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ANALYSIS OF PROCESS VARIABLE EFFECTS ON THE ROLLER IMPRINTING PROCESS

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Roller Imprinting, Process Modeling, Finite Element Analysis, Microfluidics

ABSTRACT
Efficient and cost-effective manufacturing methods are needed for the widespread adoption of microfluidic devices. This paper focuses on the roller imprinting process, which is a new method for fabricating microfluidic devices. In this process, a cylindrical roll with raised features on its surface creates imprints by rolling over a fixed workpiece substrate and mechanically deforming it. Imprint precision is a function of the imprint roll features, the substrate material, and process parameters. This paper presents an analysis of the effects of process variables on the imprint using finite element (FE) simulations of the roller imprinting process.

INTRODUCTION
Microfluidics is the science and technology of systems that manipulate small amounts of fluids (in the pico-liter range) using channels with dimensions in the microns domain (Whitesides, 2006). Microfluidic devices (MFDs) are being increasingly used in a number of applications ranging from bio-defense to molecular biology (Whitesides, 2006). Efficient and cost-effective manufacturing methods are needed for the widespread adoption of these devices. This paper focuses on the roller imprinting process, which is being developed for the fabrication of microfluidic devices. In this process, a cylindrical roll with raised features on its surface creates imprints by rolling over a fixed workpiece substrate (see Figure 1).

FIGURE 1: SCHEMATIC OF ROLLER IMPRINTING PROCESS
To reduce the process development time and eliminate the need for post-processing operations, it is important that imprint rolls are designed and manufactured such that they create precise imprints. Microfluidic devices are composed of networks of fluid flow pathways. Precision is determined by the positional accuracy of the pathways, the form error in the pathway channels, and the profile of the channel surfaces. Roll design is very important here, as the features on the roll have the greatest influence on the precision of the imprints. Other parameters which influence the imprint precision include the material properties of the substrate, and the process parameters of the imprinting operation. Prior work by the authors on selecting a methodology for the design of imprint rolls has been discussed in Vijayaraghavan and Dornfeld (2007).

In order to design rolls which create precise imprints, it is first necessary to understand the mechanism of feature creation during the roller imprinting process as a function of the process variables. Given the wide range of variables to study, it is cumbersome and time-consuming to experimentally determine their effect. In this paper, simulation studies of the roller imprinting process using finite element analysis are performed to understand the effect of workpiece material properties, process parameters, and imprint roll features on the precision of the imprinting process.

This paper discusses the development of 2D simulations of the imprinting process, which are a necessary precursor to the more complex 3D simulations. As 2D simulations have considerably shorter run times than 3D simulations, a larger parameter space can be easily tested. The results from these simulations can be applied in understanding 3D behavior as well.

The next section presents a background on microfluidic devices, and makes the case for the development of the roller imprinting process.

**BACKGROUND**

**Application Area: Microfluidic Devices**

Microfluidic devices exploit both small feature sizes and the properties of liquids at this scale, such as laminar flow. In a recent review, Whitesides (2006) discussed the problems that need to be addressed for the widespread development and adoption of microfluidic technology, highlighting the importance of good design and manufacturing processes for the commercialization of these devices. MFDs vary widely in scale and application (see Figure 2), and processes need to be customized to scale and application.

![Figure 2: Feature Complexity in MFDs](image)

The most common process used for MFD fabrication is soft lithography (Ziaie, 2004). Features are created by casting an elastomer over a silicon master and allowing it to cure. Elevated temperatures speed up the curing, and the elastomer is removed and used to create the device, leaving the master for reuse (Becker, 2002). The most common material used in this method is Polydimethylsiloxane (PDMS) and the silicon masters are created using standard lithography processes. Soft lithography-based
methods are popular because of the small feature scales possible and the potential for reusability of the silicon masters (McDonald, 2000). Other materials used for microfluidic device fabrication includes Poly-methyl methacrylate (PMMA) and Polystyrene (PS).

However, lithography-based methods have significant equipment requirements and tend to have a long lead-time due to the multiple steps involved (mask-making, photo-resist preparation, baking etc.). Moreover, though semiconductor processes can create very precise features, the features are in 2.5-dimensions due to the physics of the lithography process, resulting in fixed-depth channels in the devices. Due to the small feature scales in MFDs, flows have a low Reynolds number making the mixing of fluids difficult. Efficient mixing of fluid streams is required for biological applications where fast analysis is needed (Kim, 2005). Due to the limitations of soft-lithography, rapid mixing is enabled by creating complex out-of-plane features in the MFDs. While these methods have been successful (Nguyen, 2005), the manufacturing processes required to realize them tend to be complicated and involve multiple fabrication steps. Semiconductor processes are also sub-optimal for creating features larger then 100 µm due to long lead-times; several applications of MFDs are in this scale (Yager, 2006).

**Suitability of Roller Imprinting**

Roller imprinting is a suitable manufacturing process for large-featured MFDs (with features larger than 100µm). It is significantly easier to set up than soft lithography-based methods as it is completely mechanical and does not require the use of process chemicals. It is also a room-temperature process and the equipment required to create the imprints can be compactly fabricated. The capital costs for this process are significantly lower than the costs for semiconductor processes (Trybula, 2006). Batch processing is also easy to setup by adding multiple sets of features on the roll. It is important to note that the size of the features that can be created with roller imprinting is limited by the precision used to create the imprint rolls. The imprint rolls developed as part of this research are being fabricated by micromachining technology, therefore micron-scale features are achievable (Dornfeld, 2006).

With micromachining it is possible to machine contoured free-form surfaces which can be used to create MFDs with contoured flow fields, which can help in improving the mixing rates. Micromachining research has focused on creating accurate surfaces by minimizing machining artifacts and errors (like burrs) (Dornfeld, 2006) and these results can be applied in creating accurate imprint rolls. Injection molding using micro-machined imprint rolls is also being developed to create MFDs, but is limited by the materials which can be used (Hartnet, 2007). Xu et al. (2000) discuss the development of a room-temperature imprinting process for PMMA (Polymethyl methacrylate) and report that this was successful in accurately creating micron-scale features. As roller imprinting uses the same physical principles as this process, it is reasonable to expect that similar accuracy is possible.

**Related Work**

Roller embossing methods have been used in creating micro-scale features. Chang et al. (2006) discussed the use of roller embossing in fabricating lens arrays in a UV-curable photopolymer. These methods, however, have only been used in creating simple patterns and features. Also, there has not been extensive work in designing the roll features to create specific embossed features.

Finite element analysis (FEA) has been used extensively in studying metal forming. While analytical methods can also be applied to understand the mechanism of metal forming, FEA offers the most flexibility and accuracy as a wide range of boundary conditions and material models can be tested; parametric analysis of the process is also easy. Hartley and Pillinger (2006) discuss at length the application of various numerical methods (including the finite element method) in studying the metal forging process. 2D and 3D FE-analysis has been used in the design of both process parameters and process equipment (such as tool and die design) (MacCormack, 2002). Antonio et al. (2004) discuss the formulation of the metal forging process as an optimization problem and use this to select geometric and process design variables. Inverse methods are applied to design dies and set parameters based on the outcomes of the optimization algorithms. Sousa et al. (2002) also use a similar approach in designing dies. Fourment et al. (1996) combined shape
optimization methods with FE-analysis to design the initial workpiece shape as well as the die for forging operations.

SIMULATION STUDY

2D simulations of the roller imprinting process were implemented in the Abaqus finite element analysis package. 2D simulations are a good starting point as they are adequate for understanding the fundamental material deformation dynamics. They are also useful in eliminating process parameter choices which are clearly sub-optimal, and help in decreasing the size the parameter space for subsequent 3D simulations of the process.

FIGURE 3: SCHEMATIC OF SIMULATION SETUP SHOWING POSITION OF ROLL AND WORKPIECE.

Figure 3 shows a schematic of the simulation setup, indicating the relative position of the roll to the workpiece. The roll is created with a linear array of regularly spaced features (w is the feature spacing). Multiple features are used so that edge effects can be eliminated. The imprints created by the middle features are more consistent than those created in the lead-in and lead-out features. The imprints created by the middle features are used in the analysis, which is discussed in a later section. The features on the roll are described using b-spline curves, and the roll itself is a part of a circle. The roll is modeled as a rigid body in the simulations. This is a reasonable assumption as the roll is usually made of metal and is significantly harder than the polymer workpiece.

Quadrilateral elements are used to mesh the workpiece. The element size was decided such that it would be small enough to capture the features of the roll being imprinted, but not smaller so that the simulation time remained acceptable. Based on this, the element size used in the simulations was 40µm x 40µm. An explicit time-increment scheme was used by the FEA-solver and the time increment was selected to give a stable, converging solution. Different time steps were tested, and a small enough time-step to provide convergence was selected.

The workpiece is constrained along its bottom surface, and the roll is rotated by applying linear (Vx) and rotational velocities (ω) to its center. The roll is positioned vertically such that the circular regions barely touch the workpiece during imprinting. Care is taken to position the roll just away from touching the workpiece to minimize the “air-time” in the simulations. The position of the workpiece in the horizontal direction is calculated based on the roll-radius to ensure the imprint is created in the center of the workpiece with an equal length of undeformed material on both sides. The height of the workpiece is set nominally as 2.5 times the maximum feature height (when the workpiece was taller than this, no stresses is seen in the bottom nodes).

The effect of the following process variables on the quality of the imprints was studied: feature shape, feature spacing, roll radius, roll velocity, and substrate material properties. A base-case of parameters was first chosen, and the process parameters were varied about the base-case. One parameter was varied while keeping the other parameters at the base-case. A full-factorial experiment was not performed as this would have resulted in too many cases to analyze. The limited parameter space which was explored in this study was adequate for capturing the effect of all the parameters on the imprint quality.

The base-case was representative of common fabrication process parameters and material properties. In the base-case, the rolls had a radius of 50mm and were moving at a linear speed of 25 mm/sec. The rotational speed of the roll was set to induce a no-slip condition at the point of contact between the roll and the workpiece. Feature A was used in the base-case (see Figure 4), which is a hemisphere-like feature representative of simple fluid pathways channels. The spacing of the features on the roll was equal to the width of the feature. The
material used for these initial simulations was PMMA modeled as an elastic perfectly-plastic material with a modulus of 2 GPa and a yield-stress of 100 MPa. Following the base-case, the process parameters which were varied are listed below in Table 1. Figure 4 shows the features that were varied in the roll design. These features are representative of those used to create contoured fluid channel surface.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feature Spacing</td>
<td>0.5, 0.75, 1.0, 1.25, 1.5 times the feature width</td>
</tr>
<tr>
<td>Roll Features</td>
<td>See Figure 4</td>
</tr>
<tr>
<td>Roll Radius</td>
<td>25mm, 50mm, 100mm</td>
</tr>
<tr>
<td>Roll Velocity</td>
<td>10mm/sec, 25mm/sec, 40mm/sec</td>
</tr>
<tr>
<td>Materials</td>
<td>PMMA, PS</td>
</tr>
</tbody>
</table>

The quality of the imprints was calculated using two metrics: (1) feature transformation (2) imprint-gap (see Figure 5). (1) The feature transformation metric was chosen to capture the transformation of the feature from the roll to the substrate. This was calculated as the optimal linear transformation between a goal and the deformed configurations (Demmel, 1997). The goal configuration was calculated based on the b-spline control points of the feature required to be imprinted. The deformed configuration was extracted from the simulation results (the middle feature was used as this had the least edge-effects). (2) The imprint-gap is the difference in height between the top of the imprint walls and undeformed substrate. It is an important metric as features with zero imprint-gaps are needed for leak-free lamination of the substrates.

RESULTS AND ANALYSIS

Changing the feature spacing had the largest impact on the quality of the imprints. The imprint-gap decreased with increasing feature spacing until the spacing was equal to the width of the feature. For features spaced wider than their width the imprint-gap was negligible. Figure 6 shows this trend for the four different features. Features A and B were narrower than Features C and D and the plot also indicates that the wider features had a slightly smaller normalized imprint-gap at the same normalized feature spacing. Figure 7 shows the deformation behavior when the feature spacing is varied for one type of feature. Tighter feature spacing restricts the flow of material as the workpiece is deformed, and this results in the material between features being squeezed to a lower height than their original. The elastic relaxation is also not adequate for the material in the gaps to return to their original height. On the other hand, when the spacing is wide enough, the flow of the material in the gaps is not constricted and the original height is restored in the gaps.
FIGURE 7: EFFECT OF FEATURE SPACING ON THE IMPRINT GAP

The feature transformation was calculated for different roll features, with the process parameters being held the same as in the base case. When the process parameters were held constant, the deformation behavior (and thereby the transformations) for all the features was comparable. The transformation was in the form of a 2x2 matrix (since it was a 2D linear transform) and in all the cases terms were present only for the cases of deformation in the $x$ and $y$ directions (the shear terms were close to zero, and were ignored). Moreover, these terms were smaller than 1, which indicated that there was some shrinkage happening to the roll features when imprints were created with them. Figure 8 shows the relative deformation to the imprinted features in the $x$ and $y$ directions.

Intuitively, this denotes that there is a finite elastic relaxation which results in the imprinted feature being smaller than they were intended to be. As numerically equivalent transforms were seen for different features, this implied that the feature transformation was not a function of the feature itself, and was instead dependant on the material properties and the process parameters. From the perspective of designing features on the roll which can guarantee a specific imprint, it is important to take this effect into account as the features on the roll need to be larger than what is required in the substrate.

FIGURE 8: IMPRINT DEFORMATION IN X AND Y SHOWING SMALL VARIATION WITH ROLL FEATURE

The imprinting forces also did not vary much when the features were changed. Figure 9 shows that the peak workpiece reaction force from the simulations was similar for different features. This reinforces the observation earlier that the feature shape does not significantly affect the deformation behavior. The roll radius, however, had a significant impact on the workpiece reaction forces and larger roll radii resulted in larger reaction forces. Figure 10 shows the peak reaction force for increasing roll radii and also shows the peak force when the same features had to be created by stamping. Stamping can be imagined as a rolling process with a roll of infinite radius, and correspondingly requires more force than rolling. It is important to note here that the die used in the stamping process had the same number of features as the rolls. The maximum rolling force will not increase with the number of features as the features in contact at any point of time is only a function of the roll radius; but with stamping the force required will increase with the number of features being imprinted.

FIGURE 9: PEAK IMPRINTING FORCE FOR DIFFERENT FEATURES
Material properties had a significant influence on the quality of the imprints. To study the effect of workpiece material properties on the imprints, three properties of PMMA which was used to model it in Abaqus were varied independently, keeping the other parameters constant. These parameters were density, elastic modulus, and yield strength. Increasing the elastic modulus (at a constant yield strength) reduced the elastic component of the strain, leading to less relaxation, resulting in imprints which match the roll feature more closely. Increasing the yield strength (at a constant elastic modulus), on the other hand, increased the elastic component of strain, resulting in an imprint which matched the roll feature less closely. Changing the density had no effect on the imprint quality. These results closely followed theoretical expectations.

**DISCUSSION**

The 2D FE-analysis of the rolling process helped understand the material deformation during imprinting. The effect of the feature spacing on the quality of the imprints has strong implications in 3D simulations, as features will have “neighbors” in all directions and spacing between all of them will affect the imprint precision. It was also interesting to observe that the feature spacing effect was uniform for different features when simple material models were used. This indicates that analysis can be performed on a small set of features and extrapolated to more complex ones as the trends seem relatively insensitive to feature shape. Of course, this has to be validated with more complex material models as well.

As the feature transformation from the roll to the imprint was a linear transform, it is possible to take the inverse of this transform and apply it to modify the roll features. Preliminary results indicate that the rolls with modified features were very effective in creating the required imprint on the substrate. This opens the possibility of using iterative methods to optimize the roll design.

Preliminary 3D simulations of the imprinting process also revealed that the cross-sections of the 3D features (when taken far from the edges) corresponded very closely to the 2D imprints. This validated the hypothesis made earlier that 2D simulations can be used to better understand 3D behavior.

**FUTURE WORK**

Future work for this research includes expanding the simulations to model the fabrication of 3D features and pathways. The material models used in the simulations will be improved and the workpiece material will be modeled using visco-elastic and visco-plastic constitutive models. Appropriate constitutive models of visco-plastic polymers will be applied (Hasan, 1995). Optimization routines will be formulated based on these results and will be applied to design imprint rolls which guarantee precise features for a given range of process parameters and material properties. Future work will also include experimental validation of the simulation results by using micro-machined imprint rolls to create features in PMMA.

Ultimately, the simulation studies will contribute to the development of CAD tools to assist in process design and planning for roller imprinting. Effective design tools are essential for the widespread adoption and commercial success of the roller imprinting process.

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