Numerical simulation of the polymer forming by hot embossing process

G. CHENG, J.C. GELIN, T. BARRIERE

FEMTO-ST Institut, Applied Mechanics Department, 24 Rue de l'épitaphe, 25000 BESANCON

Résumé:

Ce travail concerne la modélisation thermomécanique par éléments finis du procédé d'estampage à chaud des polymères thermoplastiques. Le principe consiste à chauffer une plaque de polymère à une température au-delà de la température de transition, entre deux plateaux rigides indéformables, dont l'un possède des motifs microstructuraux. Différents paramètres matériaux ont été testés lors de la simulation du procédé de compression à chaud afin d'étudier leurs influences au cours de procédé de mise en forme. Les résultats numériques obtenus sont très encourageants.

Abstract:

This work concerns the numerical modelling of the hot embossing process by using finite element method. The process consists to the upsetting of a thermoplastic plate with an adapted temperature and to replicate the microstructures between two rigid die structured moulds. The different material characterisations of polymers have been taken into account in order to determine the main processing parameters. The hot embossing simulation has been realized by FEM. The results obtained are in proper agreement with the experts.

Mots clefs: **Hot embossing process, polymers**

1 Introduction

In the development of micro technologies, the size of the microstructures continuously decreases from micro and sub-micro to nano scales with the fast development of the micro systems and devices. The topographical surface state of the functional components becomes more and more complex and the materials used also become more complex. Well-known conventional technologic such as injection moulding, hot embossing and casting process have been extensively used at the micro-replication scale. Hot embossing is now becoming a promising manufacturing processes, which is well suited for producing dedicated microstructures with high aspect ratios and small distortions [1-2].

However, larger diffusion of the hot embossing process is limited due to the lack of adequate characterisation and process optimization. To face the future requirements, reliable computer models and simulation tools for hot embossing processes are necessary [3]. Due to the high processing temperature in embossing conditions, the visco-elastic properties of the polymer may have an effect on the forming process. In this paper, a reliable constitutive model is applied to describe the material properties of PMMA during the hot embossing process by using COMSOL® Multiphysics© software.

2 Description of hot embossing process

Hot embossing process is a polymer replication process that is investigated in different laboratories [1][4]. This process is especially well suited for manufacturing small and medium batch of micro-components [2]. This process can be divided into four sequential stages (figure 1):

- Heating stage: Heat a polymer plate to glass transition temperature between lower and upper micro structured plates,
- Compression stage: The upper mould move down and embosses the polymer plate with an imposed pressure at the hot embossing temperature,
- Cooling stage: Cool down the polymer plate to the demoulding temperature,
- Demoulding stage: Open the mould to obtain the polymer plate with micro structured cavities.

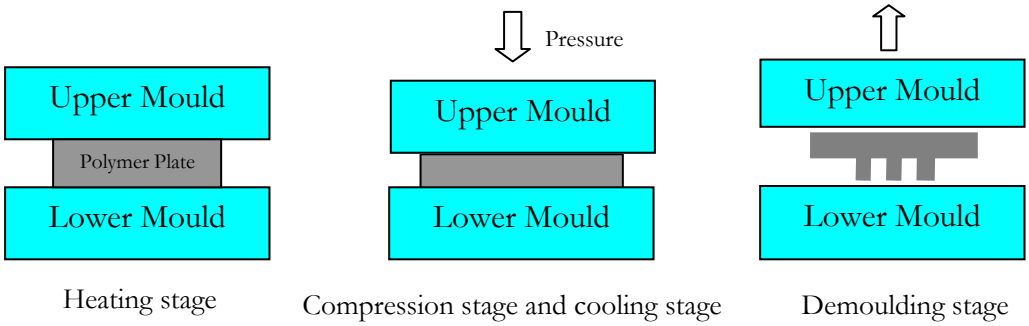


FIG. 1 – The different stages of hot embossing process: heating, compression, cooling and demoulding stage

A polymer plate is inserted between two compression plates. The thickness of the polymer plate depends on the depth of the cavities. The surface of the polymer must cover the structured part of the moulds. The moulds and the polymer plate are heated up to the glass transition temperature in vacuum, which is above the polymer's softening temperature. The upper mould moves down to compress the polymer plate into the micro-structured cavities until the maximum embossing force is reached. During the replication period, the temperature is always kept up to the hot embossing temperature. The variation of the temperature and pressure during the hot embossing process is related in figure 2 [5]. After the filling of the cavities, the polymer plate is cooled down below the softening temperature. In order to avoid the shrinkage and sinking marks, the embossing force is maintained during the cooling stage. The upper mould lift and the structure part can be demoulded.

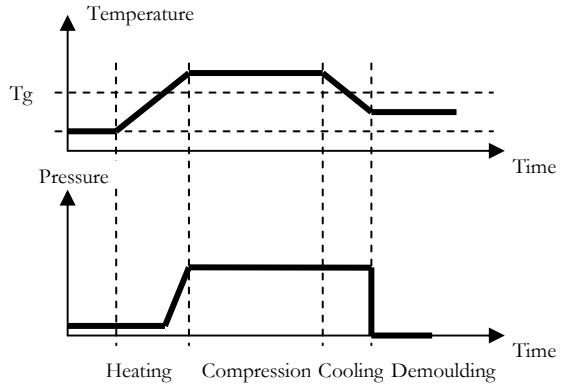


FIG. 2 – Profile of the hot embossing pressure and temperature, which shows the variation of temperature and pressure during hot embossing process [5]

The hot embossing process is more flexible, compared to other micro manufacturing processes, such as injection moulding and casting. Different moulds can be used in hot embossing process and the experimental processing conditions are more extended compared to injection moulding process. Due to the fact that the highest temperature in hot embossing is above the softening temperature, and the polymer need to be heated above the melting temperature in the injection process. Nowadays, the research activities are focused to find low-cost production processes, so the hot embossing process is well suited for that [2].

2.1 Modelling of the hot embossing process

The simulation of the hot embossing process is one of the most popular subjects in the microstructure field in recent years. Thanks to the quick developing of the FEM simulation tools, the hot embossing process can be analysed with various FEM software, such as Abaqus©, Comsol©, Ls-dyna©. The hot embossing process is complex and is difficult to define only one FEM tool to simulate the whole process [6]. The simulation of the hot embossing process can be divided into several steps: the heating process simulation, the embossing process simulation and the demoulding process simulation. The hot embossing process simulation covers the material behaviour, the characterization of contact friction between polymer and moulds, the mechanical and thermal conditions [7]. The demoulding process step is the most important one, because the risk of destroying microstructures is highest during this processing [6]. Due to the complexity of the hot embossing process, the work involved in the heating and compression stage, not include the demoulding one. In order to simplify the modelling process, the linear viscoelastic model has been applied for taking into account the evolution of the material behaviour. The contact and friction between polymer and moulds have been

taken into account during the process modelling. The thermal conditions have been treated by using a variable Young due to the softening of the polymer at high temperature. The modelling of the hot embossing process has been carried out by using COMSOL® Multiphysics© software.

2.2 Definition of behaviour law

A thermoplastic polymer Poly (methylmethacrylate) (PMMA) has been selected in the simulation of the hot embossing process. The deformation of the polymer occurs principally at the compressing stage. Therefore the modelling of the mechanical behaviour needs to be able to describe the evolution of the viscoelastic behaviour beyond the glass transition temperature. A linear viscoelastic model has been selected to describe the material behaviour at the compressing stage, for which the stress depends linearly on the strain and its time derivatives (strain rate). It is assumed that the viscous part of the deformation is incompressible, so that the volume change is purely elastic. The total stress tensor is in the form of:

$$\sigma = K[\varepsilon_{vol} - 3\alpha(T - T_{ref})]\mathrm{I} + \sigma_d \tag{1}$$

where K is the bulk modulus, α is the coefficient of thermal expansion, the strain tensor is decomposed as:

$$\varepsilon = \frac{1}{3}\varepsilon_{vol}\mathrm{I} + \varepsilon_d \tag{2}$$

where the volumetric strain is defined as:

$$\varepsilon_{vol} = trace[\varepsilon_{ij}] \tag{3}$$

The stress deviator is expressed as follows:

$$\sigma_d = 2\int_0^t \Gamma(t-t')\frac{\partial \varepsilon_d}{\partial t'}dt' \tag{4}$$

where the function $\Gamma_{(t)}$ is called the relaxation modulus function that can describe the evolution of the material shear modulus during the relaxation time. The generalized Maxwell model, which is the most general form of the linear model for viscoelasticity, has been introduced for this approach. The model can be represented by a purely viscous damper and a purely elastic spring connected in series. It takes into account that the relaxation does not occur at a single time, but at a distribution of times. The function can be expressed as:

$$\Gamma(t) = G + \sum_{m=1}^{N} G_m \exp(-\frac{t}{\tau_m}) \tag{5}$$

where G is the shear modulus of material, τ_m is the relaxation time constant of the damper and G_m represents the stiffness of the spring in the same branch.

2.3 Simulation of the hot embossing process

The compression modelling has been realized under 2 dimensions axisymmetric geometrical assumption (figure 3). A polymer plate has been compressed between two rigid and non deformable plates, which have a Young's modulus and a Poisson ratio corresponding to those of structure steel (table 1). The three blocks in the model are constructed respectively in the software. The interfaces between the polymer and steel plates are treated as contact pairs. The dimensions of the polymer disc equals to 40 mm in diameter and 5 mm of thickness. A suitable Young's modulus has been applied for the polymer disc, in order to properly account the thermal conditions at high temperature. Therefore, the polymer Young's modulus is equal to 2380 MPa and the Poisson ratio is equal to 0.4 (table 1). The processing geometry model has been meshed with free triangular elements. The rigid plates have been supposed to be undeformable, so a much more coarse mesh size has been applied. The deformation of the PMMA plate is more important for the modelling. Therefore, the element size of the polymer plate is much finer in order to improve the simulation accuracy. The element size for the polymer and two plates is related in table 2.

Material	Density (Kg/m³)	Young's modulus (MPa)	Poisson ratio
Upper and lower mould (in steel)	7850	200000	0.33
Polymer plate (PMMA)	1190	2380	0.40

Table. 1– Viscoelastic parameters for PMMA plate and moulds

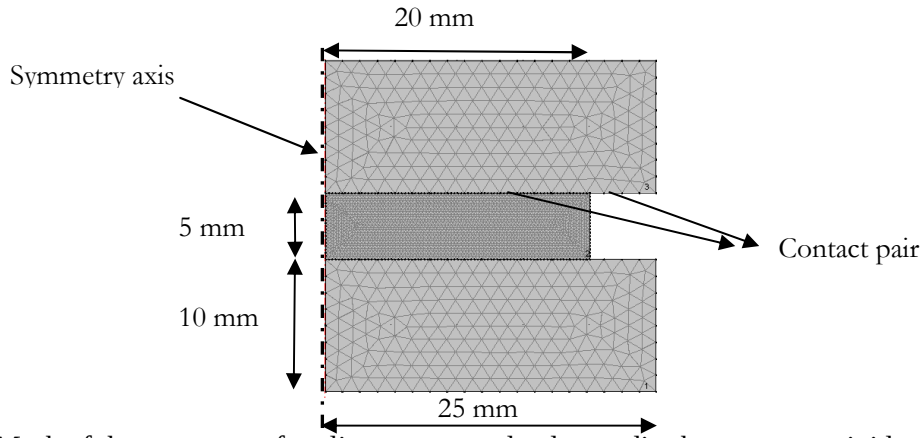


FIG. 3 – Mesh of the geometry of tooling system and polymer disc between two rigid moulds used for simulation of hot embossing process

Material	Element type	Max. element size (mm)	Min. element size (mm)	Element number
Upper and lower mould	Free triangular(three nodes)	1.33	0.0075	772
Polymer plate	Free triangular(three nodes)	0.25	0.0005	4036

Table. 2– Description of element size of the PMMA plate and the steel moulds

2.3.1 Simulation of the heating process

The heating stage has been simulated using COMSOL® Multiphysics© software for Heat Transfer physic modelling, which is used for simulating the evolution of temperature in the PMMA and upper and lower plates during the heating stage. The PMMA glass transition temperature is equal to 105 °C [8]. The aim of the heating stage is to heat the PMMA to the temperature above the glass transition temperature. In the simulation of the heating process, the polymer plate is heated by two steel moulds, which have an initial temperature 160°C. The time-dependent study is selected in order to see the evolution of temperature in the polymer plate. The boundary thermal conditions during the heating stage are described as follows:

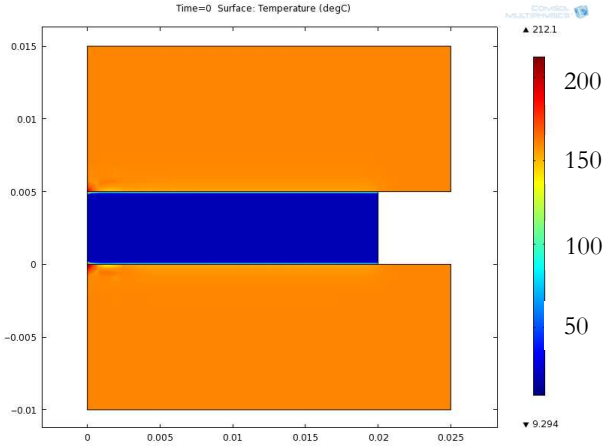
- The initial value of ambient temperature has been fixed to 20°C, so as the polymer plate
- The initial value of temperature in the steel moulds has been fixed to 160°C
- The whole model is axisymmetric with the reference axis R=0.

The thermal material properties of the polymer plate and the discs are described in table 3. These parameters describing the physical behaviour of the materials used could be obtained directly in the database of the COMSOL® software.

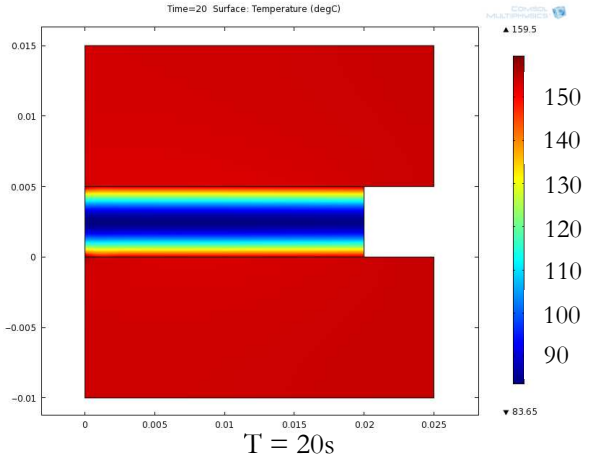
Material	Glass transition temperature [°C]	Heat capacity at constant pressure [J/(Kg*°C)]	Thermal conductivity [W/(m*°C)]
Upper and lower mould (in steel)	-	475	44.50
Polymer plate (PMMA)	105	1420	0.19

Table. 3– Physical parameters of the polymer plate and discs

A Time Dependent Solver has been used to calculate the internal temperature of the polymer PMMA during the whole heating stage. The heating time has been defined in the range from 0 to 100s with a step equal to 10s. The temperature contours in the tools and embossed material can be observed as follows (figure 4):



T = 0s



T = 20s

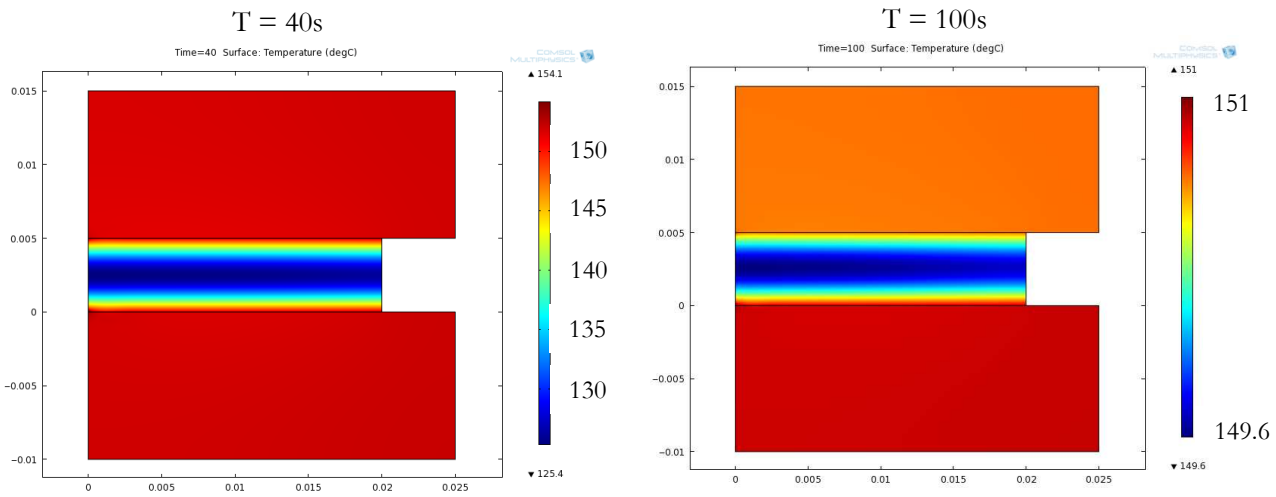


FIG. 4 – Temperature contour in the embossed plate and moulding plates when T=0s, T=20s, T=40s and T=100s

According to the figure 4, at the beginning of the heating process (T=0s) the temperature in the moulds and polymer plate corresponds the initial conditions of the model. During the heating process, the distribution of the temperature in the model is symmetric because of the symmetric boundary conditions imposed. At the end of the process (T=100s), the polymer plate has been heated to nearly 150°C and the whole model has almost the same temperature.

2.3.2 Simulation of the compression process

The compression stage has been simulated by applying a constant pressure at the external surface of the upper disc. In order to obtain the rigid and undeformable moulding plates, a much larger value of the Young's modulus has been applied in the compression process. The contact friction between the polymer surface and the mould disc surface has been taken into account by using the contact pair in the software. The value of the Young's modulus is equal to 2380 MPa, which corresponds the PMMA proprieties at high temperature. The alternative form of Equation (5) is

$$\Gamma_{(t)} = G_0[\mu_0 + \sum_{m=1}^{N} \mu_m \exp(-\frac{t}{\tau_m})] \tag{6}$$

where the constant μ_m are such that

$$\sum_{m=0}^{N} \mu_m = 1 \tag{7}$$

In the simulation, a four-term Generalized Maxwell material has been applied in order to describe the viscoelastic property of the polymer. The parameters for the model are as follows: $\mu_0 = 0.54$; $\mu_1 = 0.04, \tau_1 = 30s$; $\mu_2 = 0.08, \tau_2 = 300s$; $\mu_3 = 0.09, \tau_3 = 3000s$; $\mu_4 = 0.25, \tau_4 = 12000s$.

The viscoelastic properties have a strong dependence on the temperature for many polymers, therefore an assumption is used in these materials. A change in the temperature can be transformed directly into a change in the time scale. A WLF (Williams-Landel-Ferry) equation has been applied in order to describe the relaxation time $\alpha_T(T)$:

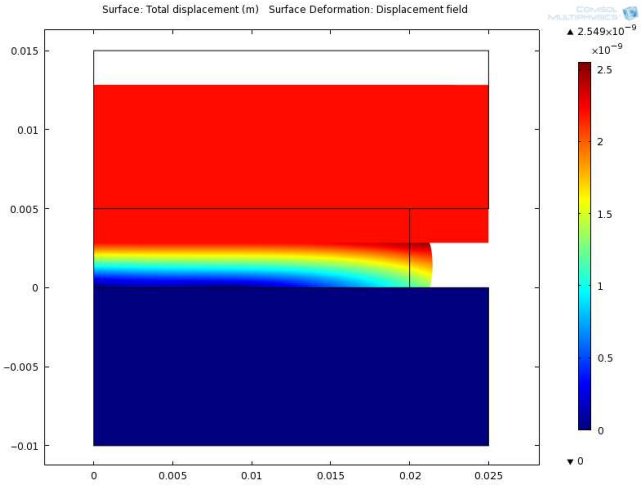
$$Log(\alpha_T) = \frac{-C_1(T - T_0)}{C_2 + (T - T_0)} \tag{8}$$

where T_0 is the glass transition temperature of the material, C_1 and C_2 are material constants: $C_1 = 17.44$, $C_2 = 51.6$.

The boundary conditions in the simulation of the compression process are as follows:

- The lower mould die is fixed during the embossing process
- A upsetting load $P = -1500\, N/m^2$ has been applied in the exterior surface of the upper disc
- The whole model is considered as axisymmetric with the reference axis R=0.
- The viscoelastic material date (instantaneous) for the polymer: $G_0 = 1700MPa$, $K_0 = 3966.7MPa$

- The reference temperature for the viscoelastic material is 150°C
- The contact friction coefficient for the contact pair is 0.1.



. FIG. 5 – Total displacement for an imposed pressure equal to P=1500N/m^2 applied to the exterior surface of the upper disc

In the compression stage, both discs have been supposed rigid and non deformable, this is clearly observed in figure 5. During compression by the rigid disc, the polymer plate exhibits a significant deformation. The free boundary surface of the polymer plate exhibits a large displacement in the horizontal direction. The contact friction conditions have been taken into account for the simulation, so a slip movement of the polymer plate in the contact surface could be observed in figure 5. The deformation of the PMMA plate is not symmetric with the horizontal axis, due to the pressure applied on the external surface of the upper disc when the lower disc is always fixed. The PMMA layers closed to the upper disc exhibit more displacement than the lower PMMA layers.

3 Conclusions

The developments presented in that paper corresponds to a first investigations for the numerical simulation of the hot embossing process based on COMSOL® Multiphysics© software (4.0a). The heating process and the compressing process have been simulated in this analysis. A viscoelastic material model has been applied for the polymer in order to describe the material properties at high temperature. The contact and friction conditions between the polymer plate and the mould tool are taken into account in order to be close to the reality conditions. Remaining problems associated the hot embossing process simulation are now in progress in the laboratory.

References

[1] Heckele M., Schomburg W.K., Review on micro molding of thermoplastic polymers, Micromech Microeng. Journal, 14, 1-14, 2004.
[2] Worgull M., Hétu J.-F., Kabanemi K.K., Heckele M., Modeling and optimization of the hot embossing process for micro- and nanocomponent fabrication, Microsy. Techno., 12, 947-952, 2006.
[3] Worgull M., Heckele M., New aspects of simulation in hot embossing, Microsy. Techno., 10, 432-437, 2004.
[4] Sahli M., Millot C., Roques-Carmes C., Khan Malek C., Barriere T., Gelin J.C., Quality assessment of polymer replication by hot embossing and micro-injection moulding processes using scanning mechanical microscopy, Materials Processing Technology. Journal, 209, 5851-5861, 2009.
[5] Liu C., Li J.M., Liu J.S., Wang L.D., Deformation behavior of solid polymer during hot embossing process, Microel. Eng., 87, 200-207, 2010.
[6] Worgull M., Kabanemi K.K., Marcotte J.-P, Hétu J.-F., Heckele M., Modeling of large area hot embossing, Microsystem Technology., 14, 1061-1066, 2008.
[7] Jena R.K., Chen X., Yue C.Y., Lam Y.C., Viscosity of COC polymer (TOPAS) near the glass transition temperature, Experimental and modeling, 29, 933-938, 2010.
[8] Lin C.-T., Kuo S.-W., Huang C.-F., Chang F.-C., Glass transition temperature enhancement of PMMA through copolymerization with PMAAM and PTCM mediated by hydrogen bonding, Polymer, 51, 883-889, 2010.