Defectivity prediction for droplet-dispensed UV nanoimprint lithography, enabled by fast simulation of resin flow at feature, droplet and template scales

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February 23, 2016

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Outline: droplet-dispensed NIL simulation

• Modeling objectives and key phenomena in droplet-dispensed NIL (JFIL)
• Capillary-driven droplet-spreading model
• Scalable model for merging of droplet arrays
• Integrated full-field simulation of JFIL
  • Template edge effects
  • Wafer edge effects
  • Template curvature and avoiding gas entrapment
Droplet-dispensed simulation involves template approach, spreading and holding phases.

1: Template approach (Constant velocity)

2: Relax template curvature (constant load)

3: Hold template load constant

Optimize through simulation for speed and defectivity
The key to the simulation technique: model the impulse response $g(x,y,t)$ of the resist layer

Spatial response of resist

Mechanical impulse applied uniformly over small region at time $t = 0$

Resist layer

Wafer

Temporal response

Newtonian: impulse response constant in time for $t > 0$

Viscoelastic: impulse response is function of time.

Change in topography is given by convolution of impulse response with pressure distribution $p(x,y,t)$.

$$\frac{\Delta}{\Delta t} = \left[ p(x, y, t) \ast g(x, y, t) \right] \Delta t = 1$$
Layer-thickness reductions and cavity filling are represented through time-stepping.

Tall cavities: no filling

Finite-height cavities

Limiting value of $r$: cavities completely filled
Elastic stamp deformations are composed of local deflections, shear, and plate bending.

Local deflections
- Modulus-dependent
- Largely thickness-independent

Local and bending deflections
- Modulus-dependent
- Thickness-dependent

Local deflections:
- $E_{\text{stamp}}$
- $E_{\text{substrate}}$
- $\lambda$
- $t_{\text{stamp}}$

Local and bending deflections:
- (log axes)
- Relative stamp deflection
- Bending
- 1 µm

Examples:
- e.g. bit-patterned hard disk
- e.g. microprocessor

Typically $t_{\text{stamp}} \sim 0.5$ mm
The model captures spatial interactions in the imprinting of heterogeneous patterns

**NIL test pattern**
(broad mixture of feature shapes, sizes, and densities)

- **Cavities** (~500 nm deep)
- **Protrusions**

Simulated RLT

**PMMA 35 kg/mol**

**Residual layer thicknesses (nm)**

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Simulation</th>
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<tbody>
<tr>
<td>150 °C, 6 min, 5 MPa</td>
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<tr>
<td>165 °C, 4 min, 3.5 MPa</td>
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<tr>
<td>180 °C, 2 min, 5 MPa</td>
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- **Long rectangles, 0°**
- **Long rectangles, 90°**
- **Square holes**

Feature pitch 100 µm

Protrusion density (% area)
Droplet spreading is driven by capillary and external loads, and can be highly directional.

- Feature, droplet and chip length scales span 6 to 7 orders of magnitude – multiscale modeling is essential.
- *Virtual work* concept used to capture work done by capillary forces.
Droplet spreading is driven by capillary and external loads, and can be highly directional.

- When droplet spreads beneath arrays of parallel lines, the resist impulse response is anisotropic, modeled with the following proportion of resist displacement directed parallel to the lines:

\[ k_{\text{parallel}} = 0.75 + 0.25 \tanh \left( 1.5 \log_{10} \frac{0.5h}{r} \right) \]

\[ \text{Cavity height} \quad \text{RLT} \]

- Key parameters:
  - Extent of pattern on stamp
  - Protrusion density
  - Feature pitch (μm)
  - Residual layer thickness
    - ≥ 100 nm
    - 10 nm
    - ≤ 1 nm

- Elapsed imprinting time:
  - 0.01 s
  - 0.1 s
  - 1 s
  - 10 s
  - 30 s
The spreading and merging behavior of regular arrays of droplets can be aggregated.

Example shown:
- Resin viscosity: 10 mPa.s
- External load: 40 kPa
- 1 pL droplets on 120 μm pitch
- Resin-template and resin-wafer contact angles: 15°
- Relationship captures both filling and RLT changes with time
Gas entrapment between merging droplets can be avoided by controlling template curvature

- Fix curvature, bring stamp down under constant load, and droplets merge.
- If gas is entrapped, dissolution model would be needed; but aim is to avoid entrapment.
The time evolution of residual layer and cavity filling can be compared for multiple processes.

- Example pattern, 30 mm x 40 mm template = single imprint field
- 1 pL droplets; target RLT 25 nm
- Constant approach velocity of 50 μm/s until load of 50 N reached
- Load then maintained while template curvature relaxed over 1 second
The time evolution of residual layer and cavity filling can be compared for multiple processes.
Extrusion of resist at template edge can be simulated and optimized

- Material squeezed out from edge of template costs silicon real estate: simulations can predict this
- A slight surplus of template cavity volume in the border may be used to suppress resist extrusion
Outlook

- JFIL simulation algorithm incorporating effects of pattern-dependent capillary pressures, external loads, and template bowing. Easily scales to >10,000 droplets.
- Predicts RLT uniformity and template filling evolution
- Provides insights into template edge extrusion and likelihood of gas entrapment
- Simulation speed and resolution can be tuned
  - For a 30x40 mm field simulated on an Intel i7, 8 GB RAM:
    ~5 seconds at 1 mm resolution; ~5 mins at 0.1 mm resolution
- Detailed (pre-)production data needed for model calibration
  - Locations and frequencies of defects within imprint fields, and spatial maps of RLT
  - Data needed for multiple template curvature relaxation cases and spread/hold times
Upcoming developments include integrated multiscale simulations and user-defined models.

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<tbody>
<tr>
<td>Company founded</td>
<td>Spun-on UV-NIL simulation</td>
<td>Droplet-dispersed UV-NIL module</td>
<td>Roll-to-roll module</td>
<td>Support for user-defined filling models</td>
<td>Process Advisor</td>
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<th>Dec 2010</th>
<th>Dec 2014</th>
<th>March 2016</th>
<th>Early 2017</th>
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<tr>
<td>First product: chip-scale TNIL simulation</td>
<td>Multi-layer template module; multi-height cavities</td>
<td>Simprint Multiscale (integrated feature-to-wafer-scale simulation) and Gas dissolution and condensation module</td>
<td>Design Advisor</td>
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\[^1\text{Youn et al., Jpn. J. Appl. Phys. 52 06GJ07}\]
Collaborators and acknowledgements

• **MIT**
  - Duane Boning
  - Matt Dirckx
  - Eehern Wong
  - Melinda Hale
  - Aaron Mazzeo
  - Lallit Anand
  - Shawn Chester
  - Nici Ames
  - James Freedman

• **NILT, Copenhagen**
  - Theodor Nielsen
  - Brian Bilenberg
  - Kristian Smistrup

• **UC San Diego**
  - Yen-Kuan Wu
  - Andrew Kahng

• **HTL Co Ltd, Japan**
  - M. Kato and M. Tsutsui

• **NTU, Singapore**
  - Lam Yee Cheong

• **IBN, Singapore**
  - Ciprian Iliescu, Bangtao Chen, Ming Ni

• **Funding**
  - The Singapore-MIT Alliance
  - Danish National Advanced Technology Foundation

• **Helpful discussions**
  - Hella Scheer, Andre Mayer, Derek Bassett, Roger Bonnecaze, Siddharth Chauhan, Grant Willson, Yoshihiko Hirai, Wei Wu, S.V. Sreenivasan