Energy-based geometry evolution and 3D simulation of thermal polymer reflow

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The ability for 3D manufacturing is crucial for future devices, especially in the field of fluidics and photonics. Polymers and their patterning techniques are promising for these areas of application due to a broad spectrum of available polymers, the ability for efficient tuning of their properties and the usability of respective emerging technologies. Electron beam grayscale lithography has demonstrated its potential for multi-tier structures down to the nano-scale.[1] Polymer reflow has recently proven its ability to transform such multi-tier structures into complex convex and concave patterns on the micro-scale.[2] The combination of these two methods can be exploited in the master origination for replication processes like nanoimprint lithography and molding.

The manufacturing of complex 3D patterns with this combined approach (Figure 1) primarily requires a high predictability for an efficient design flow, especially for its quick adoption in large scale manufacturing. This work discusses the main reflow effects and their implementation in an energy-based simulation approach. Therefore, the free software Surface Evolver[3], being based on a minimal-energy soapfilm-method, was investigated for its applicability. The goal is to provide an efficient simulation tool for predicting polymer reflow patterns.

A selective reflow process is typically based on temperatures at maximum 20°C above the glass transition temperature T_g. This process was intensively studied in representative experiments using poly (methyl methacrylate) (PMMA). The time-evolution of the apparent contact angle between polymer and substrate (Figure 2a) was found to be the dominating effect for reflow temperatures T_r about 10°C above T_g. At or below T_g, the contact angle evolution is rather slow and the reflow process is mainly dominated by the trend towards constant curvature surfaces ("shape optimization") (Figure 2b). This quickly removes sharp corners of multi-tier grayscale patterns and is exploited in a recently published topography equilibration process.[4]

Knowledge about these two effects enabled the simulation of the reflow of single lines in the micro-scale (Figure 3). As a generalized concept, this simulation approach will be extended to the reflow of grayscale patterns at a much smaller scale (Figure 4a) and the prediction of freestanding 3D patterns (Figure 4b).

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[1] F. Hu and S.-Y. Lee, J. Vac. Sci. Technol. B (26) 2003, pp. 2672-2679
[2] A. Schleunitz and H. Schift, J. Micromech. Microeng. (20) 2010, pp. 095002
[3] K. A. Brakke, Experimental Mathematics (1) 1992, pp. 141-165
[4] A. Schleunitz et al., Nano Convergence, 2013 (accepted for publication)

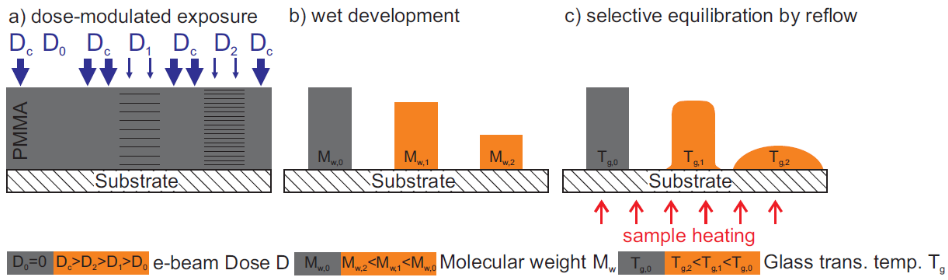

Figure 1: Schematic of the process flow combining electron beam grayscale lithography and polymer reflow for selective pattern equilibration.

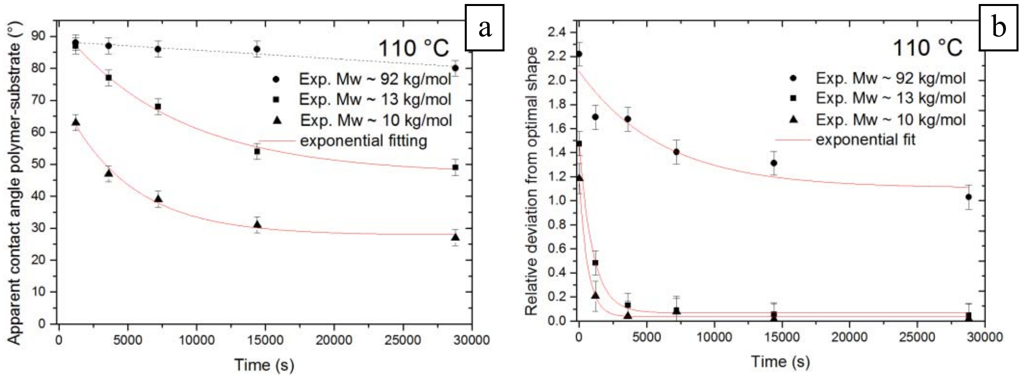

Figure 2: Evolution of a) the apparent contact angle and b) the geometries relative deviation from the ideal geometry. This knowledge was obtained from representative experiments and is required for the material simulation.

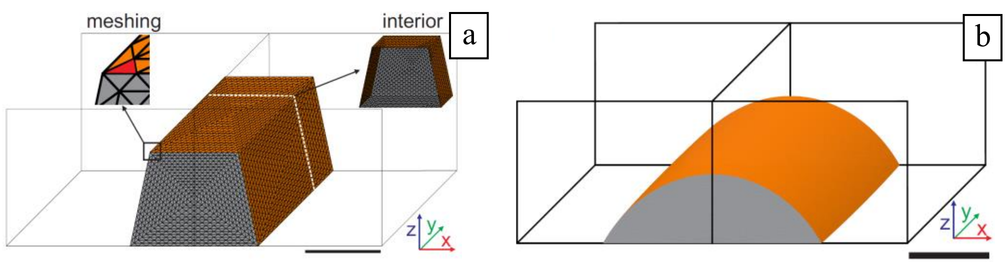

Figure 3: a) Initial geometry for the reflow simulation of a single line demonstrating the triangular meshing and the soapfilm approach (hollow interior) and b) simulated line after reflow. (scale bars 1 µm)

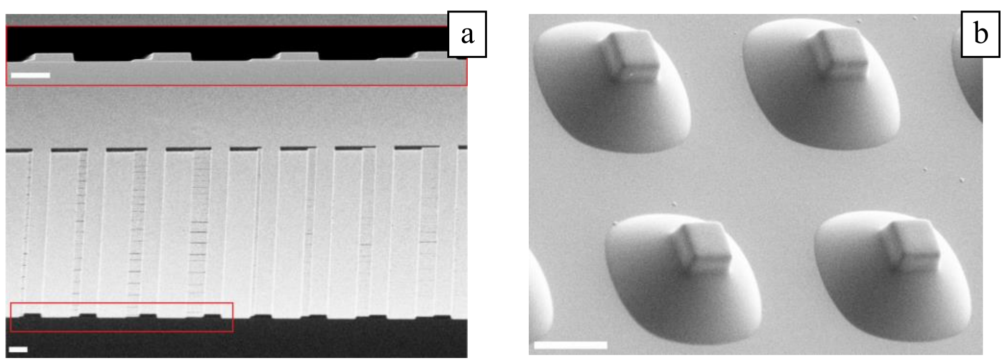

Figure 4: a) Grayscale patterning of several steps in a 450 nm thick PMMA film (inset 120 and 450 nm high steps of several widths) and b) selective reflow of 3D structures with a central stabilizing pillar. (scale bars 2 µm)