627. Simulation of hot imprint process of periodic microstructure using elasto-plastic material model

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Abstract. Hot imprint process for thermoplastic polymers is one of the technologies for manufacturing of micro-fluidic and micro-optical components. It combines both microscale resolution and high throughput. In a hot imprint process a rigid stamp is pressed onto a polymer substrate so that micro-patterns can be replicated. Polycarbonate is one of the most important engineering materials in this process. However, nonlinear relationship between temperature and elasto-plastic behavior of this material has not been very well understood until now. This paper explores the development and application of finite element model for studying of polycarbonate substrate behavior under thermal load in order to evaluate temperature and displacement fields as well as stresses formed during hot imprint process. The model of this process includes heat transfer, structural mechanics as well as contact analysis and supports nonlinear structural-thermal analysis with contact, large deformations, and the use of temperature-dependent elasto-plastic material formulation. The thermal loads are applied by means of convective boundary conditions. Simulations were performed with COMSOL Multiphysics software using heat transfer transient and structural plane strain parametric analysis types.

Keywords: elasto-plastic, hot imprint, thermo- mechanical coupling, thermal contact.

1. Introduction

Recent advances in nano-fabrication technologies have given great attention to processes based on imprint forming (Fig. 1). The exceptional capabilities of this technology in terms of highly parallel throughput, low cost, ease of implementation and ability for achieving high resolution are among the main reasons driving the interest for researching, establishing and applying such manufacturing capabilities [1]. Fine nano- and micro-scale structures and patterns are required for the production of a wide range of components and heterogeneous systems such as mini-fluidics and bio-chemical sensors, optoelectronics, photonics and health monitoring systems.

Although several techniques exist for imprint forming such as hot embossing, laser pulse assisted nano-imprint lithography, etc. they all utilize the same basic process steps outlined above. Hot embossing is an effective method to fabricate micro- and nano-structures on a polymer substrate. However, to apply hot embossing to submicron- or nano-structure fabrication, it is important to better understand the physical and chemical mechanisms of polymer deformations and fillings [2]. Furthermore, to fabricate nano- and micro-combination structures by hot embossing it is essential to investigate the fabrication process in order to obtain defect-free components [3]. Whereas these typical applications use thermoplastic

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polymers as the standard formable material, the imprint forming is indeed possible for a wider range of materials. Thermoplastic material such as PolyMethyl-MethAcrylate (PMMA), PolyCarbonate (PC), Cyclic Olefin Copolymers (COC), and Cyclic Olefin Polymers (COP) are emerging as materials of choice for the hot imprinting. The generality of this process calls, therefore, for a study of the risk of potential defects of the formed pattern and the quality of the manufactured structures that can occur as the result of the melting of the material and the release of the structure from its mould. These defects include, for example, material shrinkage, inaccuracies in shape replication, cracks, etc.
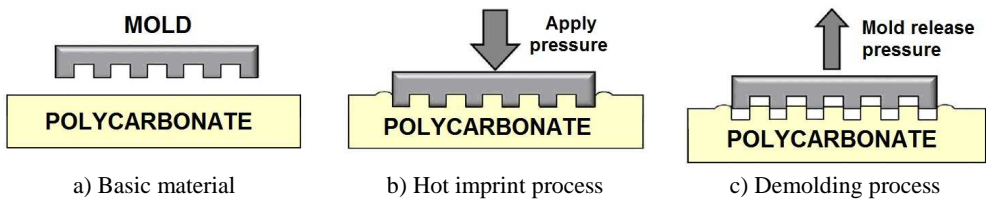
a) Basic material   b) Hot imprint process   c) Demolding process
Fig. 1. Steps of imprint process of periodical microstructure

Mechanical properties and material behavior of the formable material in hot imprint are extremely important when identifying optimal process conditions for the manufacture of defect-free nano-structures. Most applications in hot imprint are based on polymeric materials that have suitable properties for the particular method of softening the material. An accurate determination of the critical material parameters below and above the T_g of the material is a key requirement for the numerical simulation. This study investigates the process with polycarbonate, one of the most common polymers used in the fabrication of fine patterns.

The imprint pressure is another process parameter that has a major impact on the quality of the replication. An insufficient pressure would result in an incomplete filling of the pattern grooves and may lead subsequently to shape defects. Conversely, high imprint pressures should also be avoided as this will cause high residual stresses in the cured polymer during the subsequent process steps.

The main issue at the final step of hot imprint is associated with defects resulting from the mold removal. Ideally, the polymer should have higher adhesion to the substrate and much lower adhesion to the mould to secure defect-free removal of the mold.

A parameter that defines how strong two surfaces are adhered to each other is the adhesion energy. It is the energy required to de-bond the surfaces and depends typically on the surface energies of the polymer and the mould material. To promote easy release of the mold from the polymer, the mould should have lower surface energy compared with the surface energy of the substrate, or should be subjected to an anti-friction layer treatment [4].

In this paper, finite element method (FEM) was used to build a model of hot imprint process in order to understand the behavior of the polycarbonate in each step.

2. Mathematical model of the hot imprint process and results

Majority of hot embossing processes include three steps. The first is heating and applying the pressure step, the second is maintaining the temperature and pressure step and the third is the demolding step [5]. Hot imprint process model includes heat transfer, structural mechanics and contact analysis. The model is capable of nonlinear structural-thermal analysis with contact and large deformations. Temperature-dependent material properties were used in the model [6]. The thermal loads were applied using convective boundary conditions.

The simulations were performed using COMSOL Multiphysics finite element software. Fig. 3 presents a schematic illustration of the FE model, which comprises the rigid mold and the polycarbonate substrate. As shown, both the mold geometry and the loading conditions are symmetrical (Fig. 2), and thus the simulation model can be simplified to a 2-D plain strain model with symmetric boundary conditions (Fig. 3) [7,8]. Also, the material behavior of the polycarbonate is defined as elastic-plastic.

In the Fig. 3 $h_m = 100$ nm is the depth of the cavity of the periodic microstructure and $h_p = 3$ mm is the thickness of the polycarbonate. The initial temperature of the stamp and polycarbonate is 293 K. Molding temperature $T = f(T,t)$ is a function of heating temperature (T – temperature (Kelvin)) and time (t – time (second)). The imprint temperature is 421 K.
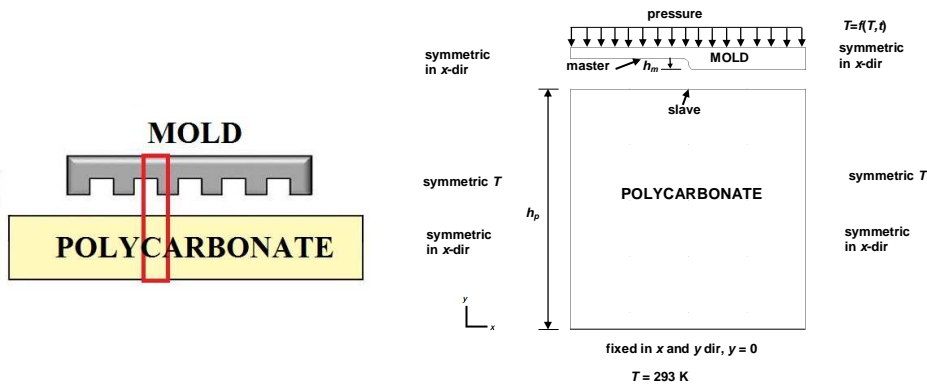
Fig. 2. Geometric definition of the hot imprint process

**Fig. 3.** Computational domain and boundary conditions

In this model hot imprint process is divided into three steps: heating, imprinting and demolding. In hot imprint process a polycarbonate is heated below its glass transition temperature and the mold is pressed into the polycarbonate.

At the heating step the polymer is linearly heated from $T_0 = 293$ K to $T = 421$ K and the polymer is assumed to be elasto-plastic body.

During the process of imprint, polycarbonate deforms and contact forces appear between polycarbonate and stamp. The lamellar microprofile of the stamp is partially filled with heated deformed polycarbonate.

The process of demolding lasts a very short period of time at the working temperature of 421 K. Therefore temperature reduction in the polycarbonate may be neglected.

In this model displacement in horizontal and vertical directions of the polycarbonate in contact edge (Fig. 4) was analyzed in each hot imprint process step. Heating process lasts only $3 \cdot 10^{-7}$ s (Fig. 5). At the beginning of this process ($0 < t < 1.5 \cdot 10^{-7}$) the integral displacement in x direction is equal to zero because at this time the temperature of the polycarbonate is still near the initial temperature. The shifts of the polycarbonate were observed from $1.5 \cdot 10^{-7}$ s to $2.7 \cdot 10^{-7}$ s. Polycarbonate is elastic therefore polymer from the contact with mold areas shifts to the empty cavity of the mold. The cavity of the mold is partially filled with heated polycarbonate. At the time of $2.7 \cdot 10^{-7}$ s deformations of the polycarbonate cease. It means the heating process is steady.
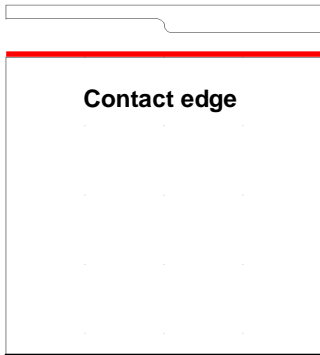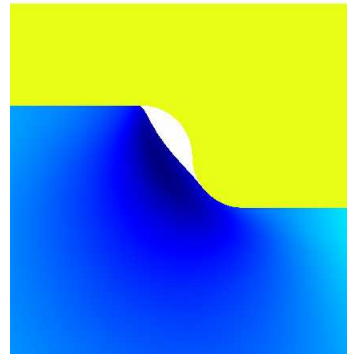
Fig. 4. Contact edge in the model
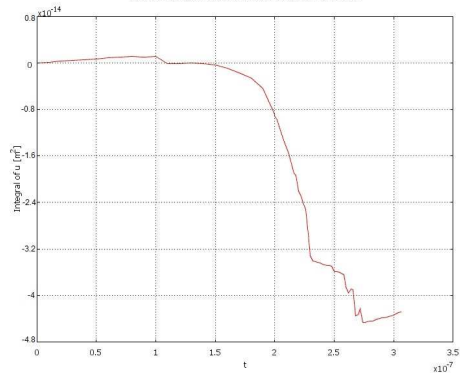
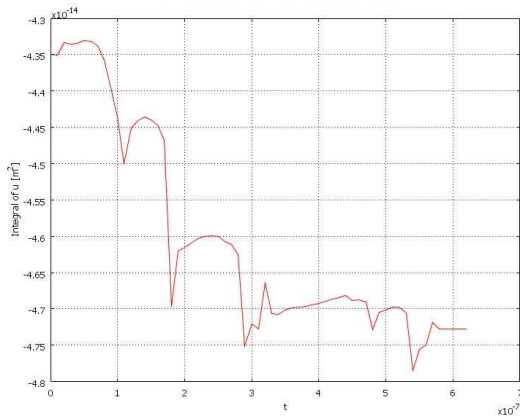**Fig. 5.** Integral displacement in *x* direction of contact edge in heating step
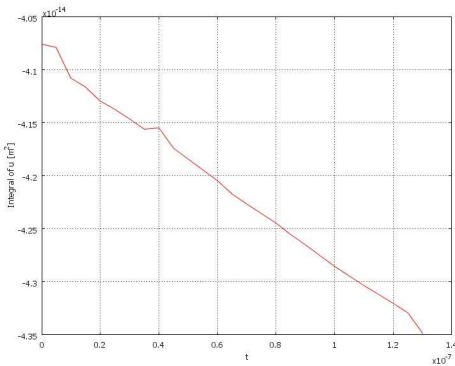
Fig. 6. Integral displacement in *x* direction of the contact edge in the imprint step

Fig. 7. Deformed polycarbonate after imprint step

In the imprint step ($0 < t < 1.4 \cdot 10^{-7}$ s) the integral displacement module in *x* direction increases linearly (Fig. 6). After imprint step an empty area remains between the mold and the polycarbonate (Fig. 7).

Fig. 8. Integral displacement in *x* direction of the contact edge in demolding step

In the demolding step the integral displacement module in *x* direction increases step by step (Fig. 8). It is because the mold goes up discreetly.

3. Conclusions

The deformation behavior of the polycarbonate during hot imprint process was analyzed using COMSOL Multiphysics software. A constitutive model was presented to evaluate the deformation behavior of the polycarbonate during hot imprint process. A finite element analysis was conducted to observe the deformation behavior of polycarbonate during hot imprint process. In this study, the developed numerical model is based on elasto-plastic material formulation and enables effective prediction of polymer behavior during imprinting. The model has been proposed to predict the profiles of polymer including simulation of polymer filling and its recovery after demolding. The deformation analysis in each hot imprint step allows identification of polymer behavior in each time instant. Simulations revealed that after the imprint step an empty area remains between the mold and polycarbonate.

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