Polymeric microembossing and nanoimprinting: computationally inexpensive process models for designing inline optical metrology

Hayden Taylor

Department of Mechanical Engineering, University of California, Berkeley
hkt@berkeley.edu — telephone 510 642-4901

We have developed a set of extremely fast computational techniques for simulating the imprinting and embossing of micro- and nano-scale patterns into layers of polymeric materials. The techniques are scalable to complex geometries containing many millions of features and can be used to guide the design of processes for manufacturing microfluidics, integrated circuits, photonics, and functional surfaces.

Conventional techniques for simulating imprinting and embossing include finite element modeling, which is excellent for studying feature-scale effects but not readily scaled to the complex patterns of complete integrated circuits, for example. Meanwhile, simplified solutions of the Navier-Stokes equations offer much faster simulation but have been demonstrated only for Newtonian resist models. Our method offers yet faster simulation speeds and the capability to model the embossing of any linear viscoelastic material.

We encapsulate the polymer's mechanical behavior using an analytical function for its surface deformation when loaded at a single location [1]. The stamp and substrate, meanwhile, are well modeled as linear-elastic and we distinguish between local stamp/substrate indentation and stamp bending, which we find to dominate when the spatial period of the pattern is more than about four times the stamp thickness. Our approach takes a discretized stamp design and finds polymer and stamp deflections in a series of steps. The compliance of the resist is gradually increased with each step, and the algorithm iteratively finds the distribution of stamp–polymer contact pressure that is consistent with the instantaneous compliances of the stamp and polymer. Incremental changes in polymer layer thicknesses are computed at each step by convolving the found pressure distribution with an appropriately scaled version of the polymer's point-load response. After each step, local polymer layer thicknesses and cavity-filling extents are re-evaluated, and the system is re-linearized for the next step. At the final step, the polymer's layer thickness distribution is reported along with the completeness of pattern replication.

We further accelerate the simulation of feature-rich patterns in the following way. We pre-compute relationships between the applied imprinting pressure–time profile and the completeness of pattern replication, for stamps patterned with uniform arrays of a variety of common feature shapes [2]. These relationships are encoded in a dimensionless form. We can then subdivide a given imprinting stamp into a coarse grid of regions, each of which is characterized as being patterned uniformly with features of a particular shape, size, and packing density. A spatially coarse simulation is then conducted.

The first application that I will describe is in the hot micro-embossing of highly entangled thermoplastics, for example for the production of microfluidic devices. Here, we use a Kelvin-Voigt model to approximate the viscoelastic behavior of the material in a rubbery state, and have experimentally calibrated models for three commonly used materials: PMMA, polycarbonate, and a cyclic olefin polymer, Zeonor 1060R [1].

The second application of the algorithms is in nanoimprint lithography (NIL) — in which a thermoplastic film or ultraviolet-curing resin is mechanically nanopatterned in contact with a solid template. NIL offers sub-10 nm patterning resolution with potentially lower capital and ownership costs than competing technologies such as extreme ultraviolet lithography. To be adopted widely in data storage and semiconductor manufacturing, however, NIL's throughput needs to increase and its defect rate needs to fall. Our model of the nanoimprint process can guide this optimization. We have extended the model to describe roller-based imprinting on continuous substrates, capturing substrate-speed and roller-load dependencies. By considering viscoelasticity of the imprinted material, we argue that there is an optimal substrate speed that maximizes the fidelity of imprinted patterns (Fig 1) [3].

Thirdly, we introduce recent work to model efficiently the directional spreading and coalescence of tens of thousands of picoliter-volume droplets of photocurable resin beneath a patterned imprint template [4]. In this extension of the model, we incorporate the mechanical work done by the surface tension of the resin droplets as they spread beneath the template. In this process, an important concern is to predict the locations of any incomplete coalescence of droplets and our analysis shows that the local curvature of the template at the location where droplets coalesce plays a crucial role in determining whether or not coalescing droplets will entrap gas bubbles (Fig 2). 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.

Finally, I will discuss how these mechanical process models can be used to design process-monitoring diffractive optical elements that could be incorporated unobtrusively into embossed/imprinted patterns. These process monitors would impart information to an illuminating laser beam about the performance of the embossing process, and could diagnose specific processing issues such as pressure nonuniformity, incomplete cavity filling (Figure 3), and demolding defects.

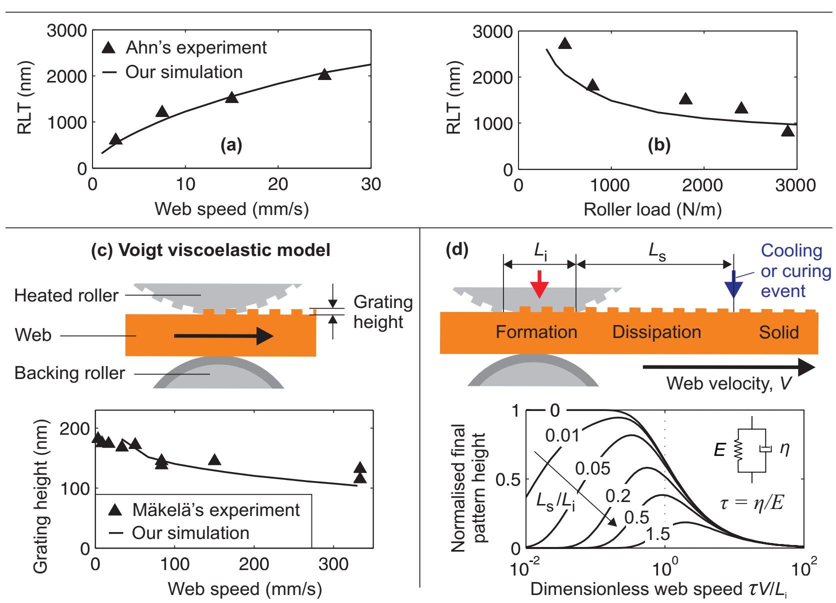

Figure 1: Our technique captures the dependencies of residual polymer layer thickness (RLT) on (a) web speed and (b) roller load seen experimentally by Ahn [5] using a polymeric roller, a solid backing plate and epoxysilicone resist. A Newtonian resist with viscosity 0.8 Pa.s is assumed. Meanwhile, by adopting a Voigt viscoelastic model (c), the technique captures the dependence of an imprinted grating's height on web speed as measured by Mäkelä [6] for a cellulose acetate web heated on one side by a metallic roller. If solidification of the imprinted material finishes after the load is removed (d), pattern dissipation can occur, implying an optimal web speed.

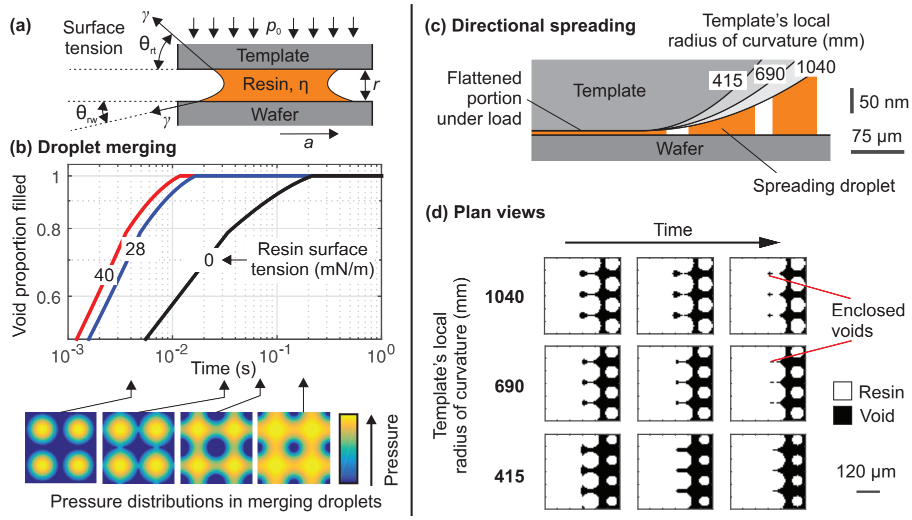

Figure 2. Model for spreading and coalescence of resin droplets beneath a template. Resin deformation (a) is driven by externally applied loads, p_0, and surface tension. For a typical square array (b) of 1 pL, 10 cP-viscosity droplets on a 120 μm pitch, merging beneath a flat template under a load of 40 kPa, capillary pressures are a major contributor to coalescence speed. 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.

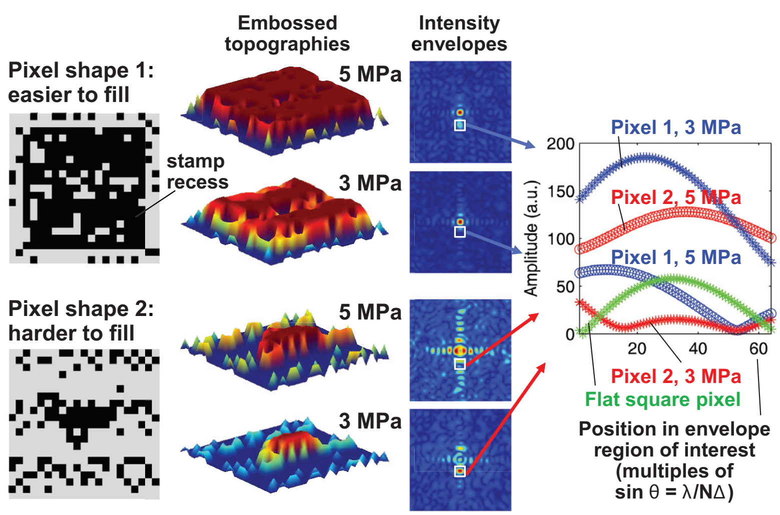

Figure 3. Example of two embossable, micro-scale holographic test structures that have been designed by simulated annealing to detect the degree of completeness of stamp cavity filling by polymer. In this example, as the simulated embossing pressure varies between 3 MPa and 5 MPa (for a typical thermoplastic such as PMMA embossed in a rubbery state above the glass transition temperature), pixel design 1 directs a decreasing amount of optical radiation to the target angular range in the far-field diffraction pattern, while pixel design 2 directs an increasing amount of light to the same far-field region. Patterns composed of these two pixel designs could be combined to yield a simple-to-read inline process monitor.

References

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