Towards nanoimprint lithography-aware layout design checking

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Nanoimprint is the mechanical patterning of resist spun or sprayed on to a wafer

- Resist viscosity \( \geq 10^3 \) Pa.s
- Applied pressures \( \sim 5 \) MPa
- Thermoplastic or UV-curing
- Viscous resist squeezing
- Elastic stamp deflections

- Resist viscosity < 0.1 Pa.s
- Applied pressures \( \sim 5 \) kPa
- Droplets tailored to pattern
- Key figure of merit: filling time
- Gas trapping and dissolution


www.molecularimprints.com
Nanoimprinting of spun-on layers exhibits pattern dependencies

Pattern density already constrained to a modest range (typ. 40-60%)

Not realistic in semiconductors
Nanoimprinting of spun-on layers exhibits pattern dependencies

Two relevant timescales for pattern formation:

- Local cavity filling
- Residual layer thickness (RLT) homogenization
Nanoimprinting of spun-on layers exhibits pattern dependencies

Objective for nanoimprint-friendly design:

*Limit time to bring residual layer thickness variation within spec.*

NIL for planarization

*Similarly, limit time to bring NIL-planarized surface within spec.*
Nanoimprint modeling and simulation needs

- **Cell-level**
  - Hundreds of features
  - Guide iterative layout design
  - Desktop processing in minutes

- **Chip-level**
  - Many millions of features
  - Pre-fabrication check: overnight?
  - Guide process selection

- **Need for flexibility**
  - Rapid innovation in resist and stamp materials
  - Richness of geometries
### Nanoimprint compared to photolithography modeling

<table>
<thead>
<tr>
<th>Feature-scale</th>
<th>Photolithography</th>
<th>Nanoimprint</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PROLITH; “TCAD”</td>
<td>Hirai¹; Rowland²; Scheer³; Reddy⁴</td>
</tr>
<tr>
<td>Chip-scale</td>
<td>OPC software</td>
<td>Mendels/Zaitsev⁵; <em>and this work</em></td>
</tr>
</tbody>
</table>

We need a unified simulation approach for micro- and nano-embossing/imprinting

Initial polymer thickness, $r_0$

- 10 mm
- 1 mm
- 100 µm
- 10 µm
- 1 µm
- 100 nm

Cavity width, $w$

- 1 nm 10 nm 100 nm 1 µm 10 µm 100 µm

- Biological micro-/nano-devices
- Tissue engineering
- Diffractive optics
- Flat-panel displays
- Photovoltaics
- Photonics
- Metamaterials
- Semiconductors
- Hard-disk drives
- Planarization
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Cavity width, $w$

- Single-peak filling
- Dual-peak filling
Key: model impulse response \( g(x,y,t) \) of resist layer

Model in space:

- Mechanical impulse applied uniformly over small region at time \( t = 0 \)

Model in time:

- 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.

\[ \Delta = \Delta ty * p(x, y, t) \]

- **Small, unit disp.**
- **Stamp**
- **Resist**
- **Substrate**

**Time increment**

\[ \left[ p(x, y, t) * g(x, y, t) \right] \Delta t = 1 \]

- **Pressure**
- **Impulse response**
- **Unit displacement in contact region**
Contact pressure distributions can be found for arbitrary stamp geometries

2.3 µm-thick polysulfone film embossed at 205 °C under 30 MPa for 2 mins

Stamp design  Simulated pressure  Optical micrograph

Cavity  

0  160 MPa  

200 µm

Taylor et al., SPIE 7269 (2009).
Successful modeling of polysulfone imprint

2.3 µm-thick polysulfone film embossed at 205 °C under 30 MPa for 2 mins

Taylor et al., SPIE 7269 (2009).
Representing layer-thickness reductions

Tall cavities

-limiting value of $r$ : cavities completely filled

Shallower cavities
Modeling stamp and substrate deflections

Indentation

Magnitude of stamp deflection

Indentation and bending

\( \lambda \)

\( t_{\text{stamp}} \)

\( \lambda / t_{\text{stamp}} \)

1 and 4

(log scales)

\(~4\)
Simulation method: step-up resist compliance

**Experiment**

- PMMA 495K, c. 165 °C, 40 MPa, 1 min

**Simulation**

- RLT (nm)
- Scale: 0.1 mm
- Scale: 200 nm
Abstracting a complex pattern

Local relationships between pressure-compliance and RLT:

\[ r \rightarrow p_g \]

\[ r \rightarrow p_g \]

\[ r \rightarrow p_g \]

\[ r \rightarrow p_g \]
Simulation results: abstracted pattern

Test-stamp pattern  

Simulated residual layer thickness

Experimental topography
495K PMMA, 10–15 MPa, 170 °C

Simulation
Simulation time

Simulation time (s)

Expected:
\[ \text{time} \sim O(N^2 \log N) \]

Simulation size, \( N \)

Stamp 1
Feature-scale

Stamp 2
Abstracted
The physical insights of simulation can be encapsulated in design rules

- **Keep protrusion density** $\rho$ **uniform**
  - Dummy fill insertion
  - Importance *grows* with lateral length-scale (unlike CMP)
  - Could vary cavity *heights* spatially*: expensive

- **Minimize transient stamp deflections**: uniform $F_1\rho a^2$
  - Care to avoid capillary bridging$^+$ if some cavities unfilled
  - Impose upper limit on $F_1\rho a^2$ to limit filling time
  - Trenches quicker to fill than square holes $\Rightarrow$ impose grid

- **Link to other process steps**
  - Exploit RLT variation to counteract etch nonuniformity

- **Pattern density rules**, RLT variation target, stamp flexibility and substrate/stamp smoothness will be interrelated

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Varying stamp’s bending stiffness: simulations

Stamp thickness:
- 5 mm
- 0.5 mm
- 0.12 mm

Features
- 200 nm

Residual layer thickness
- 4 mm
Summary: fast nanoimprint modeling

• Contributions
  • Flexible modeling approach
  • Pattern abstraction optional
  • Suited to cell and chip scales
  • 1000+ times faster than finite element modeling

• Outlook
  • We will need NIL-aware design checking
  • Can use as an engine for “Mechanical Proximity Correction”
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