FlexPAET

Analysis of the temperature distribution during embossing of diffractive optical elements by numerical simulation

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SEVENTH FRAMEWORK PROGRAMME

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  - **Process issue**
- **Field tests**
- **Conclusions**

Flexible Patterning of Complex Micro Structures using Adaptive Embossing Technology

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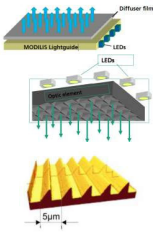
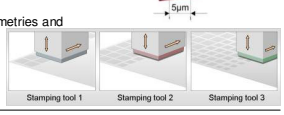
Introduction

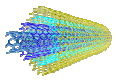
- **Objective :** Development of a production chain using micro embossing, surface structuring and mass replication for the production of large area micro structured optical components
- **Process**
  - Multiple embossing steps are used in order to structure large surfaces up to 2m²
  - Typical structure size in the range of 2 … 100 µm with optical surface quality
  - Structuring process using various structure geometries and orientations

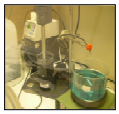


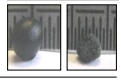


Material

- **Polymer : neat / filled**
  - PA6 / PMMA
  - Filled with Carbon Nanotube (CNT) for higher thermal conductivity
- **Filled polymer with DOPE® process**
  - for a better CNT distribution
  - for enhanced properties
- **DOPE® Process**
  - Mixture of Multi Wall CNT & Alginate
  - Reticulation of capsule from the fall of a droplet in to a cation solution
  - Frizzing of the capsule in frozen nitrogen
  - Drying with freeze-dryer

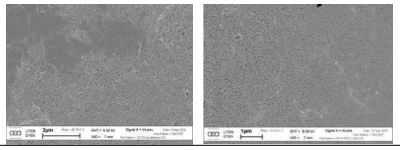




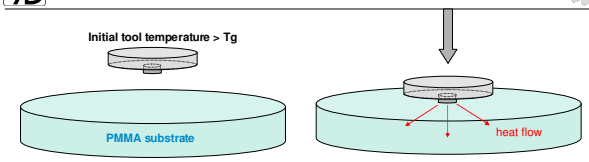


Material

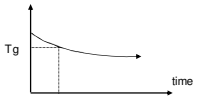
- **Filled polymer**
  - Extrusion of neat polymer + capsules
  - Sample produced by Injection Mouling
  - CNT repartition improved by DOPE®



Numerical simulation - Objectives



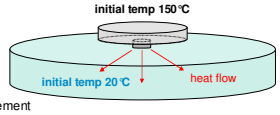
- **Is it possible to obtain a cooling effect just by the heat transfer through the substrate ?**
- **What are the material properties required for the substrate (thermal conductivity) ?**



⇨**Thermal transient analysis of the embossing step have been performed by finite element method**
- **2D axisymetrical CEA (Castem software)**
- **3D IMT Bucharest (ConventorWare)**

Simulation - Input data

- **Boundary and initial conditions**
  - tool preheated at 150 °C
  - tool and substrate in contact at t=0
  - substrate bottom surface at 20°C
  - tool upper surface at 150°C or heating management
  - adiabatic conditions elsewhere



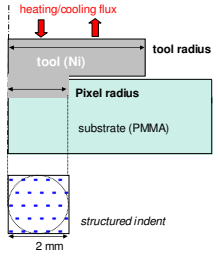
- **Material properties**

	specific mass	thermal conductivity	specific heat	Tg
Substrate (PMMA)	1.2 g/cm3	**0.1 W/m/K** to **1 W/m/K *optimized value***	1.5 J/g/K	115 °C
Tool + indent (Ni)	8.88 g/cm3	60.7 W/m/K	0.46 J/g/K	/

Simulation - Input data

- **Geometry (2D/3D)**
  - **single pixel tool**

	radius	thickness
Substrate	7,5 mm	4 mm
Tool	**0,5 to 7,5 mm**	0,3 mm
Pixel (single)	**0,05 to 1,5 mm**	0,01 mm



  - **Multi-pixel tool**

Simulation - Material

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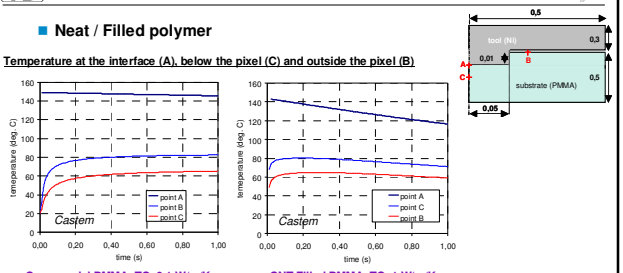
- **Neat / Filled polymer**

Temperature at the interface (A), below the pixel (C) and outside the pixel (B)



Commercial PMMA, TC=0.1 W/m/K

CNT Filled PMMA, TC=1 W/m/K

⇨ A faster cooling of the interface tool-polymer is predicted only for the more conductive material: CNT filled polymer

Simulation - Tool size

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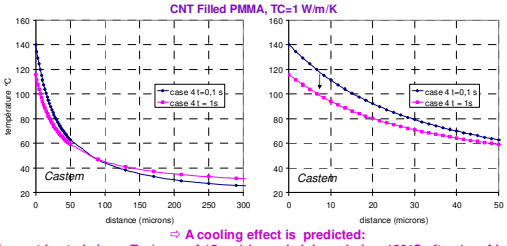
- **Ni Shim radius = 0,5 mm**

Temperature along the upper face of the substrate (from the tool edge)

CNT Filled PMMA, TC=1 W/m/K



⇨ A cooling effect is predicted:
the part heated above Tg (zone of 15 µm) is cooled down below 120°C after 1 s of holding

Simulation - Tool size

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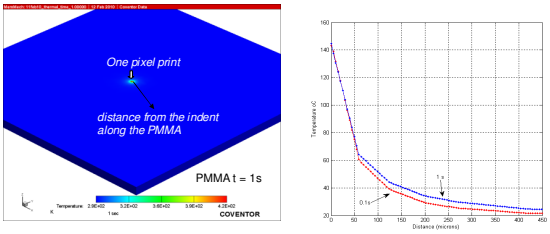
- **Ni Shim radius = 7.5 mm, temperature map after 0.1 and 1s**



⇨A cooling effect is not observed in this case even if the thermal conductivity is optimized (up to 1 W/m/K) : the ratio between the tool volume and contact area is to high

Simulation - Tool size

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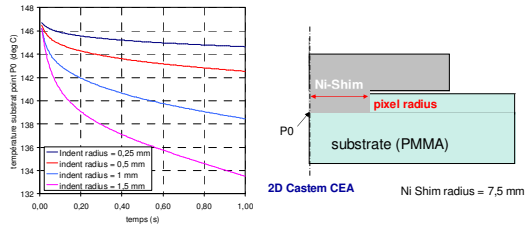
- **Ni tool = 0.25, 0.5, 1 and 1,5 mm**

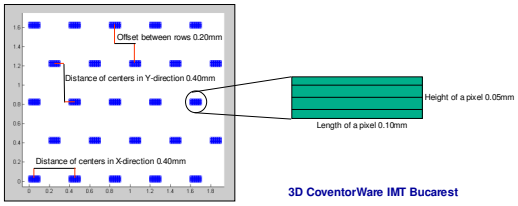
Temperature histogram at the center of the tool (point P0)



⇨ A cooling effect is predicted as the radius of the tool is rising to large values (> 0,25 mm)

Simulation - Tool shape

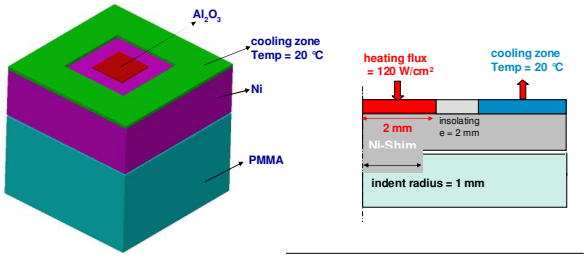
- **Case of tool with 25 pixels**



3D CoventorWare IMT Bucarest

Simulation - Process (heating/cooling system)

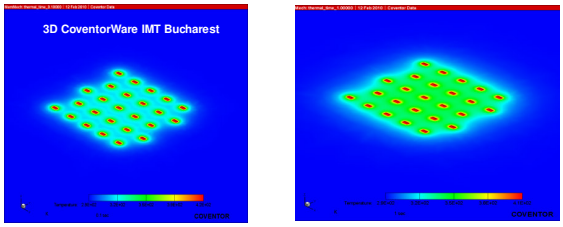
- **Input parameters**
  - step 1 : before embossing, tool is pre-heated
  - step 2 : during embossing heating flux is maintained or interrupted



Simulation - Tool 25 pixels

- **Temperature map**

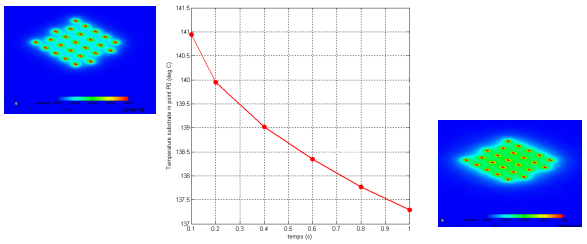
Temperatures in the substrate after embossing at 0.1 and 1 s



IMT-Bucharest

Simulation – Tool 25 pixels

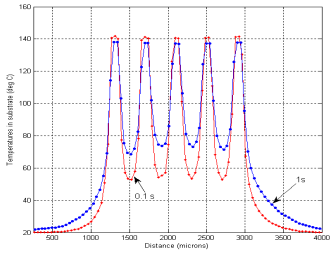
- **Temperature histogram at the center of the Tool (point P0)**

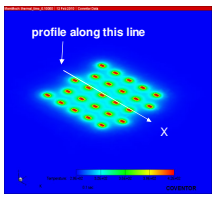


⇨ A slight cooling effect is observed for this geometry,
but insufficient after one second to reach a temperature below the Tg

Simulation - Tool 25 pixels

- Temperature profile along the print

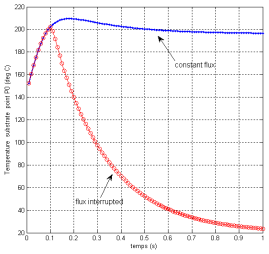


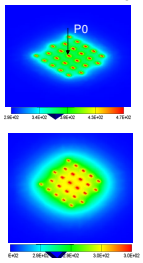


⇨ Further cooling is required to decrease the temperature between pixels bellow Tg (to not deform the existing pixels) - 3D analysis

Simulation - Process (heating/cooling system)

- Temperature histogram of the substrate at the center of the central pixel (P0)

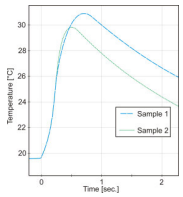




⇨ A cooling effect is predicted only when the heating flux is interrupted during embossing

Field Tests

- Experiment performed on neat & filled polymer
- Temperature measured by fast respond thermal sensor at 1.5mm below the surface



⇨ General behavior in good agreement
⇨Obvious interest of filled polymer (thanks to thermal conductivity)

Conclusions

- The time evolution of temperature in the substrate depends on:
  - thermal properties of materials
  - size and heating/cooling management of the Ni tool (process/design parameters)
- A cooling effect can be achieved:
  - if the thermal conductivity of the substrate in increased to 1 W/m/K but **also** if the ratio between the contact area (heat transfer) and the tool volume (stored heat) is increased
    - reduction of the size of the Ni Shim (15 mm to 1 mm)
    - augmentation of the size of the Ni tool (0.1 mm to values higher than 0.5 mm)
  - or with an appropriated management of the heating/cooling sequence of the tool
    - interruption of the Ni-Shim heating during embossing (0,1 s)
- Predicting tool can be used for machine designer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Thank you for your attention
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