Mold machining and injection molding of diffractive microstructures

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A R T I C L E  I N F O

Article history:
Received 23 November 2016
Received in revised form 9 February 2017
Accepted 16 February 2017
Available online 17 March 2017

Keywords:
Injection molding
Diffractive microstructure
Diamond turning

A B S T R A C T

Diffractive microstructures are used for many applications due to their unique optical functionalities, e.g. as security features on banknotes or documents. By developing more complex microstructures which almost cannot be copied, the protection against counterfeiting can be improved. This paper introduces a modified diamond turning process to machine such kind of functional microstructures. A fast-tool-servo assisted diamond turning process is presented, which enables machining of holograms consisting of diffractive microstructures with an overlaying pattern. The resulting structure is capable of shaping incident light into a defined intensity distribution. Such holograms could be used as security tags or be embossed in plastic packaging of valuable products. In order to make this technology accessible to mass production, replication of the microstructures by injection molding is essential. To investigate the replicability by injection molding, a blazed structure was diamond turned into a mold, identical to the basic structure of the holograms. Three optical polymers (polymethylmethacrylate PMMA, cyclic olefin copolymer COC, cyclic olefin polymer COP) were used for injection molding experiments to investigate the filling behavior of the mold and the replicated quality of the diffractive microstructure.

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1. Introduction

Diffractive microstructures offer unique optical properties and are used for a wide variety of applications. Ranging from classical spectroscopic gratings and intra-ocular lenses to security features on banknotes, complex optical functionalities can be achieved [1]. Especially for security applications, constantly improved and highly functional microstructures are required to ensure a sufficient protection against counterfeiting. The complexity and thus the functionality of the microstructure largely depend on the kinematic options and precision of the machine tool. Common manufacturing processes for machining of diffractive structures are lithography, laser machining or diamond machining, which are distinguished by small structure sizes and short working wavelength [2].

Diamond machining processes have proven to be suitable for machining discontinuous microstructures and freeform surfaces. The high machining accuracy enables this process to machine advanced functional optical surfaces [3,4]. Typical diamond machined structures consist of mainly constant features in feed direction. One example are blazed gratings which can be a reliable alternative to electron beam lithography in terms of holographic fabrication [5,6]. Another example are Fresnel lenses. By using of non-rotational diamond cutting tools even multiple-focus micro Fresnel lenses can be machined with higher accuracy than lithography processes [7,8]. Both examples are having structure sizes ranging from a few hundred nanometers to several micrometers. More complex structures can be generated by an additional in-process tool movement, in order to adjust the depth of cut dynamically. Such a fast tool servo assisted turning process would enable the machining of even multi-leveled as well as freeform diffractive optical elements. The inexpensive, fast and extremely flexible machining process can be used also in the prototype fabrication for injection molding [9,10]. The technology used in the paper is based on a nano Fast Tool Servo (nFTS) as proposed by Brinksmeier et al. [11], which modulates the depth of cut in the nanometer range for machining of diamond turned holograms (DTH).

Previous research in this field has demonstrated that an excellent geometrical precision can be achieved by diamond turning [12]. However, in order to make this technology accessible to mass production, a replication of the structured surfaces is essential. In this paper, fundamental experiments are carried out to investigate the replicability of diamond turned blaze gratings by injection molding. Experiments were conducted using the different optical
polymers (polymethylmethacrylate PMMA, cyclic olefin copolymer COC, cyclic olefin polymer COP). The filling behavior of the mold and the replicability of the diffractive microstructure were of primary interest and thus evaluated by measuring the structures with an atomic force microscope (AFM) as well as with a white light interferometer (WLI).

2. Machining of diffractive surfaces

The manufacture of the diamond turned holograms (DTH) is achieved by a face turning process, implemented on a Precitech Freeform 3000 ultra-precision machine tool. Due to the local height levels, diffractive holograms are capable of modulating the phase of laser radiation to generate a defined intensity distribution (cf. Fig. 1 cross section A-A). As the local height levels are ensuring the functionality of the resulting holographic structure, the depth of the cut needs to be dynamically adjusted. Therefore, the classical diamond turning process is combined with a piezo driven nano Fast Tool Servo (nFTS) with a frequency of up to 10 kHz. The maximum stroke of the nFTS measures 350 nm and it is able to modulate the depth of the cut with a positioning accuracy less than 4 nm, which is required to achieve the high quality of the holographic structures. In combination with a spindle speed of \(n = 100 \text{ min}^{-1}\), the nFTS is able to generate 2000 segments per revolution, each having a specific height level depending on their radial position \(q\) on the helical tool path. The radial position of each segment is derived from the angular encoder of the main spindle, which is used as a trigger for initiating the nFTS movement.

The tool is a monocrystalline diamond with a wedge-shaped geometry, having a nose angle of \(\varepsilon = 84^\circ\) and a structure angle \(\kappa = 6^\circ\) (cf. Fig. 1 cross section A-A). This specific tool geometry combined with the process kinematics is generating the spiral-shaped blaze structure on the surface. The clearance angle \(\alpha\) is limiting the maximal angle which the tool can generate while moving into the workpiece. To obtain higher structure accuracy the clearance angle \(\alpha\) needs to be relatively large, in this case \(\alpha = 20^\circ\).

There are several requirements regarding the workpiece material, in order to achieve diffractive optics with excellent surface finish. The material needs to be machinable by diamond turning and the resulting surface has to meet optical quality (i.e. roughness \(Sa < 10 \text{ nm}\)). The functionality of holographic structures is highly depending on the contouring accuracy and a minimal Burr formation. In former investigations, several nickel silver alloys, which have been proven to be machinable by diamond turning, were examined for applications in the field of visible light. Nickel silver shows a high hardness as well as no significant tool wear and thus, it is advantageous for machining of sharp edges. From a wide range of alloys with specific characteristics CuNi8Zn42Pb4Mn1 (N31) has been chosen, because of its excellent machinability. The relatively high percentage of lead (4%) leads to low cutting forces and little burr formation. Together with the formation of short chips, this results in significantly less tool wear and an excellent surface finish [12]. The high content of Zinc (42%) is also advantageous for diamond turning, inducing a better machinability and less deformations [13]. These improvements are resulting in less surface defects, a high contouring accuracy and lower roughness values \((Sa = 5 \text{ nm} \text{ on top of the optical effective surfaces of the blaze structure})\) [11]. The optical effective surface is the surface which is showing the provided structure angle \(\kappa\) as well as the specific height level and is reflecting the incident light in the intended way by shifting the phase of the reflected wave front (cf. Fig. 1 cross section A-A).

3. Mold machining

For the assessment of the replication process, continuous blaze structures without height modulation were diamond turned on an ultra-precision machine tool. Table 1 shows the process parameters as well as the material and geometry of the cutting tool. For cooling, a paraffin spray mist was chosen. As discussed in chapter 2, nickel silver N31 was adjudged to be the most suitable mold material.

Under these machining conditions, the blaze structure was transferred into the mold by diamond turning. In Fig. 2(a) the mold insert is shown. The surface topography of the blaze structure is shown in Fig. 2(b). A white light interferometer (Talysurf CCI HD, Taylor Hobson) was used to measure and evaluate the geometry of the blaze structure, which will be compared with the molded surfaces in chapter 4.

The surface topography is smooth and sharp edges can be detected, which are required for high performance optical applications. In Fig. 2(c), the surface profile A-B is shown. Based on this profile, the structure height \(h\), the length of the optical effective surface \(s\) and the structure angle \(\kappa\) have been measured on each structure element. Afterwards, the average and the standard deviation were calculated over the measured values for each parameter respectively. In Table 2 the results of this analysis are listed. It can be seen, that the average structure angle equals 6.6°. This deviation from the desired structure angle \(\kappa = 6^\circ\) is not decisive for the finally
desired optical functionality. The actual structure can be assessed by pre-machining and measuring of a witness sample and will be considered in the optical design algorithm. Therefore, the diamond tool in the machining process can be adjusted more roughly and not perfectly to that specific nominal angle. Optional the structure angle can be set in advance to a fixed value for the optical design calculation; then a very accurate alignment for the diamond tool to that angle is required. Here, the first method which is much easier to handle from a practical point of view was applied. The structure height was measured to 0.96 μm with a standard deviation of 0.02 μm and the structure width as 8.36 μm with a standard deviation of 0.18 μm, thus the intended geometry was achieved within good agreement to the nominal structure.

4. Replication by injection molding

The replication experiments were carried out on an “Arburg Allrounder 221k” screw-type injection molding machine with a cold-runner and pre-heated tool, using Polymethyl Methacrylate (PMMA), Cycle-Olefin-Copolymer (COC) and Cycle-Olefin-Polymer (COP). In Fig. 3 the machining setup can be seen. The movable plate of the tool holds four cavities for exchangeable cylindrical tool inserts with a diameter of 40 mm each [14].

In these experiments, one cavity is equipped with the blaze insert, while the opposing cavity produces a plane cylindrical disc of comparable size in the same injection cycle. The other two inserts were not active in this injection molding setup. Two opposing molds on the same runner were chosen to enable a symmetric melt flow, originating from the runner at the center of the plate.

Injection molding requires carefully adjusted parameters, such as melt and tool temperature, filling speed and packing pressure. Table 3 gives an overview of parameter settings, which were used in these experiments. Weighing and visual inspection of the molded parts established a suitable packing time of 5 s, regardless of the material [13]. The overall shot-weight per injection is approximately 14 g for both parts and the runner. No releasing agent was applied.

<table>
<thead>
<tr>
<th>Structure height (h_s)</th>
<th>Length of the optical effective surface (s)</th>
<th>Structure angle (\kappa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average</td>
<td>0.96 μm ± 0.02 μm</td>
<td>8.36 μm ± 0.18 μm</td>
</tr>
<tr>
<td>Standard deviation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table 2**

Average geometry of the mold before injection molding.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA</td>
<td>80</td>
<td>240</td>
<td>20</td>
<td>650</td>
</tr>
<tr>
<td>COP</td>
<td>100</td>
<td>245</td>
<td>20</td>
<td>300</td>
</tr>
</tbody>
</table>

**Table 3**

Injection molding parameters.

![Fig. 2. (a) Diamond turned mold insert, (b) Surface topography measured with a white light interferometer and (c) extracted surface profile A-B.](image1)

![Fig. 3. Injection-Molding Machine (left) and movable tool plate with blaze insert (right).](image2)
5. Molded parts and tool inspection after molding

Generally, it is expected that polymers with a very low viscosity at melting temperature (e.g., COP) are very suitable for the replication of microstructures [14]. In these studies, however, the best replicating results were achieved by using PMMA with a significantly higher viscosity at melting temperature.

The surface topography of the molded parts was measured at a point distant to the gate by using an atomic force microscope. The topography of the molded PMMA part in Fig. 4(a) appears to be a true negative representation of the mold with evenly tilted optical effective surfaces and sharp edges, whereas the replications in COP and COC reveal blunt edges and curved flanks. The 10 μm lateral spacing of the blaze is well visible in each material.

The geometric trueness of the moldings is indicated by the replicated length of the optical effective surface (s) and the overall height (h) of the structures as shown in the cross-sections in Fig. 5. The optical effective surface corresponds to the part of the structure, which meets the original structure angle κ. The length of the optical effective surface is approximated by Pythagoras’ theorem as

$$s = \sqrt{s_1^2 + s_2^2}. \quad (1)$$

A perfect replication would yield exactly the same structure height and flank angle (cf. Fig. 2(b) and Table 2) as turned into the tool.

The parts molded from PMMA reveal the best geometric trueness with an average structure height of 0.97 μm and an average structure angle of 6.7°, with a small fluctuation. The structures molded in COC and COP, however, do not match the negative geometry of the tool insert well. The average height of the profile is found to be 0.78 μm in COP and 0.73 μm in COC, respectively. The edge radius is also larger, which leaves a significantly shorter useable flank (cf. Table 4).

Considering the length of the optical effective surface, Table 4 shows that all injection molded surface are deviating from the original height of 0.96 μm to a large extend. The PMMA surface shows an average length of about 6.39 μm with a standard deviation of 0.57 which is the closest approach of the required surface. The large discrepancy between the desired and the produced surfaces with regard to the length of the optical effective surface is critical, considering the high optical demands on the generated surfaces. It is conspicuous that for all injection molded surfaces, the replicated structure angle equals the original structure angle κ significantly (cf. Table 4), which has a positive effect on the optical effectiveness of the molded surfaces.

In Fig. 5, also an edge radius is marked for one structure-element for each material. It is to be noted, that the radius of the circle drawn does not comply with the real edge radius. It is meant only for direct comparison of the different materials. It can be seen, that the COP surface (Fig. 5(b)) as well as the COP surface (Fig. 5(c)) are showing large edge radii. For the PMMA surface (Fig. 5(a)) in contrast, the edge radius is smaller, thus the edges of the PMMA surface are the sharpest.

The tool insert was inspected after the molding experiments visually (Fig. 6 and Table 5). Except from minor burrs at the top

### Table 4

Geometry of the surface profile.

<table>
<thead>
<tr>
<th></th>
<th>PMMA</th>
<th>COP</th>
<th>COC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Average</td>
<td>Standard deviation</td>
<td>Average</td>
</tr>
<tr>
<td>Height h&lt;sub&gt;1&lt;/sub&gt;</td>
<td>0.97 μm</td>
<td>± 0.05 μm</td>
<td>0.78 μm</td>
</tr>
<tr>
<td>Length of the optical effective surface s</td>
<td>6.39 μm</td>
<td>± 0.57 μm</td>
<td>5.59 μm</td>
</tr>
<tr>
<td>Structure angle κ</td>
<td>6.7°</td>
<td>± 0.21°</td>
<td>6.3°</td>
</tr>
</tbody>
</table>

### Table 5

Average geometry of the mold after injection molding.

<table>
<thead>
<tr>
<th></th>
<th>Structure height h&lt;sub&gt;1&lt;/sub&gt;</th>
<th>Length of the optical effective surface s</th>
<th>Structure angle κ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average</td>
<td>0.97 μm</td>
<td>8.24 μm</td>
<td>6.6°</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>± 0.05 μm</td>
<td>± 0.77 μm</td>
<td>± 0.04°</td>
</tr>
</tbody>
</table>

**Fig. 4.** Atomic force microscope image of the injection molded (a) PMMA surface (b) COC surface (c) COP surface.

**Fig. 5.** Surface profile of the injection molded (a) PMMA surface (b) COC surface (c) COP surface.
edge of the triangular grooves, no significant tool wear was found and no adhesive polymer material was observed.

6. Summary and conclusions

In this paper, a modified diamond turning process was presented to machine highly functional diffractive microstructures. The optical functionality of these structures has already been proven under reflective conditions [see Ref. [11]]. In order to make this technology accessible for mass production, the replication of the microstructures by injection molding was investigated. To do so, a mold was diamond turned with a blaze structure. Because of its excellent machinability, N31 was chosen as material for the mold. Subsequently, three optical polymers, PMMA, COC and COP, were used in injection molding experiments to investigate the replicability of diffractive structures. The produced surfaces have been investigated according to the filling behavior of the mold and the replicability of the diffractive microstructure.

The best replications were achieved in PMMA, while the molded structures in COC and COP appeared to be blunt and the length of the optical effective surface was undersized compared to the tool. Packing pressure and mold temperature were well chosen to yield useful replications in PMMA. In the molding of the olefin polymers, however, shrinkage in the final polymerization stages of the material may have led to the geometric deviations observed.

It has been seen, that in any case shrinkage occurs in a molding process. This will influence the replicated structure, and thus the optical functionality of the molded part. For a perfect replication, the mold design, in our case, mainly the blaze angle, should be adjusted in an iterative design of machining and measuring loops, in order to obtain the intended angle on the molded part. Also, active cooling (quick-freezing) or the application of a compression-injection tool [15] will have to be considered. Generally, melt rheology, heat convection and heat conduction for tools with microscopic structures have to be further investigated. Finally, the optical functionality of these molded parts will be shown in future investigations.

Acknowledgements

This research paper was conducted as a cooperative work of the Laboratory for Precision Machining in Bremen and the Beuth University of Applied Sciences in Berlin, Germany.

The authors gratefully acknowledges the Volkswagen Foundation for funding this work (I/83 979, I/83 980, I/83 981) within funding initiative “Innovative Methods for Manufacturing of Multifunctional Surfaces”.

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