Study on the Characteristics of Multilayer Dielectric Grating Mask Profile by the RCW Method

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ABSTRACT

The fabrication of multilayer dielectric gratings was theoretically and experimentally investigated. The RCW (rigorous coupled-wave) method was adopted to theoretically analyze the influence, which is caused by the gratings profile and multilayer dielectric stack, on the diffraction efficiency. Researches on detecting principle and methods of the multilayer dielectric gratings were also tried to be carried out here. The spectral distributing of the zero order diffraction efficiency was used to judge the gratings profile, basing on the theoretical research and the calculating results by the RCW method. Detecting experiments have been conducted to compare the theoretical analyses; the results of this comparison may be helpful to instruct the detection of the gratings profile.

Key words: diffraction and gratings, detection of gratings mask, RCW method, multi-layer dielectric stack

1. INTRODUCTION

Contemporary the developments of ultra-short high-energy lasers, which are often based on the application of chirped-pulse amplification, have renewed the demand for high-efficiency diffraction gratings that also exhibit a high threshold for laser damage. The grating pairs used for pulse compression are typically planar reflection gratings used in first order near the Littrow angle. Conventional metallic gratings have high reflectivity with diffraction, so they are often used as pulse compression gratings. However, they have an inherent disadvantage of low threshold for optical damage, because metallic gratings owe their reflection to conductivity, which leads to the absorption of radiation causing heating and damage. The multi-layer dielectric gratings 5,6,7 compose of dielectric structures with periodic grooves to create diffraction, and the multi-layer dielectric substrate to create high reflection. Transparent dielectric materials have much smaller absorption coefficients than do metals. So multi-layer dielectric gratings have potential for withstanding more intense radiation, and this brings about high threshold for damage. Researches in this field have been widely conducted since 1990s 6,7, and some products with good properties have been reported in recent papers 5.

The production of high-efficiency multi-layer gratings is based on the photo-resist grating mask. The fabrication procedure of the multi-layer grating consists of two basic steps: the holographic generation of a grating mask in photo-resist layer and the transfer of this grating mask into top layer of the multi-layer dielectric substrate by ion beam etching. So the perfectly made ion beam etching gratings require a high quality grating mask, that is to say, the mask should have certain groove depth and duty cycle to adapt to the requirement. What merits our attention is that the groove region of the resist-grating mask must be exposed to the substrate. Otherwise the residual resist will severely influence the etching technique, and hence results in the deteriorated property. So the detection of the characteristics of grating...
mask is very important. This paper attempts to introduce a new method, which is based on the RCW (rigorous coupled-wave) method\textsuperscript{1,2,3,4} to detect the profile of the grating mask by the spectral distributing of the zero order diffraction efficiency. This method, avoiding the damage to the grating mask caused by the SEM detection, is effective to detect the profile.

2. THEORY

The purpose of theoretical and experimental research on the gating mask is to find out the relationship between diffraction efficiency and grating profile, and thus to direct the fabrication of the multi-layer dielectric grating mask. The accurate method of detection is the SEM, but unfortunately the SEM will cause damages to the grating mask that is not reparable. A new method is introduced in this paper to detect the profile of the grating mask without causing damage, which uses large sum of numerical results as criterion. The computer programs based on the RCW method worked out these results.

2.1 DIFFRACTION EFFICIENCY OF MULTI-LAYER DIELECTRIC GRATING MASK

The relationship between diffraction efficiency and grating profile as well as multi-layer dielectric substrate is analyzed for TE polarization (incident plane-wave polarization perpendicular to the plane of the incidence) by the RCW method in this paper. The implementation for TM polarization is straightforward if corresponding changes are adopted. The structure of a conventional multi-layer dielectric grating mask is shown in Fig.1. Without any loss of generality, we choose the coordinates as shown in Fig.1, where D is the groove depth, \( \Lambda \) is the grating period, and \( t_r \) is the residual thickness of photo-resist. The polarized electromagnetic wave is obliquely incident at the angle of incidence \( \theta \). The grating is bound by two different media with refractive indices \( n_1 \) and \( n_2 \) and in this paper is photo-resist and atmosphere respectively.

![Fig.1 Geometry for the diffraction grating analyzed herein](image_url)

The incident normalized electric field for TE polarization is given by

\[
E_0 = \exp[-jk_0n_1(sin \theta x + cos \theta z)],
\]

(1)
where \( k_0 = \frac{2\pi}{\lambda_0} \) and \( \lambda_0 \) is the wavelength of the light in free space. The normalized solutions in region 1 \((0 < z)\) are given by

\[
E_i = E_0 + \sum_j R_j \exp[-j(k_{i,\lambda}x - k_{i,\lambda}z)].
\]  

(2)

where \( k_{i,\lambda} \) is determined from the Floquet condition and is given by

\[
k_{i,\lambda} = k_0[n_i \sin \theta - i \frac{\lambda_0}{\Lambda}],
\]

(3)

and where \( k_{i,\lambda} = k_0[n_i^2 - (k_{i,\lambda}/k_0)^2]^{1/2} \) if \( n_i < k_{i,\lambda}/k_0 \), the negative square root of \( k_{i,\lambda} \) is adopted. \( R_i \) is the normalized electric-field amplitude of the \( i \)th backward-diffracted (reflected) wave in region 1.

The detailed theoretical analysis and calculation by computer program are based on [3] and [4]. What is different with the surface-relief dielectric grating analyzed in [3] and [4] is that the changes of the boundary conditions between region 2 and grating region should be considered here, which are caused by the multi-layer dielectric substrate with high reflection. In region 2, there are not only the transmitted diffractive amplitudes of the electromagnetic field but also the reflected amplitudes of the transmitted wave caused by the multi-layer dielectric substrate. A change is made to the dielectric stack in theoretical calculation. We regard the residual resist as the top layer of the dielectric stack, and thus a new stack is formed. In this case the normalized solutions in region 2 are given by

\[
E_2 = \sum_i T_i \exp[-j(k_{i,\lambda}x + k_{2,\lambda}(z - D))] + \sum_k T_k r_k \exp[-j(k_{k,\lambda} - k_{2,\lambda}(z - D))],
\]

(4)

where \( T_i \) is the normalized electric-field amplitude of the \( i \)th transmitted wave (including those have imaginary wave vectors). \( T_k \) is the normalized electric-field amplitude of the real transmitted wave in region 2, and \( r_k \) is the reflective coefficient of the \( k \)th transmitted amplitude caused by the new dielectric stack. \( \sum_k T_k r_k \) is the total contribution to the region 2 under the function of the dielectric stack. The normalized magnetic-field amplitude is straightforward according to the Maxwell’s equations. We programmed to calculate the amplitudes of the reflective diffracted fields \( R_i \) that are of practical use by matching the tangential electric- and magnetic-field components at the two boundaries. And then the diffraction efficiencies are defined as

\[
DE_{ni} = |R_i|^2 \text{Re}(\frac{k_{i,\lambda}}{k_0 n_i \cos \theta})
\]

(5).

The numerical results have been compared with [7] to confirm the correctness of the computer programs.

### 2.2 NUMERICAL CALCULATION AND ANALYSIS

The structure of multi-layer dielectric stack analyzed in this paper is S|A1B1(A1B2)9 A1B3A2|C, where S stands for the
material of the substrate (glass K9), C for atmosphere, A1 for layer of HfO2 with thickness of 0.104µm, B1 for layer of SiO2 with thickness of 0.393µm, B2 for layer of SiO2 with thickness of 0.262µm, B3 for layer of SiO2 with thickness of 0.066µm, and A2 for the top layer of HfO2 with thickness of 0.205±0.005µm. (A1B2)9 indicates there are 9 pairs of such layers. The actual refractive index is variant with the change of incident wavelength. The refractive index of SiO2 used in this paper is 1.4557, and the HfO2 1.9519.

![SEM photos](image1)

No.1

No.2

![SEM photos](image2)

No.3

No.4

Fig.2. SEM photos of grating masks analyzed herein

Four multi-layer dielectric grating masks manufactured under the same conditions are analyzed in this paper, and these 4 grating masks have the same period of 0.676µm. SEM photos of them are shown in Fig.2. According to the analysis to these photos, the parameters of these grating masks are educed in Table1.

<table>
<thead>
<tr>
<th>Grating Number</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Groove Depth (nm)</td>
<td>515</td>
<td>532</td>
<td>483</td>
<td>436</td>
</tr>
<tr>
<td>Duty Cycle</td>
<td>42.8%</td>
<td>36.5%</td>
<td>31.7%</td>
<td>27.4%</td>
</tr>
<tr>
<td>Residual Thickness (nm)</td>
<td>65</td>
<td>55</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
The curves of 0 order diffraction efficiency are educed based on these data at the incident angle of $51.2^\circ$, and the area of incident wavelength considered here is 900nm~1200nm. These curves, both for TE and TM polarization, are shown in Fig.3.

What we really detect in experiments is the response to the distribution energy of the diffracted light, not the real distribution of the diffraction efficiency. So the profile characteristics of the diffraction efficiency curves are mainly analyzed here. According to the above two figures, the profile characteristics for TE polarization is more explicit, while the profile characteristics for TM polarization change little with various profiles of the grating mask. So the TE mode is adopted in the experimental detection.

3. EXPERIMENTAL DETECTION AND ANALYSIS

![Experimental devices used herein](image_url)

According to the above theoretical analysis, the devices shown in Fig.4 were adopted in the experimental detection. What the detector really detects is relevant to the energy of the lamp-house, to the diffraction efficiency of the grating,
and the response of the total optical system (including the spectrum device). $T(\lambda)$ is defined as the signal that the detector eventually detects, $I(\lambda)$ as the light intensity of the lamp-house, $\eta(\lambda)$ as the diffraction efficiency of the grating, and $M(\lambda)$ as the response of the total optical system. The conclusion is drawn here that $T(\lambda) = I(\lambda) \cdot \eta(\lambda) \cdot M(\lambda)$. In order to eliminate the influence to detection results caused by the light intensity of the lamp-house and the response of the total optical system, we take following steps. We substitute dielectric stack without grating mask for grating mask to conduct another detection. And now the signal detected is defined as $T_i(\lambda)$, and the conclusion is $T_i(\lambda) = I(\lambda) \cdot R(\lambda) \cdot M(\lambda)$, where $R(\lambda)$ is the reflectivity of the dielectric stack. The light intensity of lamp-house $I(\lambda)$ and the response of the total optical system $M(\lambda)$ are supposed to be what they were. From these two equations, the following equation can be given by $\eta'(\lambda) = \frac{T(\lambda)}{T_i(\lambda)} = \frac{\eta(\lambda)}{R(\lambda)}$, where $\eta'(\lambda)$ is defined as the relative diffraction efficiency. The same process was implemented to the theoretical diffraction efficiency and the reflection of the dielectric stack which are calculated by the computer programs based on the RCW method, so that the theoretical relative diffraction efficiency is educed to compare the experimental relative diffraction efficiency.

The curves of relative diffraction efficiency shown in Fig.5 are detection results of the grating masks shown in Fig.2 by the optical system shown in Fig.4. The corresponding theoretical curves are shown in Fig.6. The experimental curves in the area of 950nm~1130nm are corresponding to the theoretical curves in the area of 970nm~1170nm. This area is the main function area with high diffraction efficiency at +1 order. The other areas are areas of side-lobe current laminations.
The experimental curves are not identical with the theoretical ones in the main function area; and imparities in side-lobe areas are very large. We think the errors in the process of the formation of the dielectric stack should answer for these negative results. The further theoretical calculation indicates that the random error of each layer in dielectric stack influences the results severely. The total error of the dielectric stack will lead to the minor shift of the main function area and also cause the variety of the width of this area. From the results of detection, we found the reflection peak of the dielectric stack in grating2 is of little difference with other gratings. The theoretical curve in Fig.6 has been corrected. Despite the imparities of the theoretical and experimental curves, the following conclusions can be made in the main function area by comparison with Fig.5, Fig.6 and Fig.2.

(1). The curves of relative diffraction efficiency approximately correspond to the variety of the grating profiles.

The variety of the curves is sensitive to the variety of the residual thickness of the photo-resist according to the analysis of Fig.5. The curves of grating1 and grating2 are very similar in the situation that both of them haven’t been exposed to the substrate. And the curves of grating3 and grating4 are also of very little difference when they are exposed to the substrate. According to the experimental results shown in Fig.5, the distinguished discrimination of the curves concerning whether they are exposed to the substrate or not is the relative height between the left and right peak. Before being exposed to the substrate, the relative height is not so large as is exposed to the substrate. If the mask is exposed to the substrate, the left peak falls greatly and the relative height is therefore very obvious.

(2). The experimental curves are approximately identical to the theoretical ones.

The same conclusions can be made in Fig.6 as in Fig.5 on the relative height. What’s more, from these two figures we find that the right peak will shift to left slightly if the mask is exposed to the substrate, and the experimental results are more distinguished than theoretical ones. So the tendency of change of the experimental and theoretical curves is identical with each other on the matter that whether the mask is exposed to the substrate.

The groove depth and duty cycles seem to have little influence on the experimental curves, and more accurate experiments and larger data-base are necessary to judge these two parameters.

4. CONCLUSION

This paper theoretically analyses the relationship between dielectric grating profile and the diffraction efficiency by the RCW method. Computer programs based on this method educed the diffraction efficiency distribution of the gratings. And according to these results, 0 order diffraction light for TE polarization is adopted to detect the grating mask. This method has been proved to be effective. However, the accuracy of the detection experiments still need to be improved further.

REFERENCES


Proc. of SPIE Vol. 5636 107


