Chapter 4

Simulated Results

4.1 Introduction

The design of the sub-wavelength grating is presented in this section. For accurately calculating the efficiency of TE-mode and TM-mode light, the software, GSOLVER based on RCWA, is utilized to perform the simulation. According to Eqs. 2.2.5 and 2.2.10, the effective refractive indices of a sub-wavelength grating are much dependent on its dimension and material. First, the proposed structure of the sub-wavelength grating is briefly introduced. However, owing to the limitation of our fabrication equipments, the light separation efficiency of the sub-wavelength grating is not as good as ideal. Thereafter, the tolerance analysis for the fabrication is also demonstrated.

4.2 Design of the Proposed Sub-wavelength Grating

The sub-wavelength grating with smaller period is able to produce a higher efficiency of light separation; however, fabrication remains an issue. To achieve high efficiency and do-able fabrication simultaneously, parameters of the grating including period, duty cycle, thickness and material have to be optimized. For display technology and infrared applications, the proposed sub-wavelength grating is designed with a quartz substrate, photoresist gratings and aluminum gratings. The period, thickness, and duty cycle of the grating layer are 0.2 um, 0.05 um, and 50% respectively, as shown in Fig. 4.1. The efficiencies of light separation are

then simulated with the parameters listed in Tab. 4.1. As the results shown in Fig. 4.2, the reflection efficiency of TE-mode is greater than 90 %, whereas the transmission efficiency of TM-mode is greater than 41 % over the visible spectra (0.4 um \sim 0.8 um) and the near infrared spectra (0.8 um \sim 2.5 um).



Tab. 4.1 Simulation parameters of the proposed sub-wavelength grating

Substrate	Quartz ($n = 1.54$)	
Period of grating (um)	0.2	
Duty cycle (%)	50	
Thickness of metallic layer (um)	0.05	
Material of grating layer	Aluminum	
Material of dielectric layer	Photoresist	
Polarization angle	0° (TE-mode) & 90 $^{\circ}$ (TM-mode)	
Wavelength (um)	0.4 ~ 1.5	
Incident angle	$0^{\circ} \sim 40^{\circ}$	
Diffraction orders	15	



Period of a grating is the most important parameter to determine the diffractive efficiency. It is selected according to what kinds of applications for. For example, form birefringence appears when the period of the grating is much smaller than wavelength of incident light. Period of sub-micrometers is needed to provide visible spectra with a high efficiency of light separation. Thus, period of the sub-wavelength grating interested will be taken into consideration first.

In simulation, metallic layer, aluminum which is selected because of its high reflectivity. To consider the effect of incident angle of the incident light on diffraction efficiency, various incident angles are taken into account. After that, several periods of the sub-wavelength grating, which are selected to be smaller than visible spectra, are simulated with both p ray and s rays. The simulation parameters are listed in Tab. 4.2.

Substrate	Quartz (<i>n</i> = 1.54)			
Period of grating (um)	0.1 ~ 0.4			
Duty cycle (%)	50			
Thickness of metallic layer (um)	0.05			
Material of metallic layer	Aluminum			
Polarization angle	0° (s ray) & 90° (p ray)			
Wavelength (um)	0.4 ~ 1.5			
Incident angle	0° ~ 40°			
Diffraction orders	15			
1896				

Tab. 4.2 Simulation parameters for determining period of metallic layer

We can notice that both p ray transmission and s ray reflection efficiency are higher and higher as the period of the sub-wavelength grating becomes smaller and smaller from the simulated results shown in Figs. 4.3 and 4.4. For the purpose of having the highest efficiency in the visible spectra (0.4 um ~ 0.8 um) and the near infrared spectra (0.8 um ~ 2.5 um), one can choose period of the grating to be 0.4 um, or smaller. Nevertheless, the smaller the period of the grating is, the harder the fabrication will be. Therefore, we trade-off the diffraction efficiency and limitation of fabrication instruments, and select period of the sub-wavelength grating to be 0.2 um where the reflection efficiency of TE-mode is greater than 90 % and the transmission efficiency of TM-mode is greater than 41 % over the visible spectra (0.4 um ~ 0.8 um) and the near infrared spectra (0.8 um ~ 2.5 um).



Fig. 4.3 Simulated results of TE-mode reflection efficiency versus wavelength of incident light with various periods of the sub-wavelength grating.



Fig. 4.4 Simulated results of TM-mode transmission efficiency versus wavelength of incident light with various periods of the sub-wavelength grating.

4.4 Surface Profile Effect

Characteristics of birefringence are essential to separate the polarization of TE-mode and TM-mode. In addition to asymmetry of material or incident angle, variation of interface profile is another way to produce asymmetry. In a surface relief grating, it is obvious that TE-mode and TM-mode encounter different boundary condition. In this section, another structure with different surface profile which is compared with the original model in section 4.2 is proposed to discuss the surface profile effect.

The other proposed sub-wavelength grating is designed with a quartz substrate, photoresist gratings and aluminum gratings, as shown in Fig. 4.5. The surface profile is changed from rectangular profile to triangular profile. The period, thickness, and duty cycle of the Al grating layer are 0.2 um, 0.05 um, and 50% respectively. As the simulated results shown in Figs. 4.6 and 4.7, the reflection efficiency of TE-mode is greater than 60 %, whereas the transmission efficiency of TM-mode is greater than 35 % over the visible spectra (0.4 um \sim 0.8 um) and the near infrared spectra (0.8 um \sim 2.5 um). Compared with the case of rectangular profile, both efficiencies of reflection and transmission are reduced in the visible spectra and the near infrared spectra. Therefore, the closer the rectangular surface profile is, the higher light separation efficiency will be.



Fig. 4.5 Structure of the sub-wavelength grating with triangular profile.



Fig. 4.6 Simulated results of TE-mode reflection efficiency versus wavelength of incident light with various structures of the sub-wavelength grating.



Fig. 4.7 Simulated results of TM-mode transmission efficiency versus wavelength of incident light with various structures of the sub-wavelength grating.

4.5 Tolerance Analysis of Thickness Inaccuracy of Each Grating

As mentioned above, the sub-wavelength grating is designed with the period of 0.2 um, the duty cycle of 50% and the material of aluminum. However, owing to the limitation of the fabrication instruments, the surface profile of grating may not be as ideal as the simulated cases. For example, the imperfect contrast of interference fringes may reduce the resolution of the nano-pattern during the interference. Furthermore, the mold releasing process in UV-nanoimprint lithography also probably brings defects to the transferred nano-structure. As a result, these issues may cause the fabricated gratings with non-uniform line-width and then degrade the beam-splitting efficiency of the sub-wavelength grating.

Therefore, the tolerances analysis is necessary for fabricating the sub-wavelength grating. Assume the line-width variation of each grating layer is $\pm 10\%$, the efficiencies of light separation are then simulated with different line-width of the sub-wavelength grating. The simulation parameters are listed in Tab. 4.3. As the results shown in Figs. 4.8 and 4.9, the reflection efficiency of TE-mode is greater than 96%, whereas the transmission efficiency of TM-mode is greater than 94% over the near infrared spectra. Compared with the ideal model, both deviations of TE-mode reflectance and TM-mode transmittance are of less than 1% over the near infrared spectra. Ideally, the transmitted light of TM-mode over the near infrared spectra = TM-moed_{transmit}+ (TE-mode converted to TM-mode)_{transmit} = $94\% \times 0.5 + 96\% \times 0.5$ \times 0.9 (quarter wave plate conversion factor) \times 94% = 87.6%. As for the case of ±10% line-width variation, the transmitted light of TM-mode over the near infrared spectra = $93\% \times$ $0.5 + 95\% \times 0.5 \times 0.9$ (quarter wave plate conversion factor) $\times 93\% = 86.2\%$, which deviates the designed value by 2%.

	El	E	SVE	1E	
E			7/	ZE	
	EL			× اع	

Tab. 4.3 Simulation parameters for tolerance analysis

Substrate	Quartz ($n = 1.54$)	
Line-width variation of grating	±10%	
Period of grating (um)	0.2	
Duty cycle (%)	50	
Thickness of metallic layer (um)	0.05	
Material of metallic layer	Aluminum	
Polarization angle	0° (TE-mode) & 90° (TM-mode)	
Wavelength (um)	0.4 ~ 1.5	
Incident angle	$0^{\circ} \sim 40^{\circ}$	
Diffraction orders	15	



Fig. 4.8 Simulated results of TE-mode reflection efficiency versus wavelength of incident light with the line-width variation of grating



Fig. 4.9 Simulated results of TM-mode transmission efficiency versus wavelength of incident light with the line-width variation of grating

4.6 Summary

By optimizing transmission and reflection efficiencies, the sub-wavelength grating herein is constructed by a quartz substrate, photoresist grating, and aluminum grating, while the period, thickness and duty cycle are 0.2 um, 0.05 um and 50%, respectively. From the simulation results, the reflection efficiency of TE-mode is above 90% and the transmission efficiency of TM-mode is above 41% for the visible spectra (0.4 um ~ 0.8 um) and the near infrared spectra (0.8 um ~ 2.5 um).

Since fabricating a wide area sub-wavelength grating by e-beam writing technique is time-comsuming and costly, the integration of interferometry and nano-imprint, described in chapter 3, is proposed to enlarge the area of the sub-wavelength grating in our fabrication. Although combining interferometry and nano-imprint can increase the yield, the limitation of the fabrication instruments will reduce the profile accuracy of grating and then decay the efficiency of light splitting. Compared with the ideal model, both deviations of TE-mode reflectance and TM-mode transmittance are of less than 1% over the near infrared spectra. The beam-splitting efficiency will be affected by the line-width variation of the grating and the deviation of beam-splitting efficiency is less than 2% within 10% width variation.