# Rigorous Coupled-wave Analysis for the High Reflective Mirror Used in Multi-layer Dielectric Grating*

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**Abstract**: An enhanced, numerically stable transmittance matrix approach based on rigorous coupled-wave analysis (RCWA) was applied in the optical character of multi-layer dielectric thin film. A design of high reflective mirror used in multi-layer dielectric grating was presented using the method of RCWA. The optics spectral of the fabricated high reflective mirror presents a good agreement with the design which is optimized by employing the rigorous coupled-wave analysis.

**Key words**: High reflective mirror; Multi-layer dielectric grating; Rigorous coupled-wave analysis

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## 0 Introduction

Multi-layer Dielectric Thin Film (MDTF) has been widely used as antireflection coating, high-reflection coating, edge filter and band-pass filter, neutral mirror and beam splitters to modulate the propagation of wave[1]. The basic functions of the multi-layer optical thin film are as follows: energy distribution, beam splitting, beam polarizing and the other special function such as Indium-Tin Oxide (ITO)[2]. As far as we know, there are several efficient approaches such as matrix method, graphical technique and effective admittance technique to calculate the performance of the thin-film optical coating. As for graphical technique, it is not useful for the multi-layer optical thin film. Meanwhile, for effective admittance technique, it is difficult to understand its physical sense. Therefore the matrix method has been widely used to design and optimize the structure of multi-layer thin film to achieve excellent optical performance during the past years[3]. The most important of the matrix method is how to eliminate the numerical instability problem caused by the presence of evanescent field.

The rigorous coupled-wave analysis (RCWA) has been a widely used method for the accurate analysis and the design of diffraction gratings. It is an exact solution of Maxwell′s equations for the electromagnetic diffraction by the corrugated structure. The accuracy of the solution depends solely on the number of terms retained in the space-harmonic expansions of the fields, with conservation of energy always being satisfied[4].

In this paper, the RCWA and the enhanced transmittance matrix approach are employed to analyze and design the performance of high reflective mirror used in multi-layer dielectric grating. The calculated and experimental result shows that the method is a relatively straightforward and deterministic technique.

## 1 Theory mode

In the technique to analyze the diffraction from surface relief grating structures, the grating is divided into a large number of sufficiently thin planar grating slabs. The electromagnetic fields in each grating layer are determined by the coupled-wave approach. The electromagnetic boundary conditions are then applied in sequence at the interface among the input region, the individual grating layers, and finally the output region to obtain the reflected and the transmitted diffracted field amplitudes. It is well known that the evanescent fields, which are associated with successive matching of the tangential electromagnetic fields at the interface between layers, result in ill-conditioned transmittance matrices and the numerical instability problem. The inversion of this ill-transmitted matrix results in a matrix with numerically large diagonal elements that can′t be represented with sufficient numerical accuracy. Thus, the numerical inaccuracy will produce numerical instability in the calculated transmitted and reflected-field

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amplitudes[5].

Fig. 1 shows the schematic of the multi-layer optical dielectric thin film with uniform dielectric in each layer. RCWA is a deterministic technique by using enhanced transmittance matrix approach that converges to the proper solution without inherent numerical instabilities. A stable implementation of the RCWA is employed to analyze the reflection and the transmittance of multi-layer optical dielectric thin film for multi-layer dielectric gratings (MDGs) in this paper[6].

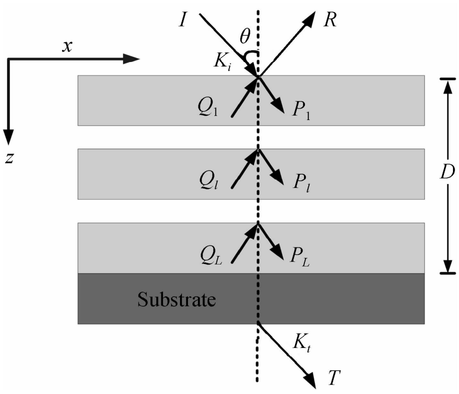


Fig. 1 Geometry for the reflection and transmission of multi-layer optical dielectric thin film

As can be seen from Fig. 1, we consider the reflection and the transmission of a TE-polarized plane wave of free-space with wavelength $\lambda_0$, incident at angle $\theta$, on $L$ uniform layers. Thin film above the high reflective films lies in $x$-$z$ plane. For analyzing, the multi-layer dielectric can be divided into $L$ layers along $z$-direction Each layer possesses the refractive index of $n_1$, $n_2\cdots$, $n_L$ and thickness $d_1$, $d_2\cdots$, $d_L$. When the TE polarized light (electric field perpendicular to incident plane) illuminate MDGs with free-space wavelength $\lambda_0$ and incident angle of $\theta$, the normalized electric field for the input and output regions can be written as

$$\begin{cases} E_{I,y}=\exp\{-\mathrm{j}k_0 n_I[\sin(\theta x)+\cos(\theta z)]\}+ \\ \sum_i R_i\exp[-\mathrm{j}(k_x x-k_{I,z}z)] \\ E_{II,y}=\sum_i T_i\exp\{-\mathrm{j}[k_{xi}x-k_{II,zi}(z-D)]\} \end{cases} \tag{1}$$

Where $R$ and $T$ are the reflected and the transmitted amplitudes of the electric fields, $k_0=2\pi/\lambda_0$ is the wave-vector magnitude in the air. The wave-vector along $x$ direction and $z$ direction in each divided layer are $k_{xi}=k_0 n_i\sin\theta$ and $k_{zi}=k_0 n_i\cos\theta$, respectively[7].

The tangential magnetic and electric fields in the $l$-th ($0<z<D$) divided layer can be expressed according to the following form

$$\begin{cases} E_{l,gy}=\sum_i S_{l,yi}(z)\exp(-\mathrm{j}k_{xi}x) \\ H_{l,gx}=-\mathrm{j}(\varepsilon_o/\mu_o)^{1/2}\sum_i U_{l,xi}(z)\exp(-\mathrm{j}k_{xi}x) \end{cases} \tag{2}$$

Here, $\varepsilon_o$ and $\mu_o$ are the permittivity and permeability of free space. $S_{l,yi}(z)$ and $U_{l,yi}(z)$ are the normalized amplitude of the $i$-th space-harmonic fields that satisfy Maxwell's equation in each divided layer[8].

As is in the uniform homogenous layer, the reflected and transmitted amplitudes can be solved by matching tangential electromagnetic fields at the boundaries between the two divided layers. At the boundary between the input region and the first dielectric layer ($z=0$), the following equation should be satisfied.

$$\begin{bmatrix} \delta_{i0} \\ \mathrm{j}n_1\cos\theta\delta_{i0} \end{bmatrix}+\begin{bmatrix} I \\ -\mathrm{j}Y_1 \end{bmatrix}[R]= \begin{bmatrix} W_1 & W_1X_1 \\ V_1 & -V_1X_1 \end{bmatrix}\begin{bmatrix} c_1^+ \\ c_1^- \end{bmatrix} \tag{3}$$

At the boundary between the $l$-1 and the $l$ divided layer ($z=D_l$)

$$\begin{bmatrix} W_{l-1}X_{l-1} & W_{l-1} \\ V_{l-1}X_{l-1} & -V_{l-1} \end{bmatrix}\begin{bmatrix} c_{l-1}^+ \\ c_{l-1}^- \end{bmatrix}= \begin{bmatrix} W_l & W_lX_l \\ V_l & -V_lX_l \end{bmatrix}\begin{bmatrix} c_l^+ \\ c_l^- \end{bmatrix} \tag{4}$$

At the boundary between the last divided layer and the substrate ($z=D_L$)

$$\begin{bmatrix} W_LX_L & W_L \\ V_LX_L & -V_L \end{bmatrix}\begin{bmatrix} c_L^+ \\ c_L^- \end{bmatrix}=\begin{bmatrix} I \\ \mathrm{j}Y_2 \end{bmatrix}[T] \tag{5}$$

Where $W$ and $V$ are matrix whose element can be deduced from the equation of (1) and (2). $Y_1$ and $Y_2$ are diagonal matrices with the diagonal elements with the value of $k_{I,zi}/k_0$ and $k_{II,zi}/k_0$, respectively, in each divided layer. $C_L$ is the unknown constant to be determined. So the following relation can be obtained as

$$\begin{bmatrix} f_L \\ g_L \end{bmatrix}T_L=\begin{bmatrix} 1 & \exp(-k_0\gamma_Ld_L) \\ \gamma_L & -\gamma_L\exp(-k_0\gamma_Ld_L) \end{bmatrix}\cdot \begin{bmatrix} a_L \\ b_L\exp(-k_0\gamma_Ld_L) \end{bmatrix}T_L= \begin{bmatrix} a_L+b_L\exp(-2k_0\gamma_Ld_L) \\ \gamma_L[a_L-b_L\exp(-2k_0\gamma_Ld_L)] \end{bmatrix}T_L \tag{6}$$

Where, $\begin{bmatrix} a_L \\ b_L \end{bmatrix}=\begin{bmatrix} 1 & 1 \\ \gamma_L & -\gamma_L \end{bmatrix}^{-1}\begin{bmatrix} f_{L+1} \\ g_{L+1} \end{bmatrix}$, and $f_{L+1}=1$, $g_{L+1}=\mathrm{j}k_{II,z}/k_0$

We can easily obtain the relation of reflected and transmitted amplitudes from the equation of (3)～(6) by using enhanced transmittance matrix approach [6] without any numerical instability as follows

$$\begin{bmatrix} \delta_{i0} \\ \mathrm{j}n_1\cos\theta\delta_{i0} \end{bmatrix}+\begin{bmatrix} I \\ -\mathrm{j}Y_1 \end{bmatrix}[R]=\begin{bmatrix} f_1 \\ g_1 \end{bmatrix}T_1 \tag{7}$$

Here $f_1$ and $g_1$ are the assistant parameters in the enhanced transmittance matrix approach. $T$ and $T_L$

must meet the following relationship

$$T = a_L^{-1} X_L \cdots a_l^{-1} X_l \cdots a_1^{-1} X_1 T_1 \tag{8}$$

From the equation of (7) and (8), we can obtain the reflected amplitudes $R$ and transmittance amplitudes $T$. So the reflectance and transmittance of the multi-layer can be solved as

$$\begin{cases} R = RR^* \operatorname{Re}\left(k_{I,z}/k_0 n_I \cos\theta\right) \\ T = TT^* \operatorname{Re}\left(k_{II,z}/k_0 n_I \cos\theta\right) \end{cases} \tag{9}$$

## 2 Design and experiment

In high-energy laser systems, multi-layer dielectric gratings have been widely used owing to their high diffraction efficiency and high damage resistant ability[9-11]. MDGs can be obtained by etching a grating structure on the top of a multi-layer dielectric thin film. The diffraction property is determined by the performance of the beneath reflective stack. According to the design and fabrication of MDGs, the multi-layer dielectric thin film must provide high transmittance during holography exposuring wavelength (413 nm), high reflectance at working wavelength (1 053 nm) and sufficient manufacture tolerance latitude of the grating design. Here we give an example of a multi-layer dielectric thin film stack used for the MDGs, which is working at 1 053 nm with TE mode and 51.2° incident[12]. Considering the exposing wavelength is chosen to be 413.1 nm with TE mode and 17.8° incident, the designed multi-layer dielectric reflective stack should have high reflectivity at working wavelength of 1 053 nm and high transmittance at exposing wavelength of 413.1 nm.

According to the above theory model, which is based on the rigorous coupled-wave analysis and the enhanced transmittance matrix approach, the numerical calculation is performed and an excellent multi-layer stack can be obtained for the use of multi-layer dielectric grating. Firstly, according to the incident angle and the TE mode, the wave vector of $x$ direction and $z$ direction can be deduced. Then the enhanced transmittance matrix is applied to get the reflected amplitudes $R$ and transmittance amplitudes $T$. In the end, the reference wavelength can be adjusted to meet the requirement of the multi-layer dielectric not only at the working wavelength, but also at the exposing wavelength. In order to eliminate the numerical inaccuracy and achieve stable implementation during the optimized process, the field harmonics should be chosen to be the proper value.

The high reflective mirror for multi-layer dielectric grating is optimized to meet the above requirement with the stack of $H_3L(H_2L)^9H0.5L$. The optical thickness of high-and low-index materials, $HfO_2$ and $SiO_2$, are one-quarter of 810 nm ($n_{HfO_2} = 1.96$ and $n_{SiO_2} = 1.46$). The optimized high reflective mirror is deposited upon the $K_9$ substrate by E-beam evaporation. The basic deposition condition is shown in table 1.

**Table1 The parameter of deposition**

| Vacuum | Temperature | Baking | Gas |
|---|---|---|---|
| $2.5\times10^{-3}$ | 300℃ | 3H | $O_2$ |

Fig. 2 give the comparison of the optical performance between the numerical calculation and experimental result at working wavelength and exposing wavelength respectively, which are corresponding to the stack of $H3L(H2L)^9H0.5L$. As can be seen from Fig. 2, both the working wavelength and the exposing wavelength meet the basic optical requirements of multi-layer dielectric grating. Furthermore, both of the wavelengths have sufficient tolerance latitude. The experiment proves that rigorous coupled-wave analysis and enhanced transmittance matrix approach are effective methods to calculate the performance of multi-layer dielectric thin film.

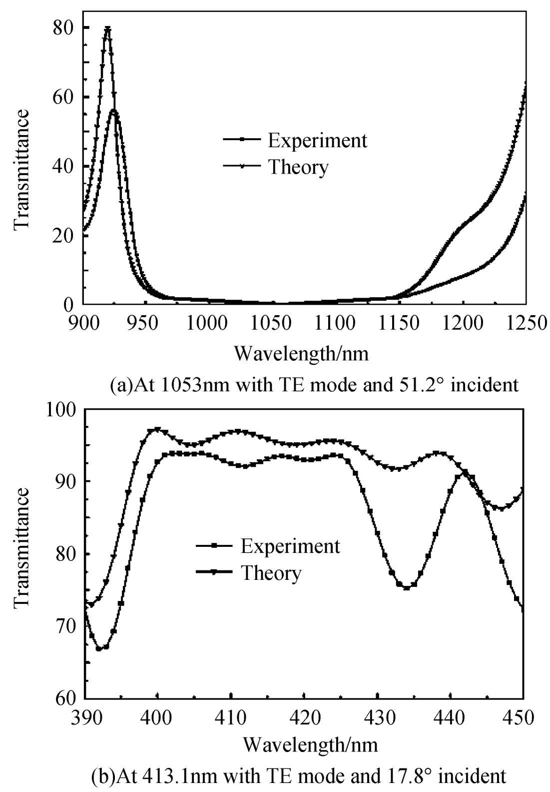


Fig. 2 Optical performance of $H3L(H2L)^9H0.5L$

## 3 Conclusion

According to the rigorous coupled-wave

analysis and enhanced transmittance matrix approach, which are used for the accurate calculation of diffraction performance of gratings, we developed a relatively straightforward and deterministic technique for the specially analysis of the optical property of high reflective mirror for multi-layer dielectric grating. Experiment shows that the designed high reflective mirror of H3L(H2L)9H0.5L presents excellent optical spectrum at working wavelength and exposing wavelength, which proves that rigorous coupled-wave analysis and enhanced transmittance matrix approach are stable and efficient numerical implementation of the analysis of multi-layer optical thin film.

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# 多层介质膜光栅用高反射镜的严格耦合波分析

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**摘 要**:基于严格耦合波和增强透射矩阵的方法,提出了一种数值稳定的求解多层介质膜光学特性的机理模型.利用该模型计算了多层介质膜光栅用高反射镜的优化设计膜系.使用电子束热蒸发方式制备的多层介质膜光谱特性和理论设计的结果符合得很好,该严格耦合波模型是分析介质膜光学特性有效的稳定的数值求解方法.

**关键词**:高反射镜;介质膜光栅;严格耦合波分析

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