PHYSICAL MODELLING OF AMORPHOUS THERMOPLASTIC POLYMER AND NUMERICAL SIMULATION OF MICRO HOT EMBOSSING PROCESS

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Abstract. Micro hot embossing process is considered as one of the most promising micro replication processes for manufacturing of polymeric components, especially for the high aspect ratio components and large surface structural components. A large number of hot embossing experimental results have been published, the material modelling and processes simulation to improve the quality of micro replication by hot embossing process are still lacking. This paper consists to 3D modelling of micro hot embossing process with amorphous thermoplastic polymers, including the mechanical characterisation of polymers properties, identification of the viscoelastic behaviour law of the polymers, numerical simulation and experimental investigation of micro hot embossing process. Static compression creep tests have been carried out to investigate the selected polymers' viscoelastic properties. The Generalized Maxwell model has been proposed to describe the relaxation modulus of the polymers and good agreement has been observed. The numerical simulation of the hot embossing process in 3D has been achieved by taking into account the viscoelastic behaviour of the polymers. The microfluidic devices with the thickness of 2 mm have been elaborated by hot embossing process. The hot embossing process has been carried out using horizontal injection/compression moulding equipment, especially developed for this study. A complete compression mould tool, equipped with the heating system, the cooling system, the ejection system and the vacuum system, has been designed and elaborated in our research. Polymer-based microfluidic devices have been successfully replicated by the hot embossing process using the compression system developed. Proper agreement between the numerical simulation and the experimental elaboration has been observed. It shows strong possibility for the development of the 3D numerical model to optimize the micro hot embossing process in the future.

1   INTRODUCTION

Micro hot embossing process is considered as one of the most promising micro replication processes for manufacturing of polymeric components [1]. It is used to elaborate the micro or nano components in diverse fields, thanks to its relatively lower cost for embossing tool, flexibility choice of embossing material and high replication accuracy for small features. In micro hot embossing process, the embossed material is always heated to a certain temperature, which allows the material flow into the cavities of mould insert. For amorphous thermoplastic polymers, the processing temperature is lightly above their glass transition temperature (Tg), which the massive changes in physical properties of polymer occur during this temperature range. More and more micro-components have been fabricated with thermoplastic polymers by micro hot embossing process during recent years, but the lack of the numerical modelling and simulation restricts the further development of the process [2]. The object of this work is to propose a 3D numerical model to investigate the effects of the hot embossing process parameters, such as embossing temperature, embossing pressure, processing time, on the replication accuracy of polymeric components.

Amorphous thermoplastic polymers have a randomly ordered molecular structure, unlike the highly ordered molecular structure of crystalline of semi-crystalline polymers. The amorphous thermoplastic polymers soften gradually as the temperature arises, allowing to a relatively larger moulding temperature range compared to the crystalline polymers. Various behaviour laws have been proposed in the literature in order to describe the physical behaviour of the amorphous thermoplastic polymers used in the micro hot embossing process [3-9]. The viscoelastic model has been widely applied in the numerical simulation of hot embossing process because of its efficiency in numerical computation and its well-fitting with the experimental characterization [10].

This paper consists to 3D modelling of micro hot embossing process with amorphous thermoplastic polymers, including the mechanical characterisation of polymers properties, identification of the viscoelastic behaviour law of the polymers, numerical simulation and experimental investigation of micro hot embossing process. Static compression creep tests have been carried out to investigate the selected polymers' viscoelastic properties. The Generalized Maxwell model has been proposed to describe the relaxation modulus of the polymers and good agreement has been observed. The numerical simulation of the hot embossing process in 3D has been achieved by taking into account the viscoelastic behaviour of the polymers. Different loads have been applied on the mould die insert and the viscoelastic responses of the polymer substrate have been investigated in the simulation. The microfluidic devices with the thickness of 2 mm have been elaborated by hot embossing process. The comparison between the numerical simulation and the experiments shows proper agreement for the prediction of the polymer substrate deformation using the hot embossing process.

2   MODELLING APPROACH

In the numerical simulation of the hot embossing process, the mould die cavity was considered as a rigid body, and the polymer substrate exhibits the viscoelastic behaviour. The related constitutive equations have been implemented in the software. The stress tensor of the viscoelastic material is separated mathematically in two parts [11], the volumetric stress and

the deviatoric stress, as shown in the following equation:

$$\sigma = K_b \varepsilon_v \mathrm{I} + \sigma_d \qquad (1)$$

where is K_b the bulk modulus, ε_v is the volumetric strain, I is the identity matrix, and σ_d is the deviatoric stress.

The strain tensor of the viscoelastic material is written as:

$$\varepsilon = \frac{1}{3}\varepsilon_v \mathrm{I} + \varepsilon_d \qquad (2)$$

where ε_d is the deviatoric strain, with the volumetric strain given by:

$$\varepsilon_v = trace\left(\varepsilon_{ij}\right) \qquad (3)$$

The general dependence of the deviatoric stress on the strain history could be expressed in the form:

$$\sigma_d = 2\int_0^t G_{(t-t')}\left(\partial \varepsilon_d / \partial t'\right) dt' \qquad (4)$$

where $G_{(t)}$ is the shear modulus, which could be obtained by the well-known relationship with the elastic modulus for homogeneous isotropic materials:

$$G_{(t)} = E^{cr} / \left(2(1+\upsilon)\right) \qquad (5)$$

where υ is Poisson's ratio, and E^{cr} is the relaxation modulus identified in the compression creep tests.

## 3   IDENTIFICATION OF VISCOELALSITC PROPRETIES THERMOPLASTIC POLYMER

The true stress vs. time and true strain vs. time curves of the amorphous polymer PMMA have been obtained from compression creep tests at the hot embossing temperature range from Tg+ 20∘C to Tg+ 40∘C. The relaxation modulus, expressed as the ratio between the true stress and true strain of the polymer specimens during the creep tests, could thereby be obtained. The relaxation moduli of the PMMA are presented in Figure 1. The relaxation modulus of the polymer decreases with respect to time at different testing temperatures in short-term compression creep tests. With the increase of the testing temperature, the relaxation modulus decreases. The relaxation modulus exhibits a sudden decline at the beginning of the compression creep tests and then decreases smoothly with time.

In this study, the Generalized Maxwell model was used to describe the relaxation modulus of the amorphous PMMA specimens with respect to time, as obtained from the compression creep tests. Two relaxation time constants have been characterized to fit the experimental data from the compression creep tests. The compression relaxation modulus E^{cr} of polymer could

be expressed as follows:

$$E^{cr} = E_{\infty}^{cr} + E_1^{cr} \exp\left(\frac{-t}{\tau_1^{cr}}\right) + E_2^{cr} \exp\left(\frac{-t}{\tau_2^{cr}}\right)$$

(6)

where E_{∞}^{cr} is the relaxation modulus when time becomes infinite, t represents time, E_1^{cr} and τ_1^{cr} are the relaxation modulus and relaxation time at 1-branch, respectively, and E_2^{cr} and τ_2^{cr} are the relaxation modulus and relaxation time at 2-branch, respectively.
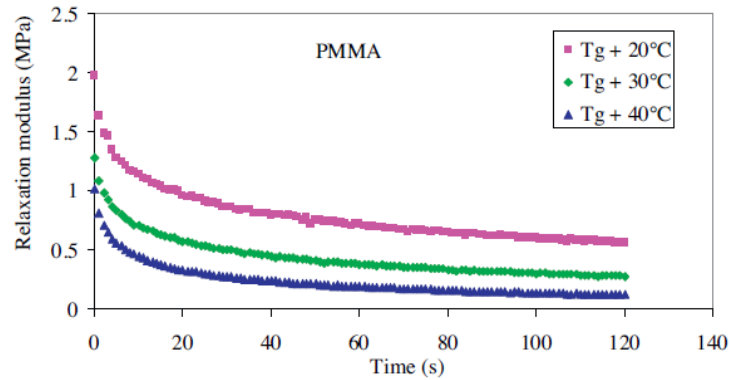
Figure 1: Relaxation modulus of PMMA at Tg+ 20◦C, Tg+ 30◦C and Tg+ 40◦C in short-term compression creep tests.

## 4 NUMERICAL SIMULATION OF HOT EMBOSSING PROCESS

In this study, a 3D model composed by the polymer substrate and the micro mould die cavity insert was created in the simulation. The mould was considered as a rigid body, which was supposed to be undeformable during the simulation. The polymers substrate was considered as viscoelastic material, described by the Generalized Maxwell model using the identification parameters obtained in compression creep tests. The simulation of the hot embossing process was effectuated at Tg+ 20◦C, Tg+ 30◦C and Tg+ 40◦C. The imposed loads were applied on the mould die cavity insert. The bottom surface of the polymer substrate was fixed, and the displacement of this surface was imposed as 0.

4.1 Hot embossing with fixed compression displacement

The polymer substrate was first compressed with a fixed compression displacement of 0.1 mm with a constant compression speed, shown in Figure 2. The compression tests lasted for 30 s at each compression temperature. Figure 2(a) presents the total displacement of the top surface of the polymer substrate. The reservoir and the channel exhibit almost the same displacement, because the displacement imposed on the mould die insert is the same everywhere. A cutting line in the reservoir zone on the top surface of the polymer substrate, which passes through the center of the reservoir, shown in Figure 2(b), has been selected in order to investigate the displacement profile. Figure 3(c) shows the displacement profile of the polymer PMMA substrate at the cutting line at different compression temperature. The initial height of the polymer substrate is approximately 2 mm and it is compressed by the

mould die insert during the simulation test. The displacement of the polymer substrate in the reservoir zone is approximately 0.1 mm, which is equal to the applied compression displacement. There is not significant difference in the displacement of the polymer substrate among the different compression temperatures. However, the displacement ofthe polymer substrate at Tg+ 40∘C is a little more significant than that at Tg+ 20∘C. This demonstrates that with the same applied compression displacement, the polymer substrate exhibits a larger displacement at a higher compression temperature.
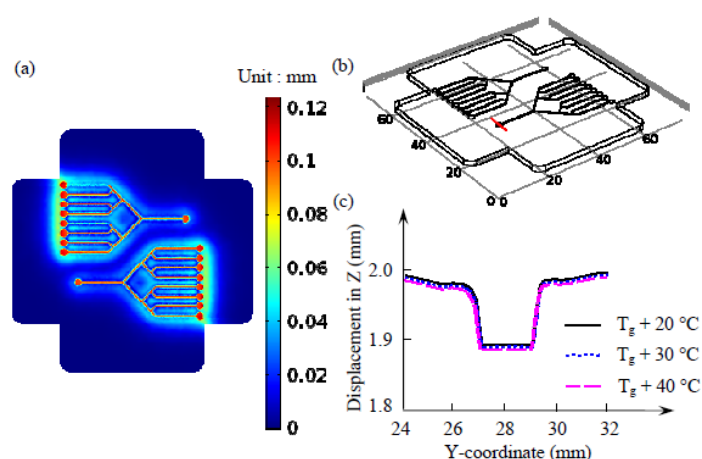
Figure 2: (a) Displacement of the polymer PMMA substrate in the hot embossing simulation with fixed compression displacement 0.1mm at Tg + 20 °C, (b) location of the cutting line on the top surface of the polymer substrate and (c) displacement profile of the cutting line at the end of the testing time at different compression temperature.

## 4.2 Hot embossing with constant pressure

The polymer substrate was then compressed with a constant pressure of 1 MPa for 30 s at each compression constant pressure of 1 MPa at different compression temperatures, shown in Figure 3. The initial height of the polymer substrate is approximately 2 mm, and it is compressed by the mould die insert at constant pressure during the simulation test. In this test, the difference in the displacement of the polymer substrate in the reservoir zone at different compression temperatures is more significant than in the previous simulation test. Figure 3(a) shows the total displacement of the top surface of the polymer PMMA substrate with applied pressure 0.1 MPa at Tg + 40 °C in the hot embossing simulation. A cutting line in the reservoir zone on the top surface of the polymer substrate, which passes through the centre of the reservoir, shown in Figure 3(b), has been selected in order to investigate the displacement profile. Figure 3(c) shows the displacement profile of the polymer PMMA substrate at the cutting line at different applied pressures. The displacement of the polymer substrate increases with the rise of the compression temperature. When the applied pressure on the mould die insert is fixed at 1 MPa, the displacement of the polymer substrate is approximately 0.8 mm at Tg+ 20∘C, and the displacement increases to approximately 1.6 mm at Tg+ 40∘C. This demonstrates that with the same applied pressure, a polymer substrate exhibits a larger displacement at a higher compression temperature.
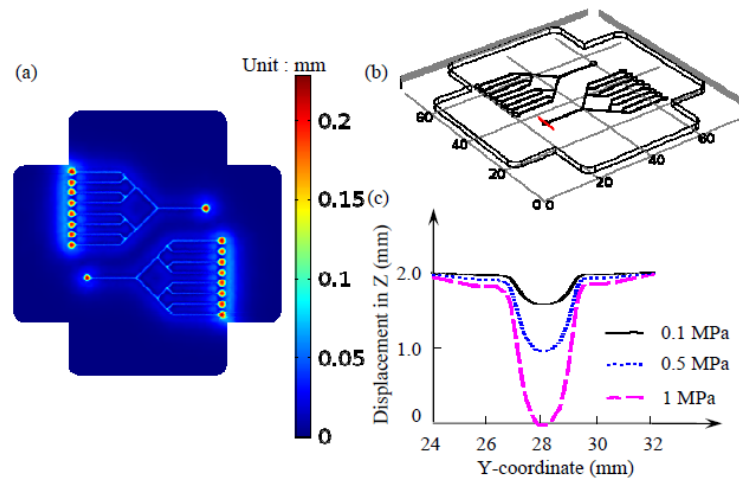
Figure 3: (*a*) Displacement of the polymer PMMA substrate in the hot embossing simulation with constant pressure 1 MPa at Tg + 20 °C, (b) location of the cutting line on the top surface of the polymer substrate and (c) displacement profile of the cutting line at the end of the testing time at different compression temperature.

5   EXPERIMENTAL INVESTIGATION WITH MICROFLUIDIC DEVICE

The replication of microfluidic devices has been effectuated with horizontal electric injection/compression moulding equipment. Mould die inserts with three different cavity dimensions have been developed in this study to obtain microfluidic devices. The height of the micro mould die cavities on the three moulds is approximately 200 μm, 100 μm and 50 μm, respectively.
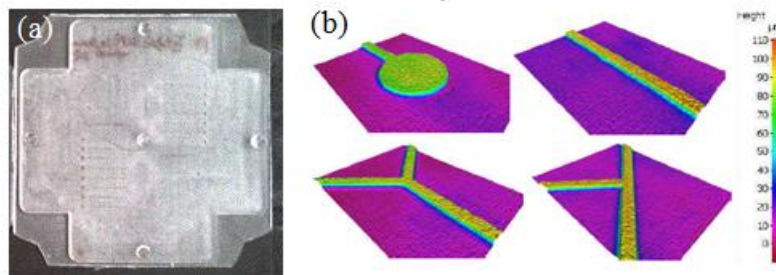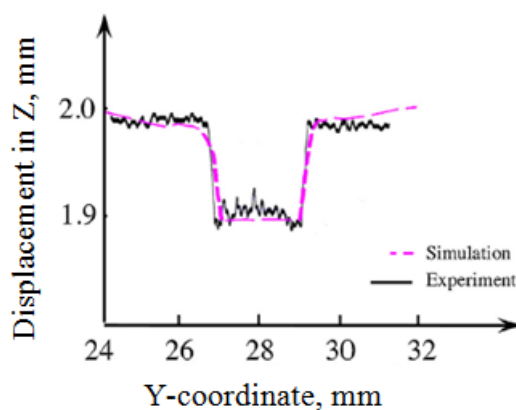

Figure 4: (*a*) PMMA microfluidic devices obtained with the mould die insert (100 μm) by the hot embossing process (b) 3D images of the selected zones of the silicone replicas elaborated from the PMMA microfluidic device.

It shows us that microfluidic devices based on PMMA substrates have been successfully obtained using the three mould die cavities. Figure 4(a) shows the microfluidic device obtained using the mould die cavities with the height of the cavities equal to 100 μm. It seems that the micro cavities in the mould die insert are well filled by the polymer flow. There are no significant replication defects visible on the microfluidic devices. The microfluidic devices produced from thermoplastic polymer substrates are optically transparent, which cause difficulties in measuring their dimensions and surface topography directly with an optical method. Therefore, room temperature vulcanizing (RTV) silicone rubber was used to replicate

the negative micro pattern on the microfluidic devices. Figure 4(b) shows the 3D images of the silicone replicas elaborated from these microfluidic devices. Four zones in the replica were observed to investigate the shape transfer efficiency using the hot embossing process. A proper replication was achieved by effectuating the comparison with the images obtained for micro mould die cavity insert.

A comparison between the numerical results and the experimental results has been made to verify the physical modelling accuracy for the hot embossing process. The identical boundary conditions have been applied for the numerical and experimental tests to make this comparison. PMMA has been compressed at the compression temperature of Tg+ 40◦C for 30 s in the hot embossing process. The displacement imposed on the polymer substrate is fixed at 0.1 mm in the numerical simulation, and the gap imposed is fixed to make sure to compress the polymer substrate by 0.1 mm for the experimental test. One cutting line on the polymer PMMA substrate, located in the reservoir zone, has been drawn to compare the micro cavity geometry after the hot embossing process. The 3D image of the reservoir zone has been obtained by an optical profilometer. The 2D contour of the reservoir has been obtained to enable the comparison of the simulation and numerical results. The 2D contours of the polymer substrate in the same position, both in the numerical and in the experimental results, has been shown in Figure 5. This shows that the diameter of the reservoir is approximately 2000 μm in the numerical simulation, and in the experimental result, the value is approximately 1980 μm. The difference between the simulation result and the experimental result is probably due to the deviation in the selections of the cutting line and the 2D con-tour of the microfluidic device. The simulation results show suitable agreement for the prediction of the polymer substrate deformation in the replication of a microfluidic device using the hot embossing process.

Figure 5: Comparison of the displacement profile on cross section of the reservoir zone of the PMMA microfluidic device obtained by hot embossing process with a fixed compression displacement of 0.1 mm at Tg+ 40◦C.

6   CONCLUSIONS AND PERSPECTIVES

This research work consists on the 3D modelling of the micro hot embossing process using the amorphous thermoplastic polymers. Uniaxial compression creeping tests on cylindrical polymer specimens were carried on in the temperature range from Tg+ 20◦C–Tg+ 40◦C. The relaxation moduli of polymers at Tg+ 20◦C, Tg+ 30◦C and Tg+ 40◦C were obtained with

respect to time. The Generalized Maxwell model with two branches was used to characterize the viscoelastic behaviour of the polymer in the compressing creep tests. Acceptable agreement has been observed by the comparison of experimental data with the fitting models. The Generalized Maxwell model using the parameters identified in the compression creep tests has been used to describe the polymer behaviour in the hot embossing process. The numerical simulation of the filling stage of the hot embossing process has been achieved by taking into account the modelling of the viscoelastic behaviour of amorphous thermoplastic polymers. Polymer-based microfluidic devices have been successfully replicated by the hot embossing process using the compression system developed in our group. Proper agreement between the numerical simulation and the experimental elaboration has been observed. It shows strong possibility for the development of the 3D numerical model to optimise the micro hot embossing process in the future.

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