

## Modeling and simulation of stamp deflections in nanoimprint lithography: exploiting backside grooves to enhance residual layer thickness uniformity

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We describe a model for the compliance of a nanoimprint stamp etched with a grid of backside grooves, as proposed by Nielsen *et al.* [1]. We integrate the model with a fast simulation technique that we have previously demonstrated [2], to show how etched grooves help reduce the systematic residual layer thickness (RLT) variations that occur when different patterns lie in close proximity on the stamp.

Our model for the deformation of a grooved stamp incorporates local indentation, transverse shearing, and bending. The backside grooves lie between feature-carrying ‘mesas’. We conducted finite-element simulations in which we varied the flexure thickness,  $t_g$ , and length,  $g$ , and the initial wafer thickness,  $t_m$ . We assumed periodic boundary conditions, with uniform unit pressure applied to every ninth mesa in both directions. A balancing uniform pressure was applied across the backside of the stamp. From these simulations we extracted the ‘lumped’ compliance of each geometry, and fit a dimensionless model describing the increase in long-range compliance enabled by backside grooves (Fig 1). A flexure-length-to-mesa-pitch ratio of just 0.1 increases the compliance by  $\sim 10$  times, relative to a groove-less stamp.

We have incorporated this compliance model into our existing nanoimprint simulation algorithm [2]. This technique describes the mechanical behavior of the resist using the response of its surface topography to a unit impulse applied at a single location. Meanwhile, deflections of structured stamps are described using two separate point-load response kernels: one that assumes a uniform stamp thickness of  $t_m$  and describes the relatively small deflections within each mesa, and a second kernel that captures additional relative displacements of mesas due to the presence of grooves. The evolution of RLT is computed in a series of steps, by convolving an iteratively-found contact-pressure distribution with the scaled impulse-response of the resist. Simulations using this enhanced algorithm (Fig 2) agree closely with the experiments of Pedersen *et al.* [3]: a structured stamp with thicker material supporting the imprinted features permits far less within-chip RLT variation than a thinner stamp that can bend across the mesa.

Thin flexures *between* mesas, however, are desirable because (i) they help the stamp to conform to random undulations of the stamp and substrate and (ii) they mechanically ‘decouple’ adjacent mesas. To illustrate flexures’ decoupling capability, we simulated transient RLT variations during the imprinting of a stamp with adjacent mesas of highly contrasting protrusion density (Fig 3). For a 500  $\mu\text{m}$ -thick silicon stamp without backside grooves ( $t_m = t_g$ ), the simulated peak RLT range is several times higher than if all mesas on the stamp were patterned identically. Reducing  $t_g$  helps adjacent mesas to move relatively to one another. Where  $s_m = 6g$  (Fig 3a–e), setting  $t_g$  to 100 or 200  $\mu\text{m}$  substantially reduces the filling-time and peak RLT range in both the 20%- and 67%-density regions. Meanwhile, a thin flexure of  $t_g = 50$   $\mu\text{m}$  allows individual mesas to behave almost as if they were independent of their surroundings. If the flexure length  $g$  is larger so that  $s_m = 3g$  (Fig 3f–j), the decoupling effect for a given value of  $t_g$  is greater. Here, a  $t_g$  of 50  $\mu\text{m}$  has little more benefit than one of 100  $\mu\text{m}$ . Cross-sections through the simulated RLT distributions after 30 s imprint-time (Fig 3c,h) show how, without etched flexures, the RLTs of 20%-density mesas are increased if they lie adjacent to 67%-density regions, and that uniformity is improved by flexures.

Introducing stamp flexures offers earlier completion of stamp-cavity filling and a tighter range of within-mesa RLT, compared to a uniformly  $t_m$ -thick stamp. Structured stamps could therefore offer faster imprinting times. We have fabricated test stamps carrying mesas with density contrasts as in Fig 3, and work is ongoing to test our predictions with experimentation.

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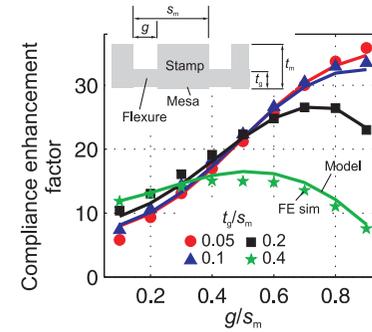


Figure 1. Stamp compliance is considerably increased by backside grooves. ‘Compliance enhancement factor’ is the ratio of pk-pk deflection of the structured stamp to that of a uniformly  $t_m$ -thick stamp, under identical loadings. Symbols: finite-element simulations; lines: semi-analytical model. Inset: stamp cross-section.  $t_m/t_g = 3.3$ .

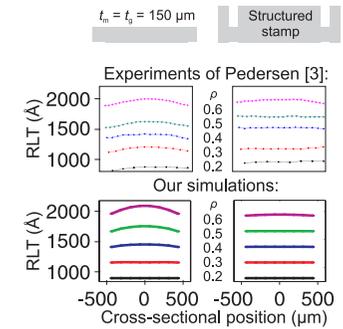


Figure 2. A structured stamp with narrow flexures separating thicker feature-carrying mesas reduces systematic RLT variation.  $\rho$ : protrusion density. Resist viscosity fit:  $2 \times 10^5$  Pa.s (within the range of literature values for this 50K PMMA).  $t_m = 525$   $\mu\text{m}$ ;  $t_g = 150$   $\mu\text{m}$ ;  $s_m = 1.5$  mm;  $g = 500$   $\mu\text{m}$ . Stamp-average pressure 0.35 MPa; imprint time 5 min.

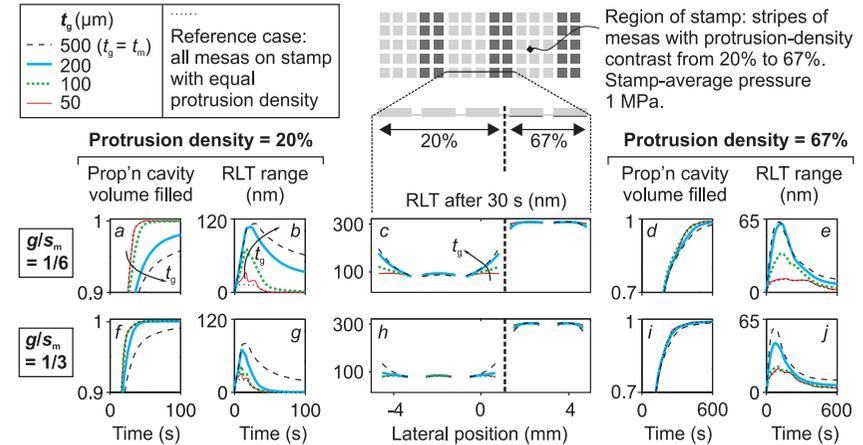


Figure 3. Simulations of imprinting an array of mesas with a strong density contrast. Thinner flexures accelerate cavity-filling and reduce peak RLT ranges by decoupling differently patterned adjacent mesas on the stamp. Longer flexures have a stronger decoupling effect. Resist viscosity:  $2 \times 10^6$  Pa.s.  $s_m = 2$  mm.