Economic fabrication of a novel hybrid planar Grating/Fresnel lens for miniature spectrometers

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Abstract: We propose a new technique to fabricate a highly specialized optical element, a hybrid planar Grating/Fresnel lens (G-Fresnel), which is particularly useful to improve or enable more-affordable miniature/portable spectrometers. Both the Fresnel and the grating surface are fabricated simultaneously by sandwiching soft PDMS between a hard grating and a pre-replicated negative Fresnel surface. Several adhesion reduction techniques are also investigated that help improve both fabrication and cost efficiency (by reducing the solidification time) as well as the lifetime of the mold. Alignment errors are systematically analyzed, and their effects on the G-Fresnel lens evaluated. A compact fabrication platform was built, which is smaller than a volume of $160 \times 140 \times 106 \text{ mm}^3$ to fit into a conventional vacuum drying oven, for the fabrication of a G-Fresnel lens with a diameter of 25.4 mm, an equivalent focal length of 25 mm, and a blazed grating pattern with 600 lines/mm spacing. The solidification time was reduced to 2 hours thanks to the improved adhesion reduction technique that permits a PDMS drying-temperature as high as 65 °C. The fabricated G-Fresnel lens was evaluated with regard to both geometrical fabrication precision and optical performance. The measured results, using a step gauge and atomic force microscopy, confirm that this replication technique produces high-quality replicates of the master surface-profile. Furthermore, a prototype spectrometer that uses a G-Fresnel lens was built and evaluated. The spectrometer fits within a volume of about $100 \times 50 \times 30 \text{ mm}^3$, and it operates across a wide wavelength spectrum (450 nm to 650 nm). Both the calculation based on the optical software ZEMAX and the experimental measurements are consistent and confirm that the spectrometer with the G-Fresnel lens can provide a spectral resolution of better than 1.2nm.

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1. Introduction

Compact and portable spectrometers are essential instruments for many biological, medical, and environmental measuring tasks [1–3]. Thanks to recent rapid progress in spectrometry research, modern spectrometers can meet the majority of today’s scientific and engineering applications. However, the typically used discrete optical components, which include a curved collimating collecting mirror and a diffraction grating, make spectrometers relatively complex devices, large, and expensive.

Attempts to tackle these limitations include the use of concave gratings, volume holographic spectrometers (VHSs), and grating/Fresnel lenses [4–12]. A concave grating combines the light collimation, collection, and diffraction in one device [4–7]. However, the two conventional methods used to fabricate diffraction gratings, mechanical ruling and holographic recording, are of limited help if devices with a larger numerical-aperture are required. The VHS design eliminates the entrance slit, and combines the collimation and the curved collection mirrors with the grating by using a volume hologram [8–10]. This hologram, however, is affected by the spatial incoherence of the incident beam. Compared to the concave gratings and the VHS, the grating/Fresnel lens (G-Fresnel) has two advantages with respect to light dispersion and focusing capability. This is because it can provide a larger numerical aperture and thus more compact dimensions without significant reduction in resolution [11,12]. In addition, its planar surface permits less expensive mass-production because replication can be done from master patterns. In other words, the G-Fresnel has good chances to produce commercial less expensive and more compact spectrometers available in the future.

During the past several years, however, not many researchers have studied the G-Fresnel systematically. One study focused on a PDMS based soft lithography technology, which was introduced to form the G-Fresnel lens and used in a spectrometer [12]. In this paper, a novel double casting technique is used to fabricate a prototype G-Fresnel lens with a resolution better than 1.2 nm. Even though the casting process is simple in principle, it is time-consuming because the double casting process requires a significant amount of time to solidify the PDMS. Moreover, its high resolution can only be achieved for a short spectral range (20 nm). There are also no reports of systematic efforts to improve G-Fresnel lens design. Here, we demonstrate a
new process to modify the soft-lithography-based fabrication process of a G-Fresnel that allows a reduction of the fabrication time to less than 5%. Furthermore, using the new G-Fresnel, we could build a spectrometer with a better than 1.2 nm resolution across a 200 nm spectrum. Fabrication process, system design and construction, as well as an evaluation of the spectrometer performance are explained and discussed.

2. Theoretical background

Figure 1 shows a schematic of a spectrometer that uses a G-Fresnel lens. An incident beam, which comes from a slit or a point source (A), is collimated at the Fresnel surface and diffracted at the grating surface. The grating surface can be characterized by the differing shapes of the surface features: rectangular, sinusoidal, or triangular. In this study, the triangular shape was selected to blaze the first order diffraction beam, so that the energy of this diffraction order can be focused to improve sensitivity.

As illustrated in Fig. 1, both light-focusing and diffraction are accomplished using both surfaces. In other words, the fabrication of high-quality surfaces is important. Among the various available fabrication methods, replication from master patterns is fast and therefore suitable for mass production [12]. Figure 2 shows details of the fabrication of these two functional surfaces. We refer to this production method as the “double casting technique” throughout this paper. The G-Fresnel lens is shaped by two molds, the grating mold on one side, and the negative G-Fresnel mold on the other side.

In the first step, a negative G-Fresnel mold is obtained from a positive Fresnel surface with the same surface-profile of the desired G-Fresnel lens-surface, see Figs. 2(a)-2(c), which is similar with that shown in [12]. To reduce the fabrication time, in our research, a high-temperature drying step was employed. Both the negative Fresnel lens and the formation material consist of PDMS, hence, adhesion is a problem. For this reason, we needed to find a coating that reduces adhesion, see Figs. 2(d) and 2(e). This anti-adhesion layer is thoroughly discussed below, and an evaluation of the fabrication results, in terms of both geometrical profile and optical performance, is presented in the subsequent Sections.
3. Design and fabrication of the G-Fresnel lens

The design and fabrication of the G-Fresnel lens are discussed in this section. The selection of the lens parameters, the spectrometer prototype, the adhesion reduction method, and the fabrication error-analysis are presented.

3.1 Lens parameters and spectrometer prototype

To design a G-Fresnel lens, we need to consider the performance and size targets as well as ensure feasibility of the fabrication. According to a survey of spectrometer specifications for research, the following target specifications were determined: a physical dimension of less than 10×10×10 cm, a spectral range of 450-650 nm, and a resolution of about 1 nm [4,5]. According to the basic imaging principle, the object distance is about half the spectrometer size. Furthermore, a Fresnel lens with an effective focal length (EFL) of 25 mm was preliminarily selected to produce the Fresnel surface mold to ensure suitable dimensions. This number was refined later using the optics design software ZEMAX. We selected a small grating-period because it provides a relatively large diffraction-angle, which helps improve the optical performance. However, a large diffraction-angle and normal incidence increases the distance from the CCD which increases the final size of the spectrometer. After balancing the optical performance and compactness, a 600 lines/mm grating constant (1.66 μm grating period) was selected based on an accurate calculation and simulation.
To evaluate the optical performance of the lens, a miniature spectrometer prototype was constructed by the optical design software ZEMAX. Figure 3 shows a schematic of the spectrometer. We set the G-Fresnel in the center of the coordinate system. The position of the light source was set to \((0, 0, r_a)\), and the distance between light source and Fresnel surface is denoted as \(r_a\). According to the fundamental principle in geometric optics, the imaging system can be most compact when the image distance equals approximately the distance to the object. Hence, we set \(r_a = 50\text{mm}\) to obtain a spectrometer-length that does not exceed 100 mm. Under this condition, the first-order diffraction position can be determined, which is where the CCD should be placed. \(C (x_i, y_i, L)\) was used to represent the center position of the linear CCD. In this paper, \(x_i = 0\text{mm}, y_i = 15\text{mm}, L = 40\text{mm}\), the CCD slope angle \(a = 40^\circ\).

After determination of the geometrical parameters, ZEMAX was used to simulate the optical performance of the spectrometer. In the simulation, 11 fields were introduced to form a slit light source of 1000 \(\times 5\mu\text{m}\), and there were fourteen different wavelengths in each field. An aperture was placed after the light source by 10 mm to control the incident energy by changing the width of the beam. The CCD position was adjusted precisely to optimize the resolution (about 1 nm) between 450 nm to 650 nm. Here the term resolution was defined as half of the smallest clearly distinguishable wavelength difference between adjacent wavelengths, which is equivalent to the full width at half maximum (FWHM) of a peak on a spectrogram. Figure 3(b) shows the spot diagram of each wavelength on the image plane, from which the resolution can be calculated. For example, the resolution at 450nm is 1nm. The simulation results confirm that the G-Fresnel lens spectrometer can resolve better than 1.2 nm spectral differences.

3.2 Fabrication error analysis

When the first negative Fresnel-mold and blazed-grating sandwich the G-Fresnel lens as shown in Fig. 2(d), alignment errors, including thickness error, tilting error, and eccentricity error affect the shape of the lens. For an optimized optical layout of a spectrometer prototype, positions of light source, G-Fresnel, and detector were fixed and these abovementioned errors will cause the lens shape change. The changed lens shape will lead to spectrometric resolution change. Calculations with ZEMAX were carried out to evaluate these differences.

Figure 4 illustrates the three types of errors. The symbols \(d\), \(\theta\), and \(\alpha\) represent the lens thickness, rotation angle, and eccentricity, respectively. The symbol \(d\) is the distance between
the two molds (the negative-Fresnel mold and the grating master), and also represents the thickness of the G-Fresnel lens, which is affected by the position accuracy of the mechanism. The target thickness is 5 mm, and the range for d was set to 0.2 mm, with a 0.1 mm interval. The light source and aperture parameters kept the same, while the position of the CCD was recalculated to optimize the resolution with the pre-set errors. The spectral range was set to 450 nm - 650 nm. The calculation results show that there is no significant difference in resolution for deviations smaller than 0.1 mm.

The angular deviation $\theta$ is a parameter used to evaluate how parallel the two molds are. There are two types of angular rotation: One is around the Y-axis, which is denoted by $\theta_Y$, and the other around the X-axis, denoted by $\theta_X$. In the simulation, the angle describing the deviation from their parallel state was set to $-1^\circ$ to $1^\circ$, which can be ensured using a commercial rotation stage. The simulated results indicate that, when the angular rotation is within 1 degree, the maximum resolution is still less than 1.4 nm.

The eccentric error $\alpha$ considers the movement between the physical centers of the negative-Fresnel surface and the grating master. Because the Fresnel surface is a centrosymmetric structure, and the periodic grating-surface has a constant grating period, the small-order eccentric error, $\alpha$, does not change the optical properties. To be compatible with other optical devices inside the spectrometer, the dimensions of the G-Fresnel lens need to be optimized. In other words, the error $\alpha$ should be as small as possible.

Based on the above analysis, a special setup for the fabrication was designed – see Fig. 5. It consists of four parts, a two-axis (X-Y) stage, a frame for the negative-Fresnel lens mold, a Z-axis stage (Thorlabs Corp.), and a mold cavity. These stages can provide positions with a minimum step of 10 $\mu$m and a repeatability of better than 50 $\mu$m in each axis. The mold cavity was designed such that the inner dimensions of the bottom section under the step are identical to the master grating ($25 \text{ mm} \times 25 \text{ mm} \times 6 \text{ mm}$). During fabrication, the master grating is first attached to the cavity, with its bottom aligned with the low surface of the cavity. Next, the whole cavity is mounted onto the two-axis stage to adjust the position of the master grating.
The negative Fresnel lens was mounted onto the Z-axis stage. Its height can be adjusted to control the height of the G-Fresnel lens.

Prior to the experiment, the accuracy of the mechanism was ensured by the CNC machine with a geometrical accuracy better than 10 μm and was calibrated to ensure that the position errors are within the values shown in the simulation above. The full size of this setup is about 140 mm × 106 mm × 160 mm. The compact size makes it easy to put it into a vacuum drying oven to solidify the PDMS.

Fig. 5. 3D model and picture of the experimental setup.

3.3 Adhesion reduction techniques

It took 2 days to cure the molding as well as avoid adhesion at room temperature [12], and the adhesion problem occurred when we tried to accelerate the solidification process by increasing the curing temperature. We overcame the adhesion problem by introducing an isolating layer that reduces adhesion, for the lower surface energy and lower static friction coefficient of the new surface were two key points in a trouble-free demolding process [13]. More specifically, two different adhesion reduction methods are investigated in this paper.

The first adhesion reduction method uses sputtering of a material called Parylene C [13–15] - see Fig. 6(a). The Parylene C layer, which is deposited via a CVD process, shows strong adhesion to the PDMS substrate, while there is no adhesion to the upper PDMS/Parylene interface. This is because there is no Parylene C on the upper bulk-PDMS and no CVD deposition occurred. This isolation causes weaker adhesion between Parylene-C and the upper PDMS, which allows a high temperature to accelerate drying of the PDMS cast. Even though a thick Parylene C layer adds some complications, this method succeeds at providing a strong durable film.

The second adhesion reduction method is illustrated in Fig. 6(b). Here, perfluoro-decyl-trichloro-silane (FDTS) was used [16,17], which is a colorless liquid chemical, and its molecules form self-assembled monolayers. The monolayers bond onto surfaces terminated with hydroxyl (-OH) groups and anchor to oxide surfaces with its trichloro-silane group to form covalent bonds. Due to the heavily fluorinated tail group, the FDTS monolayer reduces surface energy. Deposition of a FDTS monolayer is accomplished using a relatively simple process, which is known as molecular vapor deposition (MVD) [18]. This is done at room or near room temperature, which makes this process compatible with most substrates. The process is usually carried out in a vacuum chamber and assisted by the presence of water vapor. Treated surfaces can have water repelling and friction-reduction properties. The lower surface-energy helps to reduce the ejection force and the demolding of polymer parts in an injection molding, which also allows the formation of a thin layer. Thus, in this study, FDTS-based anti-adhesion coatings were used after several imprinting experiments. However, the slight toxicity of FDTS requires it to be treated carefully.
4. Results and discussion

In this section, we describe the fabrication process of the G-Fresnel lens, and evaluate the lens with respect to both geometrical parameters and optical performance. As illustrated in Fig. 2, there are four fabrication steps: first casting, adhesion reduction, second casting, and cleaning.

In the first casting step, PDMS is mixed with the curing agent in a 10:1 weight ratio. The mixture was degassed in a vacuum drying oven at room temperature for 20 minutes. The Fresnel lens was then attached to the mold with its edges aligned. The degassed mixture is poured into the mold and degassed again by putting the mold in a vacuum drying oven at 65 °C for 2 hours. The negative Fresnel lens mold is peeled off after it cooled down. As a result, we obtain a negative Fresnel surface, which is treated to reduce adhesion. The negative Fresnel lens mold was transferred into a drying can. A few FDTS droplets are dropped into the can, which is annealed in a drying oven at around 60 °C for 60 minutes. We then remove the mold in a ventilated environment. The second casting step is carried out using the treated negative Fresnel-lens mold. In this step, the PDMS mixture is prepared as described above. The PDMS is sandwiched between the negative Fresnel-lens mold and the grating, using the setup shown in Fig. 5. The equipment is then moved into the vacuum drying oven and annealed at 65 °C for 2 hours, an acceptable highest temperature and a shortest time, obtained by trial and error. Subsequently, we demold the treated negative Fresnel lens and blazed grating to obtain a G-Fresnel lens. Finally, we remove (peel off) the remaining PDMS and keep both molds clean.

Figure 7 shows a picture of the Fresnel-lens surface and the fabricated G-Fresnel lens. It can be seen that there is no damage of the replicated grating and no remaining PDMS on the master grating. In contrast, under the same drying conditions, the damage always occurred on the replicated grating when no anti-adhesion process was employed in our experiments. The Fresnel mold determines the quality of the fabricated G-Fresnel lens. Measurements were carried out to evaluate the replicating process. A step gauge (DektakXT, Bruker) was used to measure the profile of the Fresnel-lens surface. Figure 8 shows the result of the measurements. A small pit exists in the center of the Fresnel lens, which is used to determine the position of the origin. Even though it is difficult to find the same position for the master Fresnel lens and the negative-Fresnel lens (because the Fresnel lens has a centrosymmetric structure), the results show that the master was replicated with good accuracy.
The quality of the replicated blazed grating-structure was evaluated using an atomic force microscope (AFM, Bruker Dimension Icon). The target specifications were a 1.66 μm grating period, 180 nm grating depth, and a blazing angle of around 10°. Figure 9 shows the recorded AFM images. The profile of the replicated grating is not as uniform as the master grating. Both the period and the amplitude of the replicated grating is slightly longer than that of the grating master. Especially, the amplitude of the replicated grating is not as uniform as that of the master grating. The differences in profile and dimension are mainly caused by the softness of PDMS because a small deformation occurs during the peeling step. Also, the sensitivity of the AFM against to different material will also influence the measurement results. This difference is acceptable, and its effect on the spectrometer performance can be compensated by calibrating the spectrometer accurately.

A prototype spectrometer was then constructed to evaluate the actual spectrometric performance of the G-Fresnel lens. Figure 10 shows the setup we used. Three light sources, 450 nm, 532.2 nm, and 632.8 nm were co-axially mixed together and coupled into a fiber, using the optical layout shown in Fig. 10(a). At the exit of the fiber, a slit (5 μm × 1 mm) was added, which is of the same dimensions as the one used in the simulation. The fiber end with the exit was attached to a three-axis stage and the G-Fresnel lens was attached to the setup. The CCD (ILX554B, Sony) was mounted on a four-DOF motion stage so that both position and rotation angle can be adjusted. The CCD was then connected to a data processor (Torus, Ocean Optics) for data acquisition and processing.
Figure 11 shows the results of the measurements. Neither the software nor database could be used directly because the 2048-pixel CCD is calibrated for a different spectral range (400 nm – 1200 nm). Hence, a recalibration of the CCD was carried out.

A second-order function was used to fit the relationship between pixel number $x_i$ and wavelength $y_i$, based on these three measured values. The following equation was obtained:

$$y_i = 0.00004381x_i^2 + 0.3079x_i + 227.7$$

The spectral width that each pixel represents is critical for the determination of the resolution. A differential calculation was used to obtain the spectral width of a pixel.

$$y'_i = 0.00008762x_i + 0.3079$$

Using this equation, a single pixel represents a spectral width for a given pixel number, the real resolution can be calculated. For example, for a 450 nm wavelength, the pixel number is 660, and around this area, one pixel represents a spectral range of $0.00008762 \times 660 + 0.3079 = 0.3657$ nm. If this pulse signal is obtained from the CCD system, the FWHM is 3.23 pixels, and the real resolution can be obtained using $3.23 \times 0.3657 = 1.18$ nm. Similarly, the real resolutions for 532.2 nm and 632.8 nm can be obtained. Table 1 summarizes these results. The measured results are consistent with the simulation results.

Though these results are acceptable, for further improvement of the performance of the spectrometer, G-Fresnel lens shape is required to be more accurately formed. We will investigate the feasibility of our previously proposed master-replica technique, which was proposed for concave blazed grating [19]. In this technique, two hard substrates with etched...
negative Fresnel surface and grating structure are required. This will be done as a future work of this research.

| Incident wavelength (nm) | Pixels of signal FWHM | Experimental results (nm) | Simulated results (nm) |
|--------------------------|------------------------|---------------------------|------------------------|
| 450                      | 3.23                   | 1.18                      | 1                      |
| 532.2                    | 2.95                   | 1.14                      | 1.1                    |
| 632.8                    | 2.44                   | 0.99                      | 0.9                    |

5. Conclusions

We present a new technique to fabricate a hybrid planar grating-Fresnel lens. Details of the design, fabrication, and evaluation of the G-Fresnel lens are discussed. We use an adherence reduction method that effectively shortens the processing time of the required PDMS-based soft-lithography solidification step. The obtained fabrication setup is sufficiently compact (140 mm × 106 mm × 160 mm) to fit into a conventional vacuum drying oven, and it is capable of producing a G-Fresnel lens with a diameter of 25.4 mm, an equivalent focal length of 25 mm, and a blazed grating pattern with a 600 lines/mm grating constant. Both profile and dimension measurements were performed using a step gauge and confirmed with an AFM to verify that the fabrication accuracy is sufficient. Spectral measurements also confirm that the G-Fresnel lens enables a better than 1 nm first-order resolution across a spectral range of 200 nm. These outcomes will be helpful to develop high-resolution spectrometric applications that require lower cost and portability.

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