defect were acquired using SCFT.
Stability of grid defects

Mixed lamellar state is the most stable

Vertical lamellar state is the most stable

- Free energy $\Delta F$
- $\chi_{PMMA-BTM}$
- PMMA attractive neutral

• These simulation results agree with the experimental behavior.
Conformation of BCP chains

(a) PMMA chain is parallel to the bottom.
(b) PMMA chain is vertical to the bottom

We can acquire the information of the polymer chain conformation by evaluating $n_0$, $n_5$ and $n_9$ immediately above the bottom.
Conformation of BCP chain (GD-state)

Position ($L_0$)

Density

$n_0 > n_5, n_9$ immediately above the bottom

PMMA

$n_5$

$n_0$

$n_9$
PMMA blocks are nearly vertical to the bottom in the region where the vertical PMMA lamellar patterns are connected toward the bottom. This characteristic conformation of BCP chains is considered to be related with the origin of the grid defects.
• The segment density distribution acquired using SCFT was transformed into the atomic representation using the node density biased MC method.
• Using this atomic representation as initial chain conformations, we executed DPD simulations and investigated the defect annihilation dynamics.
Firstly, grid defects were observed. And finally, the grid defects disappeared and the simulation converged into the equilibrium lamellar state.
The defect annihilation dynamics of the grid defects could be understood as the change of the orientation of the BCP chains.

- **Vertically oriented**
  - Polymer chains are partially vertical.

- **Horizontally oriented**
  - Both vertically and horizontally oriented polymer chains appeared randomly.
  - The polymer chains flipped down and flopped up randomly.

- **Polymer chains are parallel**
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Polymer conformation in dislocation defects

Center node

Terminal node

Self-consistent field theory

\[ n_{\text{center}} = \text{Segment density distribution of the center node} \]

\[ n_{\text{terminal}} = \text{Segment density distribution of the terminal node} \]

\[ n_{\text{center}} - n_{\text{terminal}} \]

- Perfect state
- Single dislocation
- Double dislocation
Polymer conformation in dislocation defects

Terminal segment density is larger than the center segment density.

Terminal segment is localized in a specific region.
The delocalization of the terminal segments is effective for defect mitigation.
Summary

• We have investigated the conformations of the polymer chains in “grid defects” and “dislocation defects”.
• In both defective states, polymer chain conformations were found to play an important role in formation of the defective states.
• For practical application, it is important to understand the origin of the defective states more. We need the corporation of the simulation people more and more…!