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# Accuracy analysis of simplified and rigorous numerical methods applied to binary nanopatterning gratings in non-paraxial domain

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ABSTRACT

A set of simplified and rigorous electromagnetic vector theories is used for analyzing the transmittance characteristics of diffraction phase gratings. The scalar diffraction theory and the effective medium theory are validated with the exact results obtained via the rigorous coupled-wave theory and the finite-difference time-domain method. The effects of surface profile parameters and also the angle of incidence is demonstrated to be a limiting factor in the accuracy of these theories. Therefore, the error of both simplified theories is also analyzed in non-paraxial domain with the intention of establishing a specific range of validity for both simplified theories.



## 1. Introduction

Dielectric binary gratings are of wide interest owing to their many applications in polarization systems [1], solar energy [2,3], ultrafast optics [4], displays [5] and coherence [6]. Several investigators have analyzed the grating properties in the frame of scalar optics [7,8]. Simplified theories are commonly used and are attractive in the design and analysis of Diffractive Optical Elements (DOEs) because of their simplicity and low computational intensity [9,10]. Nevertheless, thanks to the spectacular improvements in grating manufacturing in the middle of the century due to the use of interferometry in association with servo-control systems [11,12], it becomes possible to achieve high quality gratings with more than 1000 lines/mm [13]. Here, the groove spacing and the wavelength became of the same order of magnitude and it has been demonstrated that exists a clear influence of the polarization on the efficiency curves.

The accuracy of the Scalar Diffraction Theory (SDT) has been previously compared to the Rigorous Coupled-Wave (RCW) theory in the works by Pommet et al. [14], Glytsis et al. [15] and also for perfectly conducting gratings in [16] among others. Regarding dielectric DOEs, the reliability of SDT results for the zeroth and first diffraction orders has been analyzed as a function of the normalized thickness ($h/\lambda$) in a specific range for different periods, and illumination schemes. In the area of the Effective Medium Theory (EMT) there are papers that compare EMT with the RCWA on many types of dielectric and metallic gratings such as [17–19].

Recently, Jing et al. [20,21] presented a deep analysis of the accuracy of both SDT and EMT for analyzing the transmittance characteristics of diffraction phase and sinusoidal gratings at normal incidence. The results derived from [20] concluded that SDT can accurately estimate the diffraction efficiency, even with periods of two wavelengths ($\Lambda/\lambda = 2$) and under several conditions. Regarding EMT, it is demonstrated that its precision is quite good for high spatial frequency gratings ($0.1 \leqslant \Lambda/\lambda \leqslant 0.6$). Nevertheless, the effect of the angle of incidence in the accuracy of these two simplified theories applied to binary phase gratings for a wide range of depths and grating periods has not been reported yet.

In this Letter, the Rigorous Coupled-Wave (RCW) approach with the finite difference time-domain (FDTD) method, both belonging to the rigorous electromagnetic vector theories, are used here as reference in order to analyze the behavior of the simplified theories also considering arbitrary angle of incidence. Through the comparison of the transmission efficiencies predicted by SDT and

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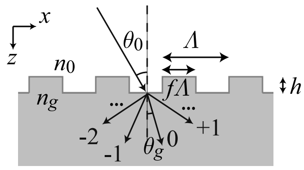


**Fig. 1.** Schematic diagram of diffraction phase grating.

EMT, with those calculated with RCW and FDTD, the limitations of simplified theories is fully determined considering the effect of the normalized period and depth and also the angle of incidence. For the RCW approach, the influence of the number of harmonics considered in the Fourier series of the contour has also been considered. Because of that, FDTD has been also implemented in order to avoid this effect in the results. FDTD is a numerical method based on a discretization of the simulation region [22]. This discretization implies some limitation when periodic media is considered. These aspects have been covered in [23–26] for instance. However, in this work an specific formalism of FDTD for periodic media has been considered. More specifically, the split-field FDTD has been implemented in order to limit the simulation size to a single period of the periodic element under analysis [27–29]. The spatial and time resolution have been chosen in order to avoid numerical instabilities with a wide decision margin. This aspect also permits to accurately describe the grating structures ensuring that results provided by FDTD are rigorous and precise. This implies greater simulation sizes and also more time steps for achieving steady-state. However, a Graphics Processing Units (GPUs) based implementation give us the opportunity to simulate in less time problems that would be unaffordable with conventional programming solutions [30,31].

To illustrate the range of validity of the simplified theories, the diffraction characteristics in transmission of binary phase gratings and their error are computed for a wide range depth and period and also for different values of the fill factor. Although the error obtained with SDT in paraxial domain is small, it grows as the gratings goes into volume region. This trend increases as the angle of incidence becomes greater, thus reducing the range of operation of this theory even with periods of five wavelengths. Regarding EMT, its accuracy is demonstrated to be more homogenous in non-paraxial domain being the best case at normal incidence and only when the zero-order wave exists. The accuracy of these theories and also the effect of the harmonics in the RCW are discussed in detail in the final section.

## 2. Theory

### 2.1. Scalar diffraction theory

In Fig. 1, $\Lambda$ and $h$ represent the period and groove depth, respectively, and $n_0$ and $n_g$ are the refractive indices of the incident medium and the grating. The light wave propagates from air ($n_0 = 1.00$) through the surface into the substrate material ($n_g = 1.50$). The diffraction efficiency of SDT can be calculated by using the scalar Kirchhoff diffraction theory, which neglects the vectorial and polarized nature of light. This theory provides reasonably accurate results when the periodicity of the surface profile is much larger than the wavelength of the incident light [20,21]. Specifically, when $\Lambda/\lambda \geqslant 20$, physical optics according to Fresnel and Snell's laws can explain the behavior of the diffraction efficiency of these optical elements [20,32]. This simplified theory is based on the general equation for diffraction efficiency $\eta$ in scalar approximation for a periodic structure as [33,20].

$$\eta = \left| \frac{1}{\Lambda} \int_0^{\Lambda} t(x) e^{-2jmx/\Lambda}\, dx \right|^2, \qquad (1)$$

where $t(x)$ is a function defined as the ratio of transmitted (or reflected) and incident wave amplitudes at location $x$, and $m$ is the diffracted order. Taking into account (1) and the geometry of the problem detailed in Fig. 1, the diffraction efficiencies for the zero and first order can be easily derived [20,33]

$$\eta_0 = (n_g \cos\theta_g / n_0 \cos\theta_0)\tau^2(\theta_0)\left[1 - 2f(1-f)(1-\cos\Delta\varphi)\right], \qquad (2)$$

$$\eta_{m\neq 0} = (n_g \cos\theta_g / n_0 \cos\theta_0)\tau^2(\theta_0)\left[\left(1/m^2\pi^2\right)\left(1-\cos(2m\pi f)\right) \times (1-\cos\Delta\varphi)\right], \qquad (3)$$

with $\theta_0$ being the angle of incidence. The rays inside the grating have an angle respect to the $x$ axes $\theta_g$ that can be obtained via Snell's Law. The Fresnel transmission coefficient is included by means of $\tau(\theta_0)$, and $\Delta\varphi = 2\pi h/\lambda(n_g \cos\theta_g - n_0 \cos\theta_0)$ is the phase difference between two parallel rays incident on the grating at an angle $\theta_0$ [20].

### 2.2. Effective medium theory

EMT considers a subwavelength grating as an anisotropic optical thin film with effective refractive indices. These indices are obtained from series expansions of transcendental functions, in terms of $\Lambda/\lambda$ [34]. Here, the zeroth-order and the second-order EMT are used to predict the diffraction efficiencies compared with the results calculated by the RCWT and FDTD.

$$n_{TE}^{(2)} = \left[ \left(n_{TE}^{(0)}\right)^2 + \frac{1}{3}\left(\frac{\Lambda}{\lambda}\right)^2 \pi^2 f^2 (1-f)^2 \left(n_g^2 - n_0^2\right)^2 \right]^{1/2}, \qquad (4)$$

$$n_{TE}^{(0)} = \left[(1-f)n_0^2 + f n_g^2\right]^{1/2}. \qquad (5)$$

To apply EMT, the diffraction grating shown in Fig. 1 can be approximated by a stack of homogenous layers. This layer is defined by a characteristic matrix.

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{ \prod_{r=1}^{k} \begin{bmatrix} \cos\delta_r & (j\sin\delta_r)/\eta_r^q \\ j\eta_r^q \sin\delta_r & \cos\delta_r \end{bmatrix} \right\} \begin{bmatrix} 1 \\ \eta_g^q \end{bmatrix}, \qquad (6)$$

where $B = E_a/E_g$ and $C = H_a/H_g$ are the ratios between the electric and magnetic fields at the front ($a$) and the substrate material ($g$) interfaces [35], $\delta_r = 2\pi h n(r)_{TE} \cos\theta_r / N\lambda$ is the phase of the $r$th layer, $n(r)_{TE}$ represents the effective index of refraction of the $r$th layer and $\eta_r = \eta_0 n(r)_{TE} \cos\theta_r$ for TE polarization, $\eta_0$ is the optical admittance in free space ($\eta_0 = \sqrt{\epsilon_0 \mu_0}$), and $\eta_g$ is the optical admittance in the substrate material. As detailed above, the angles $\theta_r$ can be calculated from Snell's Law.

### 2.3. Rigorous coupled-wave theory

In order to understand how light propagates inside a periodic medium, many numerical methods have been developed, such as the modal theory, first proposed by Wang and Tamir et al. [36–38] and applied to holography by Burkhardt [39], or the coupled-wave theory [40,41]. CWT proposed by Kogelnik [42] predicts very accurately the response of the efficiency of the first and second order for volume phase gratings. Nonetheless, the accuracy decreases when more than two orders are present in the grating. The rigorous coupled-wave theory doesn't disregard second derivatives in the CW equations and allow more than two orders. The RCW introduced by Moharam and Gaylord has accomplished the task of explaining a great number of physical situations associated with diffraction gratings of different kinds [43–46]. Since the RCW is well known only a brief description is given here.

We will study the propagation of light inside binary phase gratings. In all cases the conductivity inside the grating is supposed to