Chapter 4

Simulated Results

4.1 Introduction

We will discuss the design of the sub-wavelength grating in this chapter. First of all, the simulation tool, GSOLVER, will be briefly introduced. Because the diffraction efficiency of a grating is much dependent on its dimension, including period, thickness, and duty cycle, and material of grating, these parameters will be determined carefully by considering both diffraction efficiency and possibility of fabrication process. Although the designed sub-wavelength grating with metallic layer only is of high diffraction efficiency over the visible spectrum, a sudden decay appears in the region of shorter wavelength of the diffraction efficiency vs. wavelength curves. Thus, an addition of dielectric layer between metallic layer and substrate will be demonstrated to broaden the useful optical spectrum. Finally, a brief summary about the ultimate design of sub-wavelength grating will be given.

4.2 Simulation Tool

GSOLVER is a diffraction grating analysis tool developed by Grating Solver Development Company. It calculates diffracted fields and diffraction efficiencies from plane wave illumination of arbitrarily complex grating structures. The illumination may be from any incidence (conical mounts) with any polarization (TE, TM, circular, or elliptical). The grating structure is defined by a piecewise constant approximation which permits analysis of simple classical grating profiles (blaze, sinusoid, holographic, binary), to as complicated structures as one would like (layers, coatings, inter-weaving of material, shadows, etc). The features of GSOLVER are listed below：

- A visual grating structure editor
- Automatic generation of common diffraction grating profiles including square wave holographic, blazed, sinusoidal, trapezoidal, triangular, 3-point polyline, and others
- Full three-dimensional vector code using hybrid Rigorous Coupled Wave Analysis (RCWA) and Modal analysis
- Analysis of arbitrary grating thickness, number of materials, and material index of refraction (defined by a real and imaginary part) including dielectrics and metals
- Analysis of thin film stacks
- Three dimensional specification of incident plane wave illumination with arbitrary polarization vector, including elliptical, TE, TM, as well as conical mounts
- Linear gratings with arbitrary profiles including cusps, shadow regions, layers of multiple differing material, and arbitrary thickness
- Crossed gratings (periodicity in both X and Y directions)
- Selection of any of ten independent variables to explore grating definition parameter space, graphically and table display (lambda, theta, phi, alpha, beta, total depth, link depth, x-period, duty cycle, and orders)
- Graphing of diffraction efficiencies, fields, and phases

- Uses proprietary code that accelerates convergence for all polarization and grating depths, handles a large number of real propagating and evanescent orders (limited by computer resources, ±50 orders requires about 16 Mega of RAM for the internal arrays)
- Uses 'streamlined' code for TE and TM polarization cases
- Features a genetic algorithm for automatic grating design
- Custom parameter selection

GSOLVER employs a full 3D rigorous coupled wave algorithm which approaches to the solution of diffraction grating problems and is popularized by Thomas K. Gaylord and M. G. Moharam. We will not talk too much about the theory of RCWA here because the derivations of the equations are too complicated to be introduced here. The references of RCWA theory will be listed in the Appendix. The program calculates the diffraction efficiencies, relative field amplitude, and phases for all retained orders. Thus, the structure of the sub-wavelength grating will be analyzed by means of the calculation of diffraction efficiency in the following sections.

4.3 Dimension and Material of Metallic Layer

The effective refractive indices of a sub-wavelength grating are much dependent on its dimension and material, which have been discussed in chapter 2. The sub-wavelength with smaller period produces a higher efficiency of light separation, but is harder to fabricate. To achieve high efficiency and easy fabrication at the same time, the structure of the grating, including period, duty cycle, and thickness, has to be optimized. Thus, these parameters as well as material of the grating will be determined one by one in the following sections.

4.3.1 Period

Period of a grating is the most important parameter to determine the diffractive efficiency. It is selected according to what kinds of applications will be applied. For example, form birefringence appears when the period of the grating is much smaller than wavelength of incident light. Period of few 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, of the sub-wavelength grating with default setting of duty cycle is inserted in between quartz substrate and air. To consider the influence 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. 4.1.

Tab. 4.1 Simulation parameters for determining period of metallic layer

Substrate	Quartz ($n = 1.54$)
Period of grating (μm)	0.1 ~ 0.3
Duty cycle (%)	50 (default value)
Thickness of metallic layer (μm)	0.1
Material of metallic layer	Aluminum
Polarization angle	0° (s ray) & 90° (p ray)
Wavelength (μm)	0.4 ~ 0.8
Incident angle	$0^\circ \sim 40^\circ$
Diffraction orders	15

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. 4.1 and 4.2. For the purpose of having the highest efficiency, one can choose period of the grating to be $0.15\,\mu m$, $0.1\,\mu m$, or smaller. Nevertheless, the smaller the period of the grating is, the harder the fabrication will be. In addition, a serious decay of p ray transmission appears in the region of shorter wavelength. The solution to avoid the sudden decay is to diminish the period or employ multi-layered structure, which will be discussed in detailed in section 4.4. Therefore, we trade-off the diffraction efficiency and limitation of fabrication instruments, and select period of the sub-wavelength grating to be $0.2\,\mu m$ where p ray transmission efficiency is about 80% and s ray reflection efficiency is above 97% for the visible spectrum.

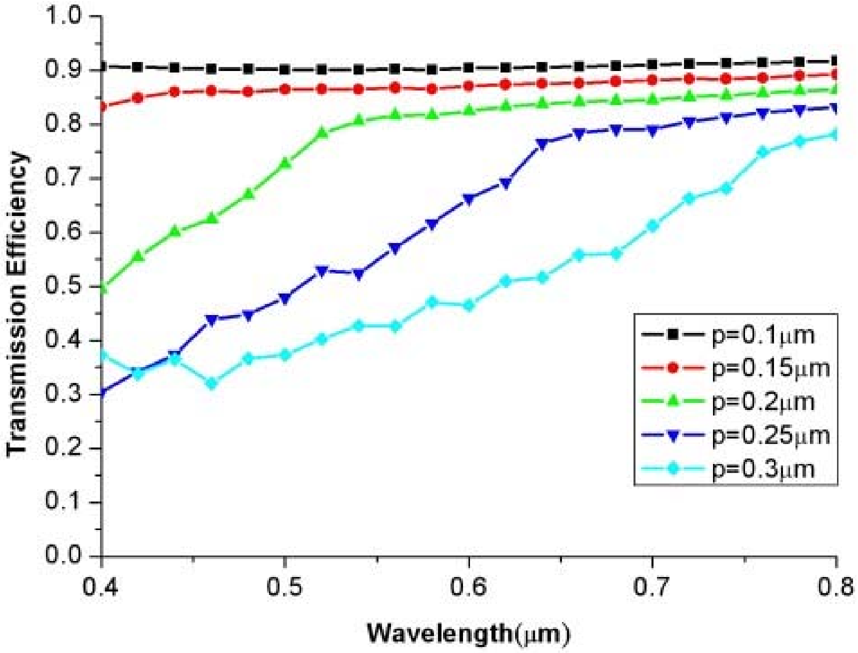

Fig. 4.1 Simulated results of p ray transmission efficiency versus wavelength of incident light with various periods of the sub-wavelength grating.

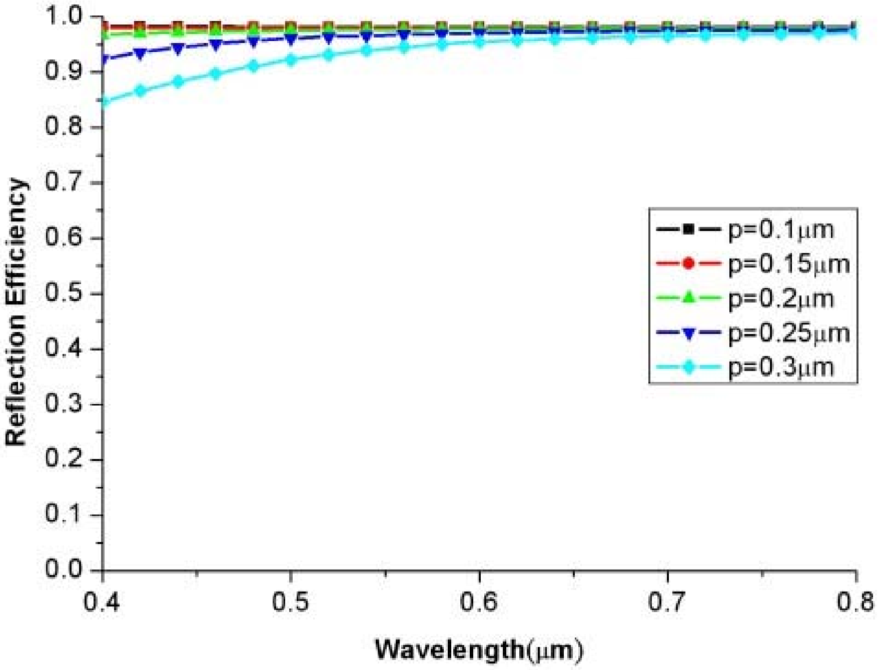

Fig. 4.2 Simulated results of s ray reflection efficiency versus wavelength of incident light with various periods of the sub-wavelength grating.

4.3.2 Thickness

Various thicknesses of a diffraction grating result in a variation of amplitude or phase of incident wave, as well as the diffraction efficiencies. A proper thickness of the grating will enhance the diffraction efficiencies; on the contrary, an improper thickness will destroy the diffraction conditions and degrade the diffraction efficiencies. Thus, we have to find a suitable thickness of the metallic layer of the sub-wavelength grating.

In simulation, aluminum grating with well-chosen period and default setting of duty cycle of 0.2 μm and 50%, respectively, is inserted in between quartz substrate and air. Afterwards, different thicknesses, range from 0.05 μm to 0.2 μm, of the metallic layer are simulated with both p and s rays. The simulation parameters are listed in Tab. 4.2.

Tab. 4.2 Simulation parameters for determining thickness of metallic layer

Substrate	Quartz ($n = 1.54$)
Period of grating (μm)	0.2
Duty cycle (%)	50
Thickness of metallic layer (μm)	0.05 ~ 0.2
Material of metallic layer	Aluminum
Polarization angle	0° (s ray) & 90° (p ray)
Wavelength (μm)	0.4 ~ 0.8
Incident angle	$0^\circ \sim 40^\circ$
Diffraction orders	15

From the simulated results, both p ray transmission efficiency and s ray reflection efficiency are increased as thickness of metallic layer becomes thicker, as shown in Figs. 4.3 and 4.4. However, the p ray transmission efficiency with thickness larger than 0.1 μm is of a more serious decay in the region of shorter wavelength even if the diffraction efficiencies are higher. Furthermore, we expect that the thickness of the sub-wavelength grating can be as thin as possible to simplify the fabrication. Consequently, thickness of 0.1 μm, which is easier to fabricate and maintain p ray transmission efficiency and s ray reflection efficiency of 80% and 97% respectively, is selected.

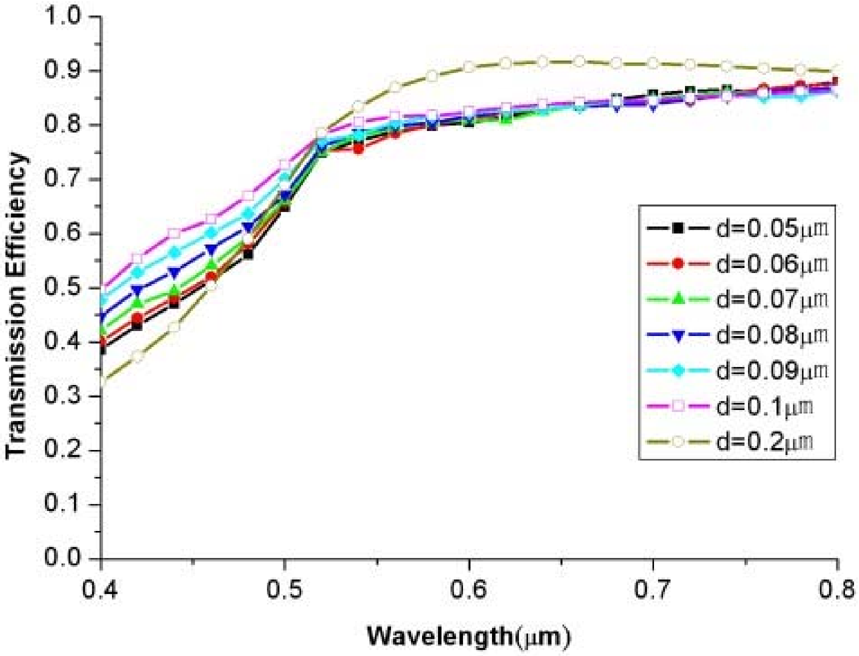

Fig. 4.3 Simulated results of p ray transmission efficiency versus wavelength of incident light with various thicknesses of metallic layer.

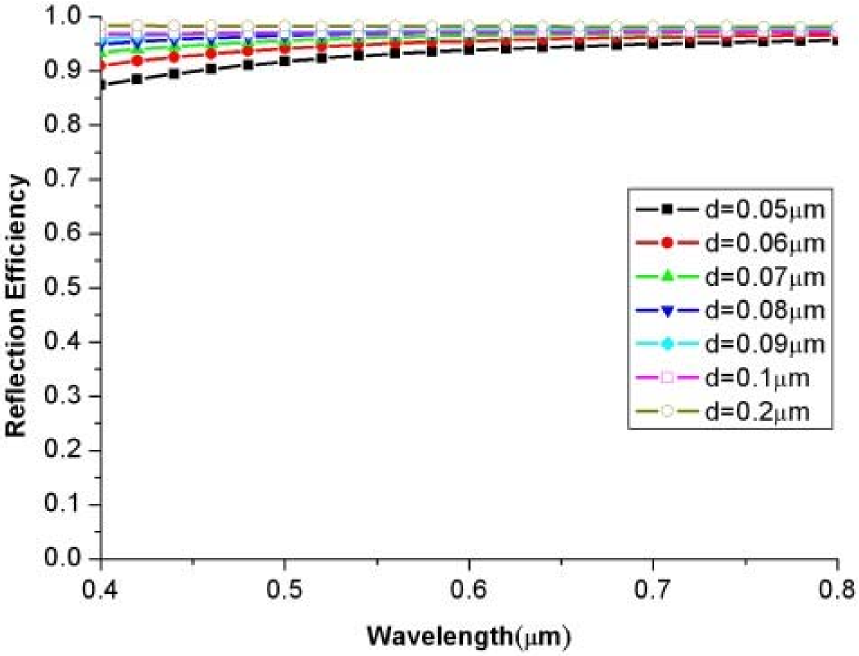

Fig. 4.4 Simulated results of s ray reflection efficiency versus wavelength of incident light with various thicknesses of metallic layer.

4.3.3 Duty Cycle

To fully describe the dimensions of a grating, duty cycle is another important parameter which will affect efficiencies of light separation. For the extreme conditions, most p rays will be transmitted as the duty cycle approximates to 0; s rays will be reflected as the duty cycle approximates to 1. Therefore, a suitable duty cycle is essential for high efficiency of light separation.

In simulation, aluminum grating with well-chosen period and thickness of 0.2 μm and 0.1 μm respectively is inserted between quartz substrate and air. Different duty cycles of the sub-wavelength grating are then simulated with both p and s rays. The simulation parameters are listed in Tab. 4.3.

Tab. 4.3 Simulation parameters for determining duty cycle of metallic layer

Substrate	Quartz ($n = 1.54$)
Period of grating (μm)	0.2
Duty cycle (%)	10 ~ 90
Thickness of metallic layer (μm)	0.1
Material of metallic layer	Aluminum
Polarization angle	0° (s ray) & 90° (p ray)
Wavelength (μm)	0.4 ~ 0.8
Incident angle	0° ~ 40°
Diffraction orders	15

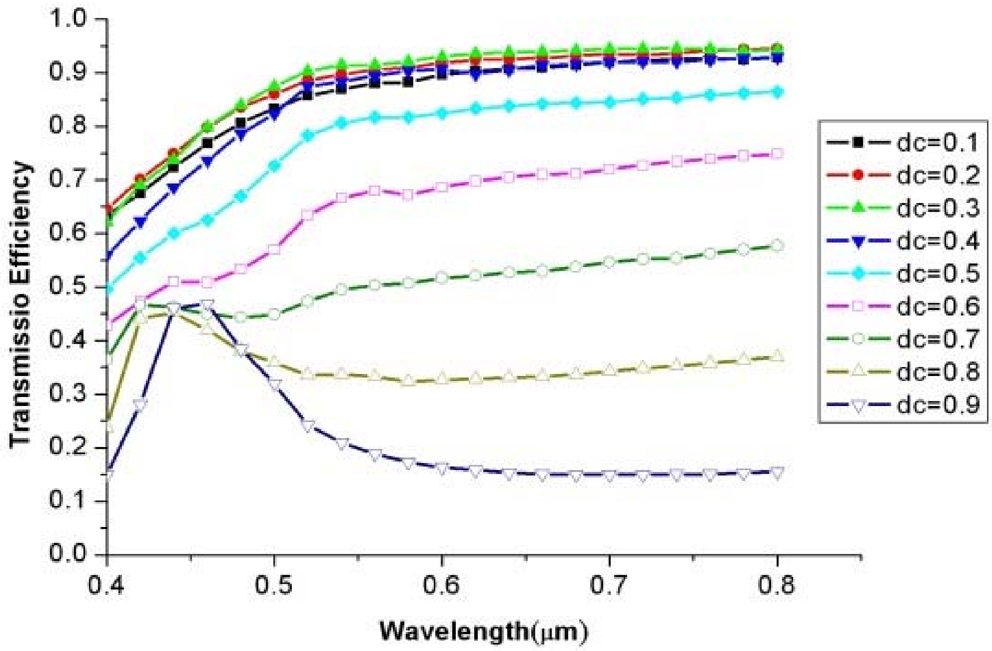

Fig. 4.5 Simulated results of p ray transmission efficiency versus wavelength of incident light with various duty cycles of grating.

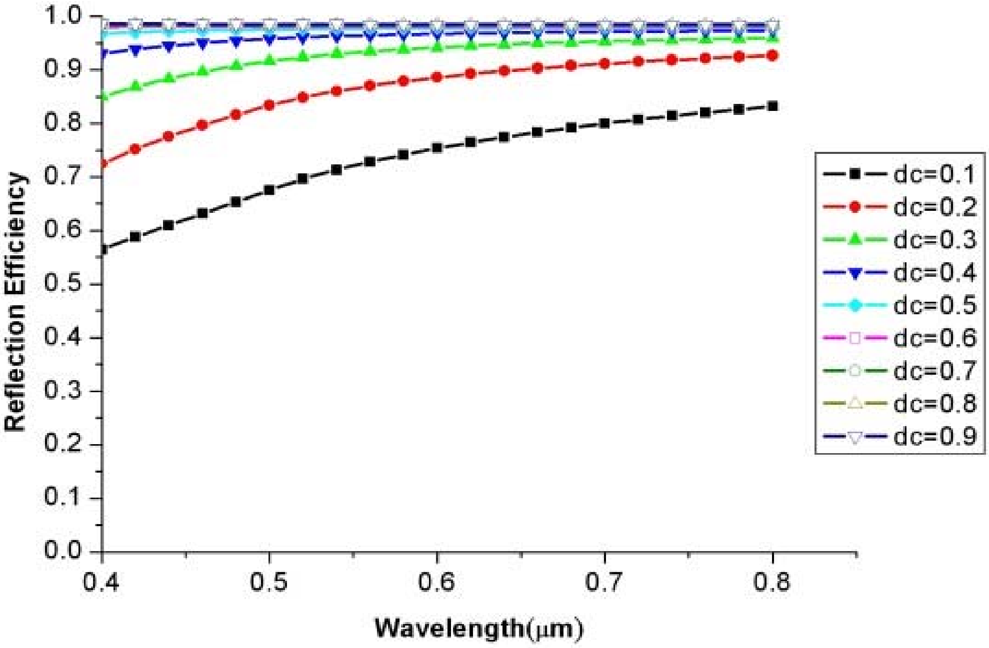

Fig. 4.6 Simulated results of s ray reflection efficiency versus wavelength of incident light with various duty cycles of grating.

It can be easily observed that the sub-wavelength grating is of higher p ray transmission efficiency, but of lower s ray reflection efficiency as duty cycle becomes smaller from the simulated results shown in Figs. 4.5 and 4.6. Among the duty cycles simulated, 40% and 50% are of the highest efficiency of light separation. Although the diffraction efficiency of duty cycle of 40% is superior to that of 50%, it is difficult to fabricate smaller duty cycle as the limitations of instruments used are taken into account. For this reason, the duty cycle of the sub-wavelength is chosen to be 50%. Ultimately, dimension of the metallic layer of the sub-wavelength grating are designed with period, thickness, and duty cycle of 0.2 μm, 0.1 μm, and 50% respectively.

4.3.4 Material

In addition to dimension, material of the sub-wavelength also plays an important role in furnishing the grating with high efficiency of light separation. From the discussions in chapter 2, the effective indices of sub-wavelength grating are extremely related to refraction index of grating bar, Eqs. 2.2.5 and 2.2.10. Thus, a suitable material is needed to fit the sub-wavelength grating for high efficiency of light separation.

Sub-wavelength grating with well-chosen period, thickness, and duty cycle of 0.2 μm, 0.1 μm, and 50% respectively is inserted in between quartz and air once more. Different metals are simulated with both p ray and s ray. The simulation parameters are listed in Tab. 4.4.

Tab. 4.4 Simulation parameters for determining material of metallic layer

Substrate	Quartz ($n = 1.54$)
Period of grating (μm)	0.2
Duty cycle (%)	50
Thickness of metallic layer (μm)	0.1
Material of metallic layer	Silver, Aluminum, Gold, Copper
Polarization angle	0° (s ray) & 90° (p ray)
Wavelength (μm)	0.4 ~ 0.8
Incident angle	$0^\circ \sim 40^\circ$
Diffraction orders	15

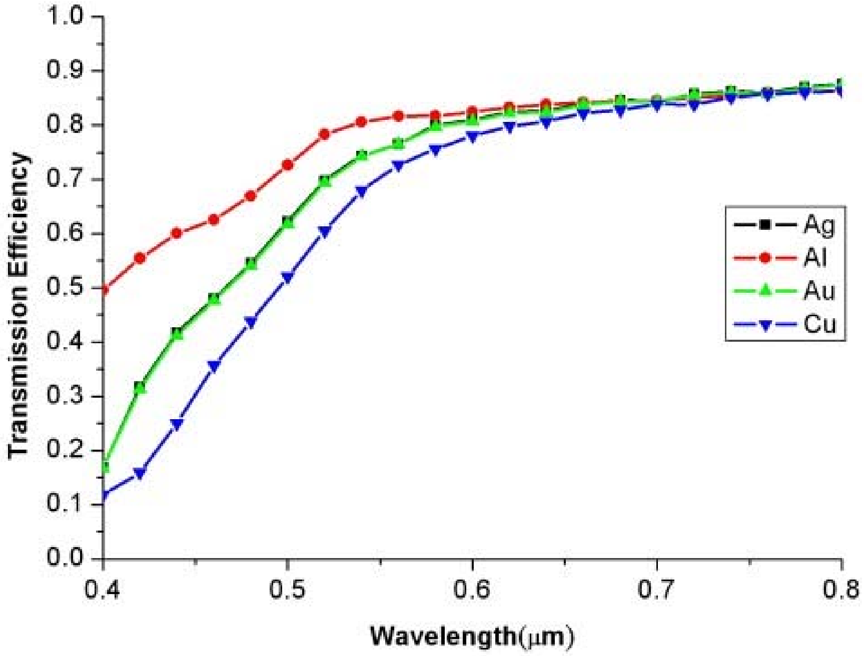

Fig. 4.7 Simulated results of p ray transmission efficiency versus wavelength of incident light with various materials of metallic layer.

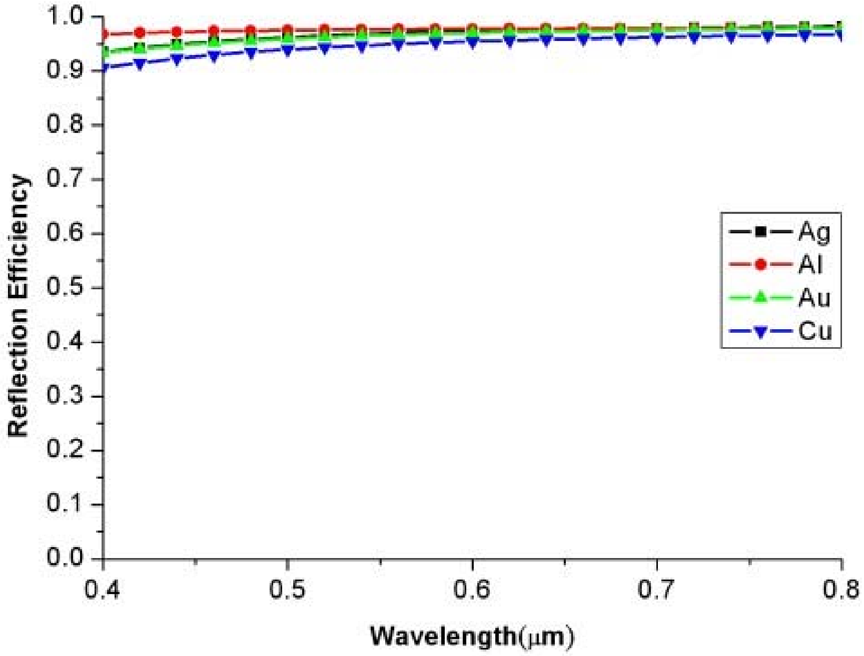

Fig. 4.8 Simulated results of s ray reflection efficiency versus wavelength of incident light with various materials of metallic layer.

From the simulated results, it is obvious that efficiencies of both p ray transmission and s ray reflection by employing aluminum are prime one. Undoubtedly, we select aluminum as the material of metallic layer of the sub-wavelength grating. As a result, the metallic layer of the sub-wavelength grating is designed with period, thickness, and duty cycle of $0.2\,\mu m$, $0.1\,\mu m$, and 50% respectively and consists of aluminum.

4.4 Double-Layered Sub-Wavelength Grating

In the simulation of the sub-wavelength grating with metallic layer only, the efficiency of p ray transmission is decreased rapidly in the region of shorter wavelength. The wavelength the efficiency decreases suddenly is called resonance wavelength, as shown in Fig. 4.9. One of the methods to condense resonance wavelength, i.e., to broaden the applicable spectrum, is to design a sub-wavelength grating with multi-layered structure. Accordingly, we will add a dielectric layer between aluminum layer and substrate to improve the decay of diffraction efficiency. The simulation of such a sub-wavelength grating with double-layered structure will be demonstrated in the following.

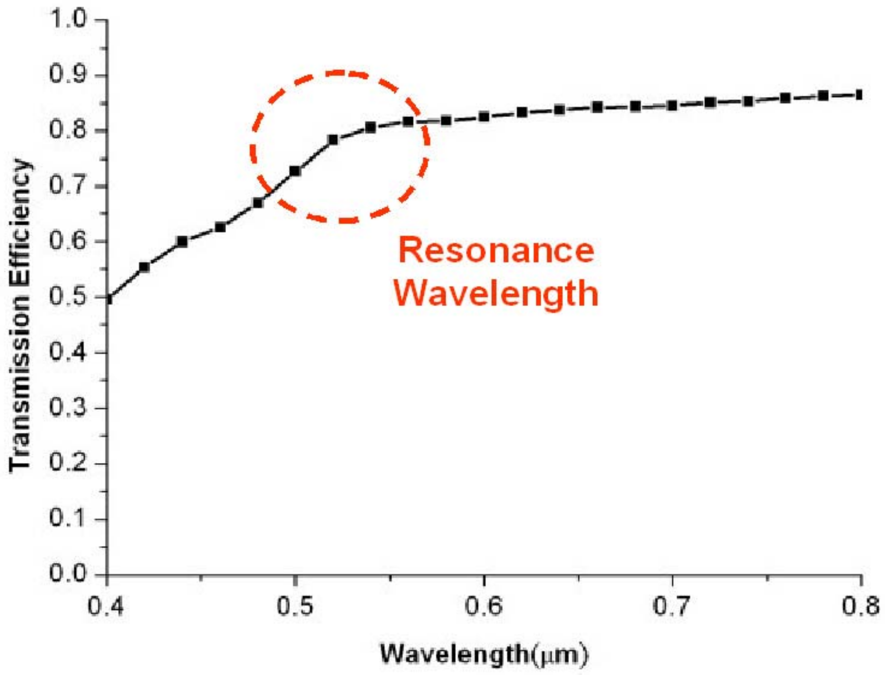

Fig. 4.9 Resonance wavelength of the sub-wavelength grating with metallic layer only and period of 0.2 μm.

4.4.1 Thickness of Dielectric Layer

Because the period and duty cycle of the sub-wavelength grating have been determined in section 4.3, we will determine thickness of the inserted dielectric layer directly.

Aluminum grating with period, thickness, and duty cycle of 0.2 μm, 0.1 μm, and 50% respectively is inserted in between quartz substrate and air first. A dielectric layer, SiO_2 which is selected randomly, with the period and duty cycle as aluminum layer is then inserted between quartz substrate and aluminum. Various incident angles are again taken into consideration in the simulation. After that, different thicknesses of dielectric layer are simulated with both p and s ray. The simulation parameters are listed in Tab. 4.5.

Tab. 4.5 Simulation parameters for determining thickness of dielectric layer

Substrate	Quartz ($n = 1.54$)
Period of grating (μm)	0.2
Duty cycle (%)	50
Thickness of metallic layer (μm)	0.1
Material of metallic layer	Aluminum
Thickness of dielectric layer (μm)	0.1 ~ 0.3
Material of dielectric layer	SiO_2
Polarization angle	0° (s ray) & 90° (p ray)
Wavelength (μm)	0.4 ~ 0.8
Incident angle	$0^\circ \sim 40^\circ$
Diffraction orders	15

There is no apparent difference in the calculated diffractive efficiencies, especially in s ray reflection efficiency vs. wavelength curve, of dielectric layers with different thickness, as shown in Figs. 4.10 and 4.11. However, the addition of dielectric layer is for the purpose of broadening optical spectrum of display applications. Dielectric layer with thickness of 0.2 μm is of the superior p ray transmission efficiency with the broadest band among the simulated thicknesses; hence, 0.2 μm is taken as the thickness of dielectric layer.

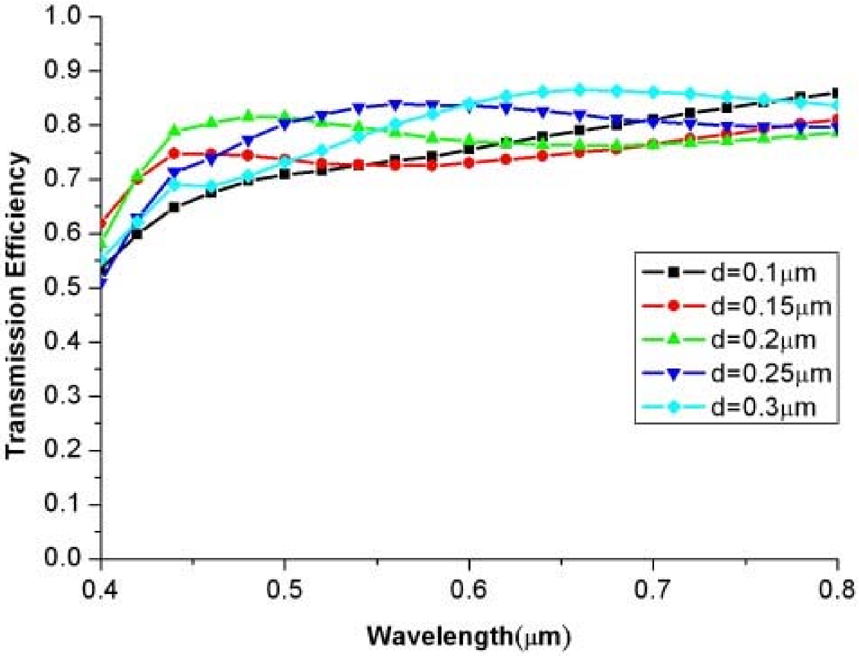

Fig. 4.10 Simulated results of p ray transmission efficiency versus wavelength of incident light with various thickness of dielectric layer.

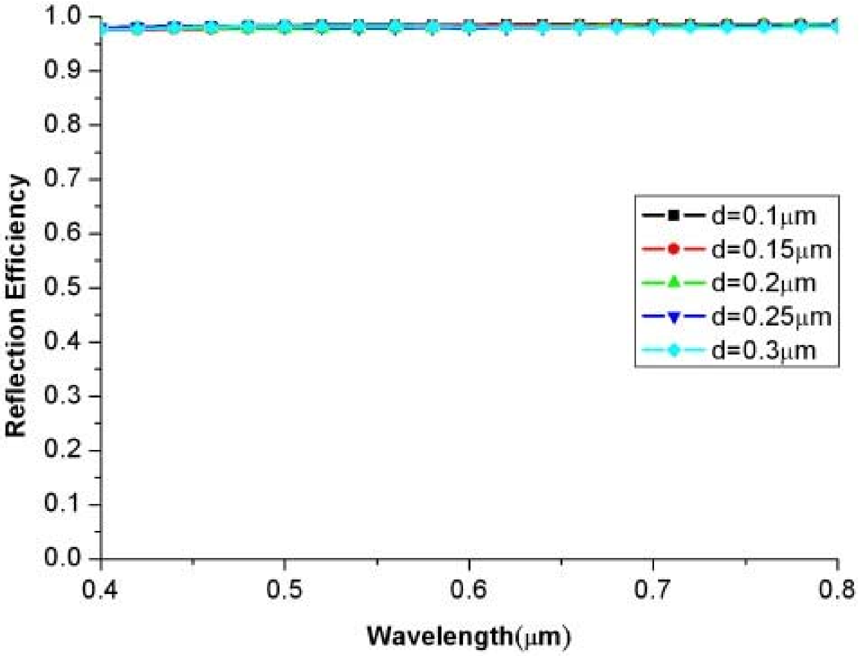

Fig. 4.11 Simulated results of s ray reflection efficiency versus wavelength of incident light with various thickness of dielectric layer.

4.4.2 Material of Dielectric Layer

Finally, we will choose the most suitable material of dielectric layer for our design. Metallic and dielectric layers with thickness of 0.1 μm and 0.2 μm, respectively, are inserted between quartz substrate and air once again. The same simulation conditions but different materials of dielectric layer are set to calculate the diffraction efficiencies with both p and s ray. The simulation parameters are listed in Tab. 4.6.

Tab. 4.6 Simulation parameters for determining material of dielectric layer

Substrate	Quartz ($n = 1.54$)
Period of grating (μm)	0.2
Duty cycle (%)	50
Thickness of metallic layer (μm)	0.1
Material of metallic layer	Aluminum
Thickness of dielectric layer (μm)	0.2
Material of dielectric layer	MgO, SiO_2, ZnS
Polarization angle	0° (s ray) & 90° (p ray)
Wavelength (μm)	0.4 ~ 0.8
Incident angle	$0^\circ \sim 40^\circ$
Diffraction orders	15

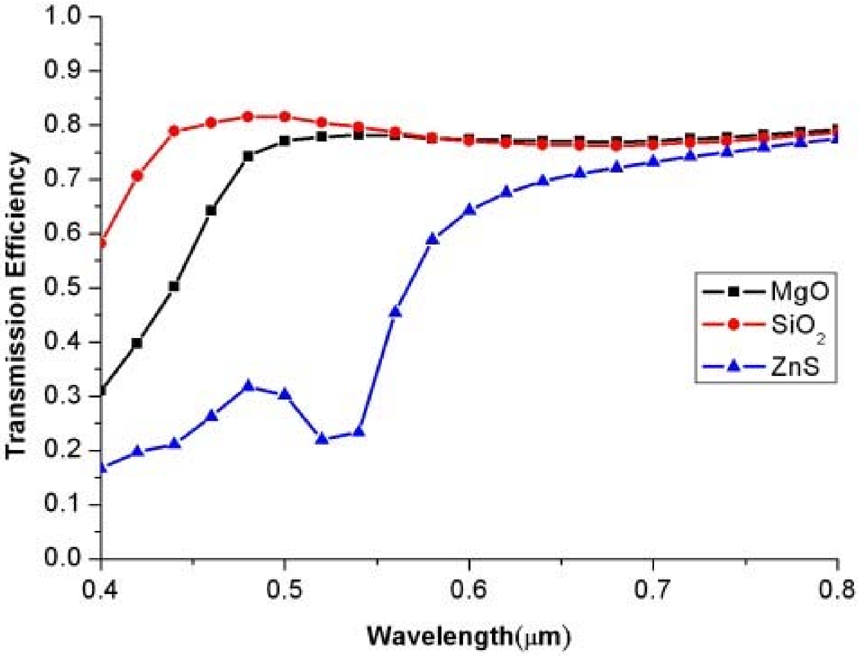

Fig. 4.12 Simulated results of p ray transmission efficiency versus wavelength of incident light with various materials of dielectric layer.

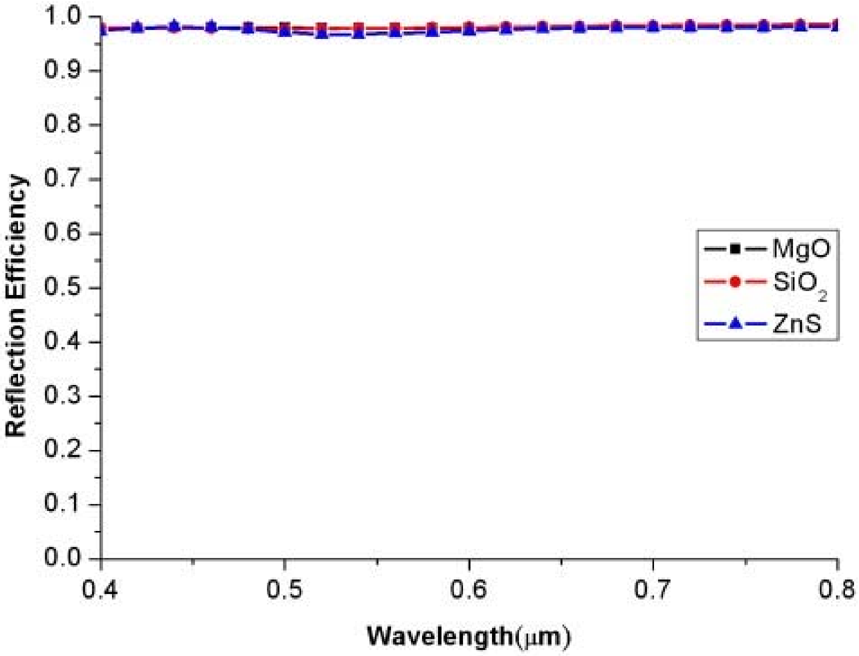

Fig. 4.13 Simulated results of s ray reflection efficiency versus wavelength of incident light with various materials of dielectric layer.

From the calculated results, a monopolized curve, which is generated by utilizing SiO_2, of p ray transmission efficiency is acquired, as shown in Fig. 4.12, and nearly identical curves of s ray reflection efficiency is obtained in Fig. 4.13. In consequence, SiO_2 is undoubtedly selected as the material of dielectric layer. Thus, the dielectric layer consists of SiO_2 with thickness of $0.2\,\mu m$ is inserted between quartz substrate and metallic layer.

4.5 Summary

In summary, we have designed a sub-wavelength grating with double-layered structure which consists of a metallic layer and a dielectric layer. By optimizing both transmission and reflection efficiencies, the metallic layer, consists of aluminum, of the sub-wavelength grating with period, thickness, and duty cycle of $0.2\,\mu m$, $0.1\,\mu m$, and 50% respectively is obtained. In order to improve the sudden decay in the region of shorter wavelength of the transmission efficiency vs. wavelength curves, i.e., to reduce the resonance wavelength, a dielectric layer, consists of SiO_2, is added between substrate and metallic layer. With this structure, most of p rays can be transmitted through the sub-wavelength grating while s rays are reflected, as shown in Figs. 4.14 and 4.15.

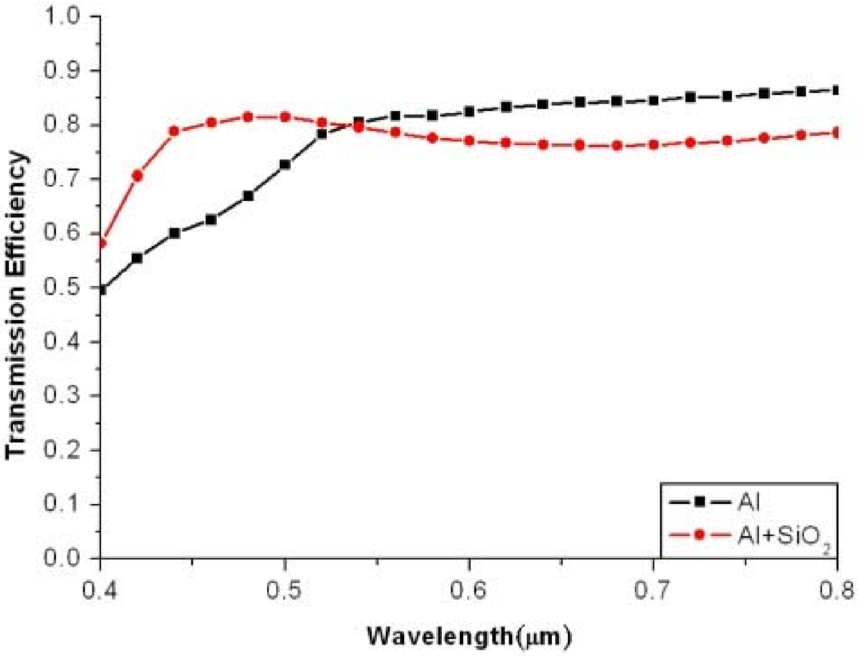

Fig. 4.14 Comparison of p ray transmission efficiency between single layer and double layer.

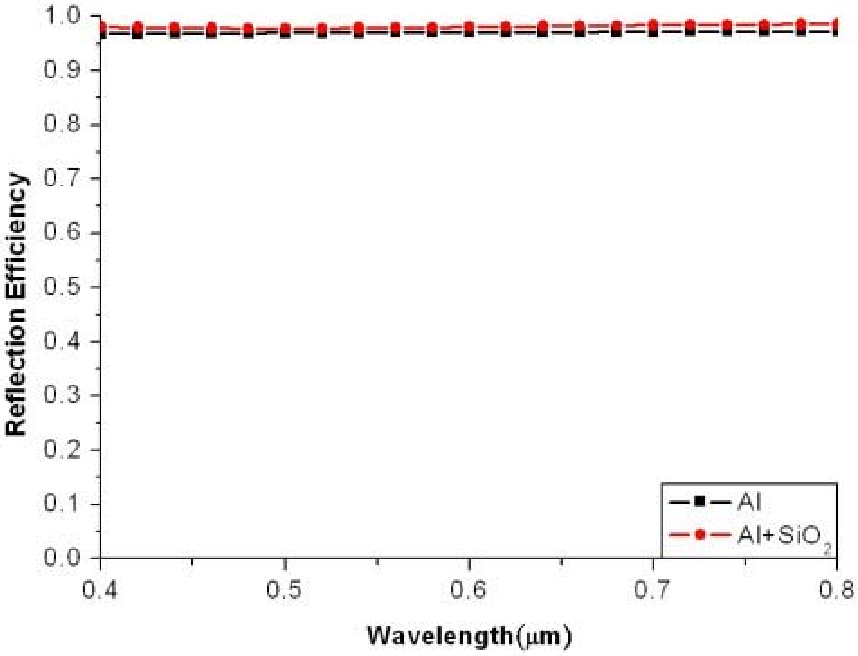

Fig. 4.15 Comparison of s ray reflection efficiency between single layer and double layer.