euspen's 21st International Conference & Exhibition, Copenhagen, DK, June 2021
www.euspen.eu

Investigation of a replication technology for nano structured diffraction optics

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Abstract
Dispersive spectroscopes are built out of at least two optical functional properties, one diffractive element and one mirror for beam shaping. The systems require precise assembly of the optical elements to avoid intensity loss, absorption and aberrations. By combining imaging and diffractive properties within one hybrid-optical element, the overall system efficiency can be enhanced while the assembly effort is considerably reduced. However, challenges are to be faced during manufacture of diffractive and hybrid-optical elements using various micro machining technologies. The requirements regarding form, structure and surface quality could reach sub-nanometre range. These requirements are costly and time-extensive for plane diffractive elements, and even more so when manufacturing hybrid-optics. To compensate these drawbacks, replication technologies are used to manufacture medium up to high size batches of various diffractive elements at reduced time and cost per part. To meet the quality demands, adequate resists, compensation of geometrical form failure by adjusted illumination and positioning, as well as appropriated casting and demoulding are essential. This requires understanding of the polymerization process and the investigation of the replication method. In this work a two-step replication procedure is proposed where a pre-form is manufactured by replication of an original master. The pre-form is used then to finally replicate optical elements. The pre-forms, transition molds of UV-PDMS and optical elements consisting of hybrid polymers with a curvature up to R = 75 mm are explored. The masters were manufactured employing ultra-precision shaping and milling processes. Nano imprint lithographic process is investigated as alternative and/or complementary processes to manufacture masters for curved structured optical elements. The preservation of geometrical and surface quality of curvature and nano structures are of highest importance. Blaze-gratings produced by means of two-step replication were analysed regarding reproduction accuracy using atomic force microscopy. The investigation proved the feasibility of the replication method proposed for manufacturing diffractive optical elements.

Hybrid polymers, Replication, Nano structure, Lithography

1. Introduction

Ultra-precision machining (UP-machining) for manufacturing optical-components has been employed since the beginning of the 70s [1]. Despite being very accurate and capable of manufacturing metallic components with excellent surfaces, UP-turning and milling are very time-consuming; even nowadays [2]. Therefore these processes are not alone suited for large scale production of optical elements in a short time.
Complex optics such as diffractive optical elements (DOE) are used in various applications and in different amounts. For instance, in aerospace industry usually single pieces of DOEs are required, while for handheld spectrometers for the mass market a large scale production of DOEs is required [3]. This large scale production can be achieved by creating a production-chain including ultra-precision machining of master structures and their subsequent replication [4]. This production-chain has the potential to significantly decrease the cost of production per single element.
For replicating curved optical elements, approaches like using a planar structured surface which is fitted to a curved substrate is feasible [5,6]. But limitations are found towards moderate curvatures due to the structural changes caused by the deformation during moulding. However, in a curvature of about 1 m, the efficiency losses due to the shape changes could be kept in a range of less than 10% [5]. Replication methods have been an important topic and focus of discussion in several investigations. However, due to the limitations of these technologies, a field of investigation for replication of micro-optics with strong curvatures remains.
This paper aims to clarify the problems involving thin-film replication of nano structured DOEs in comparison to volume replication methods. In this context, investigations of the influence of the polymerization process on the blaze-angle structure (nano structure) of a thin-film replication and the complete volume material using lithographic process in are explored.

2. Experimental set-up and methodology

To further understand the advantages of thin-film replication, a comparison of thin-film and volume replication of master nano structured workpieces were explored. Investigations started with thin-films replications of a planar nano structured workpiece with the UV-curable hybrid polymers OrmoStamp®, OrmoComp® and OrmoClear®FX (micro resist technology GmbH, Germany) and the UV-curable material polydimethylsiloxane (UV-PDMS KER-4690, Shin-Etsu Japan). Hybrid polymers were selected due to their organic-inorganic composition, which provides outstanding optical transparency, high thermal and chemical stability as well as excellent mechanical properties. UV-PDMS is used for generating soft-molds in replication technologies such as nano imprint due to its mechanical

properties. This material is useful for generating flexible transition molds that enable easy extraction.
Furthermore, the volume replication of the curved master optics with and without nano structures were conducted using OrmoComp®. At this step an UV-PDMS transition form is produced. This form is filled with liquid hybrid polymer which subsequently is polymerized by UV-light. Once the polymerization process is complete the transition form is removed. Afterwards, aluminium is deposited on the surface by a PVD process. The thin-film replication step consists of depositing a thin layer of OrmoComp® on the volume replicate, once polymerized. this process is followed by deposing an aluminium layer. **Figure 1** represents a scheme of both replication methods compared.

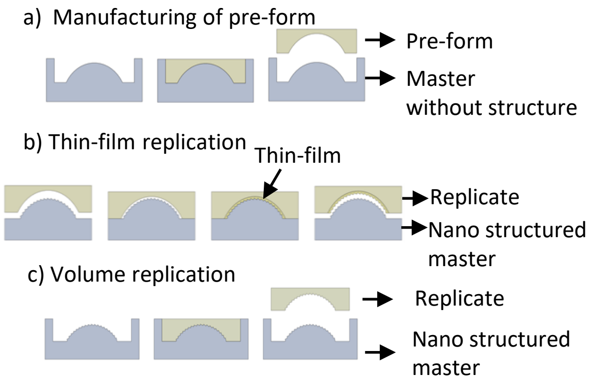

Figure 1: Replication methods compared

To discern the problems encountered during the volume and thin-layer replication methods, curved and plane nano structured master samples were manufactured by ultra-precision machining using diamond machinable materials, e.g. RSA-501 with curvature radius R = 74,9 mm, NiP with R = 20 mm, and gold, due to the capability of achieving a very precise and smooth blaze-structure surface. Curved pre-form masters were used to further understand the form deviations observed at the replication process. The curvature radii of the replicates were measured by a chromatic sensor, in which the maximum depth coordinates in X and Y axes were found, then profiles were traced in X and Y direction. These profiles are then analysed using a circle fit function using the Taubin method to approximate the curvature of the replica. **Figure 2** shows the circle fit of a measured profile. Additionally, the residual differences of the replicas to the circle fit were also calculated.

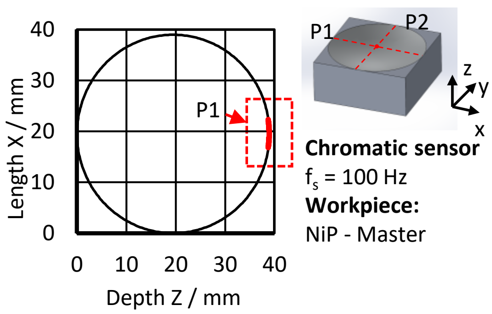

Figure 2: Example of Circle Fit analysis of a replicated optic

Plane nano structured surfaces were manufactured in a gold layer on an aluminium substrate. This master sample was used to investigate the influence of the hybrid polymers and layer thickness upon the nano structured replica. The nano structured master and replicas were measured by atomic force microscopy (AFM). **Figure 3** shows the nano structured curved master of a) RSA-501, and b) NiP. While **Figure 3** c) and d) shows the planar gold master-structures.

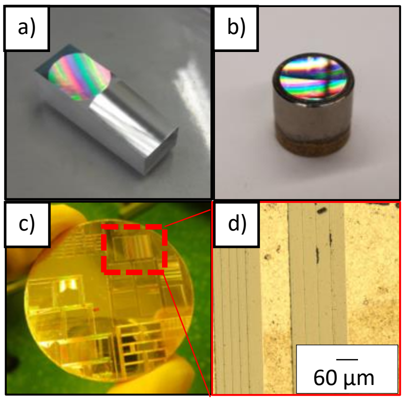

Figure 3: a) RSA-501, b) NiP master nano structured curved DOE, c) plane nano structured gold master d) microscopy image of the structures

3. Results

3.1 Thin-film replication of nano structures

To explore the influence of hybrid polymers on the nano structures, the gold master with blaze angle α = 2,72° and a separation of D = 5 µm was replicated using OrmoStamp®, OrmoComp® with and without hardbake (3 hours at 150 °C), OrmoClear®FX with hardbake (3 hours at 150 °C) and UV-PDMS. OrmoStamp® and OrmoComp® without hardbake are used for replications directly from the master, while the others are used for replications from the stamp. **Figure 4** a) shows the blaze-angle alterations and b) the roughness of the replicates and the master. The measurements were performed by AFM.

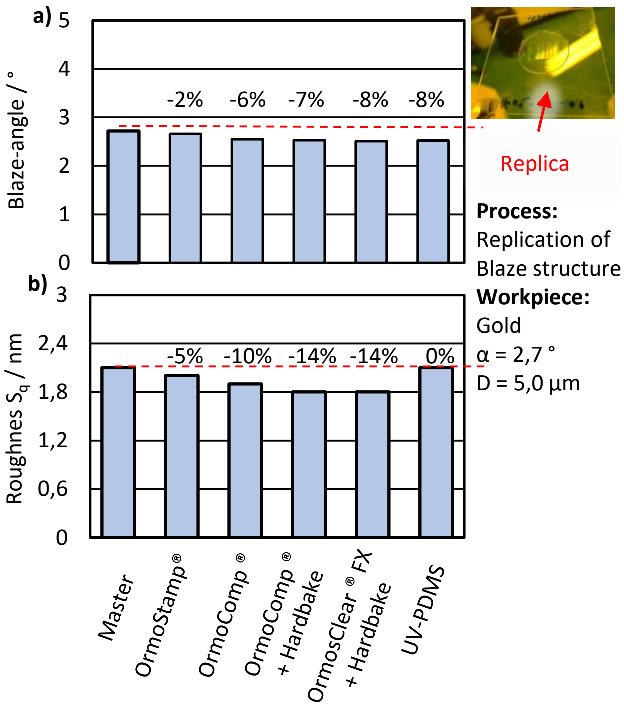

Figure 4: a) deviation of blaze angle and b) blaze roughness of a plane master grating and its replications made of different hybridpolymers and UV-PMDS

The diagram on **Figure 4** a) shows a maximum of 8 % reduction of the blaze-angle structures using polymers such UV-PDMS and OrmoClear®FX with hardbake. This data is essential and will later be used to compensate the volume reduction in future investigations. **Figure 4** b) shows an improvement of surface roughness up to 14 % as a consequence of the replication process. To further understand the influence of the layer-thickness on the process, two replicates applying thin-film layers with thickness of 70 µm and 260 µm were manufactured using the planar master workpiece. **Figure 5** represents the alterations of surface of the nano structure with a) thin-film of 70 µm and b) 260 µm, indicating a significant improvement of the surface roughness S_a using a thin-film layer of 70 µm.

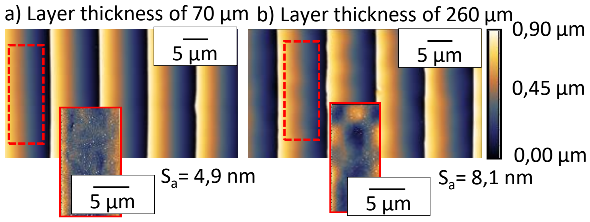

Figure 5: 2D-Plots of AFM measurments and the calculated roughness of replicas on a layer with a) 70 µm and b) 260 µm

3.2 Volume replication of curved elements

To replicate the curved optical element with and without nano structure, a transition mold is used to produce the curved pre-forms. This transition mold is a cast from the metallic master. UV-PDMS is used for the casting. UV-PDMS has an extremely low shrinkage of 0,02 % when cured at room temperature, is UV transparent, has low adhesion, is flexible, and can replicate accurately both micro and macro structures. Because of these properties, transition molds made of UV-PDMS are ideally suited. Due to the two step replication, the curvature (convex/concave) of the resulting pre-form is the same as that of the master. To produce the transition mold, the metallic master is placed in a casting mold. The UV-PDMS is mixed from two components and poured into the mold. To prevent air entrapment, the filled mold is degassed in a vacuum chamber before polymerizing. Afterwards, the filled mold is placed in a UV-chamber and, depending on the UV-PDMS quantity and thickness used, exposed for a defined time to achieve the necessary properties (**Figure 6-1**). After the exposure process, the mold is stored for several hours for relaxation at room temperature (**Figure 6-2**). As a final step, the metallic master is removed from the cured mold (**Figure 6-3**) and the resulting UV-PDMS mold is available for further process steps (**Figure 6-4**). The same steps were conducted for the NiP master structure with and without nano structures and is shown in **Figure 7**.

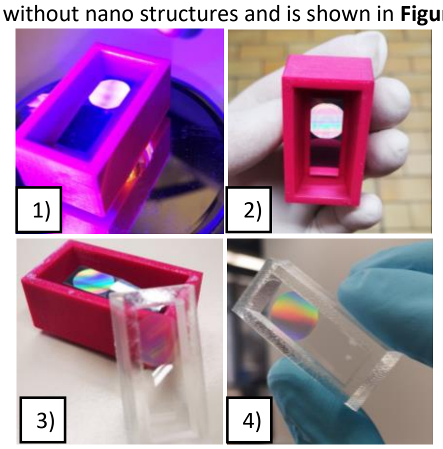

Figure 6: Steps taken to the production of a transition mould of the RSA-501 master, being 1) mold filling and polymerization, 2) relaxation, 3) removal of the mold, and 4) UV-PDMS transition mold

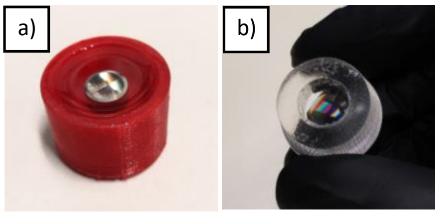

Figure 7: a) mold filling and b) transition mold of NiP master

For the following process steps, a curved master without nano structure was used, so that the transition mold also shows no structure. This mold is now molded via gravity casting. For this purpose, it is filled with a defined amount of hybrid polymer using a pipette. The material is filled in such a way that no air pockets are formed. The quantity of hybrid polymer is measured with a precision scale. The filled transition mold is sealed with an UV-permeable glass support to ensure a flat back surface. The shrinkage of the hybrid polymer (material and post treatment dependent about 3 to 9 %) must also be considered in this process step. Since the polymer shrinks most probably first where it has reached the corresponding dose, this means that the side facing the light source initiates the shrinkage and pulls material from areas that have not yet been cured. Therefore, at this step, the exposure is always from the direction where the critical structural features are. After exposure, the filled mold is also exposed to the calculated dose and then demolded. The resulting pre-form from this process is used for further considerations and for the thin-film replications.

For the analysis proposed in this section, replication experiments of a curved master with no nano structure were performed. **Figure 8** shows the residual difference from a volume-replication without nano structures.

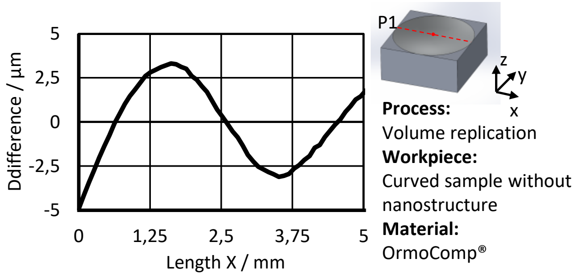

Figure 8: Deviation of the Circle-Fit of a curved replica without nano structures by volume replication

3.3 Volume replication of curved elements with nano structure

At the investigation proposed in this section, a curved nano structured master was used. The replication process was analysed by measuring the form deviations and nano structure. The form deviation is represented in **Figure 9**.

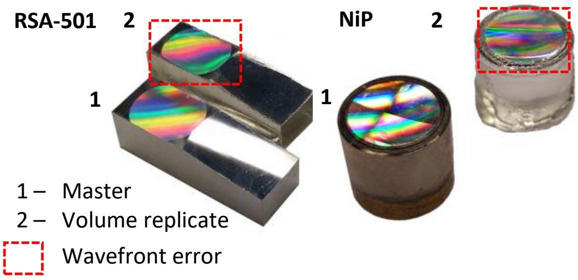

Figure 9: Wavefront error of RSA-501 and NiP curved replicas with nano structure

As presumed, the volume reduction of the hybrid polymer during polymerization has influence on the waviness of the curved surface of the optical element.

3.4 Thin film replication of curved elements with nano structure

The replication using thin-film starts with same procedure of replicating volume curved elements without nano structure. However, an extra-step is added which consists of pouring a thin layer of hybrid polymer on the volume replication once the hybrid polymer is completely polymerized. Then, the transition mold is placed on the surface of the volume replica. **Figure 10** presents the results comparing the replicate using volume and thin-film method.

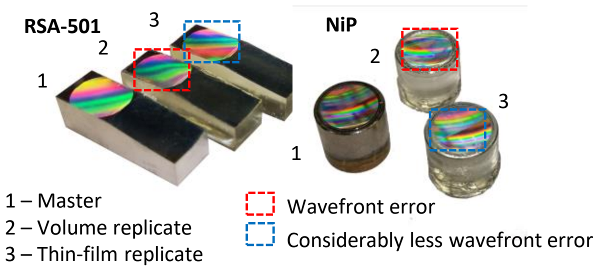

Figure 10: Example of replicas from RSA-501 and NiP masters by using the thin-film and volume techniques

With regard to form deviation, the residual difference of the curved element with nano structure and the circle fit is shown in **Figure 11**. Since the replication was conducted by manual processes, there is room for optimizing the procedure by using an automated system and compensations of the volume reduction. **Figure 12** shows the AFM measurement of the nano structures of the thin-film replicate and the volume with nano structures and master.

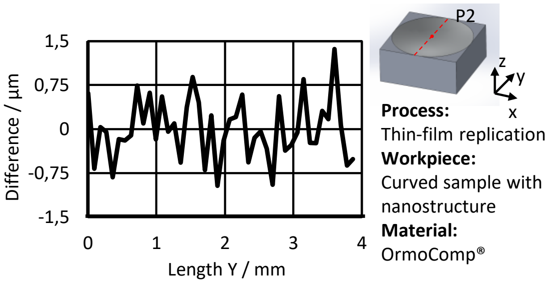

Figure 11: Deviation of the Circle-Fit of a thin-film replica with nano structures by thin-film replication

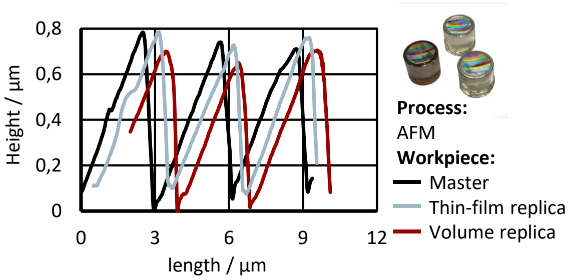

Figure 12: AFM-profiles of master, thin-film and volume replicas

4. Discussion

With regard to the replication of the nano structures, there was no indication of significant changes for a rougher surface despite using different hybrid polymer and UV-PDMS material during the replication process. However, the thickness of the deposited thin-film layer can influence negatively the process due to an increase of the waviness and roughness of the blaze grating surface. A similar result was also found by analysing the different replication techniques. It was shown that the volume of applied hybrid polymer has a negative influence on the nano structured surface of the replica. As a consequence, the polymerization process inflicts alterations and shrinkage to such an extent that the waviness of the surface can clearly be seen by the naked eye. However, a promising method to increase the quality of the replicas is by deposing a thin layer of hybrid polymer on the precedingly replicated volume and again placing it against the transition mold in order to capture the nano features in a layer of hybrid polymer which is much less impacted by shrinkage due to its comparatively much smaller volume and its uniform thin film.

However, the methods of measuring the optimal thickness of a deposited layer on a curved surface need to be significantly improved to render better results. Additionally, the replication process was mostly conducted manually. In order to have a more controlled environment, the replication of volume and also thin-film should be further investigated using a multi-axis replication machine.

5. Conclusion

Some significant alterations on the nano structures in the replication process by thin-film were observed. This volume reduction alters the blaze-grating geometry, specifically the blaze-angle $\alpha \leq 10\%$ and alterations on the surface roughness down to $S_a \leq 14\%$. This information is crucial for further compensation during the replication process or during the UP-machining of the master structure. However, due to the difference of the waviness on the surface of the volume replication of curved DOEs with nano structure elements, thin-film replication is proven to be a more promising approach in order to accurately replicate curved nano structured optical elements. To further improve the thin-film replication, the exact amount of reduced volume has to be compensated. Additionally, the replication method needs to be carried out in a multi-axis replication machine for a more controlled enviroment and to deposit thin-films with a micro meter precision.

6. Outlook

For future investigations and developments, a multi-axis replication machine will be available to generate a more precise approach to conduct both replication methods. Moreover, different UV-exposure strategies along with demolding procedures are currently being investigated.

Acknowledgement

The authors would like to acknowledge the financial contribution of the “Investitionsbank Berlin” – IBB and the support of the project partner Nano Optics Berlin GmbH. The authors also would like to acknowledge the contributions of the student Alice Wamser.

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