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Mold Filling Analysis of an Alignment Structure in Micro Hot Embossing

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Abstract: Hot embossing is one of the most popular fabrication methods to replicate polymer microdevices in the field of micro-fluidics and micro-optics. Numerical models for hot embossing were constructed to analyze the advance of flow front of the molten polymer using commercial software, DEFORM-2D. A hemisphere tipped post, used as an alignment structure in the assembly of micro devices, was modeled to demonstrate the flow behavior of the molten polymer in mold filling. Hot embossing experiments were performed to validate the feasibility of the numerical models. Most of the simulations showed agreement with experiments. The mold filling was estimated with the heights of the embossed posts in the analysis. No significant mold filling with the molten polymer was observed below the glass transition temperature of 105 °C. The mold cavity was completely filled with the polymer at the molding temperature of 137.5 °C and 150 °C while the embossing forces were 300, 600, and 900 N.

Keywords: Micro hot embossing, Mold filling, Flow stress, Molding temperature, Embossing force

Introduction

Analysis of the flow behavior of molten polymer has been widely used in the fabrication of micro-devices using hot embossing [1-5]. Numerical analysis can be utilized to understand the flow behavior of the molten polymer in the filling of the mold cavity [2-4]. The effect of individual process parameter on the mold filling [5-7] can be analyzed through parametric study. The appropriate process parameters can be selected to ensure a complete filling of the mold cavity. This can significantly increase the productivity of hot embossing while high quality of the replication can be achieved.

Hot embossing is a popular fabrication method to replicate designed patterns from a mold insert into a polymer substrate in micro-fluidics and micro-optics [8,9]. It has advantages of: low cost of operation, simplicity of the process, and easy mold exchange over injection molding [1,9]. There are three principal steps in the hot embossing process: molding, cooling, and demolding [1,8-11]. A polymer substrate is heated to a molding temperature. The molten polymer flows into the mold cavity as the embossing force is applied to the substrate during molding. The embossed pattern on the substrate is cooled down to obtain the rigidity of a replicated device after molding filling. When the demolding temperature is reached, the embossed part is separated from the mold insert.

The flow front of the molten polymer advances to fill a mold cavity during molding. A complete mold filling is a critical aspect to achieve high replication fidelity of a molded part [1-7,12]. Some analyses have been performed to analyze the flow behavior of the molten polymer in hot embossing.

Juang *et al*. [1,2] showed a stress/strain relationship of polymethyl methacrylate (PMMA). It was incorporated into the simulations of both isothermal and non-isothermal embossing processes. Mold fillings of the molten polymer were demonstrated with slip and no-slip boundary conditions at the interfacial layer between the polymer substrate and mold. The results of simulation showed uniform or non-uniform flow of the molten polymer into the mold cavity, depending on the depths of the mold cavities.

The flow of the molten polymer was correlated with the effect of heat transfer between a mold cavity and the polymer [3]. The ratio of the heat transfer dominated the flow patterns of the molten polymer, including uniform or non-uniform flow, in mold filling while the depths of the mold cavities varied from 200 μm to 1 μm.

The flow velocity of the polymer was demonstrated to understand the effect of mold structures on the mold filling [4]. A concave and convex mold was used to fabricate micro lens array. The flow stress obtained by Juang [1,2] was coupled with the numerical models in the analysis.

The strain of PMMA was considered to study the influence of embossing time on the viscoelastic behavior of the molten polymer [13]. The first order exponential decay of the strain was a more accurate model when compared to a polynomial fitting curve. The model was used to predict the recovery of the polymers [14] after demolding.

The mechanical behavior of PMMA was analyzed using a tensile test. Stress-strain curves of PMMA were characterized below and above the glass transition temperatures [15]. PMMA was hardened with large strains as the temperature increased. The characterized mechanical property was used to analyze the flow behavior of the molten polymer [2,3,5].

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The flow behavior of the molten polymer was studied to analyze the mold filling of hot embossing process. Numerical models were constructed using a finite element method (FEM). Commercial finite element software, DEFORM-2D (Scientific Forming Technologies Corp., Columbus, OH), was used to develop the finite element models. An alignment structure, used in previous studies for micro-assembly, a hemisphere-tipped post [5,8] was selected for the numerical and experimental demonstration. The models were used to predict the effect of a molding temperature and an embossing force on the mold filling. The heights of the embossed posts were characterized to assess the mold filling while the molding temperature and the embossing force varied. The results of the numerical analysis were correlated with the experimental results to validate the feasibility of the numerical models. The developed models can be used to select proper process parameters of micro hot embossing. This may lead to the reliable replication of micro-structures.

Analysis

DEFORM-2D was used to study the mold filling of hot embossing process. The flow of molten polymer was assumed as a Non-Newtonian viscous flow [3,7] in the analysis while the polymer substrate underwent a viscoplastic deformation enabling it to flow into the mold cavity. Flow stress of the polymer was defined as the functions of stress and strain under constant strain rates. It was obtained from the previous studies [1-3,15]. The flow behavior of the molten polymer was expressed by the flow stress-molding temperature relationship as shown in equation (1) [1-3]. Equation (1) defines the flow behavior of the polymer while the molding temperatures and embossing forces:

$$\sigma = cT + \varepsilon^{k} \qquad (1)$$

where σ is the flow stress, T is the molding temperature, ε is the strain rate and c and k are coefficients for the molding temperatures.

A schematic of the hot embossing and the finite element model for mold filling analysis is shown in Figure 1. Figure 1(a) shows a typical hot embossing process. A polymer substrate, Polymethyl Methacrylate (PMMA), was placed on the substrate plate. The mold cavity, a hemisphere-tipped hole, was located at the center of the mold insert. It had a depth of 925 μm and a radius of 500 μm. The polymer substrate on the plate moves upward to the mold insert to give a molding pressure on it as indicated by arrow.

The hot embossing process was modeled as an isothermal and axisymmetric model to analyze the flow behavior of the molten polymer as shown in Figure 1(b). It was assumed that the molten polymer flows identically in any cross-sectional area on the X- and Y- planes. A non-slip condition was applied on the bottom surface of the polymer substrate. The mold insert, the plate, and the platen were considered as rigid bodies. The model had 7,570 brick elements for the polymer substrate. The length of element of the polymer gradually decreased from 250 μm to 25 μm as the polymer substrate reached the boundary of the hemisphere-tipped hole. Molding temperatures were 87.5, 100, 112.5, 125.0, 137.5, and 150 °C with embossing force were 300, 600, and 900 N in the analysis. Friction, surface tension, air trap, and heat transfer were not taken into account in the analysis.

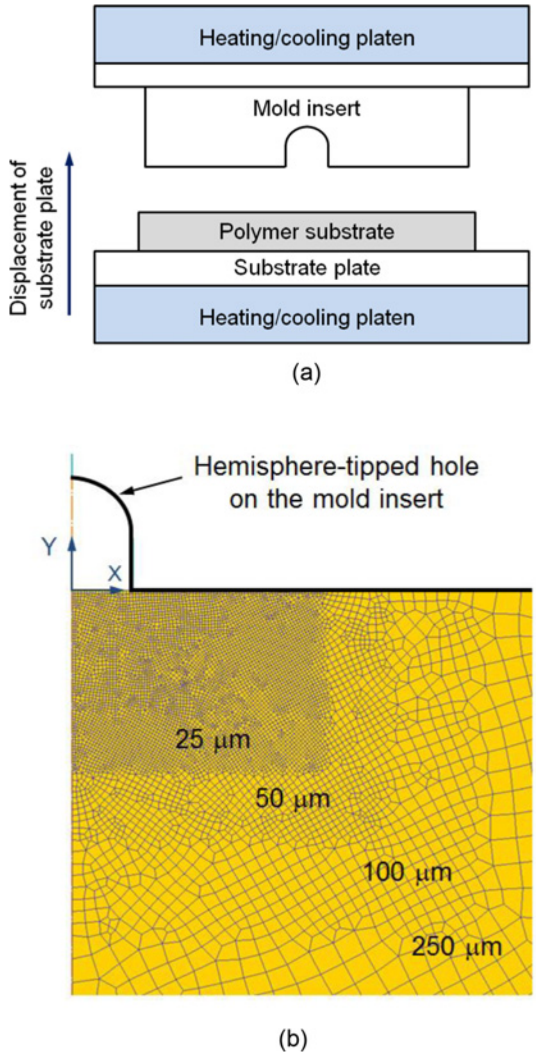

Figure 1. Schematic of hot embossing process and the finite element model for mold filling analysis; (a) schematic of the hot embossing process and (b) finite element model for the mold filling analysis.

Experimental

A brass mold insert was machined to fabricate the hemisphere-tipped hole. The tool paths were generated by computer numerical control (CNC) software, Mastercam (CNC software Inc., Tolland, CT, USA). The mold insert was machined using a CNC milling machine (Discovery 308, Hardinge Inc., Elmira, NY, USA).

A Carver thermal press (AutoFour/15-NE, Wabash, IN, USA) with heating and cooling platens and a hydraulic cylinder was used as shown in Figure 2. The mold insert was mounted at the center of the upper platen. The polymer substrate was placed on the lower platen during molding. A dial indicator with a flexible magnetic base (2YNK2, Westward, Edmonton, Canada) was used to measure the upward movement of the lower platen.

PMMA sheets (Plexiglass®, Sabic Plastics, Shanghai, China) were selected as the substrate material. The thickness of PMMA was 4.5±0.5 mm. The glass transition temperature of PMMA is about 105 °C. Prior to embossing, the polymer substrates were dried at 80 °C in a convection oven (31-350ER-1, Quincy Lab, Chicago, IL, USA) for four hours. The dried substrates were sprayed with nitrogen to remove any particulate material on the surface of the polymer substrate. A mold release agent (Mold Wiz, F-57NC, Axel Plastics research Laboratory Inc., Woodside, NY, USA) was applied to the brass mold insert and bottom platen to assist demolding of the PMMA sheet.

Embossing parameters applied in the experiments are shown in Table 1. Molding temperatures were 87.5±5, 112.5±5, and 137.5±5 °C, embossing force were 300, 600, and 900 N, holding time was 300 seconds, and demolding temperature was 92.0±5 °C.

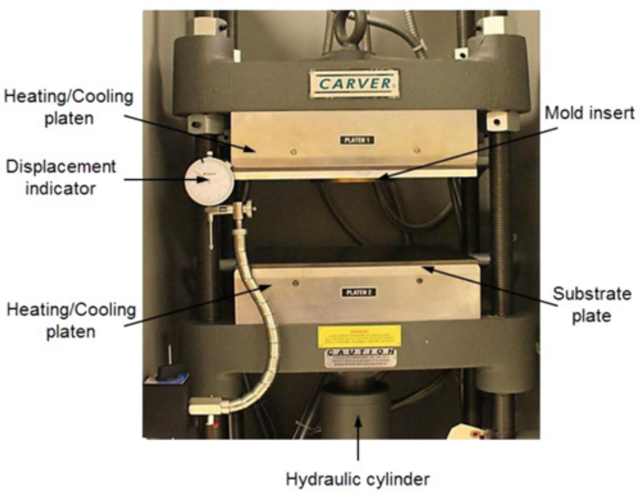

Figure 2. Carver Thermal Press 3893 4NE18 hot embossing machine.

Table 1. Molding and demolding parameters for hot embossing

Molding temperatures (°C)	87.5±5, 112.5±5, and 137.5±5
Embossing forces (N)	300, 600, and 900
Holding time (s)	300
Demolding temperature (°C)	92±5

To estimate the mold filling with the polymer, the heights of the hemisphere-tipped posts on the molded part were measured using a Measurescope (MM-800, Nikon, Kawasaki, Japan) and a focus/defocus method. Scanning Electron Microscopy (SEM) (Helios NanoLab 400, FEI, Hillsboro, OR) was used to take the side views of the molded structures.

Results and Discussion

A numerical analysis was performed to investigate the effect of the molding temperature and embossing force on the flow behavior of the polymer during mold filling. Simulation results were represented by the distribution of effective stress as shown in Figures 3 and 4. Different colors represent the effective stress of the polymer with advance of the flow front of the molten polymer.

Figure 3 shows the mold filling analysis as a function of mold displacement at a molding temperature of 112.5 °C with an embossing of 600 N. The mold displacements were 0.1, 1.0, 1.5 and 1.88 mm. High stress concentration on the molten polymer was observed at the vicinity of the edge of the mold cavity due to the geometric characteristics of the edge.

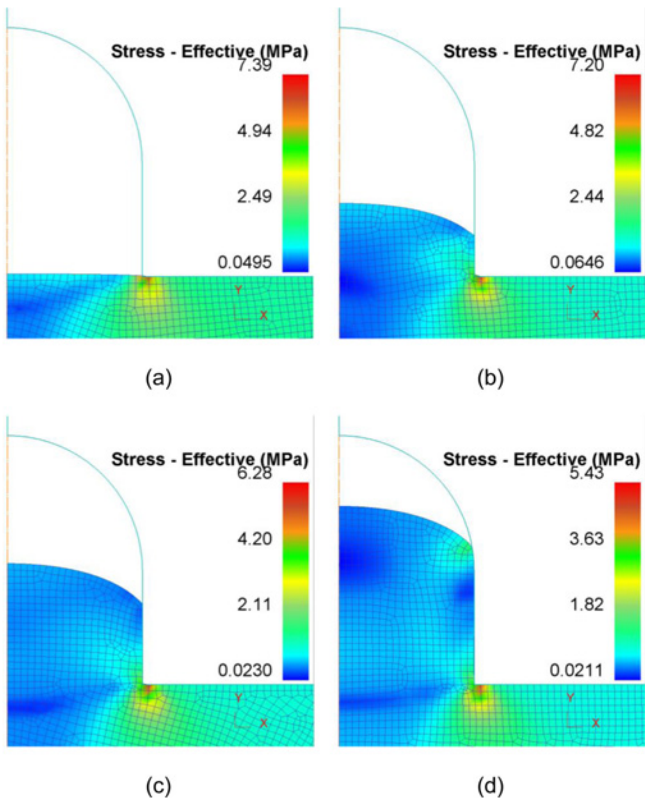

Figure 3. Flow stress of the molten polymer at a molding temperature of 112.5 °C with an embossing force of 600 N; (a) mold displacement of 0.1 mm, (b) mold displacement of 1.0 mm, (c) mold displacement of 1.5 mm, and (d) mold displacement of 1.88 mm.

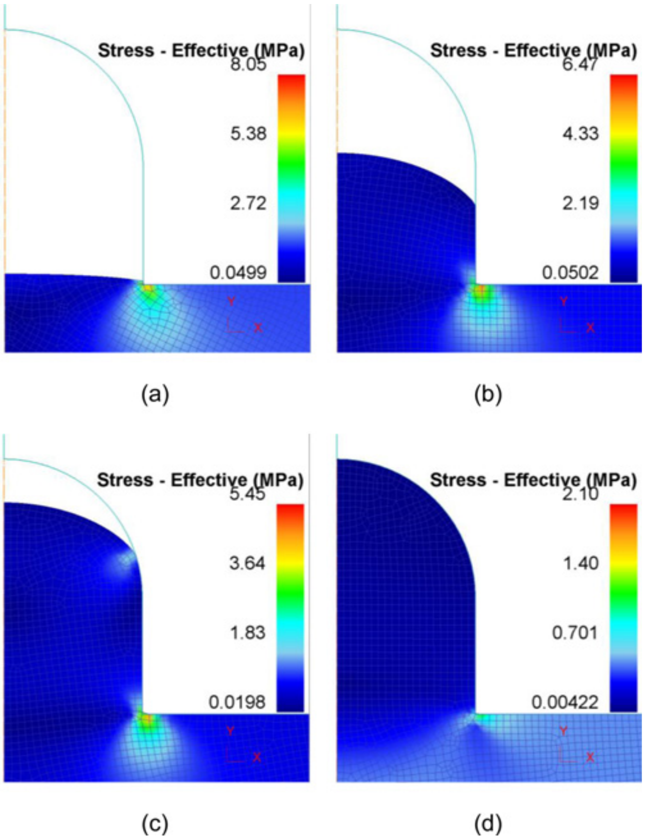

Figure 4. Flow stress of the molten polymer at a molding temperature of 137.5 °C with an embossing force of 600 N; (a) mold displacement of 0.1 mm, (b) mold displacement of 1.0 mm, (c) mold displacement of 1.5 mm, and (d) mold displacement of 2.37 mm.

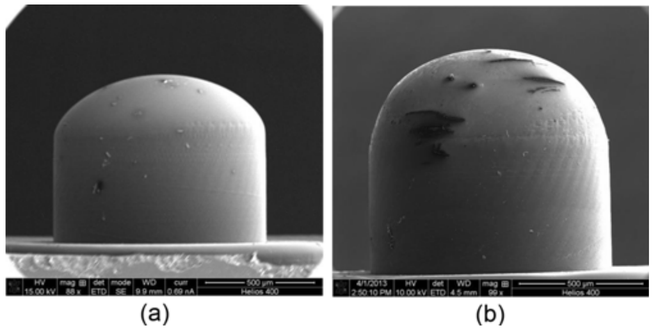

Figure 5. SEM images of the typical embossed posts; (a) molding temperature of 112.5 °C with an embossing force of 600 N and (b) molding temperature of 137.5 °C with an embossing force of 600 N.

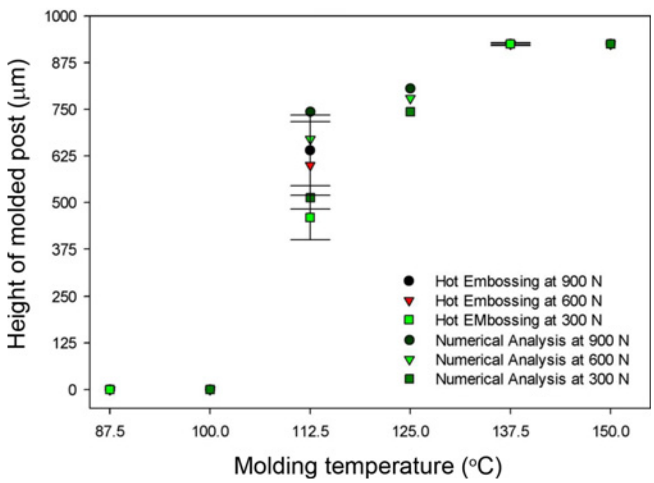

Figure 6. Estimated and measured heights of the molded posts at molding temperatures of 87.5, 100, 112.5, 125, 137.5, and 150 °C while the embossing forces were 300, 600, and 900 N.

Flow stress was significantly higher at the vicinity of the edge than the stress at the flow front as shown in Figure 3(a). The highest flow stress was 6.34 MPa at the vicinity of the edge. The flow stress was 0.892 MPa at the center of the flow front of the molten polymer. Figure 3(b) shows the mold filling at a mold displacement of 1.0 mm. The molten polymer flowed into the cavity while the mold squeezed the polymer substrate. The movement of the mold pushed the polymer into the cavity. As the mold displacement increased to 1.5 mm, the polymer filled the mold cavity further as shown in Figure 3(c). When the front flow of the molten polymer reached the boundary of the hemisphere backpressure was developed. Backpressure resulted from the reduced cavity width which increased the fluidic resistance of the molten polymer. Figure 3(d) illustrates the furthest of the molten polymer advanced into the cavity. The height of the mold filling was 0.68 mm.

Figure 4 shows the flow stress of the molten polymer at a molding temperature of 137.5 °C with an embossing force of 600 N. The advance of the flow front was represented with a mold displacement of 0.1, 1.0, 1.5, and 2.37 mm. The molding temperature of 137.5 °C yielded a complete filling of the mold cavity. The flow front of the polymer could reach further into the mold cavity when compared to the molding filling at molding temperature of 112.5 °C. When the molding temperature was increased from 112.5 °C to 137.5 °C the polymer was softened enough to completely fill the mold.

Figure 5 shows SEM images of typical embossed structures. An incomplete cavity filling was observed at a molding temperature of 112.5 °C with an embossing force of 600 N as shown in Figure 5(a). The measured height of the molded post was 690 μm. Figure 5(b) shows the embossed post at a molding temperature of 137.5 °C with an embossing force of 600 N. The estimated height of the molded post was 930 μm. The SEM images showed agreement with the simulations as shown in Figures 4 and 5.

The estimated heights of the embossed structures were shown in Figure 6 while the measured heights of the embossed structures were represented by the mean with error bars indicating the 95 % confidence interval.

No significant mold filling was observed at the molding temperatures of 87.5 °C and 100.0 °C since the polymer was not softened enough to fill the cavity below the glass transition temperature of 105 °C. The height of the embossed structure was significantly increased as the molding temperature went above 100.0 °C. This can be explained by, the increased molding temperature decreased the fluidic resistance of the molten polymer.

The complete mold filling was achieved at the molding temperatures of 137.5 °C and 150.0 °C with embossing forces of 300, 600, and 900 N. The results of simulation and experiments showed that increasing the embossing force and molding temperature promoted the advance of the flow front of the molten polymer into the mold cavity. The increase of embossing force did not improve the mold filing as much as the increase of the molding temperature did.

Conclusion

Mold filling was investigated for the realization of high replication fidelity in micro hot embossing. A numerical analysis was performed to study the advance of the flow front of the molten polymer in the mold filling. Finite element models, using DEFORM 2D, predicted the effect of molding temperatures and embossing forces on the mold filling. Hot embossing experiments were conducted to validate the numerical models. The mold filling was assessed by the heights of the embossed posts in the simulation and experiments. No significant mold filling with the molten polymer was observed below the glass transition temperature of 105 °C. A complete cavity filling was achieved at embossing forces of 300, 600, and 900 N with a molding temperature of 137.5 °C and 150 °C. The molding temperature significantly affected the advance of the flow front of the molten polymer during molding. It showed that the proper process parameters can be selected by analyzing the flow behavior of the molten polymer during mold filling. The developed models were applicable to the design of a micro hot embossing process.

Acknowledgements

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