Study of defect mechanisms in partly filled stamp cavities for thermal nano imprint control

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When an imprint process is optimized to achieve homogeneous and thin residual layers, cavities will inevitably remain partly filled when stamps with mixed structure sizes are imprinted. Unfortunately, partly filled cavities are prone to self-assembly defects (see Fig. 1). This work investigates the physical defect mechanisms leading to self-assembly with the objective to avoid such defects.

Typically, self-assembly defects feature the development of a contact angle between the polymer and the stamp ceiling or the stamp side wall. For defect control the overall situation has to be taken into account, namely the filling of the stamp cavity by external forces (pressure-induced flow, from below the stamp protrusions) and by internal forces (surface-energy-induced development of minimum energy surfaces within the cavities by capillary forces). For the latter, the interactions of the polymer with the stamp side wall, the stamp ceiling and the substrate play an important roll, as indicated in Fig. 2.

In order to differentiate between the effects of the different driving forces we made use of the different temporal length scales – due to the high viscosity of the imprint materials capillary actions are strongly slowed down. The pressure-induced flow proceeds within minutes and has been well estimated by simulations[1]. To address the surface-energy-driven flow we performed self-assembly experiments: the polymer remains (after the imprint) in a partly filled stamp cavity for several hours under imprint conditions (100 bar, 190 °C). We found that with initial layers down to 100 nm the stamp cavity acts as a capillary, thus a meniscus develops, as shown in Fig. 3a. With thinner initial layers vertical structures are formed along the stamp side walls in particular with long assembling times, Fig 3b. We suppose that a final meniscus shape allows to derive information about capillary forces between the two stamp side walls, whereas the vertical structures indicate an interaction with only one of the stamp side walls. The influence of the stamp is emphasized by the fact that the polymer transforms into a spherical shape (Fig 4), when the stamp is removed and the imprinted structures are allowed to reflow at imprint temperature. In addition, the experiments indicate a strong correlation with the roughness of the stamp side wall. An understanding of the mechanisms involved and of the conditions under which they dominate the process helps to identify processing conditions that are suitable to avoid self-assembly defects.

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[1] H. Rowland et al, J. Micromech. Microeng. **15** (2005) 2414 - 2425

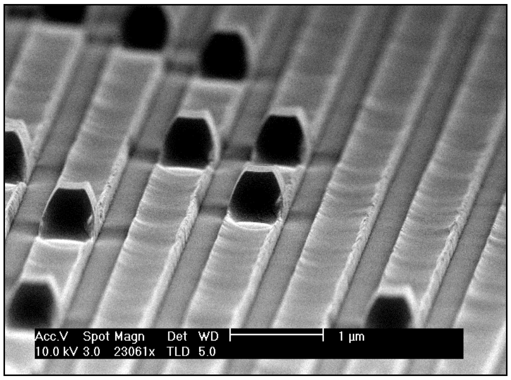

Fig 1. : Local self-assembly defects in heavily under-filled stamp cavities (width 500nm, height 500nm).

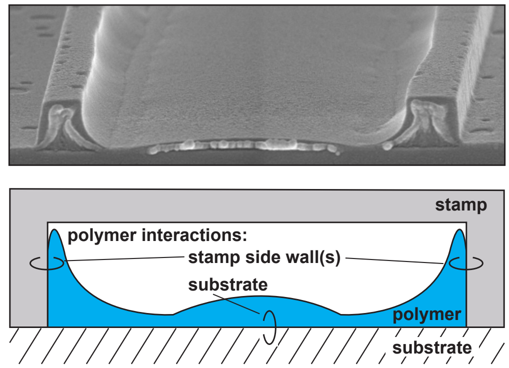

Fig 2.: Within the stamp cavity the polymer experiences a locally different interaction with the cavity side walls and the substrate.

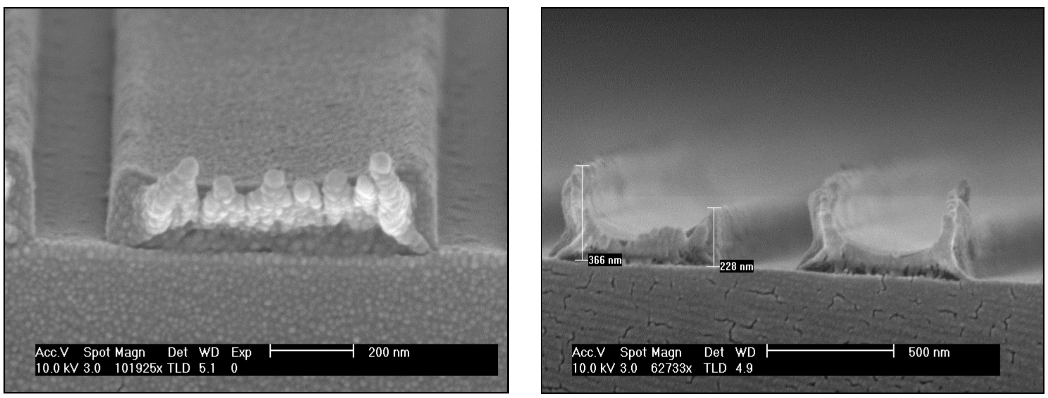

Fig 3. Shape of imprinted structures within partly filled cavities (width 500nm). Left: Meniscus shape (intial layer 150 nm) right: Vertical structures (initial layer 60 nm). Imprint details: time 90 min, temperature 190°C, pressure 100 bar.

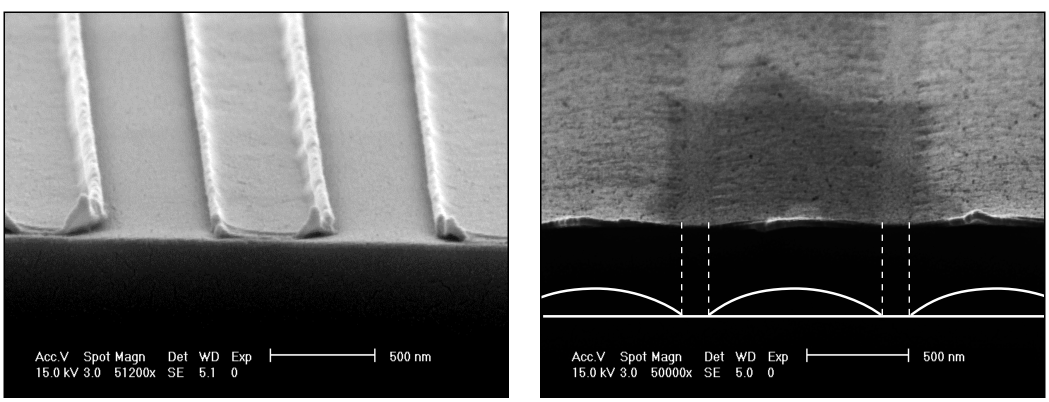

Fig. 4: Impact of stamp sidewall and substrate for pattern formation:
Left: Partly filled cavities (initial layer 30 nm) imprinted at 190 °C and 100 bar for 8 hours: vertical structures; no meniscus develops even after long imprint.
Right: Vertical structures (left) after reflow at 190 °C for 90 min without stamp: Both vertical structures transform into one single spherical cap.