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Transmittance design of internal reflection triangular-groove grating at large dimension domain

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ABSTRACT

We present that the internal reflective triangular-groove grating can be effectively analyzed and designed by the developed scalar diffraction theory and the effective medium theory at the certain feature size. This grating profile could be applied in enhancing significantly the light extraction efficiency of light-emitting diodes. The accuracy of these both uncomplicated methods is quantitatively evaluated by the comparison of diffraction efficiencies predicted from them to exact results calculated by the rigorous coupled wave analysis method. When the normalized period of a grating is more than fourfold wavelengths of emitted light, the developed scalar diffraction theory is accurate and useful to analyze the internal reflective triangle grating. As the higher order diffraction waves other than zero order wave is not to propagate, the effective medium theory can precisely evaluate the transmittance within the error of about 1.2%. Besides, the used limitation of these simple methods as a function of the normalized height is also quantitatively determined. Furthermore, the transmission characteristics of manufacturing deficiencies of an internal reflection grating as a function of the groove width are quantitatively calculated by using the rigorous coupled wave analysis.

1. Introduction

"Moth" eye structure with the tapered profile has been widely integrated in high-efficiency optoelectronic devices, such as solar cells and photodetectors [1–4]. This applied structure with an excellent antireflective property can effectively suppress the Fresnel reflection at the interface between two different refractive index materials. Also, the problem with the matching of the thermal expansion coefficient of an antireflective multilayer film can be overcome by "moth" eye structure. Therefore, the extensive research efforts have primarily focused on the external reflective structure [1–7]. However, in contrast to solar cells and other photosensitive devices, the light extraction efficiency enhancement of light-emitting diodes (LEDs) is limited crucially by the behavior of internal reflection. Especially, the total internal reflection effect occurs above the critical angle. Recently, there were few reports on the antireflective microstructure integrated in LED components [8–10]. These structure arrays on the noteworthy reduction of internal reflection demonstrated the key technology on the enhancement of the external quantum efficiency of devices. To our knowledge, recent works mostly concentrated on the external reflective property, and it is uncommon to quantitatively investigate the internal reflective performance of microstructure grating that can be applied in LED devices. Though it was reported in the experiment that the approximate triangular nanopatterning grating structure was fabricated on the contact layers of LEDs to improve the output power by 63% at 20 mA [11], the theoretical investigation is absent.

Generally, in the aspect of design and analysis of surface structure, the rigorous electromagnetic vector theories, such as rigorous coupled wave analysis (RCWA) and finite-different time-domain (FDTD), are commonly applied to yield accurate diffraction characteristics regardless of the feature size of surface profile. Nevertheless, these rigorous vector methods are difficult to be used for computationally intensive. In order to easily analyze and effectively design the transmittance characteristics of an internal reflective triangular grating structure, we propose that the uncomplicated methods, the developed scalar diffraction theory (SDT) and the effective medium theory (EMT), can be utilized. Based on the comparison of diffraction efficiencies predicted from EMT and SDT, to the results calculated by RCWA, the validity of both simple methods is quantitatively determined as a function of the normalized period and the normalized groove depth.

2. Theory and calculated results

Fig. 1 shows the schematic diagram of internal reflective grating structure. The surface structure depth is h, and the period is Λ.

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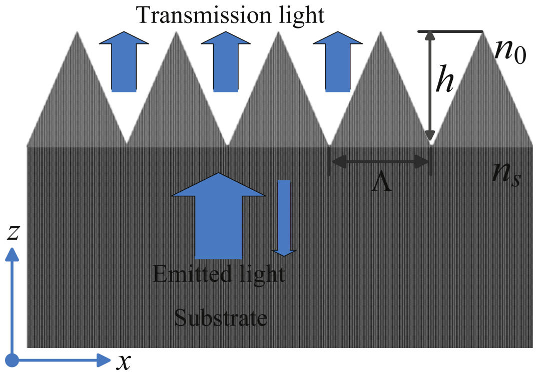

Fig. 1. The schematic diagram of the internal reflective microstructure grating with the depth h, period Λ. The refractive indices of microstructure and substrate material are n_s. The calculated transmittance of surface structure in air is emitted from the substrate material.

The refractive index of substrate material (GaN, n_s=2.5) is applied and the absorption of emitted light in structure is ignored. The emitted light wavelength of 470 nm is assumed. Although it is known that the randomization emission of photons from LEDs active layer is in all directions, the extraction light from elements can emit within the cone angle of the critical angle. For simplification, we use the plane wave instead of randomized emitted light from active layer to estimate the transmittance characteristics of triangular-groove internal reflective grating. Just vertical launch direction is considered. TE polarization light is defined as the electric field **E** parallel to the grating vector, and the electric field **E** of TM polarization is perpendicular to the grating vector. It is well known that the RCWA method has been demonstrated to be precise and effective for analyzing the diffraction efficiency of periodic surface structure [12]. Thus, in our study, the calculated diffraction efficiencies by using RCWA are utilized as the compared criterion.

2.1. RCWA method

The RCWA is a relatively straightforward technique for obtaining the exact solution of Maxwell's equations for the electromagnetic diffraction of grating structures [13]. It is a semi-analytical method in computational electromagnetics. RCWA is a widely used method for the accurate analysis of the diffraction of electromagnetic waves in periodic structures [14]. The RCWA expands mathematically the field inside the grating region with a number of Fourier series. A triangular dielectric diffraction grating depicted in Fig. 1 can be approximated by a multilayer lamellar grating. For each of the lamellar grating layers, the electromagnetic field can be obtained by using the Maxwell equations as

$$\nabla\times\mathbf{H}^j=\varepsilon^j\frac{\delta\mathbf{E}^j}{\delta t}$$
$$\nabla\times\mathbf{E}^j=-\mu\frac{\delta\mathbf{H}^j}{\delta t} \quad (1)$$

where ε^j is the relative permittivity of jth layer and μ is the relative permeability. A monochromatic plane wave of vacuum wavelength λ is incidenting on the grating at a polar angle θ and an azimuthal angle ϕ. Then the incident normalized electromagnetic field vector is

$$\mathbf{E}_{inc}=\hat{u}\exp(-i\mathbf{k}_0\cdot\mathbf{r})$$
$$\eta_0\mathbf{H}_{inc}=\hat{b}\exp(-i\mathbf{k}_0\cdot\mathbf{r}) \quad (2)$$

with

$$\mathbf{k}_0=k_0(\sin\theta\cos\phi\hat{x}+\sin\theta\sin\phi\hat{y}+\cos\theta\hat{z})$$

$$\eta_0=\sqrt{u_0/\varepsilon_0}$$

where $k_0=2\pi/\lambda$, u_0 is the permeability of free space, ε_0 is the permittivity of free space, $\hat{u}$ and $\hat{b}$ are the polarization unit vector given by

$$\begin{aligned}\hat{u}&=u_x\hat{x}+u_y\hat{y}+u_z\hat{z}\\&=(\cos\psi\cos\theta\cos\varphi-\sin\psi\sin\varphi)\hat{x}\\&+(\cos\psi\cos\theta\sin\varphi+\sin\psi\cos\varphi)\hat{y}-\cos\psi\sin\theta\hat{z},\end{aligned}$$

$$\begin{aligned}\hat{b}&=b_x\hat{x}+b_y\hat{y}+b_z\hat{z}\\&=(-\sin\psi\cos\theta\cos\varphi-\cos\psi\sin\varphi)\hat{x}\\&+(-\sin\psi\cos\theta\sin\varphi+\cos\psi\cos\varphi)\hat{y}\\&-\sin\psi\sin\theta\,\hat{z},\end{aligned}$$

where ψ is the angle between the polarization vector and the plane of incidence. For $\psi=0^\circ$ and $\psi=90^\circ$, the magnetic field and electric respectively, are perpendicular to the plane of incidence corresponding to TM polarization and TE polarization, respectively. When the azimuthal angle $\phi=0^\circ$, Eq. (2) is simplified to

$$\begin{cases}\mathbf{E}_{inc}=\hat{y}\exp[ik_0(x\sin\theta+z\cos\theta)]\\\mathbf{H}_{inc}=\frac{1}{\eta_0}(\hat{z}\sin\theta-\hat{x}\cos\theta)\exp[ik_0(x\sin\theta+z\cos\theta)]\end{cases} \quad (3)$$

for TE polarization, and

$$\begin{cases}\mathbf{E}_{inc}=(-\hat{z}\sin\theta+\hat{x}\cos\theta)\exp[ik_0(x\sin\theta+z\cos\theta)]\\\mathbf{H}_{inc}=\frac{1}{\eta_0}\hat{y}\exp[ik_0(x\sin\theta+z\cos\theta)]\end{cases} \quad (4)$$

for TM polarization. Owing to the triangular dielectric grating has the performance of periodicity, the Fourier modal expansions of basic modal field for each layer can be expressed as

$$[\mathbf{E},\eta_0\mathbf{H}]^j=\exp[ik_0(\alpha_m x+\beta_0 y)][e_{xm},e_{ym},e_{zm},-h_{xm},h_{ym},h_{zm}]^j,$$
$$\times\exp[ik_0\gamma\left(z-z^j\right)] \quad (5)$$

where $\alpha_m=\alpha_0+m\lambda/\Lambda,\quad m=0,\pm1,\pm2,\cdots\pm M,\cdots,$ $\alpha_0=\sin\theta\cos\varphi$, Λ is grating period, $\beta_0=\sin\theta\sin\varphi$, γ is the component of wave vector in the z direction, $e_{xm},e_{ym},e_{zm},-h_{xm},-h_{ym},h_{zm}$ are the coefficient of Fourier modal for electric field and magnetic field, respectively, and m is Fourier series. Using the 'inverse rule' with dramatical improvement of numerical convergence proposed by Li [15], the relative permittivity is expanded as

$$(\varepsilon)_{mn}=\frac{1}{\Lambda}\int_0^{\Lambda}\varepsilon(x)\exp\left[-i\frac{2\pi}{\Lambda}(m-n)x\right]dx$$

and

$$(\overline{\varepsilon})_{mn}=\frac{1}{\Lambda}\int_0^{\Lambda}\frac{1}{\varepsilon(x)}\exp\left[-i\frac{2\pi}{\Lambda}(m-n)x\right]dx,$$

where $m,n=0,\pm1,\pm2,\cdots\pm M,\cdots$. Therefore, the matrix equations for jth layer are derived from Eq. (1) as

$$\begin{cases}(\beta_0[e_{zm}]-[e_{ym}][\gamma_{mn}])=-[h_{xm}], & [\overline{\varepsilon}_{mn}](\beta_0[h_{zm}]-[h_{ym}][\gamma_{mn}])=-[e_{xm}]\\ [e_{xm}][\gamma_{mn}]-[\alpha_{mn}][e_{zm}]=-[h_{ym}], & -[h_{xm}][\gamma_{mn}]-[\alpha_{mn}][h_{zm}]=-[\varepsilon_{mn}][e_{ym}],\\ [\alpha_{mn}][e_{ym}]-\beta_0[e_{xm}])=[h_{zm}], & [\alpha_{mn}][h_{ym}]+\beta_0[h_{xm}]=-[\varepsilon_{mn}][e_{zm}]\end{cases} \quad (6)$$

where $[e_{xm}]$, $[e_{ym}]$, $[e_{zm}]$, $[h_{xm}]$, $[h_{ym}]$ and $[h_{zm}]$ stand for column matrices made up of $e_{xm},e_{ym},e_{zm},h_{xm},h_{ym},h_{zm}$, respectively, and $[\varepsilon_{mn}]$, $[\alpha_{mn}]$ and $[\gamma_{mn}]$ represent diagonal matrices. Then the Eq. (6) can be simplified as

$$\begin{bmatrix}I-[\alpha_{mn}][\varepsilon_{mn}]^{-1}[\alpha_{mn}] & -[\alpha_{mn}][\varepsilon_{mn}]^{-1}\beta_0\\ -\beta_0[\varepsilon_{mn}]^{-1}[\alpha_{mn}] & I^{-1}-\beta_0[\varepsilon_{mn}]^{-1}\beta_0\end{bmatrix}\begin{bmatrix}[h_{ym}]\\ [h_{xm}]\end{bmatrix},$$