# Highly improved convergence of the coupled-wave method for TM polarization

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The coupled-wave method formulated by Moharam and Gaylord [J. Opt. Soc. Am. **73,** 451 (1983)] is known to be slowly converging, especially for TM polarization of metallic lamellar gratings. The slow convergence rate has been analyzed in detail by Li and Haggans [J. Opt. Soc. Am. A **10,** 1184 (1993)], who made clear that special care must be taken when coupled-wave methods are used for TM polarization. By reformulating the eigenproblem of the coupled-wave method, we provide numerical evidence and argue that highly improved convergence rates similar to the TE polarization case can be obtained. The discussion includes both nonconical and conical mountings.

*Key words:* coupled-wave methods, rigorous grating analysis, diffractive optics. 

## 1. INTRODUCTION

In a recent publication Li and Haggans[1] provided strong numerical evidence that the rigorous coupled-wave analysis (RCWA) formulated by Moharam and Gaylord[2] converges slowly for one-dimensional (1-D) metallic gratings and TM polarization (magnetic-field vector parallel to the grating vector). They argued that the slow convergence is caused by the slowly convergent Fourier expansions for the permittivity and the electromagnetic field inside the grating. The RCWA computation is twofold. First, the Fourier expansion of the field inside the grating provides a system of differential equations. Then once the eigenvalues and the eigenvectors of this system are found, the boundary conditions at the grating interfaces are matched to compute the diffraction efficiencies. In this paper we focus on the eigenproblem of 1-D gratings for TM polarization. By reformulating the eigenproblem, we report on highly improved convergence rates even for highly conductive gratings. We also reveal that the slow convergence is due not to the use of Fourier expansions but to an inadequate formulation of the conventional eigenproblem.

In Section 2 we review briefly the previous eigenproblem formulations used in coupled-wave analysis for nonconical mountings; these include the original formulation provided in Ref. 2 and an updated formulation by the same authors.[3] In Section 3 we propose a new formulation for the eigenproblem. This new formulation can be straightforwardly extended to any modified method[4,5] that is based on a Fourier expansion of the field in the grating. Section 4 provides numerical evidence that the new formulation significantly improves the convergence rate. Two examples showing the improved convergence rate are provided. The first one is taken from Ref. 6 in which Peng and Morris showed that a very large number of orders must be retained to analyze accurately a wire-grid-polarizer problem. The second example is taken from Ref. 1, in which poor and oscillating convergence rates were observed with a highly conductive grating. In Section 5 a simple intuitive argument is used to explain the observed improvement, and in Section 6 the generalization to conical mounts is briefly derived. Concluding remarks are given in Section 7.

## 2. CONVENTIONAL EIGENPROBLEM

Let us consider a 1-D periodic structure along the $x$ axis with an arbitrary permittivity profile $\epsilon(x)$ (see Fig. 1). The $z$ axis is perpendicular to the grating boundaries. The diffraction problem is invariant in the $y$ direction. Magnetic effects are not considered in this paper, and the constant $\mu_0$ denotes the permeability of the periodic structure. $\epsilon_0$ is the permittivity of the vacuum. The period of the structure is denoted by $\Lambda$, and the length of the grating vector $K$ is equal to $2\pi/\Lambda$. An incident plane wave with wavelength $\lambda$ in the incident medium makes an angle $\theta$ with the $z$ direction in a nonconical mounting. We denote the magnitude of the wave vector of the incident wave by $k$ ($k = 2\pi/\lambda$), $\beta$ ($\beta = k \sin \theta$) is its $x$ component, and $k_0$ represents the magnitude of the incident plane-wave vector in a vacuum. A temporal dependence of $\exp(i\omega t)$ of the wave is assumed ($j^2 = -1$). $\epsilon_m$ denotes the $m$th Fourier coefficient of $\epsilon(x)/\epsilon_0$, and $a_m$ is used to denote the $m$th Fourier coefficients of $\epsilon_0/\epsilon(x)$.

Using the Floquet theorem, the $x$ component $E_x$ and the $z$ component $E_z$ of the electric field and the $y$ component $H_y$ of the magnetic field inside the grating can be expressed as[2]

 

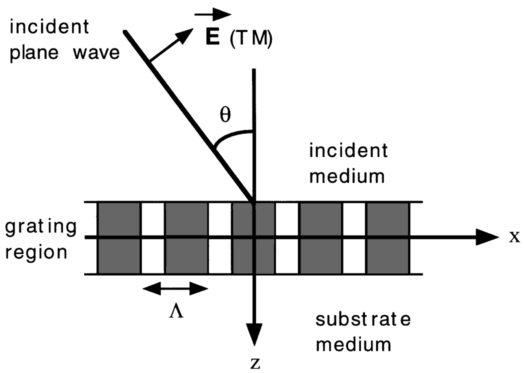


Fig. 1. Geometry for the nonconical grating diffraction problem analyzed in Sections 2 and 3 for TM polarization.

$$E_x = \sum_m S_m(z) \exp j(Km + \beta)x\,,$$
$$E_z = \sum_m f_m(z) \exp j(Km + \beta)x\,,$$
$$H_y = \sqrt{\frac{\epsilon_0}{\mu_0}} \sum_m U_m(z) \exp j(Km + \beta)x\,. \tag{1}$$

Maxwell's curl equations are

$$-\frac{\partial E_z}{\partial x} + \frac{\partial E_x}{\partial x} = -j\omega\mu_0 H_y\,, \tag{2a}$$

$$\frac{\partial H_y}{\partial z} = -j\omega\epsilon E_x\,, \tag{2b}$$

$$\frac{1}{\epsilon}\frac{\partial H_y}{\partial x} = j\omega E_z\,. \tag{2c}$$

In the following equations we denote the first derivative in the $z$ variable by a prime. Consistently a double prime denotes the second derivative. Identified in the quasi-plane-wave basis, Eqs. (1) and (2) are used to obtain

$$-j(mK + \beta)f_m + S_m' = -jk_0 U_m, \tag{3a}$$

$$U_m' = -jk_0 \sum_p \epsilon_{m-p} S_p\,, \tag{3b}$$

$$\sum_p (pK + \beta) a_{m-p} U_p = k_0 f_m\,. \tag{3c}$$

By substituting $f_m$ from Eq. (3c) into Eq. (3a), we obtain[2]

$$S_m' = -jk_0 U_m + j(mK/k_0 + \beta/k_0) \sum_p (pK + \beta) a_{m-p} U_p\,. \tag{4}$$

Equations (3b) and (4) provide a complete set of first-order differential equations and constitute an eigenproblem of size $2(2M + 1)$ when $\pm M$ orders are retained in the computation. As was noted by Li and Haggans[1] and was systematically exploited by Peng and Morris[6] and Moharam *et al.*,[3] it can be an advantage to solve the set of second-order differential equations. This solution easily takes into account the double degeneracy of the eigenproblem and decreases the computational effort. Using Eqs. (3b) and (4) we obtain the infinite set of second-order differential equations for the magnetic field:

$$U_m'' = -k_0^2 \sum_p \epsilon_{m-p} \Big[ U_p - (pK/k_0 + \beta/k_0) \times \sum_r (rK/k_0 + \beta/k_0) a_{p-r} U_r \Big]\,. \tag{5}$$

Except for minor notation disparities, Eqs. (3b) and (4) were originally introduced by Moharam and Gaylord.[2] Equation (5) can be found in Refs. 3 and 6. Equation (5) can be written in the compact form

$$k_0^{-2}[\mathbf{U}''] = [\mathbf{E}(\mathbf{K}_x \mathbf{A} \mathbf{K}_x - \mathbf{I})][\mathbf{U}]\,, \tag{6a}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{E}$ is the matrix formed by the permittivity harmonic coefficients, $\mathbf{K}_x$ is a diagonal matrix with the $i$, $i$ element being $(iK + \beta)/k_0$, and $\mathbf{A}$ is the matrix formed by the inverse-permittivity harmonic coefficients. $\mathbf{K}_x$, $\mathbf{E}$, and $\mathbf{I}$ are notations of Ref. 3. When a finite number of orders are retained in the numerical computation, the authors of Ref. 3 prefer to implement the eigenproblem by numerically inverting matrix $\mathbf{E}$ instead of directly taking the inverse-permittivity coefficients $a_m$. Replacing $\mathbf{A}$ by $\mathbf{E}^{-1}$ in Eq. (6a), we obtain

$$k_0^{-2}[\mathbf{U}''] = [\mathbf{E}(\mathbf{K}_x \mathbf{E}^{-1} \mathbf{K}_x - \mathbf{I})][\mathbf{U}]\,. \tag{6b}$$

Equation (6b) is the same as Eqs. (35) and (36) of Ref. 3. For the following comparison, the eigenproblem of Eq. (6b) is used in the RCWA implementation.

## 3. REFORMULATION OF THE EIGENPROBLEM

In this section we derive a new set of differential equations and reformulate the eigenproblem. Equations (3b) and (3c) can be written as

$$-\sum_p a_{m-p} U_p' = jk_0 S_m\,, \tag{7a}$$

$$(mK + \beta) U_m = k_0 \sum_p \epsilon_{m-p} f_p\,. \tag{7b}$$

By substituting $f_m$ from Eq. (3a) into Eq. (7b) and then eliminating $S_m$ with Eq. (7a), we obtain another infinite set of second-order differential equations:

$$(mK/k_0 + \beta/k_0) U_m - \sum_p \frac{\epsilon_{m-p}}{pK/k_0 + \beta/k_0} U_p = \frac{1}{k_0^2} \sum_{l,p} \frac{\epsilon_{m-p} a_{p-l}}{pK/k_0 + \beta/k_0} U_l''. \tag{8}$$

Note that Eq. (8) is not valid for normal incidence ($\beta = 0$) and must be replaced by Eqs. (15) as discussed in Section 5. In a compact form, Eq. (8) becomes $k_0^{-2}[\mathbf{E}\mathbf{K}_x^{-1}\mathbf{A}][\mathbf{U}''] = [\mathbf{K}_x - \mathbf{E}\mathbf{K}_x^{-1}][\mathbf{U}]$, which is written by multiplying both sides by $(\mathbf{E}\mathbf{K}_x^{-1}\mathbf{A})^{-1}$:

$$k_0^{-2}[\mathbf{U}''] = [\mathbf{A}^{-1}(\mathbf{K}_x \mathbf{E}^{-1} \mathbf{K}_x - \mathbf{I})][\mathbf{U}]\,, \tag{9}$$

with $\mathbf{E}$, $\mathbf{K}_x$, $\mathbf{A}$, and $\mathbf{I}$ being defined as in Eqs. (6a) and (6b). Since $\mathbf{A}^{-1}$ is identical to $\mathbf{E}$ when an infinite number of orders are retained, Eqs. (6b) and (9) are fully equivalent. As will be shown with numerical examples in the next Section, and as will be argued in Section 5, this equivalence is true only when an infinite number of orders is retained. When truncating the matrices for simulation purposes, we can see that the two eigenproblem formulations provide highly different convergence-rates.

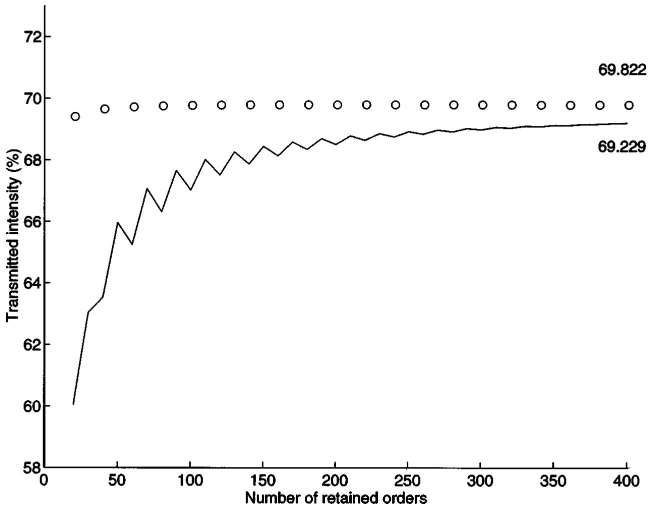


Fig. 2. Diffraction efficiency of the transmitted zeroth order of a metallic grating with TM polarized light. The solid curve is obtained by using the conventional eigenproblem formulation of Eq. (6b). The circles are provided by the new eigenproblem of Eq. (9). The grating parameters and the geometry problem are defined in Fig. 2 of Ref. 6.

## 4. NUMERICAL EXAMPLES

In our implementation of the new eigenproblem formulation, we form matrices **A** and **E** by directly using the analytical values of the harmonic coefficients $\epsilon_m$ and $a_m$. Matrices **A** and **E** are then inverted, and the eigenproblem of Eq. (9) is solved with standard library programs. When $(2M + 1)$ orders are retained in the computation, we obtain $(2M + 1)$ eigenvectors $\mathbf{u}_i$ and $(2M + 1)$ eigenvalues $\lambda_i{}^2$. Using Eq. (7a), we derive the $2(2M + 1)$ eigenvectors $\begin{bmatrix}\mathbf{u}_i \\ \lambda_i \mathbf{A}\mathbf{u}_i\end{bmatrix}$ and $\begin{bmatrix}\mathbf{u}_i \\ -\lambda_i \mathbf{A}\mathbf{u}_i\end{bmatrix}$ with eigenvalues $\lambda_i$ and $-\lambda_i$, respectively. The first numerical example is related to a metallic lamellar grating deposited on a glass substrate, which acts as a polarizer in the visible region. It was provided by Peng and Morris in Ref. 6. The lamellar grating is composed of chrome (index of refraction equals $3.18-j4.41$) and air and is acting as a zeroth-order filter for normal incidence (see the caption of Fig. 2 in Ref. 6 for more details). Figure 2 shows the transmitted intensity of the zeroth order as a function of the number of retained orders. The solid curve is obtained by solving the eigenproblem of Eq. (6b). A detailed explanation of the algorithm implementation can be found in Ref. 6. Note that a slow and oscillating convergence is obtained. The amplitude of the oscillations decreases as the number of retained orders increases. The circles are obtained by solving the eigenproblem of Eq. (9). No oscillation is observed. We are grateful to Mike Miller at the Institut d'Optique Théorique et Appliquée in Orsay, who computed for us the zeroth-order transmitted diffraction efficiency using his modal method.[7] He found a transmitted intensity of 70.28% when retaining 90 modes in his numerical computation. If we consider that 70.28% is the exact diffraction efficiency, it is clear from Fig. 2 that the new eigenproblem formulation with as few as 20 retained orders provides a more accurate result than the conventional formulation with 400 retained orders.

The second numerical example is taken from Ref. 1, where the convergence rate of a highly conductive grating on gold substrate was investigated (see Fig. 1 in Ref. 1 for additional details on the grating geometry). The diffraction configuration is a 30° incident angle, which corresponds to the first-order Bragg condition. Only the negative first and zeroth reflected orders are propagating. Figure 3 shows the diffraction efficiencies of the negative first and zeroth orders when the new eigenproblem of Eq. (9) is used for the numerical computation. As the same scale is used in Fig. 3 of this publication and in Figs. 3(a) and 3(b) of Ref. 1, a visual comparison of the convergence rates can be made. It is obvious that the convergence rate is drastically improved in that particularly stringent example. For example, when 51 orders are retained for the computation, the conventional eigenproblem provides diffraction efficiencies of 25% and 55% for the negative first and zeroth orders, respectively. With the new formulation, the diffraction efficiencies are 10% and 84%. In Fig. 3 the numerical value of the diffraction efficiencies obtained with 25, 51, 75, and 125 retained orders are given. They can be compared with the exact values 84.843% and 10.162%, obtained by Li and Haggans,[1] when 125 modes are retained in the modal decomposition of the field. When only 25 orders are retained with the new eigenproblem, the diffraction-efficiency differences between the modal method and the new eigenproblem formulation are less than 0.009 for the reflected zeroth order and 0.002 for the negative first order (relative errors less than 1% and 2%, respectively). We conclude that the new eigenproblem formulation provides highly improved convergence rates.

The improved convergence rates illustrated in Figs. 2 and 3 are not isolated cases. All our simulation results show an improvement even for dielectric and nonlamellar gratings and for small or large period-to-wavelength ratios.

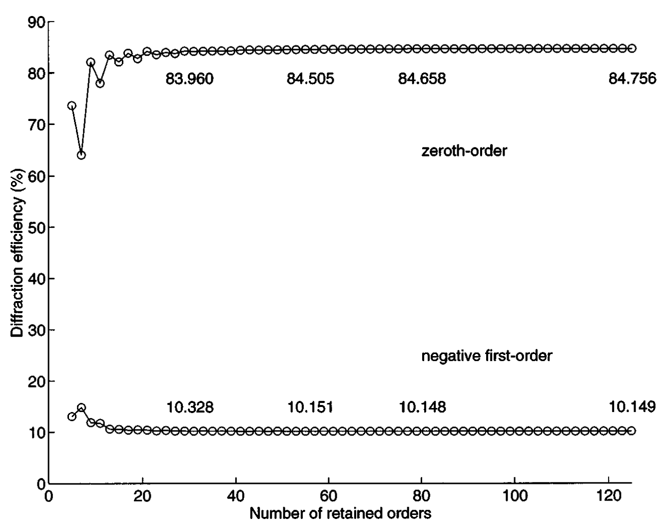


Fig. 3. Diffraction efficiencies of the reflected negative first and zeroth orders of a metallic grating with TM polarization. The circles are provided by the new eigenproblem method of Eq. (9). The grating parameters and the geometry problem are defined in Fig. 1 of Ref. 1. A direct comparison can be applied with Figs. 3(a) and 3(b) of Ref. 1, where simulation results obtained with the conventional eigenproblem and modal methods are presented.

## 5. INTERPRETATION

In this section we give a simple interpretation of the convergence-rate differences between the conventional and the new eigenproblem formulations. The interpretation is given in the quasi-static limit, i.e., when the period-to-wavelength ratio tends to zero. We show that, with the conventional eigenproblem formulation, an adequate description of the quasi-static limit requires that an infinite number of orders be retained in the computation. We also show that, with the new eigenproblem formulation, the quasi-static limit is accurately described with a finite number of retained orders.

As was shown by Li and Haggans,[1] the convergence of RCWA is directly related to the convergence of the eigensolution. Therefore any method to improve the convergence of the eigenproblem should improve the convergence of the diffraction efficiencies. Among the eigenvalues there is at least one that can be interpreted physically. It takes advantage of the equivalence between gratings and homogeneous media in the quasi-static limit. By quasi-static limit we mean situations for which the grating period is infinitely small compared with the wavelength. The equivalence was rigorously derived by Bouchitte and Petit.[8]

For the sake of simplicity we restrict the discussion to normal incidence. In the quasi-static limit and for TM polarization, the grating is equivalent to a thin layer with an effective relative permittivity equal to $1/a_0$, where $a_0$ is the zeroth Fourier coefficient of $\epsilon_0/\epsilon(x)$. The field in the grating can be written as a linear combination of two counterpropagating plane waves, namely, $\exp\, jk_0\sqrt{1/a_0}\,z$ and $\exp\, -jk_0\sqrt{1/a_0}\,z$. These two plane waves must be solutions of Eqs. (5) and (8). So in the quasi-static limit, $-k_0^2/a_0$ must be an eigenvalue of Eqs. (5) and (8). Let us note $U_m' = -jk_0 n U_m$ and $S_m' = -jk_0 n S_m$, where $-k_0^2 n^2$ is the degenerated eigenvalue expected to be equal to $-k_0^2/a_0$.

Let us first start with the conventional eigenproblem formulation. In the quasi-static limit, i.e., when $K/k_0$ tends to infinity, Eq. (4) reduces to

$$nS_0^{(0)} = U_0^{(0)}, \tag{10a}$$

$$\forall\, m \neq 0, \qquad \sum_p p a_{m-p} U_p^{(0)} = 0\,, \tag{10b}$$

where superscript (0) holds for the quasi-static notation of the fields and $\beta$ was taken equal to zero in Eq. (4). If $\pm M$ orders are retained in the computation, Eq. (10b) provides a homogeneous system of $2M$ linear equations with $2M$ unknowns, $U_p^{(0)}$ with $p \neq 0$. Except for a possible unexpected degeneracy, the solutions are zeros. So in the quasistatic limit Eq. (3b) becomes

$$\forall\, m \neq 0, \qquad \sum_{p\neq 0} \epsilon_{m-p} S_p^{(0)} = -\epsilon_m S_o^{(0)}, \tag{11a}$$

$$nU_0^{(0)} = \sum_{p\neq 0} \epsilon_{-p} S_p^{(0)} + \epsilon_0 S_0^{(0)}. \tag{11b}$$

Multiplying both sides of Eq. (11a) by $a_{-m}$ and then summing over all $m$, we obtain

$$\sum_{p\neq 0}\left(\sum_{m\neq 0} a_{-m}\epsilon_{m-p}\right) S_p^{(0)} = -\sum_{m\neq 0} a_{-m}\epsilon_m S_0^{(0)}. \tag{12a}$$

When an infinite number of orders is retained, because $\sum_m a_{-m}\epsilon_{m-p} = 0$ as **E** and **A** are inverse matrices, the left-hand side of Eq. (12a) reduces to $-a_0 \sum_{p\neq 0} \epsilon_{-p} S_p^{(0)}$. When we truncate the number of orders and retain $\pm M$ orders in the computation, this is no longer true, and we note the left side of Eq. (12a) $-a_0{}^* \sum_{p\neq 0} \epsilon_{-p} S_p^{(0)}$. Similarly, the right-hand side of Eq. (12a) can be written as $-(1 - a_0\epsilon_o) S_0^{(0)}$ when an infinite number of orders are retained and is noted as $-(1 - a_0{}^{\#}\epsilon_o) S_0^{(0)}$ during truncating. So Eq. (12a) can be written as

$$-a_0{}^* \sum_{p\neq 0} \epsilon_{-p} S_p^{(0)} = -(1 - a_0{}^{\#}\epsilon_o) S_0^{(0)}. \tag{12b}$$

In Eq. (12b), $a_0{}^*$ and $a_0{}^{\#}$ denote two slightly different values of $a_0$, which depend on the truncation rank $M$. $a_0{}^*$ and $a_0{}^{\#}$ tend to $a_0$ when the number of retained orders tends to infinity. By eliminating $\sum_{p\neq 0} \epsilon_{-p} S_p^{(0)}$ between Eqs. (11b) and (12b), we obtain

$$a_0{}^*(nU_0^{(0)} - \epsilon_0 S_0^{(0)}) = (1 - a_0{}^{\#}\epsilon_o) S_0^{(0)}. \tag{13}$$

Using Eq. (10a) to substitute $S_0^{(0)}$ for $U_0^{(0)}$ in Eq. (13), and looking for a nonzero solution in $S_0^{(0)}$, we obtain

$$n^2 = \frac{1}{a_0{}^*} + \epsilon_0\left(1 - \frac{a_0{}^{\#}}{a_0{}^*}\right). \tag{14}$$

Equation (14) shows that an infinite number of orders must be retained for the numerical computation of the exact eigenvalue $-k_0^2 n^2 = -k_0^2/a_0$. The effect of the truncation is not negligible. Figure 4 shows the real and the imaginary parts of the absolute error $e = n - \sqrt{1/a_0}$ as a function of the number of retained orders. It was obtained by solving the system of Eqs. (10) and (11) for the problem of Fig. 2. The error $e$ is quite large even when 200 orders are retained, especially for thick gratings for which a small error on $n$ is responsible for a large error on

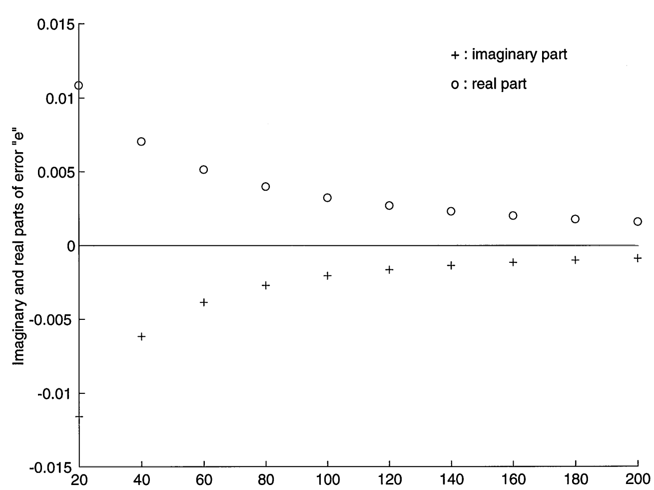


Fig. 4. Effect of the truncation on the accuracy of the conventional eigenproblem. The pluses and circles correspond to the imaginary and the real parts, respectively, of the error $e = n - \sqrt{1/a_0}$. The results are obtained by solving the system of linear equations defined by Eqs. (10a) and (11).

$\exp(-jknz)$ when the boundary conditions at the grating interface are being matched.

Let us now consider the quasi-static-limit situation with the new eigenproblem formulation. For normal incidence ($\beta = 0$) the system of second-order differential equations given by Eq. (8) is not valid. This is because $f_0 = 0$ for normal incidence. It is easily shown that Eq. (8) must be replaced by

$$\forall\, m \neq 0, \qquad m \frac{K^2}{{k_0}^2} U_m - \sum_{p \neq 0} \frac{\epsilon_{m-p}}{p} U_p = \sum_{p \neq 0, l} \frac{\epsilon_{m-p} a_{p-l}}{p {k_0}^2} U_l'' , \quad (15a)$$

$${k_0}^2 U_0 + \sum_p a_{-p} U_p'' = 0 . \quad (15b)$$

Equations (15a) and (15b) constitute the set of second-order differential equations for normal incidence. Proceeding to the quasi-static limit in Eq. (15a) results in $U_m^{(0)} = 0$ for any nonzero $m$. $n^2$ then becomes $1/a_0$ in Eq. (15b); *this result holds for any number of retained orders.*

For nonnormal incidence, a similar argument can be provided. The eigenvalue of the quasi-static limit must be equal to $-{k_0}^2(\sin^2\theta/\epsilon_0 + a_0 \cos^2\theta)^{-1}$ instead of $-{k_0}^2/a_0$; this is because, in the quasi-static limit, the equivalent homogeneous medium is uniaxial, with the optic axis parallel to the $x$ axis (see Ref. 8). The faster convergence rate of the eigenvalue problem defined by Eq. (8) was justified only in the quasi-static limit. For nonzero period-to-wavelength ratios and for TM polarization, although the eigenvalues are more difficult to interpret, it is possible to derive an eigenvalue that approximately satisfies the eigenproblem.[9] This approximate solution is expressed as a power series of $\Lambda/\lambda$. It is clear that the power series' zeroth order, which corresponds to the quasi-static limit, is given by $-{k_0}^2/a_0$. The result is that the conventional eigenproblem formulation, which is able to provide the zeroth-order term only when an infinite number of orders are retained in the computation, is also inadequate for accurately describing the eigenproblem of gratings with nonzero period-to-wavelength ratios. Although the derivation given in this section is restricted to the quasi-static limit, we believe that it provides good insight for understanding the improved convergence rates for nonzero period-to-wavelength ratios.

## 6. GENERALIZATION TO CONICAL MOUNTINGS

The new eigenproblem formulation can be generalized in a straightforward way to the case of conical mountings. We have to interpret the conical diffraction eigenproblem as a combination of TE and TM polarization eigenproblems, and we note that the conventional TE eigenproblem formulation[3] must not be changed since it provides good convergence rates. Also note that the conventional formulation for TE polarization, like the new formulation for TM polarization, provides the adequate eigenvalue in the quasi-static limit for any number of retained orders. Using strictly the notation of Ref. 3, it is then easily shown that a useful eigenproblem formulation is

$$k_0^{-1}\begin{bmatrix}\mathbf{S}_y' \\ \mathbf{S}_x' \\ \mathbf{U}_y' \\ \mathbf{U}_x'\end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{K}_y\mathbf{E}^{-1}\mathbf{K}_x & \mathbf{I}-\mathbf{K}_y\mathbf{E}^{-1}\mathbf{K}_y \\ \mathbf{0} & \mathbf{0} & \mathbf{K}_x\mathbf{E}^{-1}\mathbf{K}_x & -\mathbf{K}_x\mathbf{E}_{-1}\mathbf{K}_y \\ \mathbf{K}_x K_y & \mathbf{A}^{-1}-{\mathbf{K}_y}^2 & \mathbf{0} & \mathbf{0} \\ {\mathbf{K}_x}^2-\mathbf{E} & -\mathbf{K}_x\mathbf{K}_y & \mathbf{0} & \mathbf{0}\end{bmatrix} \times \begin{bmatrix}\mathbf{S}_y \\ \mathbf{S}_x \\ \mathbf{U}_y \\ \mathbf{U}_x\end{bmatrix} . \quad (16)$$

In Eq. (16) $\mathbf{S}_x$, $\mathbf{S}_y$, $\mathbf{U}_x$, $\mathbf{U}_y$, $\mathbf{K}_x$, $\mathbf{K}_y$, $\mathbf{E}$, and $\mathbf{I}$ are defined as in Ref. 3. $\mathbf{A}$ denotes again the matrix formed by the inverse-permittivity harmonic coefficients. The only difference between the conventional formulation [see Eq. (57) of Ref. 3] and the new formulation of Eq. (16) is in the third row of the second column, where matrix $\mathbf{E} - {\mathbf{K}_y}^2$ has been replaced by $\mathbf{A}^{-1} - {\mathbf{K}_y}^2$. In Fig. 5 the diffraction efficiencies of the negative first and zeroth orders of a conical mounting are shown as functions of the number of retained orders. The grating used to obtain the result in Fig. 5 is the same as that discussed in the second example of Section 4 (see Fig. 1 of Ref. 1). The diffraction configuration is a 30° angle of incidence, a 30° azimuthal angle, and a 45° angle between the electric-field vector and the plane of incidence. Using the notation of Ref. 3, $\theta = 30°$, $\phi = 30°$, and $\psi = 45°$. The solid curves are obtained with the conventional formulation of Eq. (57) in Ref. 3, and the dotted curves are obtained with the new formulation of Eq. (16). As in the two examples above we note that the new formulation provides faster and smoother convergence rates. For example, for the zeroth-order diffracted plane wave the numerical values of the diffraction efficiencies are 10.58%, 10.11%, 10.08%,

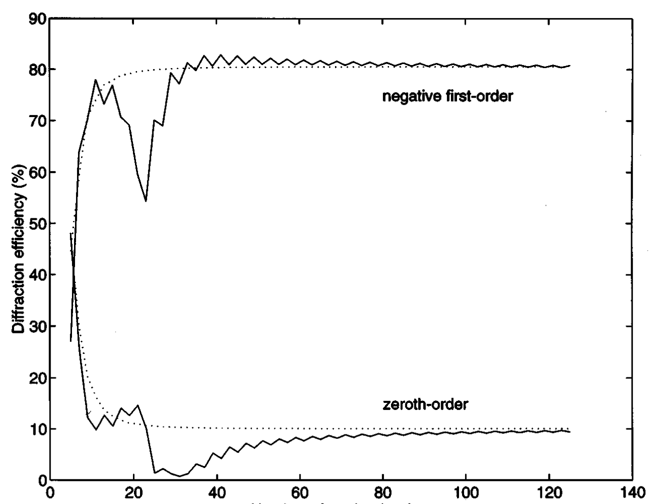


Fig. 5. Diffraction efficiencies of the reflected negative first and zeroth orders of a metallic grating for conical mount ($\theta = 30°$, $\phi = 30°$, and $\psi = 45°$). The grating parameters are defined in Fig. 1 of Ref. 1. The solid curves are obtained with the conventional eigenproblem formulation of Ref. 3. The dotted curves are obtained with the new formulation of Eq. (16).

and 10.07% when 25, 51, 75, and 125 orders, respectively, are retained with the new formulation. With the conventional formulation the corresponding diffraction efficiencies are 1.38%, 7.70%, 8.99%, and 9.42%. We conclude that the new formulation with 25 retained orders provides more accurate results than the conventional formulation with 125 retained orders. By use of the second derivative of the field vector, the eigenproblem of Eq. (16) reduces to

$$k_0^{-2}[\mathbf{U}_x''] = [\mathbf{K}_y^2 + \mathbf{K}_x^2 - \mathbf{E}][\mathbf{U}_x],$$
$$k_0^{-2}[\mathbf{S}_x''] = [\mathbf{K}_x\mathbf{E}^{-1}\mathbf{K}_x\mathbf{A}^{-1} + \mathbf{K}_y^2 - \mathbf{A}^{-1}][\mathbf{S}_x]. \qquad (17)$$

Equations (17) are new formulations of Eq. (60) in Ref. 3 and can be used to save computational time.

## 7. CONCLUSION AND DISCUSSION

By reformulating the eigenproblem of RCWA, we show that good convergence rates can be achieved for TM polarization of 1-D metallic gratings. In Ref. 1, Li and Haggans interpreted the oscillating and poor convergence rates of conventional RCWA by invoking truncation effects that are due to the slowly convergent Fourier expansions of the permittivity and the field inside the grating, but they noted that their interpretation poses a difficulty in understanding why convergence rates are much slower with TM than with TE polarization. Because the new eigenproblem is also based on a truncated Fourier expansion of the permittivity, the poor convergence rates observed for TM polarization must not be attributed to truncation effects. In Section 5, by examining the eigenproblem in the quasi-static limit, we show that the conventional eigenproblem requires an infinite Fourier expansion to provide an accurate description of the quasi-static limit diffraction problem; this can be considered to be a kind of bad conditioning of the conventional eigenproblem. However, as shown in Fig. 3, the effect of the truncation remains slightly visible with the new eigenproblem formulation. When the number of retained orders increases from 25 to 125, the zeroth-order diffraction efficiency keeps increasing from 83.96% to 84.76% and is expected ultimately to reach the approximate value of 84.84%. This convergence rate is similar to that observed for TE polarization of the same grating problem. The approach developed in this paper can be applied to any numerical techniques using a Fourier expansion and is not restricted to the implementation of RCWA.

With respect to computational effort, the new eigenproblem formulations of Eqs. (9) and (17) are more demanding than their corresponding conventional formulations [Eqs. (6b) and (60) of Ref. 3]. They additionally require the numerical computation of matrices $\mathbf{A}$ and $\mathbf{A}^{-1}$. However, for a given reasonable accuracy, the new eigenproblem formulation saves considerable time and computer memory because fewer orders have to be retained. This is especially true when continuous profile gratings or stacks of lamellar gratings are considered or when several grating depths are studied for a given diffraction problem.

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