Fast simulation of nanoimprint lithography: modelling capillary pressures during resist deformation

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We describe two computationally inexpensive techniques for simulating the role of capillary pressures in driving pattern formation during nanoimprint lithography.

We have previously developed and experimentally validated a fast technique for simulating thermal NIL with chip-scale patterns [1, 2]. Evolution of the resist's residual layer thickness (RLT) is found by convolving its surface topography's mechanical impulse response with an iteratively found stamp–resist contact pressure distribution. The technique further accelerates the simulation of complex patterns by using pre-computed relationships between pressure-history and RLT for a range of common pattern types.

In UV-NIL using spun-on resist, lower resist viscosities than in thermal NIL mean that capillary forces between the resist and the stamp can govern the speed of stamp-filling. We have adapted our simulation technique by adding a capillary pressure term that pulls the stamp down into the resist faster than under externally applied loads alone (Fig 1a). The capillary pressures are proportional to the resist's surface tension and inversely proportional to the local pitch of stamp features. Capillary pressures fall to zero in regions where stamp cavities become filled. Simulations of a typical UV-NIL process incorporating capillary pressures indicate that where stamp features have sub-micron pitch, cavity-filling and RLT reduction are about two orders of magnitude faster than if capillary pressures were to be ignored (Fig 1c–d). Increasing characteristic feature pitches by a factor of 10 reduces the contribution of capillary pressures, and for feature pitches of ~10 μm, simulations incorporating capillary pressures are indistinguishable from those ignoring them.

Where resist is dispensed as a pattern of droplets rather than as a spun-on film, components of its surface tension acting in the planes of the stamp and substrate govern droplet spreading and coalescence. Existing models of droplet spreading focus at the scale of individual features (*e.g.* [3]); yet a typical 1 pL droplet spread to a thickness of 200 nm has a diameter of ~80 μm, encompassing potentially many thousands of stamp features. Our approach uses a spatial map of a stamp's characteristic feature diameters and shapes to compute approximate capillary pressures at the edges of a specified set of droplets in contact with the stamp (Fig 2c). We iteratively find the resist pressures, p_t, consistent with uniform velocity of the stamp, subject to these boundary capillary pressures and any externally applied imprinting load (Fig 2a). An example pattern with nine droplets and a highly heterogeneous feature-size map (Fig 2b) was solved in less than 8 s (Fig 2d). The pressure distributions in all droplets are computed simultaneously, making this approach amenable to simulation of chip-scale patterns. The technique could be integrated with approximate models for the pattern-dependent entrapment of gas bubbles in stamp cavities [3], and the bubbles' subsequent rate of dissolution [4].

References

[1] H.K. Taylor and D.S. Boning, *NNT* 2009.

[2] D.S. Boning *et al.*, *NNT* 2010.

[3] S. Reddy *et al.*, *Phys Fluids* **17** 122104, 2005.

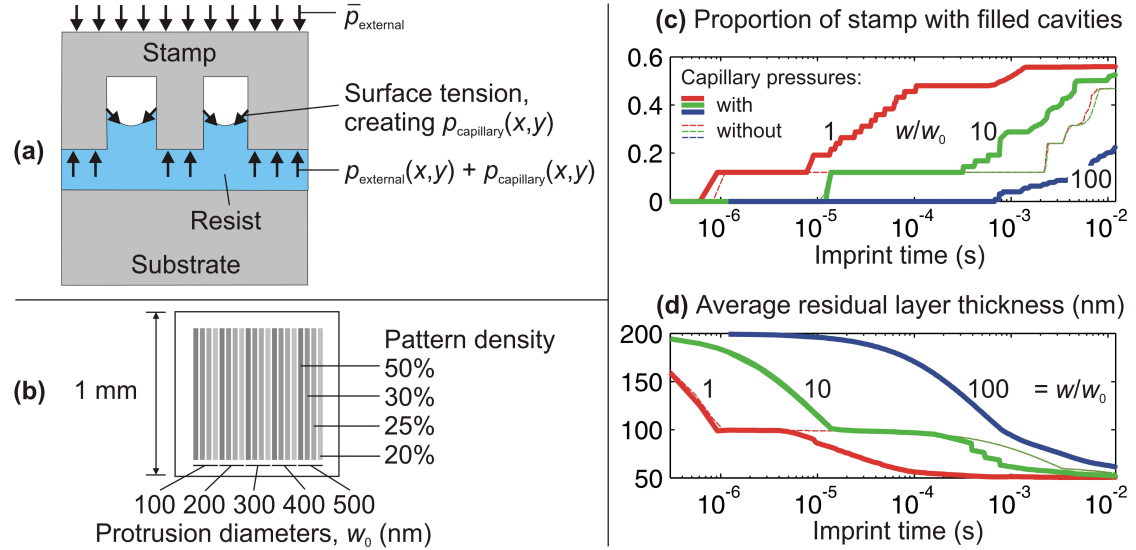[4] X. Liang *et al.*, *Nanotechnology* **19** 025303, 2007.

Fig. 1. Simulations illustrating the contribution of resist–stamp capillary forces to cavity-filling. (a) Pressures acting on the stamp in quasi-equilibrium. (b) Example pattern with arrays of parallel lines of varying diameter and areal protrusion density. (c) Time-evolution of the proportion of the stamp area with cavities completely filled. A Si stamp and substrate, a resist viscosity of 50 mPa.s and initial thickness of 200 nm, and an externally applied pressure of 0.3 MPa were assumed. Heavy lines indicate the inclusion of capillary pressures with a resist surface tension of 0.0275 N/m and a stamp–resist contact angle of 30°. Thin dashed lines show simulations ignoring capillary forces. Increasing protrusion diameters (w/w_0) diminishes the contribution of capillary pressures. (d) Evolution of average RLT for three w/w_0 values.
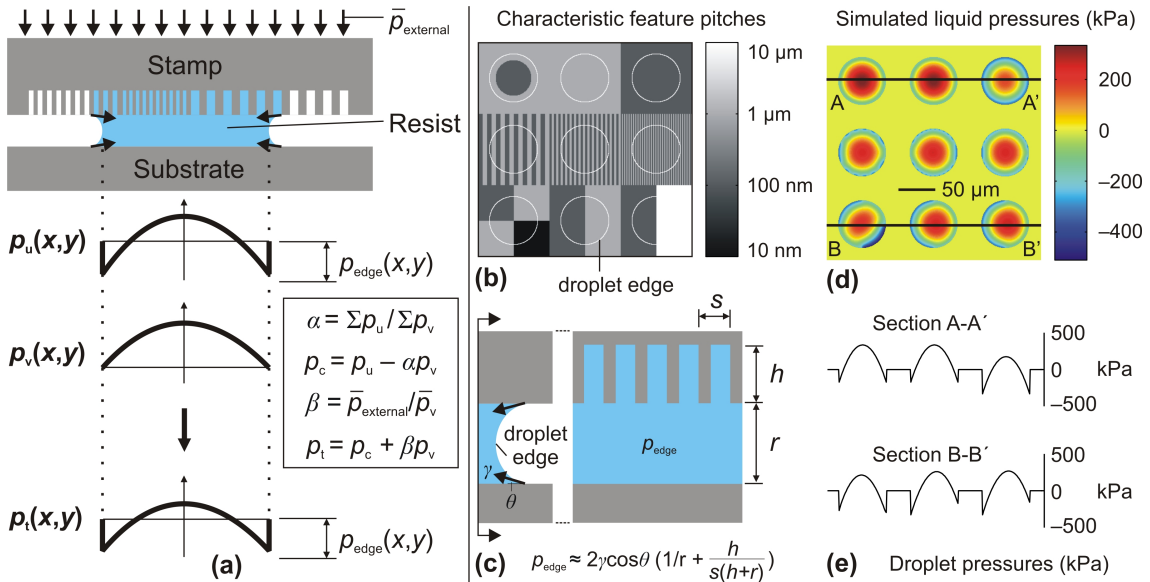

Fig. 2. Simulation of capillary-driven droplet spreading on a patterned stamp. (a) Pressure distribution is found by computing (*i*) p_u, pressures for unit stamp velocity subject to pattern-dependent capillary pressures at droplet edges; (*ii*) p_v, pressures for unit stamp velocity without capillary pressures. Total pressure p_t is a weighted superposition of p_u and p_v, satisfying equilibrium with applied stamp load $p_{external}$. (b) Demonstration pattern. (c) Scheme for approximating droplet-edge capillary pressures as a function of local pattern. (d) Simulated droplet pressures. (e) Cross-sectional plots of pressure. Resist viscosity, thickness, and surface tension are as Fig. 1. With $p_{external} = 0$, capillary-driven stamp velocity is 56 nm/ms.