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DEBONDING OF HOT-EMBOSSED POLYMERIC MICROFLUIDIC SUBSTRATE: Influence of substrate thickness on demolding behavior

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ABSTRACT

This study focuses on the influence of polymer substrate thickness on demolding of hot-embossed polymers with different sets of channel geometry via numerical simulation. It is important to understand the demolding behaviour because it has been known to pose extreme challenges that affect the overall success in the replication of polymeric microfluidic devices. Three different substrate thicknesses were analyzed on three molds with different channel depth (aspect ratio). The numerical simulations showed the significant contribution of substrate thickness to both demolding energy and plastic strain.

Keywords: polymeric microfluidic devices, substrate thickness, hot-embossing, demolding

1. INTRODUCTION

Microfluidics is the science and technology of systems that process and manipulate small amounts of fluids, typically 10^{-9} to 10^{-18} litres, by utilizing channels with dimensions of tens to hundreds of micrometers (Whitesides, 2006). This technology has emerged as a potential field to influence diverse subject areas from chemical synthesis and biological analysis to optics and information technology. The popularity in life science applications has been growing rapidly due to the unique ability in analyzing tiny quantities of samples with high throughput sampling capabilities. Besides the advantageous efficiency and speed, the microfluidic devices can also be designed to obtain and process measurements without the need of any expert operator. This factor is indeed extremely crucial in creating portable point-of-care medical diagnostic systems (Dupuy, 2005: Toner 2005). Some of the applications of microfluidic devices are lab-on-a-chip, drug screening devices, capillary electrophoresis, multi-component reactions, bio-sensors, miniaturized polymerase chain reaction (PCR), genetic analysis, single-cell analysis, cell migration, micro-reactors, and long-term culture of stem cells and neurons (Becker, 2002; Yager, 2006; Skurtys 2008).

In early days, microfluidic devices were largely made from either silicon or glass as the main materials. Nevertheless, polymer-based microfluidic devices have shown great promise as they are both cheaper and easier to be mass-produced via replication methods when compared to silicon or glass. In addition, there is a wide range of different thermoplastic polymers in such a way that it is feasible to find suitable polymers for almost every application. To mass replicate the microfluidic devices, micro-molding is one of the most promising fabrication techniques. This technique provides the ease of mass-replication once the relevant mold insert has been produced.

Injection molding is a micro-molding technique that has been well established with vast know-how and easily available machine technology. However, hot-embossing has become increasingly well-known to be one of the best candidates as it produces very little inner stress in polymer due to the short flow of polymer into the mold cavities. This is in contrast to injection molding. In addition, its simplicity in terms of set-up which is beneficial for any modification, and the suitability for producing delicate micro-channels with high aspect ratios are the other beneficial considerations to utilize this method (Heckele, 2004).

There are several steps involved in the replication of microfluidic devices via hot-embossing. Initially, mold and polymer substrate are heated to temperature above the glass transition temperature (Tg) of the thermoplastic polymer. Then, the polymer substrate is hot-pressed so that the softened polymer can flow into the mold cavities to replicate the intended micro-channels. After hot-pressing, both mold and polymer substrate are eventually cooled down to demolding temperature, followed by separation of the polymer from mold which is also known as demolding. Generally, most problems in micro-molding are not caused by the filling of polymer into the mold cavities. It is indeed the separation of the polymer substrate from the mold (demolding) that challenges the success of replications because intolerable deformation or even fracture of polymer substrate is very prone to occur.

The proneness to demolding defects is mainly contributed by the quite different thermal contraction behavior between the mold and polymer substrate. During thermal cooling from embossing to demolding temperature, polymer is constrained from thermally contracting by the mold which has a much lower coefficient of thermal contraction. The constraint further generates thermal stress that enhances the difficulty in mold-polymer separation. As demolding is generally performed by load applied on one projecting end of the embossed polymer substrate, the polymer substrate including the replicated channels will experience bending during demolding. In order to prevent any possible demolding defect, the stress experienced by the polymer substrate during the bending phenomenon should not exceed the yield or fracture strength of the polymeric material. As the polymer substrate bends during demolding, the polymer substrate thickness may play an important role in determining how severe the demolding stress will be. This is because thickness has a direct correlation to the bending stiffness property. Moreover, the effect of polymer substrate thickness to demolding has not been explored and reported yet.

Furthermore, the demolding defect issue becomes more apparent when high aspect ratio micro-channels are replicated (Worgull, 2005; Park, 2009; Yeo, 2009). There have also been reports (Guo, 2007; Saha, 2010) of experimental work showing the failure of demolded polymer substrates with high aspect ratio micro-channels (typically above 1). Knowing that higher aspect ratio micro-channels can perform better in applications, the demolding issue becomes a very crucial challenge that needs to be tackled. Hence, it may also be useful to investigate on the effect of substrate thickness to demolding of molds with varying aspect ratio that ranges from low to high.

On the whole, this paper will focus on the influence of polymer substrate thickness to demolding via numerical simulation. Several molds with different aspect ratio ranging from low to high will also be used. Then, from the numerical simulation results, both quantitative (demolding energy) and qualitative (plastic strain) results will be eventually obtained.

2. NUMERICAL MODEL

This section discusses about the different mold geometries and polymer substrate thicknesses used in the numerical study, material and interfacial properties incorporated in the numerical model, and the detailed description of the model. The numerical simulation is carried out with Abaqus/Standard.

2.1 Mold and polymer substrate

In this work, both mold and polymer substrate are made of aluminum alloy (6061-T6) and cyclic olefin copolymer (COC – Topas 8007), respectively. Aluminum alloy is chosen as the mold insert material because of its relatively low cost and simple fabrication process with excellent surface quality that has surface roughness (Ra) of about 40 nm (Tran, 2010). On the other hand, COC – Topas 8007 which is an amorphous thermoplastic polymer with glass transition temperature (Tg) of 78^{o}C is used as the polymeric material due to its superior properties such as low density, high transparency, low birefringence, extremely low water absorption, excellent water vapor barrier properties, high rigidity, high strength and hardness, very good blood compatibility, excellent biocompatibility, very good resistance to acids and alkalis, very good electrical insulating properties, and very good melt processability/flowability.

Three different polymer substrate thicknesses are used which are 1, 1.5, and 2 mm. Each of the polymer substrates is 35 mm long. There are also three different molds used in this study with identical channel width and spacing of 100 μm, but with channel depths of 50, 100, and 150 μm that correspond to aspect ratio of 0.5, 1, and 1.5. Each mold has thickness of 0.5 mm and length of 20 mm that includes 50 channels. In both mold and polymer substrate, width is not defined because the numerical model is restricted to two-dimensional with plane strain idealization. Thus, all the numerical simulation results are obtained in terms of per unit mm width.

2.2 Material and interfacial properties

In the numerical model, there are two essential parameters to be defined. They are material and interfacial properties. Material properties are required to define the material model for both mold and polymer substrate. On the other hand, interfacial property defines the bonding properties between the mold and polymer substrate.

The polymer substrate is modeled with the constitutive theory that represents the large deformation, thermo-mechanically coupled, elastic-viscoplastic behavior of amorphous thermoplastic material spanning the glass transition temperature developed by Srivastava et al. (Srivastava, 2010). And, the relevant material parameters in the constitutive theory for COC – Topas 8007 are obtained from calibration with large strain compression experiments extracted from the work of Jena et al. (Jena, 2010). On the other hand, the aluminum alloy mold is simply modeled as an isotropic linear elastic solid with the widely-known properties of aluminum alloy (6061-T6). The simple linearly elastic material model used for the mold is reasonable enough because the mold has much more superior strength when compared to the polymer substrate. Therefore, deformation is extremely less likely to occur in the mold during demolding.

The interfacial property between mold and polymer substrate is modeled as Coulomb friction interaction with a constant coefficient of friction of 0.26 using the penalty friction formulation and hard contact pressure-overclosure in Abaqus/Standard. The Coulomb friction interaction is applied to the whole contacting interfaces between mold and polymer substrate that include both horizontal and vertical interfaces (fig. 1). As demolding is performed at room temperature, the significant contribution to demolding will be from the generated thermal stress. The effect of adhesion is expected to be very weak or negligible at such a low temperature for the metallic-polymeric interfaces. Thus, it is reasonably good to apply friction interaction on the contacting interfaces in the numerical model.

The value of coefficient of friction (0.26) was calibrated and obtained from friction test based on ASTM D1894 at room temperature. In the friction test, a flat aluminum mold that has no channels with surface roughness (Ra) of about 40 nm and polymer substrate made of COC – Topas 8007 were used as the testing specimens. Prior to the friction test, the polymer substrate was hot-embossed on the flat mold, followed by cooling to room temperature. Then, the static coefficient of friction was calculated from the friction test results.

2.3 Description of model

Fig.1 shows the numerical model of mold and polymer substrate with 100 μm channel depth and 2 mm substrate thickness. The only changes subjected to the different mold and polymer substrate used in the study are simply the channel depth and polymer substrate thickness. As mentioned above, the model is based on two-dimensional with plane strain idealization. Mesh is made much denser in the regions near mold features where high stress is expected to occur, so that accurate result can be obtained.

The numerical model involves two steps which are thermal cooling and demolding. During thermal cooling process, there is a temperature boundary condition for the whole specimens, which specifies cooling from the embossing to demolding temperature (100^oC to 25^oC) within the duration of 600 seconds. In order to prevent rigid body motion during cooling process, displacement boundary condition of $u1 = 0$ is applied at node C, and $u2 = 0$ is applied at all the nodes along line AB. This means that the mold is thermally shrinking towards its own center (node C). Conversely, there is no boundary condition applied on the polymer substrate. This further suggests that free thermal contraction can be simulated so that it can reflect the real process.

After cooling to demolding temperature, demolding is eventually performed with a prescribed velocity boundary condition (50 mm/min) applied on node D at the front projecting portion of polymer substrate. Node D is located at the distance of 5 mm in front of node B. During demolding, temperature is maintained at room temperature, and all the displacement boundary conditions on mold remain the same. The displacement boundary conditions on mold can be reasonably justified because mold is usually fixed for demolding purpose. Then, the demolding load (per unit mm width)-displacement data is eventually captured from node D where prescribed velocity boundary condition is applied. From the obtained demolding load (per unit mm width)-displacement curve, the demolding energy per unit mm width is further calculated based on the area under the curve.

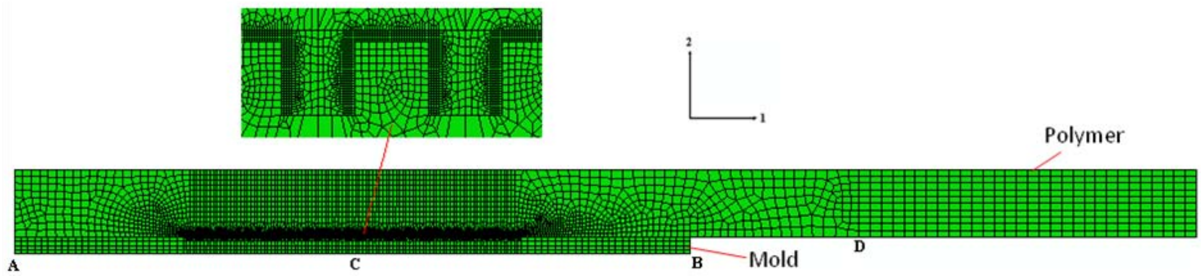


Fig.1 Numerical model (channel depth of 100 μm and 2 mm polymer substrate thickness)

3. RESULTS AND DISCUSSIONS

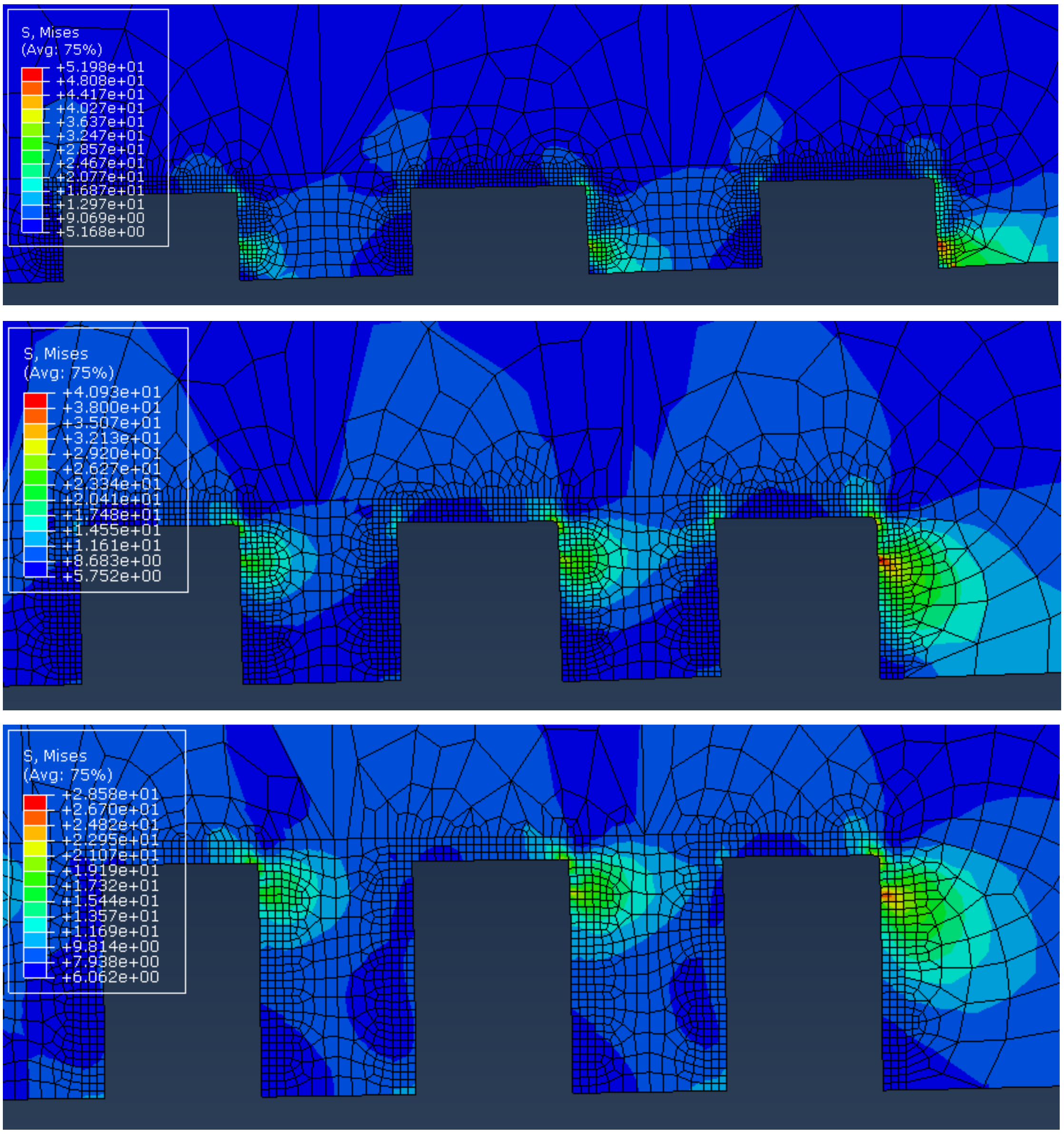
This section groups results into three different sub-sections. As there are two steps involved in the numerical simulation, the first two sub-sections discuss about the effect of polymer substrate thickness on thermal cooling and demolding. The final sub-section further correlates the influence of polymer substrate thickness to demolding on molds with the varying aspect ratio micro-channels.

3.1 Effect of substrate thickness on thermal cooling

During thermal cooling process, both mold and polymer substrate are cooled down from embossing temperature of 100^{o}C to demolding temperature of 25^{o}C. Due to the much higher coefficient of thermal contraction in polymer when compared to mold (about 4 times higher), the mold will act as a barrier to prevent polymer substrate from further thermally contracting. Thus, thermal stress will be generated.

Fig.2 shows the contour plot of Von Mises stress that represents thermal stress after cooling to room temperature for the first three channels that are located closest to node D where demolding load is applied. It can be observed that the thermal stress is only higher at the right side of the channels. This is because polymer is thermally contracting towards its own shrinkage center that is located on the left region from those first three channels.

Another important observation is that thermal stress is higher at the first rightmost channel when compared to the second and third channels, and the thermal stress at second channel is higher than that at third channel (fig.2). This obtained trend can occur because the amount of thermal stress is dependent on the relative distance between the respective channel and shrinkage center. When the relative distance is longer, thermal stress will also be greater. Similarly, the amount of plastic deformation formed due to thermal cooling process is found to have identical trend with thermal stress (fig.3). In addition, it should also be noted that the trend in thermal stress and plastic strain based on the observations mentioned above remains the same for all of the different tested molds and polymer substrates.

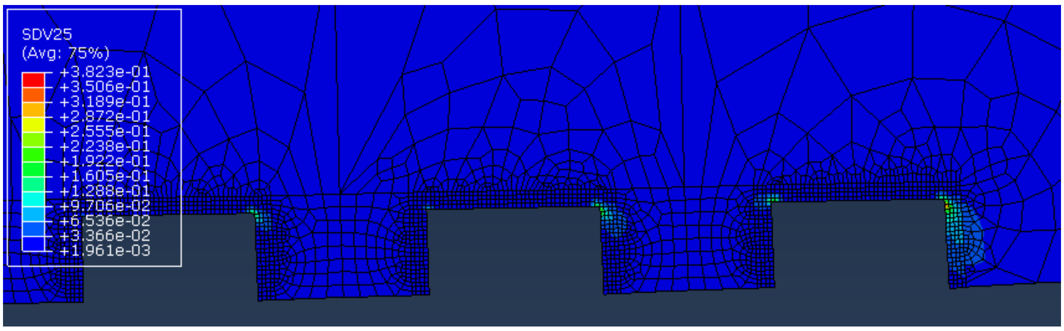


(a)

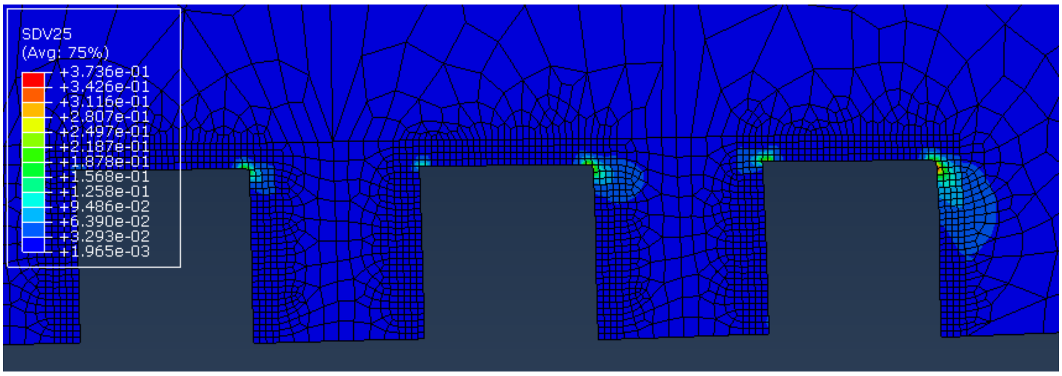
(b)

(c)

Fig.2 Contour plot of Von Mises stress (MPa) showing the first three channels closest to node D after cooling to room temperature: (a) 50 µm channel depth and 1 mm substrate thickness, (b) 100 µm channel depth and 2 mm substrate thickness, and (c) 150 µm channel depth and 1.5 mm substrate thickness



(a)



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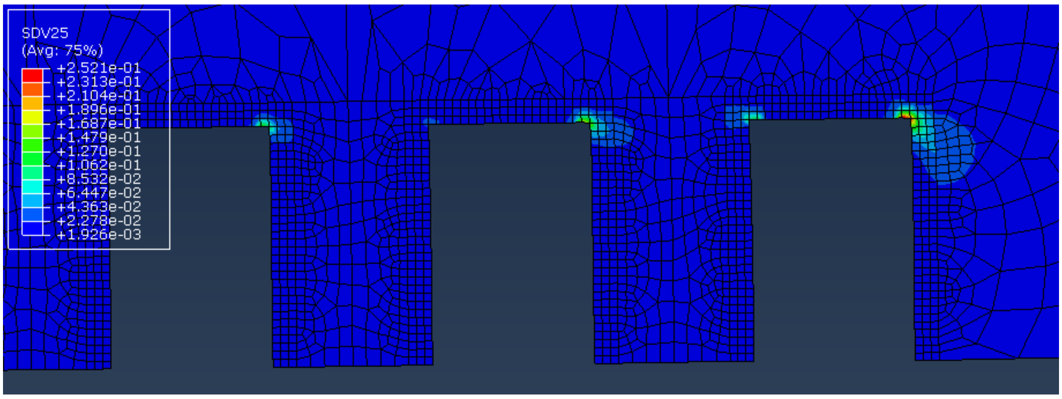


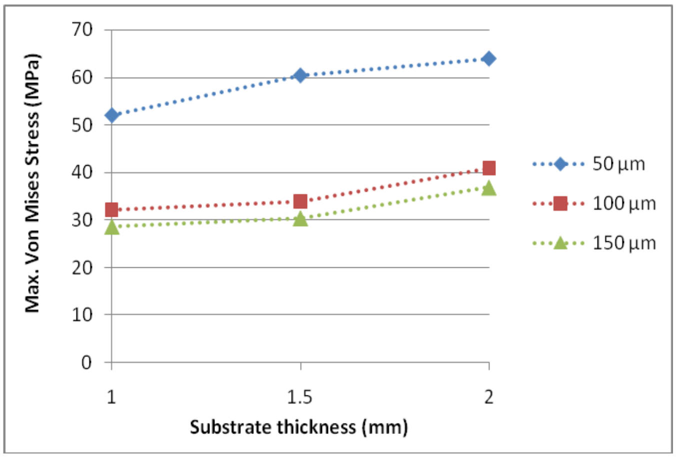
(c)

Fig.3 Contour plot of equivalent plastic strain showing the first three channels closest to node D after cooling to room temperature: (a) 50 μm channel depth and 1 mm substrate thickness, (b) 100 μm channel depth and 2 mm substrate thickness, and (c) 150 μm channel depth and 1.5 mm substrate thickness

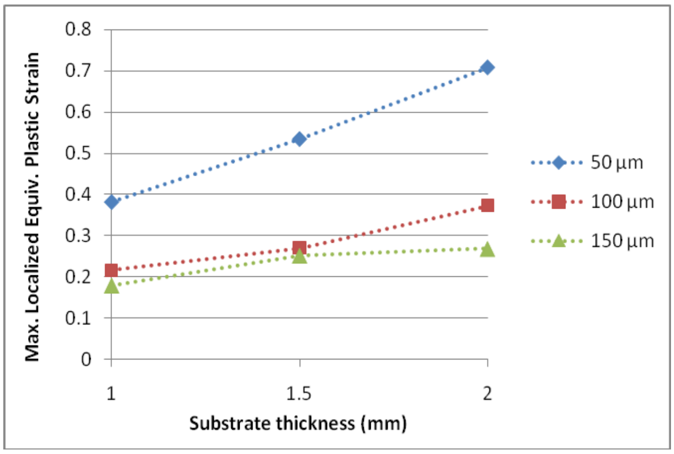
Based on the plot in fig.4a, it is found that the maximum thermal stress generated in the polymer substrate increases with the use of thicker substrate. Similarly, the maximum localized equivalent plastic strain found in the polymer substrate after thermal cooling process increases with thicker substrate as well (fig.4b). In other words, there is a general trend such that both the thermal stress and plastic strain are enhanced with the use of thicker polymer substrate.

The reasoning behind the observed increasing trend is that with thicker substrate, there is more material on the layer where the polymeric channels are standing on. Due to the existence of more material, there is more constraint in terms of thermal shrinkage provided by the layer to the replicated channels during cooling process. Hence, thermal shrinkage is more prominent with thicker substrate.

On the other hand, it can also be observed that the overall thermal stress and plastic strain are higher with shallower channels. Similar to the reasoning mentioned above, with an identical substrate thickness, there is more material on the layer above the replicated channels with shallower channels when compared to deeper channels. In this way, it can be concluded that in terms of thermal cooling process, thinner substrate is preferable to prevent huge thermal stress and severe plastic deformation from occurring.



(a)



(b)

Fig.4 Plot of: (a) Maximum thermal stress, and (b) Maximum localized equivalent plastic strain after cooling to room temperature for the three different molds

3.2 Effect of substrate thickness on demolding

The next crucial step in the whole replication process after thermal cooling to a desired temperature is to separate the replicated polymer from the mold. It is found that there is a certain trend in demolding energy when the polymer substrate thickness changes. Demolding energy is an important parameter because it can be used to determine how difficult the demolding process is. In other words, higher demolding energy means that the demolding is more difficult to accomplish.

The calculated demolding energy per unit mm width for all of the tested molds and substrate thicknesses is as shown in fig.5. For mold with 50 µm deep channel, demolding energy is found to decrease with the use of thinner substrate, whereas for mold with 150 µm deep channel, demolding energy increases drastically with the use of thinner substrate. On the other hand, there exists a minimum demolding energy when 1.5 mm thick substrate is demolded from mold with 100 µm deep channel. However, demolding at 1 mm thick substrate is more difficult to be accomplished when compared to 2 mm thick substrate.

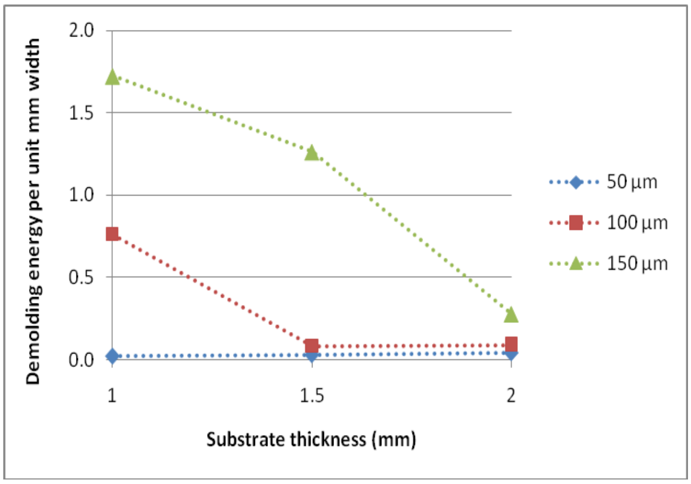
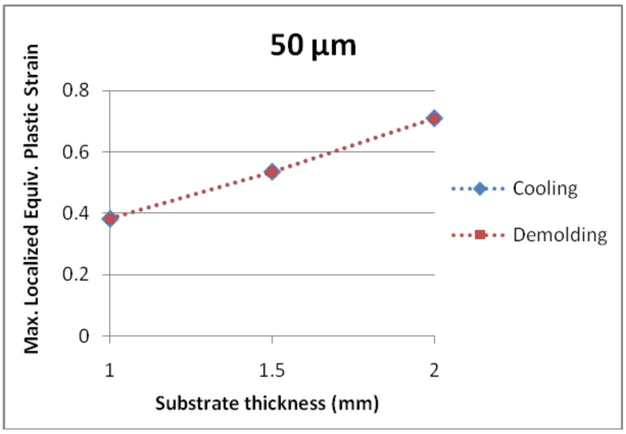


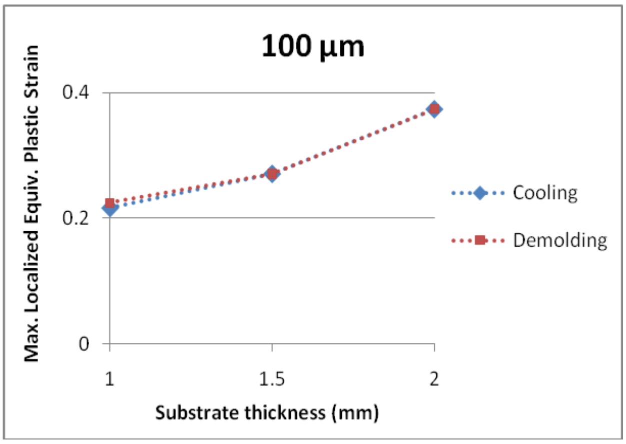
Fig.5 Plot of demolding energy per unit mm width for the three different molds

Considering the possible demolding defect in terms of plastic strain, it is found that there is no plastic deformation caused by demolding for all the three different substrate thicknesses at demolding of mold with 50 µm deep channel (fig.6a). This further means that the polymer substrate is only plastically deformed through thermal stress. Nevertheless, during demolding of mold with 100 µm deep channel and 1 mm thick substrate, there is a slight increase in plastic strain (fig.6b).

When demolding is performed at 1 mm thick substrate from mold with 150 µm deep channel, the amount of plastic strain increases quite significantly by more than double (fig.6c). Increment in thickness by 0.5 mm does help although there is still small increment in plastic strain due to demolding. In this case, demolding can only be successfully performed when 2 mm thick substrate is used.

(a)


(b)



(c)

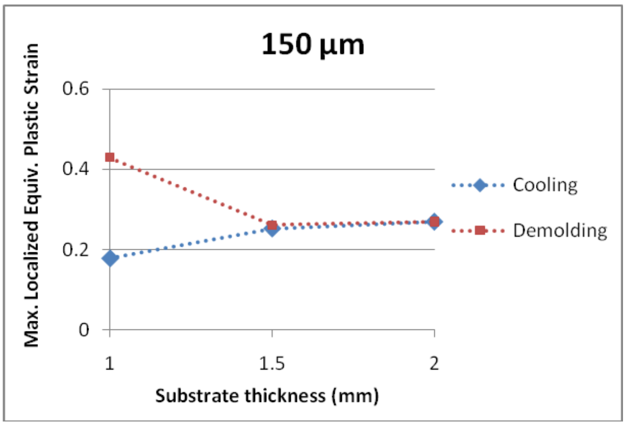


Fig.6 Plot of maximum localized equivalent plastic strain after cooling and demolding corresponding to channel depth of: (a) 50 µm, (b) 100 µm, and (c) 150 µm

In general, plastic strain formed due to demolding can be very prone to occur when polymer substrate bends too severely during demolding. This happens because with more severe bending, demolding stress generated in the polymer increases as well. As illustrated in fig.7, the success in demolding of mold with 150 µm deep channel is due to the non-severe bending experienced by the 2 mm thick polymer substrate during demolding. In contrast to the successful demolding, it can be easily observed that there is very severe bending on the 1 mm thick polymer substrate during demolding (fig.8). This further causes huge demolding stress and significant increase in plastic strain. Based on the obtained results, it can be finally concluded that polymer substrate thickness can indeed affect the bending behaviour experienced on the polymer during demolding, and most importantly, the bending behaviour can eventually affect the final demolding outcome.

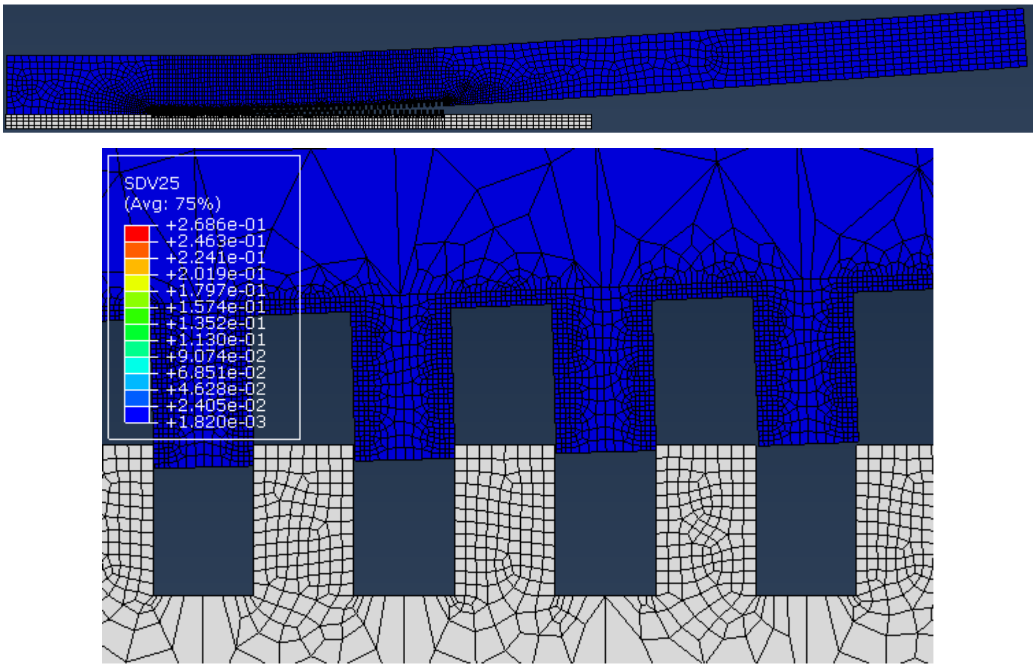


Fig.7 Contour plot of maximum localized equivalent plastic strain (150 μm deep channel & 2 mm thick substrate) showing the overall bent shape during demolding

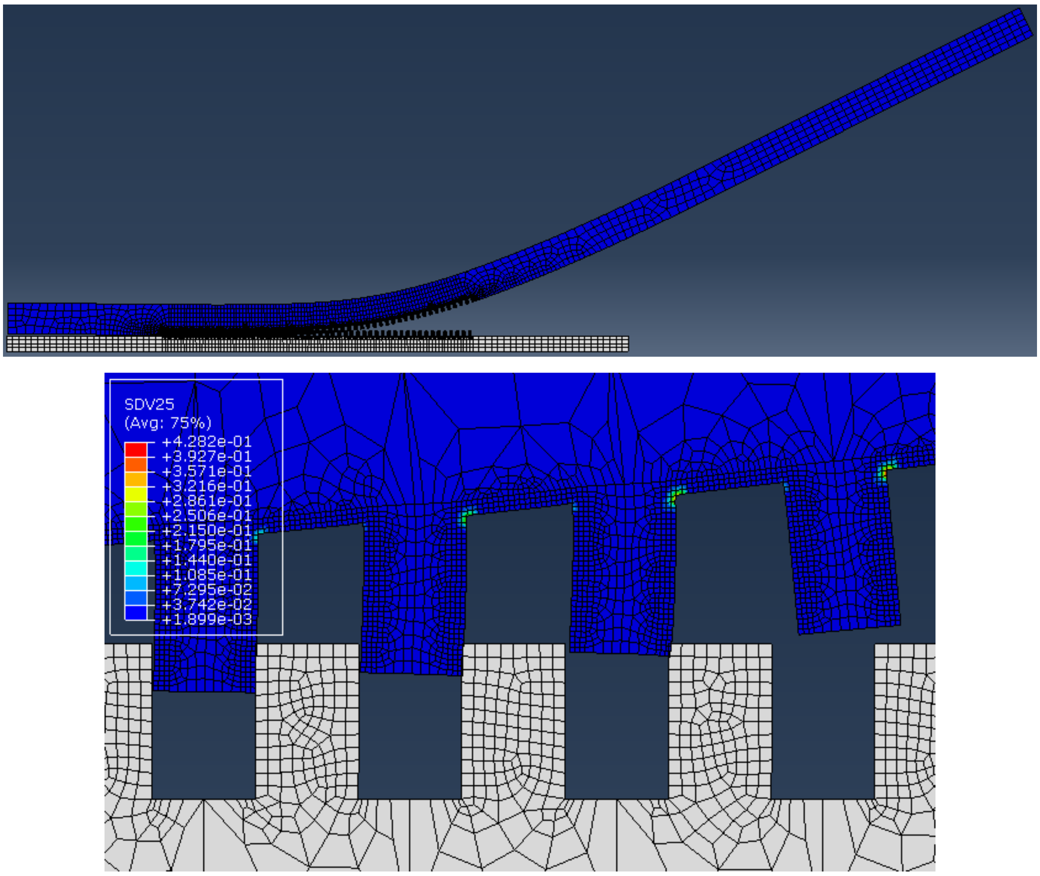


Fig.8 Contour plot of maximum localized equivalent plastic strain (150 μm deep channel & 1 mm thick substrate) showing the overall bent shape during demolding

3.3 Correlation in the effect of substrate thickness to demolding of molds with varying aspect ratio

There are three different molds used in this study that differ in channel depth. Channel depth of 50, 100, and 150 μm correspond to aspect ratio (AR) of 0.5, 1, and 1.5, respectively. Based on the findings reported by researchers, higher aspect ratio micro-channels are known to cause more difficulty in demolding. As difficulty in demolding increases, polymer substrate is expected to bend more severely during demolding. Therefore, it may be useful to investigate on the correlation between the influence of substrate thickness and demolding of molds with varying aspect ratio that ranges from low to high.

In summary to the obtained demolding results, an opposite trend in demolding energy is observed for AR of 0.5 and 1.5, while there exists a minimum demolding energy for AR of 1. It is also found that the polymer undergoes more plastic deformation during demolding of mold with AR 1 at 1 mm thick substrate, and AR 1.5 at both 1 and 1.5 mm thick substrate. Conversely, the other combinations of AR and substrate thickness are successful without any increase in plastic strain.

In the case of mold with AR of 0.5, demolding does not create any additional plastic deformation at all of the three tested thicknesses. This is due to the relatively low AR such that demolding is still relatively easy to accomplish without involving severe bending on the substrate. However, thinner substrate is found to require less demolding energy. In contrast to this, mold with a quite high AR of 1.5 causes significant difficulty in demolding. Therefore, with thinner substrate, bending stiffness decreases and the polymer substrate eventually tends to undergo much more severe bending which results in heavy plastic deformation. Nevertheless, 2 mm thick substrate is found to be suitable to achieve successful demolding of the high AR micro-channels mold.

On the other hand, there is a unique trend in demolding of mold with AR of 1. Medium thickness (1.5 mm thick substrate) eases demolding when compared to 2 mm thick substrate. However, thin substrate (1 mm) does not possess an adequate bending stiffness such that severe bending can occur. Hence, demolding stress increases quite significantly. On the whole, it can be concluded that mold with higher AR micro-channels tends to be more sensitive to substrate thickness in that bending stiffness should be adequate in order to prevent severe bending from happening, whereas mold with lower AR micro-channels has more flexibility in opting for optimum substrate thickness which results in minimum demolding energy. Based on the tested varieties in mold geometry and substrate thickness, as well as the defined testing conditions, it can be eventually concluded that it is best to use 1 mm, 1.5 mm, and 2 mm thick substrate for the replication of polymeric micro-channels with molds that have AR of 0.5, 1, and 1.5, respectively.

4. CONCLUSION

This paper has focused on the modeling of debonding process of hot-embossed polymeric microfluidic substrate and the investigation on the influence of polymer substrate thickness on demolding behavior. Three different substrate thicknesses and molds with low to high aspect ratio micro-channels have been used in the study. We have also implemented the constitutive model of the polymeric material and interfacial friction interaction in the numerical model. It is initially found that based on thermal cooling process, thinner substrate is always preferable. However, the preference in substrate thickness seems to be more dependent on the demolding outcome. In summary, this study has shown that there exists an optimum polymer substrate thickness whereby efficient and successful demolding can be obtained. Moreover, the polymer substrate thickness not only affects the overall size of the device and the amount of raw material used, but most importantly, it facilitates successful fabrication of the microfluidic device.

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