# Planar Diffraction Analysis of Homogeneous and Longitudinally Inhomogeneous Gratings Based on Legendre Expansion of Electromagnetic Fields

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Abstract-Planar grating diffraction analysis based on Legendre expansion of electromagnetic fields is reported. In contrast to conventional RCWA in which the solution is obtained using state variables representation of the coupled wave amplitudes; here, the solution is expanded in terms of Legendre polynomials. This approach, without facing the problem of numerical instability and inevitable round off errors, yields well-behaved algebraic equations for deriving diffraction efficiencies, and can be employed for analysis of different types of gratings. Thanks to the recursive properties of Legendre polynomials, for longitudinally inhomogeneous gratings, wherein differential equations with non-constant coefficients are encountered, it can also be used to analyze the whole structure at one stroke. Although this is the only case for which the presented approach is efficient from both aspects of stability and computation load, the presented approach is applied to different test cases, and justified by comparison of the results to those obtained using previously reported methods. The method is general, and can handle many different cases like thick gratings, non-Bragg incidence, and cases in which higher diffracted orders or evanescent orders corresponding to real eigenvalues, have to be included in the solution of the Maxwell's equations. In deriving the formulation, a rigorous approach is followed.

*Index Terms*—Electromagnetic diffraction by periodic structures, gratings, inhomogeneous gratings, Legendre polynomials.

#### I. INTRODUCTION

NALYSIS of wave propagation in periodic structures, A due to its wide range of applications, is faced in various cases in telecommunications, electromagnetics, 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 field profiles inside and outside of the grating. The electromagnetic theory of such structures has been extensively studied since Rayleigh's time, and different approaches such as rigorous coupled wave [1], [2], coupled mode [3], two wave methods [4], and Raman-Nath approach [5], have been reported for grating analysis. Methods for obtaining rigorous solutions can be categorized in two broad classes: integral methods and differential methods [6]. Whereas integral methods are best suited for analyzing gratings of continuous profiles, differential methods are more appropriate for the analysis of discrete-level profiles. Numerical implementation of differential methods tends to be less complicated than that of integral methods [7], due to difficulties such as logarithmic

singularities that may occur in solving the integral equation [8], [9]. Of many differential methods proposed for the analysis of volume diffraction gratings, rigorous coupled wave analysis, or RCWA, is the most precise, general, and widely used method [7], [10], [11]. It has been successfully applied to the analysis of two-dimensional and three-dimensional isotropic and anisotropic structures [12]–[15], as well as multiple grating structures [17], [18]. However, the presence of evanescent orders corresponding to real eigenvalues appearing in the solution of Maxwell's equations usually leads to numerical difficulties in applying RCWA method. This problem is also encountered in applying other conventional rigorous approaches which are based on modal expansion, where Helmholtz equation leads to a linear eigenvalue problem. This is due to the fact that evanescent orders result in the simultaneous appearance of extremely large and extremely small coefficients in the equations obtained by imposing the boundary conditions, and consequently cause numerical overflow and ill-conditioned matrices in the calculations [19]. Therefore, a robust method capable of handling evanescent orders is mandatory, especially in cases such as multiple grating structures or metallic corrugated gratings, where evanescent or complex diffracted orders cannot always be discarded. In some approximate methods based on Rayleigh hypothesis [20], the solution is divergent, and specific methods like the point matching technique are employed. The observed divergence of the solution, exacerbated by increasing the number of terms in electromagnetic field expansion in the grating region, is associated with the validity of the hypothesis and many techniques are devised to handle such an inherent problem [21]. However, such mentioned numerical instabilities are not inherent in the reflection-transmission problem solved by applying rigorous methods like RCWA. Several other techniques have been proposed and have been successfully implemented to surpass this problem, including enhanced transmittance matrix approach [10], R-matrix approach [22], [23], scattering matrix approach [24]-[26], and impedance formalism [27]. Morf has also reported a new mathematical method for the special case of lamellar gratings in [28]. That method is based on the expansion of the eigenfunctions in terms of a set of polynomial basis functions. 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 [28], [29].

In this paper, a similar yet fundamentally different approach is proposed. The electromagnetic field expressions inside the

Manuscript received January 9, 2005; revised June 21, 2006.

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grating which are the solutions of Helmholtz equation are expanded in terms of orthogonal Legendre polynomials. Then the solution is examined in a Hilbert space spanned by the polynomials. The method yields numerically stable results [19] and compared with other approaches based on modal method by Fourier expansion (MMFE), could enjoy a better convergence rate. The cost of the strong stability and generality of the proposed approach is its larger computation load in comparison to other approaches [10], [21]–[25] already devised for stabilizing conventional methods. These points are further elucidated in Section III. Therefore, the presented method can be best employed for analysis of gratings with inhomogeneous longitudinal permittivity profiles, where the computation load is cost-effective. Some examples on such structures are given in Section IV.

This paper is arranged as follows: polynomial expansion formulation of electromagnetic fields for the general case of planar slanted gratings is discussed in Section II. In Section III, numerical stability of the proposed method and its computational burden are investigated, wherein the results obtained by applying polynomial expansion method are compared to those obtained by applying the conventional RCWA modal expansion approach. Also, in this section convergence rate of the presented approach is studied in regard to the retained number of space harmonics and number of polynomial terms kept for expanding each space harmonic. Further numerical examples including frequency selective structures and inhomogeneous gratings, are investigated in Section IV. Finally, conclusions are made in Section V.

# II. POLYNOMIAL EXPANSION ANALYSIS: FORMULATION AND DISCUSSION

In this section, the electromagnetic field expressions inside the grating are expanded in terms of orthogonal Legendre polynomials [30], [31]. This novel electromagnetic field expression, in accordance with Floquet theorem, is then substituted in Helmholtz equation; appropriate boundary conditions are applied, and finally the unknown expansion coefficients and diffraction efficiencies are found. It should be noticed that expansion of the electromagnetic field expressions in a complete space spanned by orthogonal polynomial basis functions is a nonharmonic expansion [31], which has some advantages. First, the equations become algebraic rather than transcendental; being easier to manipulate. Second, this approach works properly even in those special cases in which other methods usually fail to render numerically stable results. Third, it can easily handle longitudinally inhomogeneous gratings, where the overall structure is analyzed in one stroke, eliminating the need for breaking the structure into many homogeneous sublayers.

A general form of a slanted grating is shown in Fig. 1. Here, the permittivity is assumed to be a general periodic function of x'

$$\varepsilon(x' + \Lambda_G) = \varepsilon(x') \tag{1}$$

where  $\Lambda_G$  is the grating period. Inside the grating, the Helmholtz equation can be easily derived as [32]

$$\nabla^2 E_y(x',z') + k^2 \varepsilon(x') E_y(x',z') = 0 \tag{2}$$



Fig. 1. Planar Slanted Grating.

for TE polarization, where  $k = (2\pi)/(\lambda)$  is the free space wavevector, and as

$$\nabla^2 U_y(x',z') + k^2 N^2(x') U_y(x',z') = 0$$
(3)

for TM polarization, where  $U_y x', z' = (H_y x', z')/(nx')$ ,  $k^2 N^2(x') = k^2 n^2 + (n''/n) - (2n'^2)/(n^2)$ , and *n* is the refractive index, *n'* and *n''* represent the first and the second derivative of the refractive index profile, respectively. For the case of lamellar gratings, (3) is not applicable for analysis of TM polarization and a different scheme [15], [16] need to be employed.

The relation between (x, z) coordinates and (x', z') coordinates is simply a clockwise rotation of coordinates expressed by

$$\begin{cases} x' = x\sin(\phi) + z\cos(\phi) \\ z' = -x\cos(\phi) + z\sin(\phi). \end{cases}$$
(4)

Since  $\varepsilon$  is a periodic function of x', Floquet theorem gives the general form of the solution of (2) for the TE case as [1]

$$E_y(x,z) = \sum_{i=-\infty}^{+\infty} S_i(z) e^{-j(\overrightarrow{K}_2 - i\overrightarrow{K_G}). \overrightarrow{r}}$$
(5)

where  $\vec{K}_2 = K_{2x}\hat{x} + K_{2z}\hat{z}$  is the wavevector of the refracted wave if region II were not periodic and were replaced by a medium of average permittivity, and  $\vec{K}_G = (2\pi)/(\Lambda_G)[\sin(\phi)\hat{x} + \cos(\phi)\hat{z}]$  is the grating vector. The index *i* running from  $-\infty$  to  $+\infty$  denotes the *i*th space harmonic corresponding to the *i*th diffracted order in regions I and III. Numerically, expansion of the transverse electric field in terms of infinite number of space harmonics (5) should be inevitably truncated to N number of terms. For dielectric gratings, all the space harmonics corresponding to propagating Floquet orders should be retained in the preceding expansion, where only a few of those terms corresponding to evanescent Floquet orders are needed to be included. In contrast, more space harmonics are needed to be kept for absorption gratings. Notwithstanding, this rule of thumb is seriously criticized in following sections.

The rest of this section is divided into three subsections; firstly, the expansion of electromagnetic fields inside the grating in terms of the Legendre polynomials is discussed. Secondly, this expansion is further investigated for the case of longitudinally inhomogeneous gratings, where the key properties of Legendre polynomials suitable for analyzing inhomogeneous gratings are introduced. Finally, applying the appropriate boundary conditions is commonly discussed for both homogeneous and inhomogeneous gratings.

## A. Electromagnetic Field Expansion Inside Longitudinally Homogeneous Gratings

For the case of longitudinally homogeneous gratings,  $\varepsilon$  is a periodic function and it can be expanded in terms of its Fourier series as

$$\varepsilon(x,z) = \sum_{h} \tilde{\varepsilon}_{h} e^{jh \overrightarrow{K_{G}} \cdot \overrightarrow{r}}$$
(6)

where  $\tilde{\varepsilon}_h = 2/\Lambda_G \int_0^{\Lambda_G} \varepsilon(x') e^{-jh \overrightarrow{K_G} \cdot \overrightarrow{r}} dx'$  is the Fourier component of the grating permittivity.

Substituting this form of the solution, i.e., (5) into the Helmholtz equation (2) and doing algebraic manipulations, one gets rigorous coupled-wave equations [1]

$$\frac{d^2 S_i(z)}{dz^2} - j2[K_{2z} - iK_{Gz}]\frac{dS_i}{dz} + \left[i(m' - i)K_G^2 - K_2^2\right]S_i(z) + k^2\sum_p \varepsilon_{i-p}S_p(z) = 0.$$
 (7)

Here,  $p = i - h, m' = (2K_2)/(K_G)\cos(\theta - \phi)$ , and the refracted angle  $\theta$  is defined as  $\sin(\theta) = (K_{2x})/(K_2)$ . It should be noticed that m' becomes an integer whenever the m'th Bragg condition is satisfied.

In the case of longitudinally homogeneous gratings, (7) becomes a set of constant coefficient differential equations representing a linear shift invariant system which can be solved by following the standard state variables method. That is the solution can be expanded in terms of the eigenvectors of the coefficient matrix, whose dimension is  $2N \times 2N$ , where N is the total number of retained space harmonics, i.e.,  $S_i$  (z)s. It should be noted that the exact solution is obtained by keeping infinite number of space harmonics; however, the truncation to N space harmonics is inevitable. Here, instead of following the standard state variables method,  $S_i$  (z) are expanded in terms of Legendre polynomials

$$S_i(z) = \sum_{m=0}^{+\infty} q_m^i P_m(\xi), \xi = \frac{2z - d}{d}$$
(8)

where  $P_m(\xi)$  terms are the normalized Legendre polynomials,  $q_m^i$  s are the expansion coefficients to be determined later, and in accordance with Fig. 1 and Fig. 4, d stands for the grating thickness. It should be noticed that the vector space spanned by Legendre polynomials is a complete one [31], and each  $S_i(z)$  can be expanded in terms of them. However, in practice the expansion of (8) is truncated to a finite number of polynomial terms and acceptable number of polynomial terms depends on the amount of energy coupled to each polynomial, and the required level of accuracy. Although, truncating the polynomial expansion given in (8) is inevitable, the introduced error is shown to be negligible. It should be also noticed that the interdependency of N, determining the accuracy of each space harmonic inside the grating, and number of diffraction orders outside the grating are now faded by introducing polynomial expansion bringing a new degree of freedom  $M_i$ , where the first  $M_i$  terms of the polynomial expansion (8) are retained and higher order terms are neglected. The truncated polynomial expansion is then inserted in (7) and the corresponding truncation error is minimized by projecting the resultant equation on the polynomial basis functions. Consequently, the following equation is obtained:

$$r_{m}^{i} - jd[K_{2z} - iK_{Gz}]g_{m}^{i} + \left(\frac{d}{2}\right)^{2} \left[i(m'-i)K_{G}^{2} - K_{2}^{2}\right]q_{m}^{i} + \left(\frac{d}{2}\right)^{2}k^{2}\sum_{p}\varepsilon_{i-p}q_{m}^{p} = 0 \quad (9)$$

where  $g_m^i = (2m+1) \sum_{\substack{l=m+1\\l+m \text{ odd}}}^{M_i} q_l^i$  and  $r_m^i = (2m+1)/(2)$  $\sum_{\substack{l=m+2t\\l=1,2,3,\dots}}^{M_i} (l+m+1)(l-m)q_l^i$  are the expansion coefficients of the first and the second derivatives in terms of  $q_m^i$ s, respectively.

The  $q_m^i$ s are unknown coefficients of the polynomial basis functions for each space harmonic, that is for each value of *i*, there are  $M_i + 1$  number of unknown coefficients. It should be noticed that (9) results in a set of  $M_i - 1$  equations with  $M_i + 1$ unknowns for each space harmonic. Therefore, one needs two further equations, which can be obtained by applying boundary conditions at z = 0 and z = d [19].

# B. Electromagnetic Field Expansion Inside Longitudinally Inhomogeneous Gratings

Now that the set of coupled wave equations, i.e., (7) are solved in the complete space spanned by Legendre polynomials, shift variant types of (7) can also be easily solved; this means longitudinally inhomogeneous grating for which the Fourier components of the permittivity profile are arbitrary functions of z can be analyzed. In the case of longitudinally inhomogeneous gratings the fringes are directed along the z axis, i.e.,  $\phi = 90^{\circ}$ , and the Fourier expansion in (6) and (19) are carried out along the x axis where the coefficients are left as functions of z (or  $\xi$ ), i.e.

$$\varepsilon(x,z) = \sum_{h} \tilde{\varepsilon}_{h}(z) e^{jh \overrightarrow{K_{G}}. \overrightarrow{r}}$$
(10)

where  $\tilde{\varepsilon}_h(z) = (2)/(\Lambda_G) \int_0^{\Lambda_G} \varepsilon(x) e^{-jh \overrightarrow{K_G} \cdot \overrightarrow{r}} dx$  is the z-dependent Fourier coefficient of the grating permittivity. By substituting this type of permittivity expansion in (7), the resulting equation governing the electromagnetic fields expansion coefficients inside the grating, i.e., (9), becomes shift variant. This equation reads as

$$r_{m}^{i} - jd[K_{2z} - iK_{Gz}]g_{m}^{i} + \left(\frac{d}{2}\right)^{2} [i(m' - i)K_{G}^{2} - K_{2}^{2}]q_{m}^{i} + \left(\frac{d}{2}\right)^{2}k^{2}\sum_{p}\varepsilon_{i-p}(z)q_{m}^{p} = 0.$$
(11)

Recently, we have proposed a method for analyzing one-dimensional longitudinally inhomogeneous optical structures [33], in which we have employed a recursive property of the Legendre polynomials. Here, in the same manner, this recursive property of Legendre polynomials is used to absorb any *z*-dependent coefficient of (7) in the polynomial expansion of the space harmonic amplitudes. This proclaimed recursive property is given as [34]

$$\xi P_m(\xi) = \frac{m+1}{2m+1} P_{m+1}(\xi) + \frac{m}{2m+1} P_{m-1}(\xi).$$
(12)

The above feature indicates that any power of  $\xi$  can be absorbed in Legendre polynomials by successively using of (12). It can be readily shown that

$$\sum_{m=0}^{+\infty} \xi q_m P_m(\xi) = \sum_{m=0}^{+\infty} \chi_m P_m(\xi)$$
(13-a)

where

$$\chi_m = \frac{m}{2m-1}q_{m-1} + \frac{m+1}{2m+3}q_{m+1}.$$
 (13-b)

Having arranged (13-b) in a matrix format, one obtains

$$[\bar{\chi}_m] = [\chi][\bar{q}_m]. \tag{14}$$

Therefore, once the matrix  $[\chi]$  is generated, any power of  $\xi$  can be easily absorbed in the expansion given in (13), by multiplying the corresponding power of  $[\chi]$  to the vector  $[q_m]$ .

The z-dependent Fourier coefficients of the permittivity profile in (11) being any arbitrary function of z can be interpolated by polynomials in the interval  $0 < \xi < 1$ , i.e.

$$\varepsilon_h(\xi) \cong \alpha_0 + \alpha_1 \xi + \alpha_2 \xi^2 + \alpha_3 \xi^3 + \dots + \alpha_{N_1} \xi^{N_1}$$
 (15)

where  $N_1$  is appropriately chosen so that (15) becomes an acceptable approximation. By inserting (15) in (11), any z dependence of the permittivity can be absorbed in the Legendre polynomial expansion of  $S_i(z)$ . As far as the resulting equation is still a set of algebraic constant coefficient equations, the rest of the procedure is just the same as the homogeneous case.

Therefore any inhomogeneous structure along the *z*-direction can be holistically analyzed by using the proposed method, where the need for breaking the structure into piecewise homogeneous sublayers is eliminated. This way, intensive computation load of multilayer structures analysis is leapfrogged. Some examples on gratings of inhomogeneous longitudinal permittivity profiles are given in subsequent sections.

### C. Boundary Conditions

Appropriate boundary conditions can be applied by using the electromagnetic field expressions in regions I and III given in (16) and (17), respectively [1]. They are expanded in terms of the plane waves corresponding to diffracted orders

$$\overrightarrow{E_1} = \hat{u}_y e^{-j\overrightarrow{K_1}\cdot\overrightarrow{r}} + \hat{u}_y \sum_{i=-\infty}^{+\infty} R_i e^{-j\overrightarrow{K_{1i}}\cdot\overrightarrow{r}}$$
(16)

$$\overrightarrow{E_3} = \hat{u}_y \sum_{i=-\infty}^{+\infty} T_i e^{-j \overrightarrow{K_{3i}} \cdot (\overrightarrow{r} - d\hat{z})}.$$
(17)

Here,  $R_i$  and  $T_i$  are reflection and transmission coefficients of each diffracted order, respectively. In contrast to the electromagnetic fields inside the grating which are expanded in terms of infinite set of space harmonics, i.e.,  $S_i(z)$ s, electromagnetic fields in regions I and III are expanded in terms of plane waves [35].

Applying the continuity condition of tangential electromagnetic fields by using (5), (8), (16), and (17), eliminating  $R_i$  and

 $T_i$  coefficients, and doing some algebraic manipulations result in

$$\sum_{m=0}^{M_i} (-1)^m q_m^i \left[ \frac{m(m+1)}{d} + j(K_{1iz} + K_{2z} - iK_{Gz}) \right]$$
  
=  $2jK_{1z}\delta_{i0},$  (18)

$$\sum_{m=0}^{M_i} q_m^i \left[ \frac{m(m+1)}{d} + j(K_{3iz} - K_{2z} + iK_{Gz}) \right] = 0.$$
(19)

Considering the fact that each diffracted order outside the grating must be phase matched to its corresponding space harmonic inside the grating at each boundary, one finds

$$K_{1ix} = K_{1x} - iK_G\sin(\phi) \tag{20a}$$

$$K_{3ix} = K_{2x} - iK_G\sin(\phi) \tag{20b}$$

$$K_{2x} = K_{1x} = K_0 n_1 \sin(\theta').$$
 (20c)

Now either of (9) or (11), (18), and (19) form a set of  $M_i$  +1 equations, their solution resulting in the values of  $q_m^i s$ . Consequently,  $R_i, T_i$ , and the corresponding diffraction efficiencies can be determined

$$DE_{1i} = Re\left(\frac{K_{1iz}}{K_{1z}}\right)R_iR_i^* \tag{21}$$

$$DE_{3i} = Re\left(\frac{K_{3iz}}{K_{1z}}\right)T_iT_i^*.$$
(22)

For lossless dielectric gratings, as a result of energy conservation, one finds

$$\sum_{i} DE_{1i} + DE_{3i} = 1.$$
 (23)

For the case of TM polarization, everything is similar to that of TE polarization since (3) resembles to (2). The only difference is in  $N^2(x')$  which is not simply  $\varepsilon(x')$ . However, it is a periodic function whose Fourier expansion can be used instead

$$N^{2}(x,z) = \sum_{n} a_{n} e^{jn \overline{K_{G}} \cdot \overrightarrow{r}}$$
(24)

with  $a_n$  being the *n*th Fourier component of  $N^2(x')$ .

Afterward, diffraction efficiencies can be computed by following the same approach already described for TE polarized wave incidence, just by replacing  $E_y$  with  $U_y$  defined as  $U_y = (H_y)/(n)$ .

The amount of coupling between different space harmonics is related to the harmonic content of  $\varepsilon$  (x') and  $N^2$  (x'). For a sinusoidal permittivity profile, there is more coupling between TM polarized space harmonics than in the TE case. This is due to the fact that the harmonic content of  $N^2$  (x') is richer than that of  $\varepsilon$  (x'), and the spatial variation of TM polarized waves is faster than that of TE polarized waves.

#### **III. NUMERICAL STABILITY AND CONVERGENCE PROPERTIES**

Numerical instability is one of the limitations in applying RCWA method [15]. Such numerical difficulties are exacerbated by the presence of a large number of evanescent growing and decaying fields and/or increasing the grating layer thickness both of them deteriorating the condition number of matrices involved in applying standard state variable methods.

Here, by expanding the space harmonics' amplitudes in terms of orthogonal Legendre polynomial bases, the calculation of the eigensolutions is surpassed. In other words, the process of finding eigensolutions of electromagnetic fields inside the grating and the process of applying boundary conditions are combined in finding expansion coefficients. The computation bottlenecks lie in the coefficient matrix assembling and solving the final algebraic system of equations to find expansion coefficients, i.e.,  $q_m^i$ s. The assembling process can be highly accelerated by taking into account that many parts of the coefficient matrix are the same especially when identical  $M_i$ 's are retained for each space harmonic  $S_i(z)$ . Also, the coefficient matrix mostly consists of blocks located on diagonal lines yielding a well-behaved sparse matrix. Consequently, main computational burden lies in determining the coefficients  $q_m^i$ s, i.e., the inversion process of the coefficient matrix.

In order to demonstrate the numerical stability of the proposed method, a reflection dielectric diffraction grating is analyzed as the first numerical example. The values of the grating parameters, referenced to Fig. 1, are given as: grating slant angle  $\phi = 150^{\circ}$ , the angle of incidence satisfying the first Bragg condition  $\theta' = 20^\circ$ , the grating permittivity in region II given by  $\varepsilon(x') = 2.25(1 + 0.33\cos(K_G x'))$ , and dielectric permittivities of regions I and III,  $\varepsilon_I = \varepsilon_{III} = 2.25$ , and the incident wavelength  $\lambda = 1.9284\Lambda_G$ . In Fig. 2, diffraction efficiencies are plotted versus the normalized thickness  $(d/\Lambda_G)$ , by using conventional RCWA (solid line), and polynomial expansion method proposed in this paper (dashed line). Both TE and TM polarizations are analyzed and an excellent consistency with those results obtained by Gaylord et al. [1] is observed. However, it should be noticed that conventional RCWA becomes unstable for grating thicknesses larger than  $5\Lambda_G$ . The results of the proposed method in Fig. 2 are obtained by keeping 8 polynomial terms for TE and 12 polynomial terms for TM polarization.

As another example, a transmission grating is considered with the following parameters:  $\phi = 120^{\circ}, \theta' = 42^{\circ}$  (the angle of incidence satisfying the first Bragg condition),  $\varepsilon(x') = 2.25(1 + 0.12\cos(K_G x'))$  in region II,  $\varepsilon_I = \varepsilon_{\text{III}} = 2.25$ , and the incident wavelength  $\lambda = 0.6237\Lambda_G$ . In Fig. 3, diffraction efficiencies corresponding to the zeroth and the first transmitted orders are plotted versus normalized thickness  $(d/\Lambda_G)$  by employing RCWA (solid line), and polynomial expansion method proposed in this paper (dashed line). Again, these results show good agreement with those already reported by Gaylord *et al.* [1]. The proposed results are obtained by keeping 7 polynomial terms for TE and 8 polynomial terms for TM polarization.

It should be noticed that conventional RCWA [1] analysis fails to handle more than four Floquet orders (N > 4) in both of these examples. In contrast, polynomial expansion method behaves well enough in handling such problems. It is obvious that increasing the number of retained spatial orders improves the achieved accuracy of the truncated expansion of electromagnetic fields given by (5). As stated earlier, it should be noticed that there exist other approaches devised for stabilizing RCWA [10], [22], [24]–[27], which, so long as homogeneous gratings are considered, find to be computationally more costeffective than the proposed method. It should be noticed that the results of Figs. 2 and 3 can be obtained by using such methods



Fig. 2. Diffraction efficiencies of a reflection grating ( $\phi = 150^\circ, \varepsilon_I = \varepsilon_{III} = 2.25, \varepsilon_{II}(x') = 2.25(1+0.33\cos(K_Gx'))$  and  $\theta' = 20^\circ$ ) versus  $d/\Lambda_G$  computed by polynomial expansion (dashed line) with N = 7 and M = 8 for TE and M = 12 for TM and RCWA method (solid line) with N = 5.



Fig. 3. Diffraction efficiency of a transmission grating ( $\phi = 120^{\circ}, \varepsilon_I = \varepsilon_{III} = 2.25, \varepsilon_{II}(x') = 2.25(1 + 0.12\cos(K_G x'))$  and  $\theta' = 42^{\circ}$ ) versus  $d/\Lambda_G$ , computed by polynomial expansion (dashed line) with N = 7 and M = 7 for TE and M = 8 for TM polarization and RCWA method (solid line) with N = 5.

without facing the depicted numerical stabilities. Such stabilized schemes are later used to obtain the data plotted in Fig. 5, where 120 harmonics are retained.

Though the observed numerical instability usually encountered in dealing with deep and/or thick gratings has been successfully surpassed by introducing a couple of modified methods [10], [22], [24]–[27], slow convergence rate of applying coupled wave methods or any other modal method by Fourier expansion approach is still left to overcome [11]. In following RCWA or any other modal method by Fourier expansion, both the permittivity and the electromagnetic fields inside the grating are expanded in 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 an infinite number



Fig. 4. Surface relief grating with rectangular grooves.



Fig. 5. Relative error in the first forward diffracted order DE<sub>31</sub> versus the total number of space harmonics (N), for the RCWA method (triangles) and the polynomial method (circles) for a lamellar grating with f = 0.5,  $\varepsilon_I = \varepsilon_{III} = 1.5$ ,  $\varepsilon_{\text{groove}} = 1.5$ ,  $\varepsilon_{\text{ridge}} = 8$ ,  $\theta' = 0^\circ$ , and TM polarization.

of 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 number of them. This conspicuously shows how strongly twisted are the convergence rate of the permittivity expansion and that of the electromagnetic field expansion and the number of required space harmonics. In contrast, such a strong dependency is now abated by introducing a new factor  $M_i$ . The proposed method can be categorized as a non-modal method by Fourier expansion, where each one of diffraction efficiencies, i.e., the power of each scattered harmonic denoted by  $DE_{3i}(N, M)$  for transmitted orders in region III and  $DE_{1i}(N, M)$  for reflected orders in region I, is a function of both N and M. Here, M is a vector containing N values of  $M_i$ , the number of polynomial basis functions. The subscript i denotes the index of diffracted Floquet orders. Consequently, the convergence rate can be studied from two aspects, the convergence rate as a function of N and the convergence rate as a function of M. In this section, these two different convergence rates are studied and it has been shown that polynomial expansion could partially ameliorate the



Fig. 6. Relative error in the first forward diffracted order  $DE_{31}$  versus the number of polynomial basis functions (M) for N = 81 indicated in Fig. 5. Parameters of the grating are the same as those used in Fig. 5.

inevitable truncation error of space harmonics. As a numerical example for studying the convergence rate, a lamellar dielectric grating is chosen with the following parameters:

In accordance to Fig. 4, the duty cycle of the binary grating (f) is 0.5, dielectric permittivity in region I and region III  $(\varepsilon_I, \varepsilon_{III})$  is 1.5, dielectric permittivity of grooves  $(\varepsilon_{groove})$  is 1.5 and that of ridge is  $(\varepsilon_{ridge})$  8, incident angle  $(\theta')$  is 0° (normal incidence), and grating periodicity  $(\Lambda_G)$  being equal to the wavelength of the incoming light in free space  $(\lambda_0)$  is equal to the grating thickness and all are normalized to 1, the incident polarization is TM. This structure has three forward and three backward diffracted orders. Most of the incident power is forward transmitted. The convergence of both the presented method and that of the RCWA is demonstrated in Fig. 5 by plotting the relative error for the first forward diffracted order defined in (21) and (22) versus N-the number of retained space harmonics

$$\varepsilon = \frac{|DE_{31}(N) - DE_{31}(201)|}{DE_{31}(201)} \times 100$$
(25)

for RCWA and

ε

$$=\frac{|DE_{31}(N,M) - DE_{31}(201)|}{DE_{31}(201)} \times 100$$
(26)

for polynomial expansion method.

In the definition of relative error, the exact diffraction efficiency is assumed to be that of N = 201. For the polynomial expansion method, M is fixed at 20, i.e., a uniform distribution is assumed for all  $M_i$  such that each  $M_i$  is 20. It should be noticed that the converged results, as Fig. 5 indicates, are obtained beyond N = 71 terms, whereas only three propagating orders exist. This remarkably denounces the rule of thumb according to which retaining only a few number of cutoff modes (evanescent orders) guarantees the convergence of the solution. Moreover, the numerical results obtained by following polynomial method

 TABLE I

 Comparison of the Diffraction Efficiencies and the Relative Error Obtained by Using the Polynomial Expansion Method and RCWA at

 Point A of Fig. 5

	Polynomial Method (N=81, M=20)	RCWA (N=81)	RCWA (N=201)
DE30	0.269012	0.271026	0.265298
DE31	0.297091	0.295604	0.299104
Error <sub>30</sub>	1.40%	2.16%	
Error <sub>31</sub>	0.67%	1.1%	

converge faster than those obtained by applying RCWA. All the same, so long as computational burden is considered, the observed effect cannot outstrip stabilized RCWA schemes already devised for analysis of homogeneous gratings. This point is further clarified in next section, where computation time of homogeneous and longitudinally inhomogeneous grating profiles are compared.

In Fig. 6, relative error defined by (21) for the first forward diffracted order is plotted versus the number of polynomial terms, namely basis functions, wherein the presented results correspond to the point A indicated in Fig. 5, i.e., N is fixed at N = 81 and each space harmonic amplitude is expanded based on M Legendre polynomials, i.e.,  $M_i = M$ . This figure shows how the solution uniformly converges beyond the point M = 20, where the error becomes negligible. As a matter of fact, keeping more than 17 orthogonal Legendre basis polynomials pins the error beneath the value of 1%. However, it should be noticed that expanding each space harmonic amplitude in terms of  $M_i = M$  terms is not necessarily the optimum choice, where different space harmonic amplitudes each of them enclosing different harmonic contents can be satisfactorily expanded by retaining different values of  $M_i$ . Therefore, finding the optimum values of  $M_i$  can potentially reduce and simplify the pertinent computation burden.

Diffraction efficiency  $DE_{31}$  and  $DE_{30}$  computed by RCWA [15] having N = 81 space harmonics, and polynomial expansion method having N = 81, and M = 20, are compared with the results obtained by RCWA having N = 201 [15] terms yielding the least numerical error and the results are summarized in Table I.

#### **IV. FURTHER EXAMPLES**

In this section, some examples of homogeneous and longitudinally inhomogeneous gratings are given.

The frequency selective behavior of dielectric and metallic periodic structures has found many applications in electromagnetics. They are used as filters, polarizers, radomes and subreflectors in patch antennas [36], [37]. Here, a lamellar dielectric frequency selective surface (DFSS) is analyzed. In accordance with Fig. 4, the parameters are as follows:

The duty cycle of the binary grating (f) is 0.5, region I and region III are free space ( $\varepsilon_I, \varepsilon_{III} = 1$ ), relative dielectric permittivity of grooves ( $\varepsilon_{\text{groove}}$ ) is 1.44 and that of ridge is ( $\varepsilon_{\text{ridge}}$ ) 2.56, incident angle ( $\theta'$ ) is 45°, grating periodicity ( $\Lambda_G$ ) is normalized to 1, and the grating thickness is  $1.713\Lambda_G$ . The incident polarization is TE. Reflectance is plotted in Fig. 7 versus normalized frequency  $K_0 d$  (solid line), where  $K_0$  is the free space wavenumber. Total reflection occurs at two resonant normalized frequencies of 5.32 and 5.83. The result obtained by N = 9 and

0.8 0.6 Reflectance 0.4 m = +0.1m = -00.251 5.4 5.5 5.6 5.8 59 5.253 5.7 6.1  $K_0 d$ 

Fig. 7. Reflectance versus the normalized frequency for the dielectric frequency selective grating: f = 0.5,  $\varepsilon_I = \varepsilon_{III} = 1$ ,  $\varepsilon_{\rm groove} = 1.44$ ,  $\varepsilon_{\rm ridge} = 2.56(1 + mz/d)$ ,  $d = 1.713\Lambda_G$ , and  $\theta' = 45^{\circ}$ . Solid lines: Homogeneous case (m = 0), Dashed lines: m = -0.1, Dotted lines: m = +0.1.

M = 8, perfectly agrees with that presented in [38] by Bertoni *et al.* and [36] by Coves *et al.* 

It has been reported that the spectral response of such frequency selective structures can be altered by using inhomogeneous dielectrics in the structure of a metallic grating [39]. Inhomogeneous gratings are also investigated in [40] by Forslund *et al.*, where a wave-splitting approach is used for analysis. Here, a specific example of such a structure having an inhomogeneous ridge permittivity of linear variation from z = 0 to z = d:  $\varepsilon_{\text{ridge}} = 2.56(1 + m(z/d))$  is analyzed, where the capability of tuning the reflection spectrum by altering *m* is clearly demonstrated. Other parameters are the same as the previous example. In Fig. 7 the reflectance is plotted for m = -0.1 (dashed line) and m = +0.1 (dotted line). It can be seen that the location of the resonant frequencies is moved towards higher frequencies for positive *m* and towards lower frequencies for negative *m*.

As already discussed in Section II-B, each Fourier component of the permittivity profile is a function of z, and the set of coupled wave (7) becomes a shift variant one, for which a general closed form solution is not always available. However, the set of shift variant coupled wave (7) can be solved by breaking the inhomogeneous structure into approximating homogeneous sublayers. Here, by using a recursive property of Legendre polynomials introduced in Section II-B. B, the z dependent coefficients can be absorbed in the Legendre expansion of space harmonics. This way the structure is holistically analyzed and computationally intensive multilayer analysis is not needed anymore. The



Fig. 8. Permittivity profile of a two-dimensional grating.

computation time of the overall response with 0.001 normalized frequency steps using a Pentium IV 2.4 GHz personal computer is 372.06 s for the homogeneous case, i.e., m = 0, and 510.61 s for the inhomogeneous cases of m = -0.1 and m = 0.1. It can be seen that the extra computational burden demanded for the analysis of inhomogeneity is not so much. In contrast, so long as conventional methods like RCWA are applied, introducing longitudinal inhomogeneity in the refractive index profile of gratings calls for considerable extra computational load compared to the run time of homogeneous structures. This can be explained by considering how the extra time is imposed by staircase approximation of the permittivity profile and the corresponding multilayer analysis of the inhomogeneous structure. As already emphasized, the RCWA method is superior to the proposed approach in the case of homogeneous grating. In this particular example, RCWA can be stably employed to obtain the reflectance within a much less computation time of 8.45 s for m = 0. Yet, the run time of analyzing the inhomogeneous case, i.e.,  $m \neq 0$ , by applying RCWA method is at least expected to be comparable with that of our proposed method.

Another example is a two-dimensional grating of finite thickness. The permittivity of the proposed structure, shown in Fig. 8, varies as

$$\varepsilon(x,z) = 2 + \left(0.1 + 0.2\sin\left(\frac{6\pi z}{d}\right)\right)\cos(K_G x).$$
(27)

Here, the incident angle  $(\theta')$  is 45°, grating periodicity  $(\Lambda_G)$  is normalized to 1, and  $d = 1.713\Lambda_G$ . Reflectance and transmittance are plotted in Fig. 9 versus normalized frequency  $K_0 d$ , where  $K_0$  denotes the free space wavenumber. The numerical results are obtained by N = 5 and M = 15, where the whole structure is analyzed by using the methodology introduced in Section II-B. The spectral response of Fig. 9 obtained in 52.46 s for 0.0003 normalized frequency steps using a Pentium IV 2.4 GHz personal computer, shows the efficacy of the proposed approach for analyzing such structures. This structure, with its sharply selective reflection and transmission response, can find applications in designing notch filters and multiplexers.



Fig. 9. Reflectance and transmittance of the two-dimensional grating introduced in Fig. 8, obtained by N = 5 and M = 15.

### V. CONCLUSION

In this paper, a polynomial expansion of electromagnetic fields amplitudes for grating diffraction analysis has been reported, and the formulation for the general case of planar slanted gratings has been derived. Both TE and TM polarizations have been addressed where any other incident polarizations can be considered as a superposition of these two orthogonal polarizations. This new method is based on Legendre polynomial expansion rather than the conventional modal analysis in which space harmonic amplitudes of the fields are expanded in terms of the eigenvectors of the coefficient matrix defined by rigorous coupled wave equations. To verify the proposed method, the results of our analysis have been compared with other results previously reported. It is also shown that the proposed polynomial expansion method yields reliable and stable results. Convergence rate of the proposed method is studied and is compared with that of RCWA, where the conventional rule of thumb for choosing the total number of space harmonics is criticized. Frequency selective structures and absorption gratings are also investigated to demonstrate the applicability of the proposed method. This method is particularly useful for analysis of inhomogeneous gratings, where shift variant state space equations do not have a general closed form solution. Though such inhomogeneous gratings can be decomposed into approximative gratings of homogeneous profiles, the total structure can be wholly analyzed by solving the shift variant equations using the proposed polynomial expansion approach. Such an entire analysis of inhomogeneous structures can be carried out within a reasonable time. This is the case in which the proposed approach shows especial efficiency from different aspects of computation burden, numerical stability, convergence, and generality.

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