Guiding chart for initial layer choice with nanoimprint

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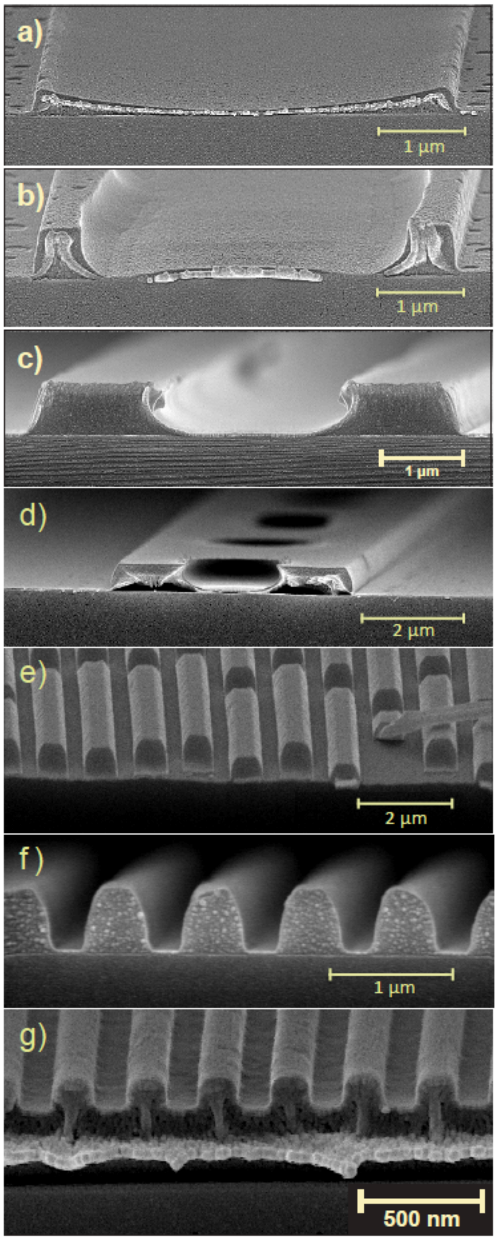
Nanoimprint, thermally operated (T-NIL) or UV-assisted (UV-NIL), has become a valuable technique for defining nanometer-scale patterns in a simple way, by replicating a template or stamp [1]. However, though claimed to be simple in application, we learn in praxis that this mechanical patterning technique often produces 'strange' results [2]; counter-measures are hard to plan without profound experimental and theoretical experience at hand. By now this is the case when nanoimprint is just the technique used to define a specific pattern, but certainly the main interest of the user is in the functionality the pattern shall provide. For such a typical situation it would be nice to have a guideline at hand how to choose specific parameters so that the imprint process proceeds successfully. With respect to the obvious processing parameters (temperature, pressure, time) such guidelines exist [1]; this is not the case with respect to less obvious parameters as the initial layer thickness or the stamp geometries.

To bridge the innovation from academia to application with nanoimprint we address the parameter 'initial layer thickness' here, taking the example of a frequently met situation, the definition of nanometer-scaled periodic gratings. Then the stamp pattern dimensions are well-defined (elevated pattern size s, recessed pattern size (cavity width) w, stamp height H, size of the patterned area A and overall stamp size A_{tot}). Then, depending on the initial layer thickness chosen, the imprint result will feature either (i) fully filled cavities with a continuous residual layer h_r below or (ii) partly filled stamp cavities without a residual layer. Fig. 1 gives examples of the imprint results obtained with various initial layer thicknesses. When the cavities are not completely filled, a number of different situations may occur, depending on the polymer volume available and on the wetting/de-wetting with respect to the stamp and substrate.

With a simple grating it is easy to calculate the minimum initial layer height to fill the cavities, as volume conservation applies for the polymer. Whether complete filling is envisaged or not depends on the specific application. With partially filled cavities the calculation becomes more challenging, but is still based on simple geometrical relationships. Fig. 2 displays the different regimes, as calculated for a pitch ratio of s:w = 1. Though helpful at first glance, this chart has to be modified to account for (i) de-wetting with thin films and (ii) physical self-assembly that may occur in partly filled stamp cavities [3].
We will quantify the chart and will discuss the modifications required, aiming to provide a chart that meets practical necessities and can serve as a 'key enabler' for successful nanoimprint.

[1] H. Schift, J. Vac. Sci. Technol. B 26 (2008) 458
[2] K.Y. Suh, H.H. Lee, Adv. Mater 14 (2012) 346; D.Y. Khang, H.H. Lee, Langmuir 24 (2008) 5459
[3] A. Mayer et al., Appl. Phys. A 121 (2015) 405



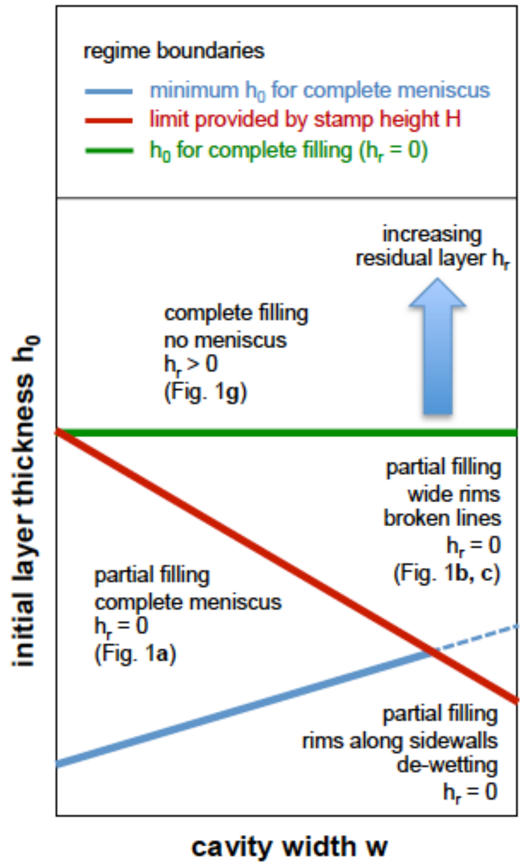


Figure 2.
Chart of imprint regimes for differing initial layer height h_0 and differing cavity width w.

Regime boundaries for linear gratings (s:w = 1:1) with given stamp height H, self-assembly not yet considered.

Figure 1. Polymer shapes obtained in cavities with increasing relative initial layer thickness from top to bottom.

a) complete meniscus
b) rim at sidewalls and center residue
c) sidewall rim only
d) almost complete filling, wide lines
e) almost complete filling, narrow lines
f) compete filling, no residual layer
g) complete filling on residual layer with increasing thickness