Fast simulation of pattern dependencies in thermal nanoimprint lithography

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Nanoimprint modeling 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
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
100 nm
1 nm
10 nm

Weed hard-disk drives

Photovoltaics

Metamaterials

Photonics

Planarization

Flat-panel displays

Tissue engineering
Diffractive optics

Biological micro-/nano-devices

Cavity width, $w$

Initial polymer thickness, $r_0$

10 mm
1 mm
100 µm
10 µm
1 µm
100 nm
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Biological micro-/nano-devices

Cavity width, $w$
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Initial polymer thickness, $r_0$

- Biological micro-/nano-devices
- Tissue engineering
- Diffractive optics
- Flat-panel displays
- Photovoltaics
- Planarization
- Photonic
- Semiconductors
- Hard-disk drives
- Metamaterials

Cavity width, $w$

1 nm 10 nm 100 nm 1 µm 10 µm 100 µm

Single-peak filling
Dual-peak filling

100 nm 100 µm 10 µm 1 µm 1 mm 10 mm
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.

After Nogi et al., Trans ASME: J Tribology, 119 493-500 (1997)
Change in topography is given by convolution of impulse response with pressure distribution:

\[
[p(x, y, t) \ast g(x, y, t)] \Delta t = 1
\]

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

Time increment

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

\( p_g \) defined in terms of:

- True pressure \( p(x, y, t) \)
- Material compliance \( J(t) \)

\[
p_g(x, y, t_h) = (1 - v^2) \int_0^{t_h} p(x, y, t') \frac{dJ(t - t')}{dt'} dt'
\]
Modeling stamp and substrate deflections

Indentation

Indentation and bending

Elastic point-load responses

Indentation

Bending
Modeling stamp and substrate deflections

Indentation

Indentation and bending

\[ \log(\lambda/t_{\text{stamp}}) \approx 4 \]

\[ \log(\text{magnitude of stamp deflection}) \]

Indentation

Bending
Simulation method: step-up resist compliance

PMMA 495K, c. 165 °C, 40 MPa, 1 min
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  | cavity
---|---
![Test-stamp pattern image](image1)

Simulated residual layer thickness

180 nm

20 nm

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

Simulation

3 min
5 min

PMMA

Silicon

200 nm

1 mm
Simulation time

Simulation time (s)

Expected: time \( \sim O(N^2 \log N) \)

Simulation size, \( N \)

Stamp 1
Feature-scale

Stamp 2
Abstracted

\( N \)
Strengths of the simulation method

- **A unified simulation approach**
  - Can cope with any layer thickness
  - Can integrate feature sizes ranging over many orders of magnitude

- **Can model any linear viscoelastic material**

- **Speed**
  - At least 1000 times faster than feature-level FEM

- **Implicit periodic boundary conditions are useful**
  - Realistic representation of whole-wafer imprint of many chips
  - Can use edge-padding for non-periodic modeling

- **Suited to quick adaptation for new NIL configurations**
  - Use to explore the use of flexible stamps and substrates
  - Explore the imprinting of non-flat substrates
  - Micro-contact printing; roll-to-roll
Varying stamp’s bending stiffness: simulations

Stamp thicknesses:

- 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 FEM

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