

Fast simulation of pattern dependencies in thermal nanoimprint lithography

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We present an extremely fast method for simulating the deformations of a polymeric layer when imprinted with an arbitrarily patterned stamp. Existing techniques for nanoimprint simulation include finite element modeling (e.g. [1]), which is excellent for studying feature-scale effects but not readily scaled to the complex patterns of complete chips. Meanwhile, simplified solutions of the Navier-Stokes equations (e.g. [2]) 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 linear viscoelastic resists.

We encapsulate the resist's mechanical behavior using an analytical function for its surface deformation when loaded at a single location (Fig. 1b). 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 resist 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-resist contact pressure that is consistent with the instantaneous compliances of the stamp and resist. Incremental changes in resist layer thicknesses are computed at each step by convolving the found pressure distribution with an appropriately scaled version of the resist's point-load response (Fig. 1b). After each step, local resist layer thicknesses are re-evaluated and the system is re-linearized for the next step. At the final step, the modeled compliance of the resist equals the true resist compliance at the end of the imprinting cycle, and the distribution of the resist's residual layer thickness is reported.

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. 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 solution for residual layer thickness is then found.

The technique is implemented in Matlab and the convolution uses fast Fourier transforms. We have faithfully simulated the imprinting of an experimental test-pattern reported by Kehagias *et al.* (Fig. 2) [2]. In the experiment simulated, a 340 nm layer of 75 kg/mol PMMA was imprinted by Kehagias at 190 °C under 6 MPa for 5 min. The stamp design has arrays of rectangular cavities of depth 300 nm and with chirped pitches all exceeding 10 μm . This pattern is represented in our simulation using a 48×48 matrix of regions, each characterized by an approximate local cavity pitch and width. Running on a standard personal computer with a 2 GHz Pentium processor and 3 GB RAM, the simulation completes successfully in less than 50 s, which is approximately 20 times faster than other simulations reported in the literature. Residual layer thicknesses simulated using our fast method match experimentally measured values to within 10–15 %.

Our nanoimprint simulation technique builds on our previous work [3] modeling the micron-scale embossing of thermoplastic polymer plates, and could be further extended to model the spreading and coalescence of inkjet-dispensed resist droplets in step-and-flash imprint processes.

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- [2] N. Kehagias, V. Reboud, C.M. Sotomayor Torres, V. Sirotkin, A. Svintsov, and S. Zaitsev, *Microelectronic Engineering*, vol. 85, 2008, pp. 846-9.
- [3] H. Taylor, Y.C. Lam, and D. Boning, *J. Micromech. Microeng.*, vol. 19, 2009, 075007.

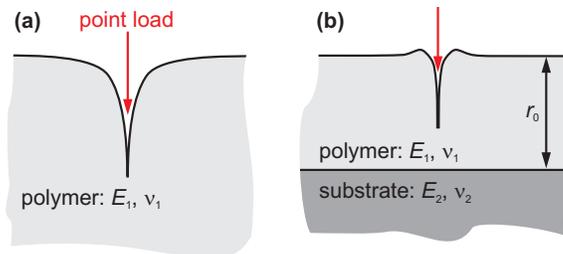


Fig. 1: Illustration of the point-load responses of polymeric layers. In our earlier work on the embossing of thick polymeric plates [3], the response of the surface topography to loading at a single location took the form shown in (a). Meanwhile, in thermal nanoimprint, a different function shape is required, to represent the lateral transport of resist material (b). For a viscoelastic material, the point-load response is a function of time as well as of position.

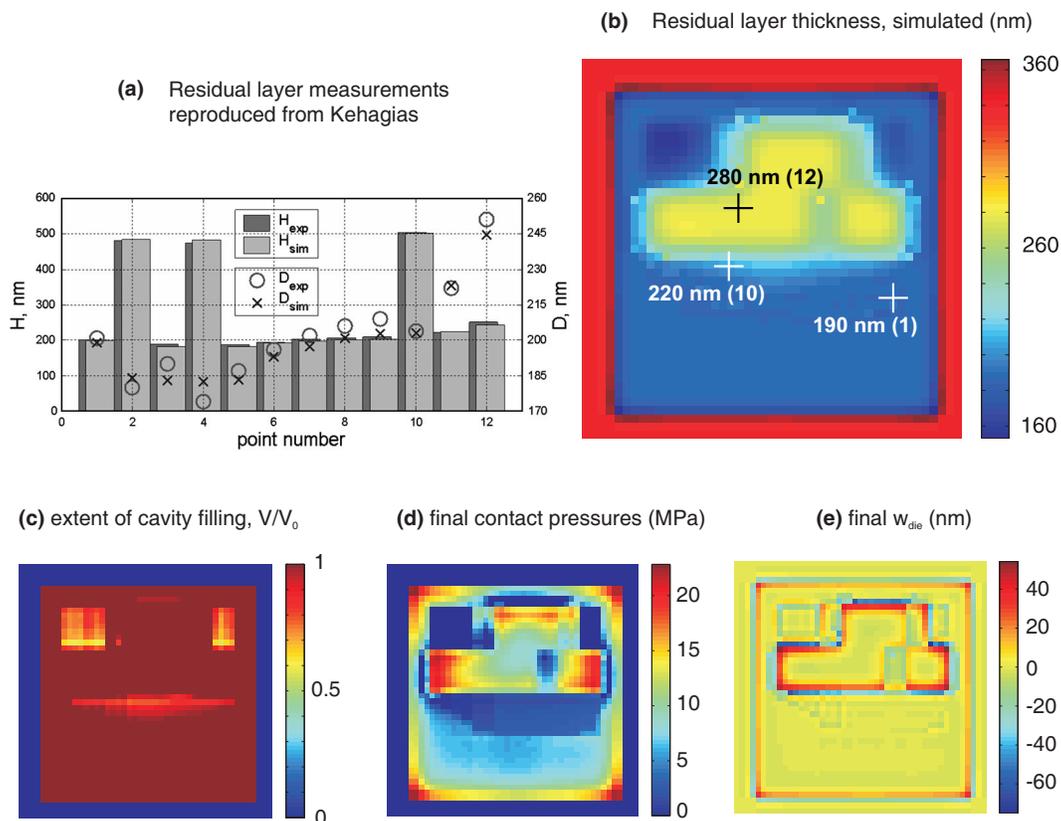


Fig 2: The result of applying our simulation technique to the experimental test pattern reported by Kehagias [2]. Plot (a) is reproduced from Kehagias: D_{exp} and D_{sim} are, respectively, their experimental and simulated values of residual layer thickness at 12 locations on the sample. Residual layer thicknesses simulated using our fast method are shown in (b). Values at three particular locations are indicated, together with the location number corresponding to pane (a). In (c), the simulated proportion of cavity volume filled is mapped. The contact pressure distribution simulated for the end of the five-minute loading cycle is shown in (d). The intra-die displacement of resist (positive out of the region) at the end of the imprinting cycle is mapped in (e).