Optimizing Filling of Anisotropic Templates in UV Nanoimprint Lithography

Yang Ban, Akhilesh Jain and Roger T. Bonnecaze

McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, Texas 78712, United States

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Abstract

UV nanoimprint lithography (UV-NIL) offers a potentially effective and low-cost nanoscale patterning method at resolutions better than photolithography. Acceptance of UV-NIL for integrated circuit (IC) manufacturing requires increased throughput and reduced defects, which are both significantly determined by the template filling process. UV-NIL involves filling a patterned template with a photocurable monomer. After UV curing, the template is removed to leave the desired pattern. Waiting for expulsion or dissolution of gas slows throughput, and trapped gas in the cured polymer leads to defects. The challenge is to optimally place the droplets on the substrate under the template. This is particularly challenging for anisotropic templates, such as lines and spaces, where the filling process is highly directional. Here we present a theory and simulation for fluid filling for anisotropic templates. The theory includes an anisotropic permeability to account for the variation in flow resistance parallel to the template. It also includes a varying capillary pressure that depends on the position of the gas-liquid interface relative to the orientation of the template. This theory is integrated into a simulation of template filling and droplet motion and merging for up to 1000 droplets to optimize droplet positions under different anisotropic templates.

Introduction

Nanoimprint lithography (NIL) is an emerging technique which is an effective and low-cost nanoscale patterning method and a promising solution to the practical limits of photolithography[1-2]. NIL's remarkable replication resolution is unmatched by any other process and approaching molecular scale[3]. While UVNIL has been deployed in the hard disk industry[4-5] and display photonics[6] as patterning tools, UVNIL is not ready for an advanced semiconductor manufacturing. In implementing UVNIL, people faces a dilemma between the defect density and

throughput. Furthermore, stringent requirements and cost of ownership demand UVNIL to be both defect free and high throughput process.

A key to the successful deployment of UVNIL to ICs manufacturing will need to break the bottleneck of UVNIL. There are several experimental observations and analysis which indicates template fluid filling, the bottleneck, is strongly related to the structure of a template and the configuration of droplet placement. Therefore, through the insights gained from a comprehensive model which captures major physics involved with fluid flow, rational design of a template or a droplet pattern could be employed in the future to achieve a low defectivity and high throughput UVNIL process. Thus, our research problem is finding an optimal UVNIL process setting which run at the shortest fluid filling time that leads to an acceptable defect density.

While optimal tunings are known for simple line-space patterns, templates for practical applications contain a range of template patterns, often adjacent to one another. It is interesting to note that the defects are highest at boundaries where pattern densities were significantly different. Optimization with experiments is expensive and laborious, and every new template requires a new optimal pattern of droplet placement. Computer simulations offer a faster and inexpensive means to optimizing droplet placements. The challenge is to be able to simulate fluid flows across centimeters in features on the scale of 10 nanometers involving over 10,000 droplets.

Methods

From experimental observations, it is found that the optimized droplet placement can significantly reduce defect density while not compromising the throughput of UVNIL. Currently, these optimized droplet placement is found by trial and error which is expensive and laborious. Our ultimate research goal is development of computer simulations which is a faster and inexpensive means to find optimizing droplet placements. A schematic of imprint droplets between a patterned template and a substrate is shown in Fig. 1. Typically, the initial radii of the droplets are about 10–100 *μm*. Thus, the droplets are many orders of magnitude larger than the nanoscale patterns. Since each droplet cover hundreds or thousands of individual patterns, the resistance to flow can be described as an effective permeability. The equation describing the pressure and velocity fields in the drop for UVNIL with patterned template are given by the Reynold's lubrication theory:

$$\frac{\partial H}{\partial T} = \nabla \cdot \left(\mathbf{K} \cdot \frac{\nabla p}{\mu} H \right), \tag{1}$$

$$\mathbf{u} = -\mathbf{K} \cdot \frac{\nabla p}{\mu}, \tag{2}$$

where H is the gap between substrate and template, P is the pressure in the droplet, $\boldsymbol{u}$ is the vertically averaged fluid velocity and μ is the viscosity of the imprint resist. The pressure profile in the fluid is calculated using Eq. (1). The capillary pressure at the liquid air interface is used as boundary condition to solve Eq. (1). The pressure boundary condition at the liquid air interface can be found by the Young–Laplace equation. Young-Laplace equation describes the capillary pressure difference sustained across the interface between resist and air:

$$\Delta P = \gamma \left(\frac{1}{R_1} + \frac{1}{R_2} \right), \tag{3}$$

$$P_{boundary} = P_{atm} - \Delta P, \tag{4}$$

where ΔP is the pressure difference across the fluid interface, γ is the surface tension, R_1 and R_2 are the principal radii of curvature, $P_{boundary}$ is the pressure at the boundary, and P_{atm} is the atmospheric pressure. The equations (1 and 2) are solved using the volume of fluid (VOF) method. The domain is discretized into cells, and the fluid content in each cell is tracked as droplet spreading simulation advanced.

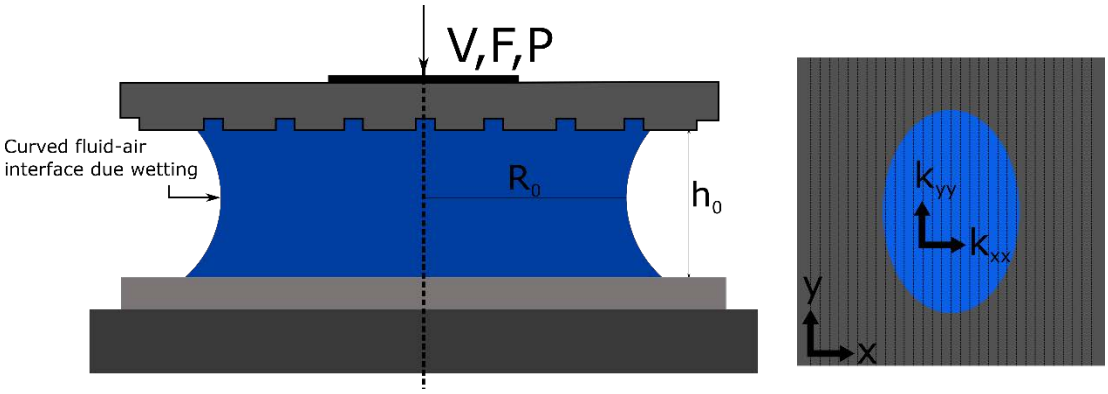

Figure 1. Droplets between a substrate and a template. The initial radius of the drop is R_0 and the initial height is H_0.

Furthermore, two physical systems, permeability and capillary pressure, must be studied in order to accurately simulate flow driven by nanopattern on the template. There a numerous studies which studied effects of structure on permeability, and we can use their approach to calculate effective permeability of various template. For capillary boundary conditions, we can use a software called Surface Evolver. Surface Evolver can generate surface created by nanostructures and calculate various parameters such as pressure and curvature involved with the particular surface.

Results

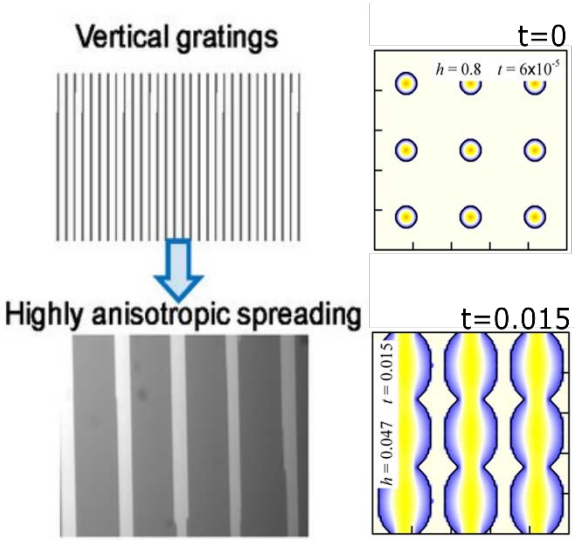

Figure 2. Fluid spreading with a patterned template with vertical grating. In experiment, straight channels of fluid and unfilled cavity formed (left figure). Simulation result also shows an anisotropic flow (right figure), qualitatively similar to the experimental result [9-10].

Simulation of UVNIL using a template with line and space patterns with nine droplets dispensed in a square arrangement is shown in Fig. 2. The droplet spreading and merging is simulated as the gap between the substrate and the template closes from an initial gap of height of 1 to a final gap height of 0.01[7]. It was founded that the droplets are stretched when UVNIL is carried out with templates having line and space patterns. The non-circular shape is a result of the difference in flow permeability in x and y directions[7]. The higher permeability in *y*-direction compare to *x*-direction (Fig. 1) leads to the droplet spreading faster in the *y*-direction compared to the *x*-direction and forming straight channels (Fig. 2).

However, the simulation result shown in Fig. 2 is not completely satisfactory because straight channels of unfilled regions was not observed in simulation. We believe the discrepancy exists between the experimental result and simulation can be mitigated by considering more accurate capillary pressure boundary condition. In the simulation[7], the capillary pressure at the fluid-air interface was calculated as if the template was a flat plate (Fig. 3). We believe this capillary pressure boundary condition caused a discrepancy. A complex surface created by nanostructures should be considered more carefully. The capillary pressure was calculated by averaging the gap height between the substrate and the template accounting for vertical grating pattern, but the interface created by vertical gratings is quite different from a flat plate (Fig. 3). From our surface simulation observation, the previous model might have under estimated the capillary pressure boundary condition.

Using Surface Evolver, the surface created by nanostructures was generated (Fig. 3). These results generated by Surface Evolver can be used to accurately calculate the capillary pressure boundary condition. The capillary pressure calculated by Surface Evolver is shown in Fig. 4. For each simulation, we set the template height into a certain value and changed the height to see the variation in capillary pressure. The template width was always fixed to 1 and

the width was fixed to 0.5. In general, as we reduce the length of any parameter the capillary pressure which propels fluid front increased. This trend was expected, because the negative capillary pressure at the boundary will increase as the radius of curvature is reduced. There are two major points that we need to mention about the result generated by Surface Evolver. First, the capillary pressure calculation was not carried out further because above a certain length scale the fluid-air interface is no longer stable, and resist fluid spontaneously flows into a nanostructure. Second, the template height did not change capillary pressure by much, since interface created by template is small. However, as the template height increases, the stable interface only exists in a small window as shown in Fig. 4.

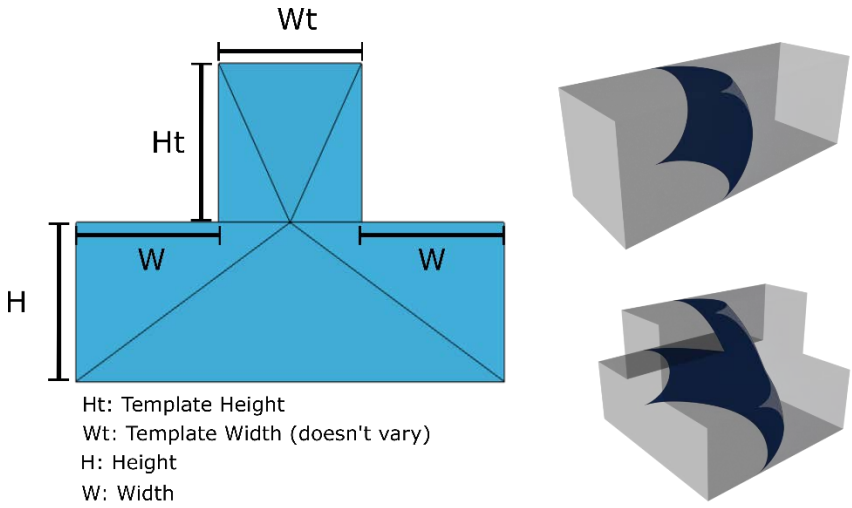

Figure 3. Fluid-air interfaces between substrate and flat template (top-right) and substrate and structured template (bottom-right), generated using Surface Evolver. The left figure shows parameters used in the simulation.

Conclusion and Future Work

In previous simulation, principal radii of fluid air interface was not exactly calculated. Rather the pressure difference, ΔP, is approximated based on the template structure and contact angles. This seems to be a poor approximation of capillary pressure and caused the discrepancy between the experimental result and the simulated result. We would like to resolve this discrepancy by calculate the exact values of principal radii. The result produced from the permeability and capillary pressure calculation will be integrated into the previous simulation which simulated droplet spreading by solving the equations (1 and 2) using the volume of fluid (VOF) method. By adding the new physical parameter, capillary pressure, the simulation can more accurately describe the fluid flow behavior in UVNIL. Furthermore, we will enhance the code to simulate spreading of 10,000 droplets less than an hour to be a practical means to find optimizing droplet placements.

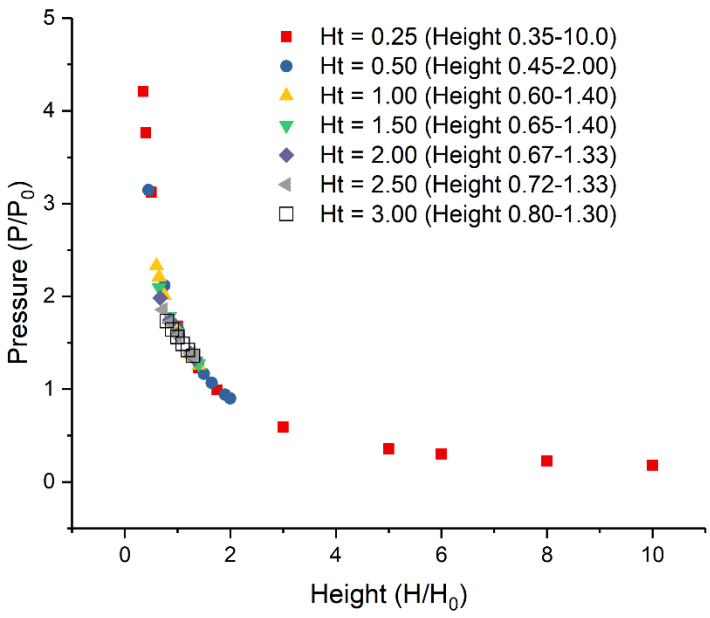

Figure 4. Capillary pressure calculated under various configuration created by vertical grating template. The comment next to legend present the range of height where stable interface existed in Surface Evolver simulation.

The enhanced simulation will be validated using published results which experimentally determined the optimal droplet placement. After the validation, the simulation will be used to determine the optimal droplet placement for various template structure and at the boundary between two different template patterns. From our research, we expect to generate several results. The first is more accurate capillary pressure boundary conditions and approach to calculate the capillary pressure. The second is more accurate and faster multi-droplet simulation for anisotropic templates. Lastly, the optimal droplet placement for various template patterns will be found.

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