Three-dimensional diffraction analysis of gratings based on Legendre expansion of electromagnetic fields

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Three-dimensional vectorial diffraction analysis of gratings is presented based on Legendre polynomial expansion of electromagnetic fields. In contrast to conventional rigorous coupled wave analysis (RCWA) in which the solution is obtained using state variables representation of the coupled wave amplitudes, here the solution of first-order coupled Maxwell’s equations is expanded in terms of Legendre polynomials, where Maxwell’s equations are analytically projected in the Hilbert space spanned by Legendre polynomials. This approach yields well-behaved algebraic equations for deriving diffraction efficiencies and electromagnetic field profiles without facing the problem of numerical instability. The proposed approach can be applied in the analysis of two cases: first, arbitrarily oriented planar gratings with slanted yet homogeneous fringes; second, nonslanted but longitudinally inhomogeneous gratings. The method is then applied to various test cases within the above-mentioned two categories, comparison to other methods already reported in the literature is made, and the presented approach is justified. Different aspects of the proposed method such as numerical stability and convergence rate are also investigated. Special attention is given to how the resonant frequency of frequency-selective structures varies with introducing tilt angles and/or longitudinal inhomogeneity in the permittivity profile. © 2007 Optical Society of America

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1. INTRODUCTION

The analysis of wave propagation in periodic structures, due to its wide range of applications, is seen in various systems and design processes for telecommunications, electromagnetism, optics, and acoustics [1]. Consequently, it is essential to have an exact, efficient, and stable way to find reflection and transmission coefficients, diffraction efficiencies, and electromagnetic field profiles both inside and outside of gratings. In this regard, various rigorous approaches have been reported for the analysis of such structures. Virtually all available computational techniques, which have been developed mainly since 1970, can be roughly grouped into two categories [2, 3]. The first category, viz. integral methods, comprises those techniques, which start from the integral form of Maxwell’s equations. These approaches are best suited for analyzing gratings of continuous profiles. On the other hand, the second category encompasses those techniques, which start from the differential form of Maxwell’s equations and are more suitable for the analysis of discrete-level profiles. Both integral and differential methods have been extensively studied and numerically implemented. However, of the many methods proposed for the analysis of volume diffraction gratings, rigorous coupled wave analysis, or RCWA, is the most precise, the most general, and the most widely used method [4–6]. This method, being widely used since the 1980s [7], is successfully applied to different types of gratings, e.g., two-dimensional and three-dimensional isotropic and anisotropic gratings [8–11], together with multiple grating structures [12, 13]. Nevertheless, the use of RCWA is inherently restricted to particular situations, in which a set of shift invariant coupled equations, i.e., a system of linear differential equations with constant variables, is obtained [7]. This fact calls for the obligatory use of the staircase approximation for the analysis of longitudinally inhomogeneous gratings, where the inhomogeneous profile of a grating is approximated with a number of cascaded homogeneous profiles, each of them yielding shift invariant coupled equations. However, these structures can be analyzed by applying either R-matrix [14], scattering matrix [14, 15], or the so-called wave-splitting approach [16]. In this paper, RCWA is combined with the polynomial expansion method, where the encountered eigenvalue problem of standard RCWA and the likely need for applying staircase approximation are both shunned by using a nonmodal method, i.e., Legendre polynomial expansion. Thanks to the recursive properties of Legendre polynomials, our proposed approach is also capable of manipulating longitudinally inhomogeneous gratings, where no excessive computation burden, as opposed to the case of analyzing homogeneous gratings, comes along. This makes our approach well suited for analyzing gratings of longitudinally inhomogeneous refractive index profiles.

Historically, using the polynomial expansion method for the analysis of the special case of lamellar gratings was reported by Morf [17]. His method is based on the expansion of eigenfunctions in terms of ordinary polynomial basis functions. However, the aforementioned polynomial expansion approach is applied only in the transverse di-
rection, and separately, at each region of constant refractive index. Even though the Gibbs phenomenon was avoided in following that approach, the method still needed a subtle and delicate handling of propagating electromagnetic fields, where numerical instabilities similar to those usually encountered in applying transfer matrix methods were expected [17,18]. In this paper, a similar, yet fundamentally different approach is proposed, where the coupled Floquet harmonics of electromagnetic fields inside the grating are expanded in terms of orthogonal Legendre polynomials. Then, the solution is examined in a Hilbert space spanned by the polynomials. This approach has already been reported for the analysis of planar diffraction gratings [19] and is now extended to analyze arbitrarily oriented three-dimensional homogeneous and longitudinally inhomogeneous gratings. However, in contrast to the nonconical case of planar diffraction gratings, where a single second order Helmholtz equation was solved [19], the coupling of TE and TM components of all the forward- and backward-diffracted waves in this case calls for direct solving of the two first-order Maxwell’s equations. Furthermore, the Fourier factorization as given in [20–22] is now employed to ensure the proper convergence rate.

The case of conical diffraction has been treated by using different methods [9,23–25] and they have found many applications in free space filters, monochromators [26,27], and can be used as polarization insensitive filters [28]. In view of that, a robust method capable of analyzing gratings in conical mounting without encountering numerical problems is mandatory, and the proposed method is well suited for the analysis of such cases, especially when the transversally periodic refractive index profile happens to be longitudinally inhomogeneous.

This paper is arranged as follows: Legendre polynomial expansion formulation of electromagnetic fields for the analysis of gratings in conical mounting is discussed in Section 2. In Section 3, the convergence rate of the proposed method is studied. In Section 4, the computational complexity of the proposed approach is briefly discussed. In Section 5, a metallic grating case is presented to fully demonstrate the applicability of the proposed method. In Section 6, a typical frequency selective structure is analyzed and special attention is given to how the resonant frequency of frequency selective structures varies with introducing tilt angles and/or longitudinal inhomogeneity in the permittivity profile. Finally, conclusions are made in Section 7.

2. FORMULATION

In this section, electromagnetic field expressions inside and outside the grating are expanded in terms of orthogonal Legendre polynomials [29,30], and uniform plane waves, respectively. This novel electromagnetic field expression, being in accordance with the Floquet theorem, is substituted in Maxwell’s equations; appropriate boundary conditions are then applied, and finally the unknown expansion coefficients and diffraction efficiencies are found. It should be noticed that expanding the electromagnetic field expressions in orthogonal complete space of polynomials is in fact a nonharmonic expansion [29,31], i.e., it is not a linear combination of intrinsic eigenvectors. Nonetheless, it has some advantages over eigenvector expansion and other previously mentioned methods. First, the equations involve algebraic rather than transcendental functions; therefore, they can be manipulated easier. Second, this approach works properly and is unconditionally stable. Third, it can be easily applied for the analysis of inhomogeneous gratings, i.e., gratings with longitudinally inhomogeneous refractive index profiles. Thanks to the holistic nature of the proposed approach, the need for applying the staircase approximation of the longitudinal variations of the permittivity profile is eliminated.

A. Electromagnetic Fields Outside the Grating

The structure to be analyzed, i.e., an arbitrarily oriented grating, is shown in Fig. 1. Here, the permittivity is a periodic function:

$$\varepsilon(r + \lambda_G) = \varepsilon(r),$$

where $\lambda_G = \lambda_G (\sin(\phi)\hat{x} + \cos(\phi)\hat{z})$, $r = x\hat{x} + y\hat{y} + z\hat{z}$, and $\lambda_G$ denotes the value of grating period. Therefore, the grating vector can be written as

$$\mathbf{K}_G = \frac{2\pi}{\lambda_G} [\sin(\phi)\hat{x} + \cos(\phi)\hat{z}] = K_G \hat{x} + K_G \hat{z}. \quad (2)$$

In accordance with Fig. 1, the normalized total vector electric field in region I ($z < 0$) and in region III ($z > d$) can be expanded in terms of uniform plane waves corresponding to different diffracted orders [9]:

$$\mathbf{E}_1 = \hat{u} e^{\pm jk_{11}z} + \sum_{l=-\infty}^{+\infty} \mathbf{R}_l e^{-j k_{1l}z}, \quad (3)$$

$$\mathbf{E}_3 = \sum_{l=-\infty}^{+\infty} \mathbf{T}_l e^{-j k_{3l}z}, \quad (4)$$

with $\mathbf{k}_{1l}$, i.e., the $l$th forward-diffracted and $\mathbf{k}_{3l}$, i.e., the $l$th backward-diffracted wave vector, given as

$$k_{1x} = k_{x1} = k_1 \sin \alpha \cos \delta - iK_G \sin \phi,$$

$$k_{1y} = k_{y1} = k_1 \sin \alpha \sin \delta,$$

$$k_{1z} = \sqrt{k_1^2 - k_{1x}^2 - k_{1y}^2} \quad (7)$$

for $l = 1, 3$ (representing region I or III).

Fig. 1. General form of a slanted grating in conical mounting.
Here the index \( i \), which is running from \(-\infty \) to \( +\infty \), denotes the \( i \)th space harmonic corresponding to the \( i \)th diffracted order in regions I \((z < 0)\) and III \((z > d)\) in Fig. 1. \( \mathbf{R} \) and \( \mathbf{T} \) are reflection and transmission coefficients of the \( i \)th diffracted order, respectively. The \( z \) component of the wave vector, \( k_{z,i} \), is either negative real (propagating wave) or positive imaginary (evanescent wave). Likewise, for region 1, \( k_{z,1} \), is either positive real (a propagating wave) or negative imaginary (an evanescent wave). Furthermore, \( \hat{u} \) stands for the incident wave polarization unit vector and is given by

\[
\hat{u} = (\cos \psi \cos \alpha \cos \delta - \sin \psi \sin \delta) \hat{x} + (\cos \psi \cos \alpha \sin \delta + \sin \psi \sin \alpha) \hat{y} - \cos \psi \sin \alpha \hat{z}.
\] (8)

In the above-mentioned equations, \( \phi \), \( \alpha \), \( \delta \), and \( \psi \) all of them depicted in Fig. 1, stand for the grating slant angle, the incident angle, the tilt angle, and the angle between the polarization vector and the plane of incidence, respectively.

B. Electromagnetic Fields Inside the Grating

Inside the grating, the Maxwell’s equations can be written as

\[
\nabla \times \mathbf{E} = -j \omega \mu \mathbf{H},
\] (9)

\[
\nabla \times \mathbf{H} = j \omega \varepsilon_0 \varepsilon_r(x,z) \mathbf{E}.
\] (10)

In these equations, \( \mathbf{E} \) and \( \mathbf{H} \) can be expanded in terms of space harmonics as \( [9] \)

\[
\mathbf{E} = \sum_i \left[ S_{xi}(z) \hat{x} + S_{yi}(z) \hat{y} + S_{zi}(z) \hat{z} \right] \exp[-j \alpha \mathbf{\hat{r}}],
\] (11)

\[
\mathbf{H} = \sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_i \left[ U_{xi}(z) \hat{x} + U_{yi}(z) \hat{y} + U_{zi}(z) \hat{z} \right] \exp[-j \alpha \mathbf{\hat{r}}],
\] (12)

where \( \alpha = k_{x} \hat{x} + k_{y} \hat{y} - j K_{G} \hat{z} \).

The above-mentioned coefficients \( k_{x} \) and \( k_{y} \) being determined from phase matching condition, are given in Eqs. (5) and (6). On the other hand, \( \varepsilon \) and \( \varepsilon^{-1} \), which are both periodic functions, can be expanded in terms of their Fourier series as

\[
\varepsilon(x,z) = \sum_k \varepsilon_k e^{j \mathbf{k}_G \mathbf{r}},
\] (13)

\[
\varepsilon^{-1}(x,z) = \sum_k \varepsilon_k^{-1} e^{j \mathbf{k}_G \mathbf{r}},
\] (14)

where \( \varepsilon_k = \frac{1}{A G} \int_{\lambda_z} e^{-j \mathbf{k}_G \mathbf{r}} d \mathbf{r} \) and \( \varepsilon_k^{-1} = \frac{1}{A G} \int_{\lambda_z} \frac{1}{\varepsilon(z)} e^{-j \mathbf{k}_G \mathbf{r}} d \mathbf{r} \) represent the \( h \)th Fourier component of above-mentioned expansion. These Fourier components are scalars for arbitrarily oriented planar gratings with homogeneous fringes and are \( z \) dependent functions for longitudinally inhomogeneous gratings, where the permittivity profile is separable in the Cartesian coordinate system, i.e., \( \varepsilon(x,z) = \varepsilon_1(z) \varepsilon_2(z) \).

Now, after substituting Eqs. (11)–(14) in Eqs. (9) and (10), the proper Fourier factorization technique should be followed to secure the fast convergence rate of numerical results with respect to the number of retained spatial harmonics \([7] \). Here, the Fourier factorization method as reported in \([20–22] \) is employed, the \( z \) components of the electromagnetic fields are eliminated, and the following set of four first-order coupled differential equations is derived. Although the presented set of equations works well to ensure the fast convergence of rectangular lamellar gratings, it fails to handle slanted metallic lamellar gratings, for which the fast Fourier factorization method should be applied\([7,32,33]\):

\[
\frac{dS_{xi}(z)}{dz} = -j \left\{ iK_{Gz}S_{xi}(z) + \frac{k_{xi}}{k_0} \sum_p \left[ [\varepsilon]_{zp}^{-1} \left[ k_p U_{xp}(z) - k_{xp} U_{yp}(z) \right] \right] + k_0 \sum_p \left[ [\varepsilon]_{zp} \right] S_{xp}(z) \right\},
\] (15)

\[
\frac{dS_{yi}(z)}{dz} = -j \left\{ iK_{Gy}S_{yi}(z) + \frac{k_{yi}}{k_0} \sum_p \left[ [\varepsilon]_{yp}^{-1} \left[ k_p U_{xp}(z) - k_{xp} U_{yp}(z) \right] \right] - k_{xp} U_{yp}(z) \right\},
\] (16)

\[
\frac{dU_{xi}(z)}{dz} = -j \left\{ iK_{Gz} U_{xi}(z) + \frac{k_{xi}}{k_0} \left[ k_p S_{xi}(z) - k_{xi} S_{yi}(z) \right] + k_0 \sum_p \left[ [\varepsilon]_{zp} \right] S_{xp}(z) \right\},
\] (17)

\[
\frac{dU_{yi}(z)}{dz} = -j \left\{ iK_{Gy} U_{yi}(z) - \frac{k_{yi}}{k_0} \left[ k_p S_{xi}(z) - k_{yi} S_{yi}(z) \right] + k_0 \sum_p \left[ [\varepsilon]_{zp} \right] S_{xp}(z) \right\}.
\] (18)

Here, \( [[\varepsilon]] \) and \( [[1/\varepsilon]] \) denote the Toeplitz matrices, whose \((i,p)\) entries are \( \varepsilon_{i-p} \) and \( \varepsilon_{i-p}^{-1} \) as given in Eqs. (13) and (14), respectively. It should be noticed that in the special case of longitudinally inhomogeneous gratings, where the grating vector \( \mathbf{K}_G \) is along the \( x \) direction and the Fourier coefficients \( \varepsilon_k \) and \( \varepsilon_k^{-1} \) become \( z \)-dependent functions, the aforementioned Toeplitz forms happen to be nonconstant \( z \)-dependent matrices, and therefore Eqs. (15)–(18) will not necessarily be shift invariant coupled differential equations to be solved analytically. However, this latter case can still be easily handled by using the following polynomial expansion.

This set of linear differential equations is solved by following the Galerkin’s method, where each component of the space harmonic amplitudes is now expanded in terms of Legendre polynomials:

\[
S_{zi}(z) = \sum_{m=0}^{\infty} q_m^z P_m(\xi),
\] (19)
where, \( \xi = (2\pi - d)/d \), \( P_m(\xi) \)'s stand for the normalized Legendre polynomials, and \( d \) is the grating thickness as shown in Fig. 1.

It should be noticed that the vector space spanned by Legendre polynomials is a complete one [30], and therefore each one of the space harmonic amplitudes can be expanded in terms of such a basis. Although truncating the polynomial expansions given in Eqs. (19)–(22), are then substituted in Eqs. (15)–(18), where the polynomial expansions of space harmonics, Eqs. (19)–(22), are then substituted in Eqs. (15)–(18), where the first \( M_1 \) terms of the expansion are retained:

\[
\sum_m q_m^i \frac{d}{dz} P_m(\xi) + \sum_m P_m(\xi) \times \left\{ i K_\xi q_m^i + k_x \sum_p [i \xi]_{ip} \left[ k_y t_m^p - k_x p_m^p \right] - k_\xi p_m^i \right\} = 0, \tag{23}
\]

\[
\sum_m h_m^i \frac{d}{dz} P_m(\xi) + \sum_m P_m(\xi) \times \left\{ i K_\xi h_m^i + k_x \sum_p [i \xi]_{ip} \left[ k_y t_m^p - k_x p_m^p \right] - k_\xi h_m^i \right\} = 0, \tag{24}
\]

\[
\sum_m t_m^i \frac{d}{dz} P_m(\xi) + \sum_m P_m(\xi) \times \left\{ i K_\xi t_m^i - k_x \sum_p [i \xi]_{ip} \left[ k_y t_m^p - k_x p_m^p \right] - k_\xi t_m^i \right\} = 0, \tag{25}
\]

\[
\sum_m t_m^i \frac{d}{dz} P_m(\xi) + \sum_m P_m(\xi) \times \left\{ i K_\xi t_m^i - k_x \sum_p [i \xi]_{ip} \left[ k_y t_m^p - k_x p_m^p \right] - k_\xi t_m^i \right\} = 0. \tag{26}
\]

In the case of longitudinally inhomogeneous gratings \( \epsilon_x \)'s and \( \epsilon_y \)'s are approximated by simple polynomials of \( N_1 \)th degree, and the following equations are obtained:

\[
[i \epsilon(\xi)] = [a_0] + [a_1] \xi + [a_2] \xi^2 + [a_3] \xi^3 + \cdots + [a_{N_1}] \xi^{N_1}, \tag{27}
\]

\[
([i \epsilon(\xi)]^{-1}) = [b_0] + [b_1] \xi + [b_2] \xi^2 + [b_3] \xi^3 + \cdots + [b_{N_1}] \xi^{N_1}, \tag{28}
\]

\[
([1/\epsilon(\xi)]^{-1}) = [c_0] + [c_1] \xi + [c_2] \xi^2 + [c_3] \xi^3 + \cdots + [c_{N_1}] \xi^{N_1}, \tag{29}
\]

where \( N_1 \) is appropriately chosen for having acceptable approximations in Eqs. (27)–(29). For slanted gratings with homogeneous fringes, however, \( \epsilon_x \)'s and \( \epsilon_y \)'s are scalars and need no interpolation. After substituting those interpolated Toeplitz matrices into a set of Eqs. (23)–(26), the resultant expansion is absorbed in the Legendre polynomial expansion of electromagnetic fields by using a well-known recurrence property of Legendre polynomials [34], which reads as

\[
\xi P_m(\xi) = \frac{m + 1}{2m + 1} P_{m+1}(\xi) + \frac{m}{2m + 1} P_m(\xi). \tag{30}
\]

This feature indicates that any power of \( \xi \) can be absorbed in Legendre polynomials by successively using Eq. (30). It can be easily shown that

\[
\sum_{m=0}^{+\infty} \xi \eta_m P_m(\xi) = \sum_{m=0}^{+\infty} \chi_m P_m(\xi), \tag{31}
\]

where

\[
[\chi_m] = [\eta_m]. \tag{33}
\]

Therefore, once the matrix \([\chi]\) is generated, any power of \( \xi \) can be easily absorbed in the expansion given in Eq. (31), by multiplying the corresponding power of \([\xi]\) to the vector \([\eta_m]\). Now the resultant equation can be analytically reprojected on Legendre basis polynomials and a set of coupled algebraic equations, representing the Maxwell’s equations in the Hilbert space spanned by Legendre polynomials, is analytically derived:

\[
\frac{2}{d} \left[ \frac{d}{dz} q_m^i \right] + j \left( i K_\xi [q_m^i] + \frac{k_x}{k_0} \sum_p [b_{n,ip} \chi]^p [k_y t_m^p - k_x p_m^p] \right) + k_\xi [t_m^i] = 0, \tag{34}
\]

\[
\frac{2}{d} \left[ \frac{d}{dz} h_m^i \right] + j \left( i K_\xi [h_m^i] + \frac{k_x}{k_0} \sum_p [b_{n,ip} \chi]^p [k_y h_m^p - k_x p_m^p] \right) - k_\xi [t_m^i] = 0, \tag{35}
\]

\[
\frac{2}{d} \left[ \frac{d}{dz} t_m^i \right] + j \left( i K_\xi [t_m^i] - k_x \sum_p [b_{n,ip} \chi]^p [k_y t_m^p - k_x p_m^p] \right) - k_\xi [h_m^i] = 0, \tag{36}
\]

\[
\frac{2}{d} \left[ \frac{d}{dz} h_m^i \right] + j \left( i K_\xi [h_m^i] - k_x \sum_p [b_{n,ip} \chi]^p [k_y h_m^p - k_x p_m^p] \right) - k_\xi [t_m^i] = 0, \tag{37}
\]

\[
\frac{2}{d} \left[ \frac{d}{dz} t_m^i \right] + j \left( i K_\xi [t_m^i] - k_x \sum_p [b_{n,ip} \chi]^p [k_y t_m^p - k_x p_m^p] \right) - k_\xi [h_m^i] = 0. \tag{38}
\]
\[
\frac{2}{d} [\ell_m'] + j \left\{ i K_G [\ell_m'] - \frac{k_m}{k_0} (k_m \tilde{q}_m' - k_m \tilde{q}_m') \right\} \\
+ k_0 \sum_{\nu} \sum_{m} \left[ c_{\nu} \mu_{\nu} \chi_m^p [q_m'] \right] = 0. \tag{37}
\]

In these equations, \( q_m' \), \( h_m' \), \( t_m' \), and \( \ell_m' \) are the expansion coefficients of the first derivative of the Legendre expansion in terms of \( q_m' \), \( h_m' \), \( t_m' \), and \( \ell_m' \) respectively, and can be computed analytically as

\[
x_m' = (2m + 1) \sum_{l = m + 1}^{M} x_{l}', \tag{38}
\]

where \( x \) can be substituted by \( q, h, t, \) or \( l \). Analytically obtaining the first derivative of the Legendre expansion furtheres the efficiency of the proposed method.

### C. Applying Boundary Conditions

It should be noticed that each of Eqs. (34)–(37) results in a set of \( M_i \) equations, whereas each space harmonic expanded in Eqs. (19)–(22) is determined by \( M_i + 1 \) unknown coefficients. Therefore, one needs four further equations, which can be obtained by applying boundary conditions [31] at \( z=0 \) and \( z=d \). Appropriate boundary conditions can be applied by using the electromagnetic field expressions in regions I and III given in Eqs. (3) and (4), respectively [9].

Continuity of the electromagnetic fields at \( z=0 \) calls for

\[
u \delta_0 + R_{x_i} = S_{x_i}(0), \tag{39}
\]

\[
u \delta_0 + R_{y_i} = S_{y_i}(0), \tag{40}
\]

\[
u \delta_0 (k_m u_i - k_1 \cos \alpha u_j) - k_i R_{x_i} + k_i R_{x_i} = k_0 U_{x_i}(0), \tag{41}
\]

\[
u \delta_0 (k_1 \cos \alpha u_i - k_0 u_i) + k_i R_{x_i} - k_i R_{x_i} = k_0 U_{y_i}(0), \tag{42}
\]

and at \( z=d \):

\[
T_{x_i} = S_{x_i}(d) \exp(iK_Gd'), \tag{43}
\]

\[
T_{y_i} = S_{y_i}(d) \exp(iK_Gd'), \tag{44}
\]

\[
k_{z,2d} T_{y_i} + k_{z} T_{y_i} = k_{0} U_{y}(d) \exp(iK_Gd'), \tag{45}
\]

\[
k_{z,2d} T_{x_i} - k_{z} T_{x_i} = k_{0} U_{x}(d) \exp(iK_Gd'). \tag{46}
\]

The divergence equation in regions I and III also yields the following equations:

\[
k_{z} R_{x_i} + k_{z} R_{y_i} + k_{z} R_{z_i} = 0, \tag{47}
\]

\[
k_{z} T_{x_i} + k_{y} T_{y_i} + k_{z,2d} T_{z_i} = 0. \tag{48}
\]

Eliminating \( R_i \) and \( T_i \) components from these equations and substituting for space harmonic amplitudes, four equations are obtained as

\[
\sum_{m} (-1)^{m} \left[ k_{z,2d}^{2} + k_{z}^{2} - q_{m}^{2} + k_{z} k_{y} h_{m}^{2} + k_{y} k_{m} \right] = 0, \tag{49}
\]

\[
\sum_{m} (-1)^{m} \left[ k_{z,2d}^{2} + k_{z}^{2} - q_{m}^{2} + k_{x} k_{y} h_{m}^{2} + k_{x} k_{m} \right] = 0, \tag{50}
\]

\[
\sum_{m} \left[ k_{z,2d}^{2} + k_{z}^{2} - q_{m}^{2} + k_{x} k_{y} h_{m}^{2} + k_{x} k_{m} \right] = 0, \tag{51}
\]

\[
\sum_{m} \left[ k_{z,2d}^{2} + k_{z}^{2} - q_{m}^{2} + k_{x} k_{y} h_{m}^{2} + k_{x} k_{m} \right] = 0. \tag{52}
\]

Now Eqs. (34)–(37) and (49)–(52) form a complete set of equations, through which the unknown coefficients, i.e., \( q_m', h_m', t_m', \) and \( \ell_m' \) are obtained. Consequently, \( R_i, T_i \), and the corresponding diffraction efficiencies can be determined:

\[
D E_{1i} = \text{Re} \left[ \frac{k_{1,1}}{k_{1,0}} R_{1i} \right], \tag{53}
\]

\[
D E_{2i} = \text{Re} \left[ \frac{k_{2,1}}{k_{1,1}} T_{1i} \right]. \tag{54}
\]

For lossless dielectric gratings, conservation of energy calls for

\[
\sum_{i} D E_{1i} + D E_{2i} = 1. \tag{55}
\]

### 3. CONVERGENCE RATE

In following RCWA or any other modal method by Fourier expansion, both the permittivity and the electromagnetic fields inside the grating are expanded in a Fourier series, whereas infinite Fourier expansions are truncated by keeping \( N \) terms. It should be noticed that each complete solution of electromagnetic fields in the grating region calls for infinite terms in Fourier expansion; therefore, none of the truncated modes can exactly satisfy Maxwell’s equations and appropriate boundary conditions. However, increasing the truncation order \( N \) makes the permittivity distribution, the eigenvalues, and the eigenvectors of the modal fields closer to their exact values. Increasing the truncation order \( N \), not only makes each space harmonic involved in the electromagnetic field expansion inside the grating more precise, but also increases the total number of them. This conspicuously shows how strongly interwoven the convergence rate of the permittivity expansion and that of the electromagnetic field expansion and the number of required space harmonics are. Such a strong dependence is now abated by introducing a new factor \( M \), the number of retained polynomial basis func-
tions in expanding electromagnetic fields inside the grating. In fact, in many cases, it is revealed that the slow convergence rate of the solution is not solely due to the Gibb's phenomenon and the use of Fourier expansions, but can be also imputed to the slowly convergent eigen-solutions and the inadequate formulation of the conventional eigenproblem [20]. In the proposed method, the strong correlation of permittivity Fourier expansion, electromagnetic field expansion, and the number of required space harmonics is broken. Therefore, the proposed method can be categorized as a nonmodal method by Fourier expansion and can benefit from Fourier expansion of permittivity whereas the electromagnetic fields, whose accuracies can be augmented by increasing $M$, are expanded in terms of polynomials. However, supposing that the number of spatial harmonics is $N$ and the number of Legendre polynomials is $M$, the total size of the algebraic set of linear equations for solving the unknown coefficients would be $NM$. Consequently, the inadequacy of the conventional eigenvalue problem is avoided at the expense of a heavier computational burden and a much larger set of linear equations. This point is further explained in Section 4, where the computational complexity of the proposed method is briefly discussed. In this section, the convergence rate of numerical results is studied as a function of $M$, the number of retained Legendre polynomial basis functions.

As the first example to demonstrate the convergence rate of numerical results with respect to $M$, a transmission grating is analyzed. The number of retained harmonics in this example is $N=7$. The parameters according to Fig. 1 are: $\phi=150^\circ$ (slant angle), $\alpha=20^\circ$ (the angle of incidence), $\delta=45^\circ$ (tilt angle), $\psi=30^\circ$ (polarization angle), and $\varepsilon(x,z)=2.25(1+0.33 \cos(K_{Gx}x))$ in region II, and $\varepsilon_1=\varepsilon_{III}=2.25$. The incident wavelength is 1.9284 $\mu$m and the grating period is 1 $\mu$m. In Fig. 2 the convergence of the zeroth-order diffraction efficiency is shown versus the number of required polynomial basis functions for three different values of normalized thickness ($d/\lambda_G$), where it can be seen that the minimum number of required polynomial basis functions increases for deeper gratings.

4. COMPUTATIONAL COMPLEXITY
In this section, the computational time for the calculation of diffraction efficiencies in a dielectric grating is presented to have a comparison between the computational complexity of our proposed method and the standard RCWA. The grating parameters, in accordance with Fig. 1, read as: $\alpha=20^\circ$ (the angle of incidence), $\delta=45^\circ$ (tilt angle), $\psi=30^\circ$ (polarization angle), $\varepsilon_I=\varepsilon_{III}=2.25$ in regions I, and III, and $\varepsilon(x,z)=2.25(1+0.33 \cos(K_{Gx}x))$ in region II. The incident wavelength is 1.9284 $\mu$m, the grating period is 1 $\mu$m, and the grating thickness is 1 $\mu$m.

In Fig. 3, the computation time for the calculation of diffraction efficiencies is plotted versus $M$, i.e., the number of retained Legendre basis functions. In this case, the number of kept space harmonics is fixed at $N=7$. The computation time of RCWA, plotted in a solid line, is also presented for the sake of comparison. Furthermore, the computation time for the calculation of diffraction efficiencies of the same structure is plotted versus $N$, i.e., the number of retained spatial harmonics, in Fig. 4. In this latter case, the number of kept Legendre polynomial terms is fixed at $M=6$, which is large enough to ensure the error of less than 0.1%.

![Fig. 3. Computation time versus $M$, i.e., number of retained Legendre polynomial terms](image)

![Fig. 4. Computation time versus $N$, i.e., number of retained space harmonics](image)
These figures clearly demonstrate that the inadequacy of the conventional eigenvalue problem in the standard RCWA method is avoided at the expense of heavier computational burden. Nonetheless, the proposed technique can handle the special case of longitudinally inhomogeneous gratings at virtually negligible extra computational cost. This point is also demonstrated in Figs. 3 and 4, where the computation time for a similar structure; this time with a slight inhomogeneity in the permittivity profile of the grating, viz. $e(x,z)=2.25(1+0.33 \cos(K_Gx))(1+0.1(z/d))$, is plotted versus $M$, i.e., the number of retained Legendre basis functions, and $N$, i.e., the number of retained space harmonics.

5. METALLIC GRATINGS

Conventional coupled wave methods exhibit a poor convergence rate especially for metallic gratings in TM polarization [6,20,21] and this calls for the Fourier factorization method [7,20–22,32,33]. In this section, the applicability of the proposed method for the analysis of a metallic rectangular surface-relief grating is numerically demonstrated, where the properties of bulk gold at optical frequencies are used in the calculations. It should be noticed that the complex permittivity of bulk gold is available through its complex refractive index, $n - j\kappa$, as

$$e = n^2 - \kappa^2 - j2n\kappa,$$

where the parameters $n$ and $\kappa$ for bulk gold at the wavelength of 1 $\mu$m are given by $n=0.22$ and $\kappa=6.71$ [6,20,21].

Assuming the geometry of a binary rectangular groove diffraction grating in the inset of Fig. 5, the duty cycle of the binary grating ($f$) is 0.5, the dielectric permittivity of region I ($\varepsilon_I$) is 1, the incident angle ($\alpha$) is 30°, and the grating periodicity ($\lambda_G$) is 1 $\mu$m being equal to the wavelength of the incoming light at free space ($\lambda_0$) and grating thickness ($d$). Figures 5 and 6 show the relative error of $DE_{10}$ and $DE_{11}$, versus the number of polynomial terms retained in our calculation ($M$), respectively. This error is
Khavasi et al. presented in [20]. The relative error of using RCWA, keeping \( N = 41 \) space harmonics, which happens to be worse than that of ours calculated by using the proposed method with \( M > 6 \), is also shown. Similarly, \( DE_{10} \) and \( DE_{11} \) versus the number of space harmonics retained in our calculation (\( N \)), are depicted in Figs. 7 and 8, respectively. These results are obtained by keeping nine polynomial terms (\( M = 9 \)) and are again compared with those presented in Table 1 of [21]. Finally, Fig. 9 demonstrates \( DE_{10} \) and \( DE_{11} \) in a conical mounting, where \( \delta = 30^\circ \), \( \phi = 45^\circ \). The obtained results show an excellent agreement with those presented in [20].

6. FREQUENCY SELECTIVE STRUCTURES
As a different type of example, a frequency selective structure (FSS) is investigated. FSSs are composed of binary gratings designed in such a way that the incident wave undergoes a resonance and therefore these structures are used as sharp filters [35,36]. Here, the analyzed structure, in accordance with Fig. 10, has the following parameters: The duty cycle of the binary grating (\( f \)) is 0.5, regions I and III are free space (\( \varepsilon_r,\varepsilon_{HH} = 1 \)), the relative dielectric permittivity of grooves (\( \varepsilon_{groove} \)) is 1.44 and that of the ridge is \( \varepsilon_{ridge} = 2.56 \), the incident angle (\( \alpha \)) is 45°, and the grating thickness is \( 1.713 \lambda_d \). Reflectance of an in plane incident wave (\( \delta = 0^\circ \)) versus normalized frequency \( \Omega = K_0d \), is plotted in Fig. 11, where \( K_0 \) denotes the free space wave vector. Total reflection occurs at the two normalized resonant frequencies of 5.313 and 5.83. The result is obtained by keeping 19 space harmonics and eight Legendre polynomial terms, and perfectly agrees with the results of [36]. It can be seen that the obtained results converge after keeping merely eight polynomial terms.

The observed resonant frequency shifts by increasing the tilt angle. This point is more precisely demonstrated in Fig. 12, where the overall reflectance of the structure, for different values of tilt angle (\( \delta = 0^\circ \), \( \delta = 3^\circ \), \( \delta = 5^\circ \)), is plotted versus the normalized frequency \( \Omega = K_0d \). The normalized resonant frequency, \( \Omega_\alpha \), is then calculated for those different values of tilt angle, and is tabulated in Table 1. It can be seen that by increasing the tilt angle,

**Table 1. Resonant Frequency as a Function of Tilt Angle for the Frequency Selective Structure***

<table>
<thead>
<tr>
<th>( \delta )</th>
<th>Homogeneous</th>
<th>Inhomogeneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 0^\circ )</td>
<td>( \Omega_\alpha = 5.3133 )</td>
<td>( \Omega_\alpha = 5.2848 )</td>
</tr>
<tr>
<td>( 3^\circ )</td>
<td>( \Omega_\alpha = 5.3170 )</td>
<td>( \Omega_\alpha = 5.2883 )</td>
</tr>
<tr>
<td>( 5^\circ )</td>
<td>( \Omega_\alpha = 5.3234 )</td>
<td>( \Omega_\alpha = 5.2944 )</td>
</tr>
</tbody>
</table>

*Using the following parameters: \( f = 0.5 \), \( \Lambda_d = 1 \), \( \alpha = 45^\circ \), \( d = 1.713 \lambda_d \), \( \varepsilon_r = \varepsilon_{HH} = 1 \), \( \varepsilon_{groove} = 1.44 \), \( \varepsilon_{ridge} = 2.56 \) (for the homogeneous case), and \( \varepsilon_{ridge} = 2.56[1 +0.1/(d/\lambda_d)^2] \) (for the inhomogeneous case).
the normalized resonant frequency increases. To show the efficiency of the proposed method for analyzing inhomogeneous gratings, the previous example is reworked with inhomogeneous ridges. The ridge permittivity has a parabolic variation from \( z=0 \) to \( z=d \): i.e., \( \varepsilon_{\text{ridge}}=2.56\left[1+m(z/d)^2\right] \). By changing \( m \), the reflection spectrum can be tuned. The permittivity profile in the longitudinal direction is shown in Fig. 13 for \( m=0.1 \). Here, the effect of longitudinal inhomogeneity on the sensitivity of the FSS to tilt angle is investigated by calculating the normalized resonant frequency for the same tilt angles as in the previous example. Again, the overall reflectance of the structure, for different values of tilt angle \( (\delta=0^\circ, \delta=3^\circ, \delta=5^\circ) \), is plotted versus normalized frequency \( \Omega=K_d/d \) in Fig. 14. The normalized resonant frequency, \( \Omega_r \), at the presence of the above-mentioned longitudinal inhomogeneity, is once more calculated for different values of tilt angle and is given in Table 1. It can be easily seen that the introduced inhomogeneity considerably decreases the resonant frequency, yet the sensitivity of the structure to tilt angle variation hardly changes. This example is merely intended to demonstrate the usefulness of the proposed method for analyzing inhomogeneous gratings; however, the appropriate choice of longitudinally inhomogeneous permittivity profiles can supposedly tailor the spectral response of such gratings. It should be noted that by following the proposed method, the inhomogeneous grating can be analyzed at one stroke, and this eliminates the need for breaking the structure into cascaded quasi-homogeneous sublayers in the \( z \) direction. This is an important advantage, especially when synthesis and optimization are concerned.

7. CONCLUSIONS
In this paper, a Legendre polynomial expansion of electromagnetic fields for grating diffraction analysis in conical mounting has been reported. In this case, TE and TM polarizations inside the grating are not separable, and a vectorial three-dimensional analysis is required. In the proposed method, a set of algebraic equations, which can be easily solved for diffraction efficiencies and electromagnetic field profiles, is derived. The method shows strong numerical stability, where no special handling of characteristic matrices are needed. Also, thanks to the recursive properties of Legendre polynomials, the system of coupled differential Eqs. (15)–(18) is analytically transformed into a set of algebraic equations. This analytic projection of Maxwell’s equations on the Hilbert space spanned by Legendre polynomial basis functions considerably relaxes the computational burden and also enables the proposed method to be easily employed for analyzing inhomogeneous gratings of arbitrary profiles, where the governing coupled differential equations become shift variant. The results of the presented approach are compared with those of RCWA and it has been shown that the presented approach yields numerically accurate results. Also, the convergence rate of the proposed method, with respect to \( M \), i.e., the number of retained polynomial basis functions, is numerically demonstrated, where a good convergence is observed.

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