Enabling layout and process optimization with fast, full-field simulation of droplet-dispensed UV-NIL

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We demonstrate a simulation framework that can efficiently track the spreading and coalescence of tens of thousands of picoliter-volume resin droplets beneath a nanoimprint template, predicting the evolution of feature filling and residual layer thickness (RLT) uniformity during the imprinting of geometrically complex designs as in solid-state memory.

Our new approach builds upon our existing chip-scale simulation techniques for *spun-on* thermal [1] and UV-curing [2] resists, as well as for roll-to-roll imprinting [3]. These techniques discretize the imprinted area on a square grid, and employ a mechanical impulse response that describes how the surface of the resist deforms when loaded by the template in each grid location. Template–resist contact pressures are computed for multiple timesteps.

To simulate droplet-dispensed imprinting, however, it is essential to account for the merging of multiple droplets within each grid location before template filling occurs. We have combined an analytical solution for the squeezing of disks of viscous resist with a numerical model that captures the flow of resist once droplets have touched each other but before the whole volume beneath the template is filled (Fig 1a). The mechanical work needed to deform the resist comes from an externally applied template load and from the surface tension that acts between the spreading edges of resist droplets and the template and wafer. Previous work on simulating droplet spreading has been constrained by computational requirements to only a few features or droplets, *e.g.* [4],[5]; in contrast, our abstracted approach does not need to solve for the behavior of each individual droplet and so can readily simulate the spreading of $>10^4$ droplets.

To avoid entrapment of chamber gases between the merging droplets, most processes initially bow the template and spread the resist from the center of the field outwards [6]. We have used simulation to explore the geometrical conditions for avoiding enclosed gas voids (Fig 1b). We find that for typical droplet properties, the template must have a radius of curvature of no more than about 500 mm where it meets the propagating fluid front. More gentle bowing may result in the enclosure of voids between coalescing droplets.

We have integrated our new droplet deformation model with models for elastic template deflections and fine cavity filling (Fig 2a), and have explored the imprinting of a 30 mm-by-40 mm field that is reminiscent of Flash memory and contains variations of protrusion areal density and feature pitch (Fig 2b). We confirm the importance of locally matching droplet spacing to the pattern density on the template, to ensure adequate resist supply for cavity filling (Fig 2c,d). Meanwhile, in the problematic case where only part of the template area is in contact with resist droplets because it overlaps the edge of the wafer (Fig 2e), simulations show ~2 nm greater RLT variability and less complete cavity filling after a given imprinting time. We attribute this deterioration of imprint quality to the asymmetrical pressure distribution experienced by the template in a partial field, and to greater resulting elastic deformations.

Finally, our simulation technique can be used to evaluate multiple template layouts, to help optimize, for example, the protrusion density of a border region at the edge of the template (Fig 2f). We observe that a border density of 50% offers superior RLT uniformity near the edge of the field compared with 0% or 100% densities, by controlling RLT reduction rate at the edge. Simulations on a 1 mm grid take ~5 s to run on a standard personal computer; those using a 0.1 mm grid require $\lesssim$ 5 minutes. This simulation approach thus offers NIL users a rapid method for evaluating ways of achieving production throughput targets of $\lesssim$ 1 s/field spreading time.

References

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[4] Reddy *et al.*, *Phys Fluids* **17** 122104 (2005)
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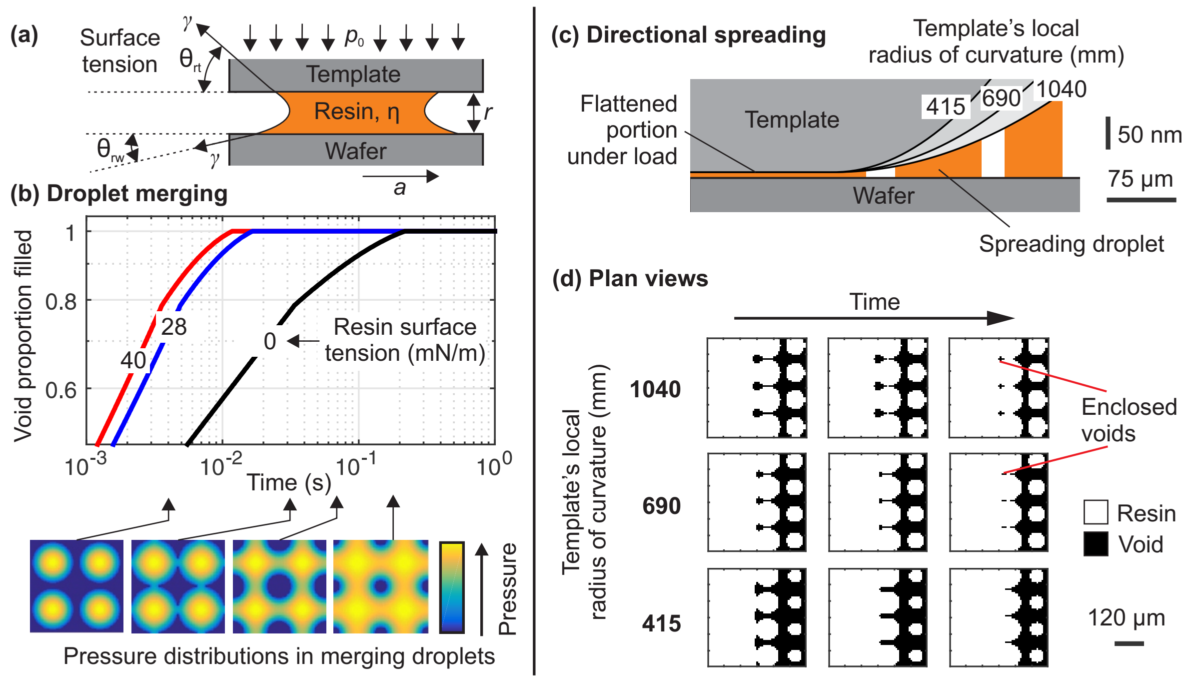

Figure 1. Model for spreading and coalescence of resin droplets beneath a template. Resin deformation (a) is driven by externally applied loads, p_0, and surface tension. For a typical square array (b) of 1 pL, 10 cP-viscosity droplets on a 120 µm pitch, merging beneath a flat template under a load of 40 kPa, capillary pressures are a major contributor to coalescence speed. In order to avoid ambient gas entrapment between merging droplets, directional resin spreading is commonly practiced by inducing elastic template curvature (c). For typical droplet parameters, simulations (d) suggest that a local radius of template curvature of at most ~500 mm is needed at the propagating fluid front in order for droplets to merge without enclosing voids of gas.

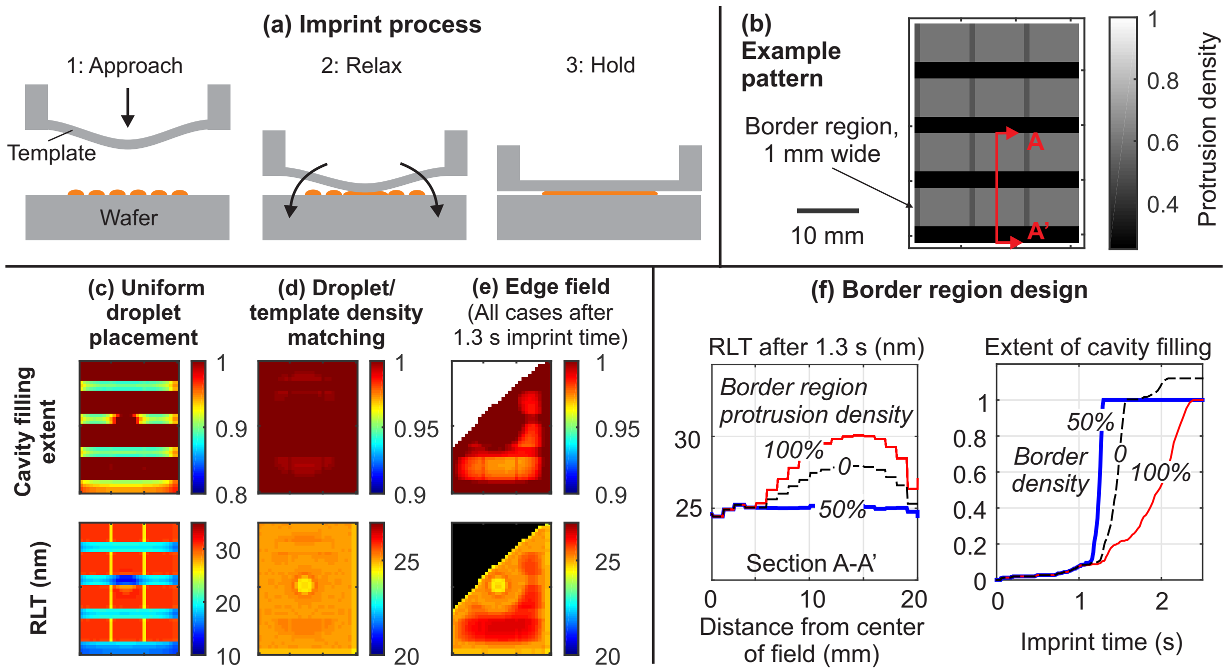

Figure 2. Full-field simulation of droplet-dispensed UV-NIL. The simulated process (a) includes (1) a constant-velocity approach until a target contact load is reached, (2) template curvature relaxation under constant load, and (3) RLT homogenization. In an example (b) of a 30 mm-by-40 mm field with 25 nm half-pitch features reminiscent of Flash memory, uniform droplet distribution (c) yields incomplete cavity filling and inferior RLT uniformity compared with locally matching droplet densities to the cavity volume on the template (d). Imprinting a partial field near the wafer edge (e) with parameters as in (d) results in an additional 2 nm of RLT variation and large areas of unfilled cavities after 1.3 s imprinting. Meanwhile (f), varying the protrusion areal density of the template border helps optimize RLT uniformity near the template edge.