Deformation of Stamp Features with Slanted Walls during Microcontact Printing

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Abstract: Microcontact printing is a method for depositing patterns of thin films or molecular monolayers surfaces on using а polydimethylsiloxane (PDMS) stamp for selective mechanical contact. Undesired deformation of the stamp features during printing affects printed pattern quality. Hence, stamps need to be well-designed to prevent erroneous prints.

Existing investigations identify the collapse modes for deformation of stamp features, develop models to predict conditions leading to stamp collapse, and reveal interdependency of these on stamp geometry [1-7]. Results of these studies are limited to stamps with straight-walled features only. However, recent work by Nietner [8] has demonstrated the ability to create PDMS stamp micro-features with adjustable wall angles.

In this study, deformation simulations are extended to cover the stamp features with slanted walls using structural mechanics module and nonlinear structural materials module in COMSOL software. Simulation results indicate that critical pressure for roof collapse increases with increasing sidewall angle and decreasing spacing of the stamp features.

Keywords: microcontact printing, roof collapse, stamp, deformation, structural mechanics, nonlinear structural materials.

1. Introduction

Microcontact printing (μ CP) is a subset of soft lithography. μ CP uses an elastic polydimethylsiloxane (PDMS) stamp to form patterns of monolayers or thin liquid films on the surface of a substrate through selective mechanical contact (Figure 1). Its applications are wide ranging including formation of etch resists at the scales of about 100 nm to be used for surface micromachining, and patterning of proteins, cells and DNA for use in cell biology and tissue engineering research.



Figure 1. Schematic describing microcontact printing.

Although the low shear modulus of the PDMS stamps allow conformal contact of its features to the substrate, it also leads to undesired stamp deformations resulting in erroneous prints at modest application pressures (Figure 2).



Figure 2. Collapse modes of stamp features: a) sidewall collapse, b) roof collapse (adapted from [1]).

Hence, studies are conducted to investigate loaddisplacement-stiffness behavior of the stamp features, identify collapse modes of the stamp and determine critical pressures leading to them. All these existing studies are limited to stamp features with straight walls [1-7]. However, recent work by Nietner [8] has shown the ability to create stamp features with controllable sidewall angles (Figure 3). The process used in this work involves centrifugalcasting a photoresist inside a rotating drum, patterning of the photoresist layer with a laser beam to obtain a mold, and casting PDMS into the mold to produce the stamp. Variations in width and sidewall angle of the stamp features could be obtained by varying the laser exposure time during patterning of the photoresist layer.

The objective of this work is to investigate how stamps containing features with slanted walls behave under loading. Pressure values leading to roof collapse are determined for various sidewall slant angle and spacing values of the stamp features.



Figure 3. Cross section of a PDMS stamp containing microfeatures with slanted walls (adapted from [8]).

Simulation results predict that stamps with slanted-walled features show greater resistance to roof collapse compared to those with straight-walled features. Collapse pressure is found to increase with increasing sidewall slant angle and decreasing feature spacing.

2. Method of Approach

Roof collapse occurs when the center of the stamp roof (Fig. 2 b) and point C in Figure 4) touches the rigid support under loading. Simulations are performed to predict roof collapse pressure for stamps having dimensions inside the range of experimentally achievable values.

Stamp dimensions used in the simulations are shown in Figure 4. Spacing and sidewall slant angle of the stamp features are varied from 100 μ m to 400 μ m, and from 90° to 150°, respectively. Default thickness value of 1 m is used in all the simulations. A fillet with a radius of 3 μ m is used at the corner of the stamp feature where it touches the rigid support.

2.1 Use of COMSOL Software

The structural mechanics module of COMSOL software is used for the simulations, which are setup with the boundary and initial conditions shown in Figure 5. The displacement is prescribed at the top stamp boundary (labeled with "5" in Figure 5) and is increased in increments of 1 μ m, until the center of the stamp roof (point C in Figure 4) is displaced by 10 μ m in the negative y direction (moment of roof collapse).

Displacement of the top stamp boundary is expressed as a boundary load by calculating the traction on this boundary. Plain strain is chosen as the 2D approximation. PDMS is defined as a hyperelastic material using the Neo-Hookean material model in the nonlinear structural materials module of COMSOL software with the parameters given in Table 1.



Figure 4. Geometry and dimensions of the simulation domain.

A free triangular mesh is used for the simulations and element size is chosen to be extremely fine

Density	970 kg/m ³
Lame parameter λ	6.93 GPa
Lame parameter µ	0.77 GPa
Poisson's ratio	0.43

 Table 1. Material properties of PDMS used in the simulations.



Domain,	Condition
Boundary,	
Point	
1	Hyperelastic material
	- Initial displacement=0
	- Initial velocity=0
2	Fixed constraint
	- Initial displacement=0
	- Initial velocity=0
(10):(6, 7, 8, 9)	Contact couple 1
	(zero friction coefficient)
(8):(9,7)	Contact couple 2
	(zero friction coefficient)
3, 4	Symmetry
5	Prescribed displacement
	(displaced in negative y
	direction with 1 micron
	increments till roof collapse
	occurs)
6, 7, 8, 9, 10, 11	Free
В	Fixed constraint
А	Prescribed displacement
	- x-displacement=0
	- v-displacement=unspecified

Figure 5. Simulation setup with boundary and initial conditions.

for all the simulations, except two of them. For stamp features with 40° sidewall slant angle and 100 µm spacing, an extra fine mesh is used. For stamp features with 60° sidewall slant angle and 100 µm spacing a custom mesh was necessary with maximum element size of 7 µm, minimum element size of 0.01 µm, maximum element growth rate of 1.01, curvature factor of 0.15, and resolution of narrow regions being 1. A mesh refinement study is performed for all the simulations involving a feature spacing of 100 μ m (See the Appendix).

3. Results and Discussion

Simulation results indicate that as the sidewall slant angle of the stamp features is increased, the critical pressure required for roof collapse increases for all feature spacing values (Figure 6). As expected, as feature spacing is increased, the critical pressure required for roof collapse decreases (Figure 7). However, it is observed that even at large spacings the angled side continues to increase collapse pressure threshold. The results also indicate that pressure required for roof collapse is not affected by feature spacing for spacing values above about $300 \,\mu\text{m}$.



Figure 6. Variation of collapse pressure with slant angle.



Figure 7. Variation of collapse pressure with feature spacing.

Since the angled sidewalls increase the collapse pressure, stamps with these features should be more tolerant of pressure variations over their area. In this way, we can conclude that angled walls improve the process robustness for microcontact printing. However, the effect of these angles on quality of ink transfer has yet to be assessed.

4. References

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6. Appendix

Sample mesh refinement analysis for the simulation containing stamp features with 100 μ m spacing and 20° sidewall slant angle is described below.

Three simulations are performed with the mesh element size being extremely fine, extra fine and coarse. Displacement of the bottom stamp boundary in the y direction is recorded for each simulation at the moment of roof collapse. No significant difference in recorded values is observed for simulations with extremely fine and extra fine mesh element size. However, displacement values differed significantly for the simulation containing the mesh with coarse element size (Figure 8). Hence, an extremely fine mesh is used in the simulations.



Figure 8. Displacement of bottom surface of the stamp in the y direction at the moment of roof collapse simulated using mesh with different fineness.