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## MODELING AND OPTIMIZATION OF THE HOT EMBOSsing PROCESS FOR MICRO- AND NANOCOMPONENT FABRICATION

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### ABSTRACT

Hot embossing, a polymer molding process conceived by Forschungszentrum Karlsruhe, is one of the established replication processes for microstructures. The process is especially well suited for manufacturing small and medium series of microcomponents [1, 2, 3, 8]. However, a wider application of the process currently is seriously hampered by the lack of adequate simulation tools for process optimization and part design. This situation is becoming more critical, as the dimension of the microstructures shrink from micron and submicron levels to the nanoscale and as productivity requirements dictate the enlargement of formats to process larger numbers of devices in parallel. The objective of a German- Canadian cooperation is to fill the gap mentioned above by developing reliable computer models and simulation tools for the hot embossing process and to incorporate these models in a user-friendly computer code. The present paper will give an overview of the activities related to material characterization, especially the development of a viscoelastic material model, the characterization of friction between polymer and mold during demolding, the development of an 8-inch microstructured mold, and the fabrication of nanostructured molds will be discussed.

### Introduction

Micromolding of thermoplastic polymers has been attracting increasing attention in recent years, because new products to be commercialized require low-cost production processes. Besides the well-known injection molding, hot embossing has evolved into a popular fabrication process. Hot embossing is especially suited for producing delicate microstructures with high aspect ratios on thin layers and with low inner stress [3]. The process is very flexible, because both mold inserts and the type of polymer can be exchanged quickly, which is why hot embossing machines are very popular for laboratory use [1, 2, 3, 8].

The vacuum hot embossing process is an open tool technique, where a semi-finished polymer sheet is put in between the upper and the lower molding tool. The complete tool is evacuated in order to ensure complete filling of the cavities of the microstructured tool, and the polymer is heated up above its softening temperature (melting temperature or glass transition temperature, depending on the polymer class). The softened polymer is pressed into the microstructured cavities. After mold filling, the polymer is cooled down below the softening temperature, while maintaining the applied force in order to avoid shrinkage and sinking marks. Finally, the machine is opened and the microstructured part can be demolded.

### Hot Embossing Process

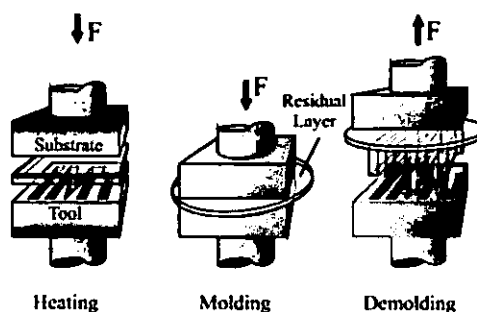


Fig. 1: The hot embossing process: Heating, molding, and demolding are the characteristic process steps. The hot embossing process is characterized by a residual layer which allows for an easy handling of the molded part.

The hot embossing process is characterized by a residual layer, a very thin layer of polymer, where the molded microstructures are fixed. The thickness of this layer depends on the process parameters of temperature and force, the polymer material, and the geometry of the mold. On the one hand, this layer allows for an easy handling of the embossed structures, on the other hand, shrinkage of the residual layer may be one reason of high demolding forces. Frequently, demolding of free-standing structures with high aspect ratios and

small cross sections on a large molding area in particular results in damage of microstructures.

## 2. Objective of the project

With regard to the scientific work [4, 5, 6], a collaboration project was started between the Institute for Microstructure Technology (IMT) of Forschungszentrum Karlsruhe (FZK) and the Industrial Materials Institute (IMI) from the National Research Council Canada (NRC). The objective of this project is to fill the gap mentioned above by developing reliable computer models and simulation tools for the hot embossing process and to incorporate these models in a user-friendly computer code. To reach the objectives, the working packages are divided between the collaboration partners).

IMT devises experiments and carries out measurements which will generate new data on the interface behavior. In detail, the following work is performed:

- Characterization of mechanical and thermal properties of the molded polymer
- Development of a viscoelastic material model of the used polymer. Determination of the WLF constants
- Measurement of friction and adhesion between mold and polymer during demolding. Determination of friction coefficients
- Fabrication of large-area microstructured molds (8 inch). Systematic replication tests for the validation of the simulation results
- Fabrication of structures on the nanoscale with high aspect ratios. Replication of these structures in polymer by hot embossing

Experiments and a new software tool will be combined to develop and optimize hot embossing of large-area tools (8 inch) and to push the replication resolution of structures down to the nanoscale.

## 3. Material Characterization

To provide reliable data for the computer model, it is necessary to characterize the polymer as well as possible. The data required for the simulation tool cannot be found in databases. Therefore, the thermal and mechanical properties have to be determined under typical hot embossing conditions. Thermal properties of the polymer are characterized by the PVT behavior measured by a high-pressure capillary rheometer. The heat capacity of the polymer used is determined as a function of temperature by a DSC measurement. Also the glass transition temperature was measured by DSC. In addition to the measurements described above, systematic tests were performed to determine the stress-strain behavior of the material during demolding. For this purpose, tensile tests of molded parts were carried out with a variation of tensile velocity and temperature. The range of the temperature for the

tensile tests was in the range of typical demolding temperatures up to the glass transition point of the polymer. The range of the tensile velocities was equal to the range of typical demolding velocities. With these measurements, rupture stress and the ultimate strain of the polymer during demolding were determined.

To describe the material behavior for the selected material (PMMA), a Maxwell viscoelastic model was developed using 10 relaxation times. Systematic DMTA measurements were investigated. Within the scope of these measurements, the WLF constants for the time-temperature shift were determined. Figure 2 shows the measured temperature-time dependency of the selected polymer.

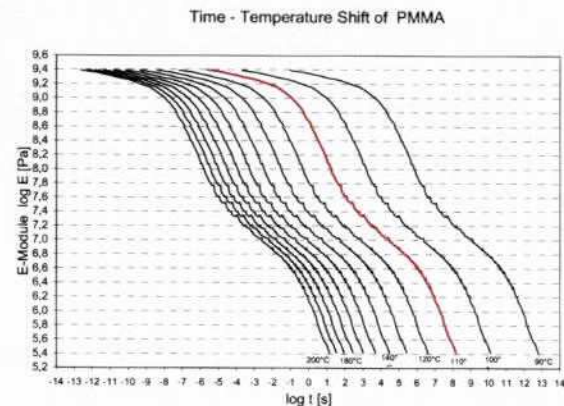


Figure 2: Measured time-temperature behavior of the selected material. The reference temperature is 110°C. In a temperature range of 170°C, the relaxation of the polymer is in the range of typical process times.

A special feature of the simulation tool is the simulation of the demolding cycle. For this, it was necessary to determine friction and adhesion between the mold and polymer under typical hot embossing conditions. Friction in a typical microstructured mold cannot be determined because of the absence of microsensors and the need for a high-resolution sensor array. Due to the lack of adequate measurement systems, a macroscopic test arrangement was built to measure static and dynamic friction as a function of the process parameters and surface quality. The sophisticated feature of this arrangement is an integrated hot embossing cycle. The polymer foil is heated up above transition temperature and pressed onto the defined surface. After cooling down to demolding temperature, a tensile test with defined velocity and contact pressure is started. The measured tensile force, in combination with the contact force and the contact area, are the variables used to calculate the friction coefficient. The advantage of this measurement arrangement is the characterization of friction and adhesion under typical embossing conditions. The influence of the process parameters like molding temperature, press force, and demolding temperature is considered as is the demolding velocity. The arrangement also allows to specify the influence of



surface roughness and mold material on friction and adhesion. In figure 3, a typical measurement curve of friction is shown.

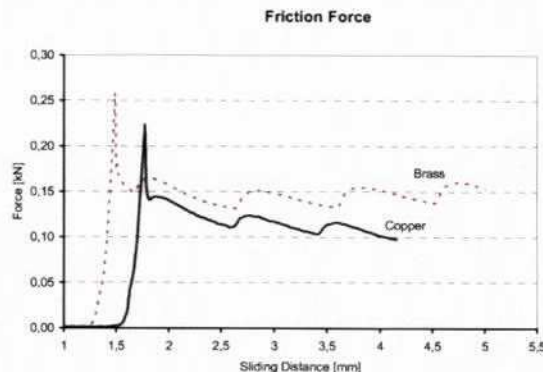


Figure 3: Friction force measured between the molded polymer and a brass and a copper mold, with the microstructured molds having a typical surface roughness. Because of the integrated molding cycle, static and dynamic friction force can be measured under typical demolding conditions. With the measurement arrangement, friction coefficients can be calculated for different material combinations

#### 4. Large-Area Replication

For verification of the simulation results and for the further development of design rules for large-area hot embossing, an 8-inch microstructured mold was developed and realized by micromachining (Figure 4). To replicate molds with these dimensions, a new generation of high-precision hot embossing machine was fabricated, specialized for industrial applications [7]. Advantages of the new embossing machine among others are short cycle times and an easy handling of molded parts. In combination with a sophisticated molding tool [9], basic prerequisites are provided for large-area replication. To obtain best molding conditions, shrinkage of molded parts and the demolding force measured are compared with the values predicted by simulation. Further design rules will focus on how small dies from the LIGA process can be integrated in a large tool [6].



Figure 4: Molded part of the 8-inch microstructured brass mold. This design is used to verify the simulation results and to optimize the hot embossing process especially for large-area hot embossing.

#### 5. Micro-Nano Interface

In addition to the design rules, research on the micro-nano interface between microstructuring by hot embossing and nanoimprinting becomes more important. Between these two replication techniques for different physical applications there is a gap. Aspect ratios of more than one are presently reached for free-standing microstructures with lateral dimensions greater than some microns only. With the support of simulations tools, this limitation is to be shifted towards the nanorange to connect the micro- and nanoworld.

Within the scope of the project, first nanostructures – honeycombs structures – with high aspect ratios were replicated in PMMA (Figure 5). The molding tool was fabricated by E-beam structuring and subsequent electroplating into a nickel mold. The result of the process chain was a 4-inch nickel shim with several nanostructured  $100 \times 100 \mu\text{m}^2$  areas. Aspect ratios in several areas vary in a wide range. For a structure height of  $2 \mu\text{m}$ , aspect ratios between 1 and 3.5 were achieved. Experiments and the simulation of shrinkage, demolding forces, and stress-strain behavior will support the development of practicable design rules for large-area nanostructured molding.

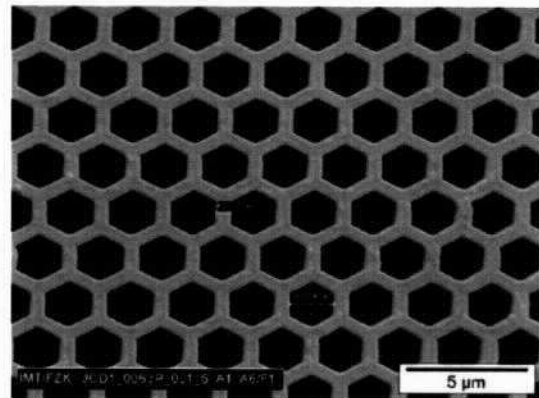


Figure 5: Detail of a nanostructured molded part with an aspect ratio of 3.5. The design of this honeycomb structure in the nanorange is also used for a verification of the simulation results.

#### Conclusion

To meet future requirements in the hot embossing technology, a German Canadian cooperation was started with the aim of improving the hot embossing process with respect to large-area molding and molding of nanoscale structures. Process development has to be supported by a process simulation. Due to the lack of adequate simulation tools, one objective of the project is the development of reliable computer models and simulation tools for the hot embossing process and the incorporation of these models in a user-friendly computer code. IMT devises experiments and carries out measurements. Within the scope of the project, PMMA as a typical polymer material was

mechanically and thermally characterized, and a viscoelastic material model was developed. For the analysis and simulation of the demolding cycle, a sophisticated measurement arrangement was used to determine friction coefficients under typical hot embossing conditions. For validation of the simulation results and adaptation of the simulation software, a large-area microstructured mold (8 inch) was fabricated. Finally, a nanostructured mold was fabricated and the structures were replicated by hot embossing so as to adapt the simulation tool also to replication in the nanorange. With the systematic measurements and process simulation, the field of application of the hot embossing process will widen.

### Acknowledgements

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