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Application of modelling tools for precise transfer of nanostructures from silicon wafers to steel injection moulding tool inserts

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Abstract
Functional nanostructures applied on various consumer products has attracted increasing attention in the industry. Examples of functional nanostructures are well known from nature, where organisms and plants possess optical, adhesive, and self-cleaning capabilities. The aim of the present work is to produce injection moulding tool inserts with the nanostructured functional surfaces as mentioned above. In order to manufacture these structures on the double-curved surfaces of the injection moulding tool inserts, a technology called nanoimprint lithography (NIL) with flexible stamps is applied. However, the resolution limit due to distortion of the stamp when applying the pressure, and complications regarding deformations of the flexible stamp, is a major concern for precise replication of the nanostructures whose functionality might change dramatically with just a few nanometres of distortion. Here, the application of modelling tools is essential in order to predict how the flexible stamp will deform during the transferring process. However, such models are quit complicated since the overall behaviour is non-linear. A review of different manufacturing and simulation cases will be presented and gives an overview of today's methodologies for transfer of nanostructures to curved surfaces.

Nanotechnology, modelling, injection moulding, nanoimprint lithography

1. Introduction

Nanostructured surfaces, both natural [1] and artificial [2] offer a broad range of advanced functionalities, such as stunning structural colours, antireflective, self-cleaning, super hydrophobic, super hydrophilic or antifogging effects. These effects are facilitated by the specific arrangement of micro- and nanostructures on the surface. Manmade nanostructured surfaces, formed by advanced microfabrication techniques such as lithography can often mimic or even exceed some of the properties found in nature. However, there is a substantial limitation, as the above mentioned fabrication techniques only apply to flat, planar surfaces. In order to manufacture these structures on curved surfaces of e.g. injection moulding tool inserts for production of polymer parts with the surface functionalities as mentioned above, the technology known as nanoimprint lithography (NIL) with flexible stamps is an opportunity. In the present work, examples on manufacturing processes and modelling tools applied for precise transfer of nanostructures will be presented.

2. Methodology

The overall concept of transferring nanostructures from a planar wafer to a double-curved injection moulding tool insert the application of NIL with a flexible stamp that is able to deform, matching the geometry of the tool insert, see **Fig. 1**. As the nanostructure consists of very small and precisely defined patterns, deformations can change their functionalities in a detrimental manner. Therefore, modelling tools for prediction these deformations are essential in further improvement of the technology. In general, two different transfer techniques have been applied experimentally and modelled by the authors: (i) transfer by etching or (ii) transfer by direct imprint.

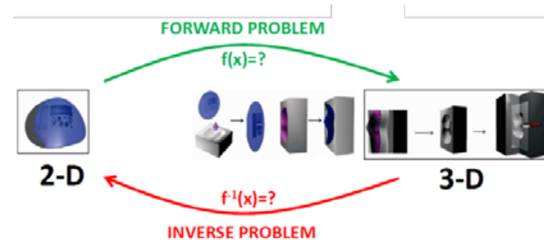

Figure 1. Illustration of the overall concept of transferring nanostructures from a 2-D planar wafer to the double-curved 3-D injection moulding tool insert.

2.1. Transfer by etching

In this process the tool insert is coated with a resist, which after NIL acts as an etching mask, see **Fig. 2**. The nanostructures are therefore transferred directly into the steel surface of the tool insert.

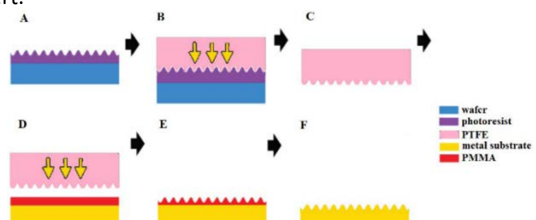

Figure 2. Schematic illustration of the manufacturing process, from nanostructures on a wafer (A), replication of the flexible stamp by hot embossing (B-C), further on to thermal-NIL into a resist material (D-E) to the final isotropic etching into the injection moulding tool substrate (F).

2.2. Transfer by direct imprint

In this process the tool insert is coated with a material (in this case hydrogen silsesquioxane (HSQ)), which will constitute the original steel surface and contain the nanostructures, see **Fig. 3**.

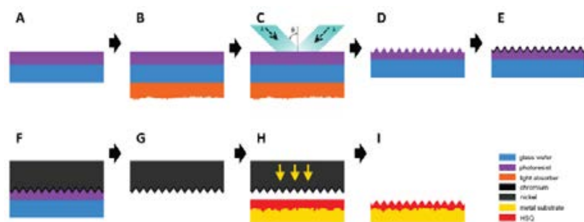

Figure 3. Schematic illustration of the manufacturing process, from preparation of the the wafer (A-D), to electroforming the flexible foil (E-G), further on to nanoimprint lithography into the material HSQ on top of the final metal substrate (H-I).

2.3. Numerical modelling tools

Modelling the deformation of an imprinting flexible stamp is not trivial, since many different non-linearities have to be taken into account in order to get proper results; large deformations make the geometrical calculations non-linear, the materials can act elasto-plastic, and finally, contact between substrate and stamp adds another non-linearity to the system of equations, which all have to be addressed. For calculation of the displacements, strains and stresses, a mechanical model based on the solution of the three static force equilibrium equations is utilized, i.e.

$$\sigma_{ij,i} + p_j = 0$$

for *i,j* = 1..3, where p_j is the body force at any point within the nickel foil and σ_{ij} is the stress tensor. Large strain theory is applied, meaning that the Green-Lagrange finite strain measure is used

$$\boldsymbol{E}^{\boldsymbol{G}} = \frac{1}{2}(\boldsymbol{X}\boldsymbol{X}^{\boldsymbol{T}} - \boldsymbol{I})$$

where $\boldsymbol{X}$ is the deformation gradient and $\boldsymbol{I}$ is the identity matrix. The constitutive model is applied via large strain elasto-plasticity, i.e. the elastic and plastic parts are decomposed by multiplicative decomposition of the deformation gradient. The transient, quasi-static mechanical models are implemented in the general purpose finite element software ABAQUS, in which the option for non-linear geometry is activated utilizing the Updated Lagrangian Formulation. Different material models (i.e. elasto-plastic or viscoelastic) have been used depending on the flexible stamp material (metal or polymer).

3. Applications

Different cases applying the two different approaches for the transfer of nanostructures have been simulated by the authors. For the transfer by etching, a polytetrafluoroethylene (PTFE) flexible stamp was used to transfer a glitter pattern into a poly(methyl methacrylate) (PMMA) resist used as a mask for futher etching into the surface of a concave injection moulding tool insert [3]. Transfer by direct imprint has also been performed, where a sinusoidal cross grating was imprinted into a HSQ resist utilizing a stamp made of nickel [4]. This approach has been further optimized with replications performed with a thick polymethylsiloxane (PDMS) stamp unto an ultra-precision diamond turned concave injection moulding tool insert with results showing a much better. In all these cases numerical modelling has been used to predict the deformed geometry and stretch of the flexible stamps, which then can be used to compensate the original 2-D wafer design.

4. Results

In **Fig. 4**, the transfer of a nanostructure consisting of plasmonic pillars from 2-D wafer to a 3-D double-curved tool insert and further on to the replicated polymer part is shown.

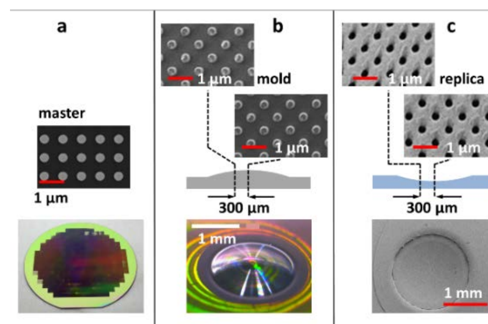

Figure 4. Photos and scanning electron microscopy (SEM) images of a) the master on a wafer, b) the mold with imprinted nanostructures and c) the replicated polymer part.

In **Fig. 5**, comparison of the period of the nanostructure measured on mold and replica, produced with the direct imprinting technique and predicted via the developed modelling tool, is shown (normalized with respect to the original period of 426.2 nm)

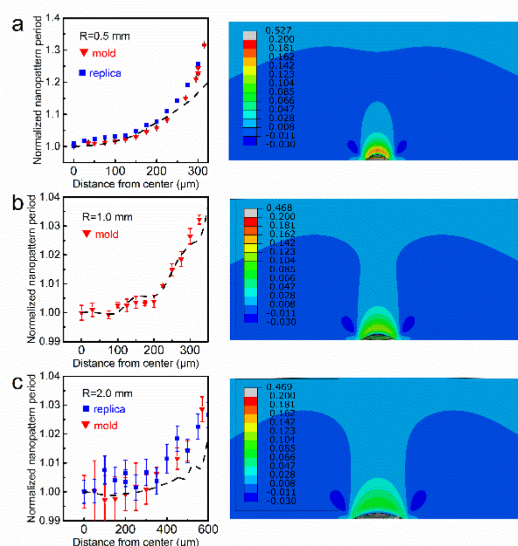

Figure 5. Comparison of measured and modelled (dashed line) changes of the nanostructures characteristics as a function of the distance from center for imprint on substrates with different radius of curvature: a) 500 µm, b) 1000 µm, c) 2000 µm.

The error bars in **Fig. 5c** indicates the combined uncertainty from the curing process and the SEM characterization. Good agreement between measurements and simulation validates that the model is able to predict the large deformations of the flexible stamp (see the contour plot of the maximum principal strain at right side of **Fig. 5**).

5. Conclusion

Modelling tools for simulating the deformation of flexible stamps in precise transfer of nanostructures from silicon wafers to double-curved tool inserts has successfully been developed, enabling the prediction of stamp deformation during the manufacturing processes.

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