# Multi-Scale Modelling Of Nano-Imprint Lithography

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One primary requirement for the industrial implementation of Nanotechnology is the ability to reproducibly manufacture nanostructures from various materials with an accuracy and overlay of or better than the nanometre. Alternative techniques to cost-intensive fabrication methods have undergone continuous development for nearly two decades, in particular where planar structures are concerned and nano-structuring is being carried-out on a surface, as opposed to a three-dimensional nano-fabrication or multi-layer assembly [1]. Among these, nano-imprint lithography (NIL) consists in embossing, at a moderate temperature, a polymer layer that has been spin-coated previously on a flat substrate. The resulting minimum size of detail reached experimentally is currently in the range of 5nm [2–4]. Scaling up the process and optimising it is, however, hampered by a number of technical intricacies. As a result, the development of NIL towards high throughput requires the appropriate modelling of the processing of nano-structures, together with their long-term dimensional and mechanical stability [1,5,6]. In parallel, mechanical and rheological measurement methods are also required, that are sensitive enough to detect instant and long-term variations of the constitutive behaviour of the material at the nano-scale.

A suite of modelling tools is being created for the European Integrated Project ”Emerging Nano-Patterning Methods”. The idea of an optimal processing window for nano-imprints is presented, together with its limiting factors. Stemming from these factors, the need for a fully integrated multi-scale modelling is identified, where the overlap is on three levels: at the wafer scale for pressure and residual layer thickness distribution, at the cavity scale for fluid dynamics, and at the sub-nanometre scale for fluid-stamp interactions. The residual layer thickness is a critical parameter for embossing large areas, and accurate modelling at various scales is needed, in order to predict simultaneously cavity filling and thickness homogeneity at the wafer level. The large number of possible filling defects pointed for the need of a full multi-scale model of NIL, where both the stamp and polymer film are modelled together. As a result, a finite element model of one single, half channel geometry, was built with the intent to use it as a representative element in a model of larger dimensions. Although the present model was only in two dimensions, a similar approach is applicable to three dimensional artifacts. ANSYS/FLOTRAN were used to solve for the fluid flow in channels of infinite length. To check that the model accurately captures all the salient features of imprinting, two studies are carried-out. Firstly, it is shown that the model reproduces well the profile of the fluid front in a cavity for a range of viscosities. Secondly, the model is successfully compared to the experimental results of load-instrumented single cavity nano-imprint (Figure 1). Finally, a larger model was built by assembling the elementary channel feature defined above, and the velocity profiles in adjacent channels were analysed (Figure 2).
Other tools have been developed during the course of the project, and the results of a large scale finite difference scheme will be presented. This lower order solution is based on a coarse grain approach, which greatly reduces the computation time and allows for rapid prediction of the quality of an imprint.

**References:**


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**Figures:**

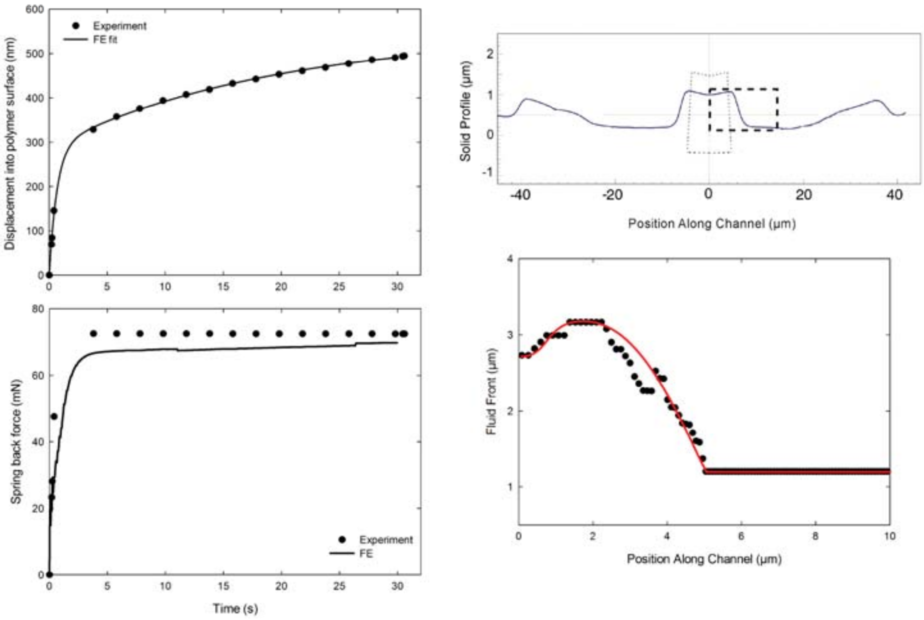


Figure 1: Left: Stamp displacement and spring-back force as a function of time, right: Solid profile after demoulding, short dashed line indicates the size of the cavity, large dashed line delimits the area for comparison with the modelled profile (top) and modelled fluid profile (bottom)

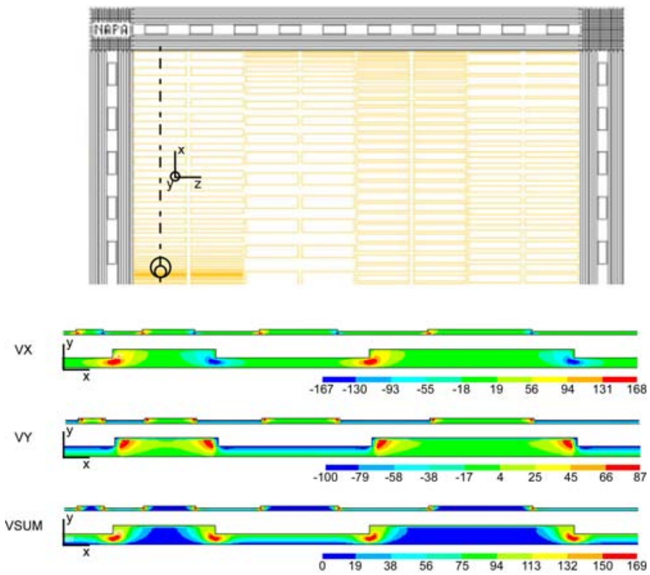


Figure 2: NaPa test stamp geometry ”Sinus 3” (top); polymer flow analysis along the line marked above, corresponding to the two regions marked by circles on the stamp geometry (bottom), taken at the end of the embossing, before relaxation - scale bar in nm/s