Differential theory for diffraction gratings: a new formulation for TM polarization with rapid convergence

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A new formulation of the differential method in TM polarization, based on correct representation of truncated Fourier series of products of discontinuous functions, is proposed. Although the derived equations are more complicated than in the classical formulation, the convergence rate with respect to the truncation parameter (with the number of diffraction orders taken into account) is much faster for arbitrary grating profiles, approaching the convergence rate in TE polarization. Numerical examples are presented for dielectric and metallic sinusoidal gratings with a 100% modulation ratio.

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Since the beginning of the 1970's, the differential theory of gratings[1] has been found to suffer from numerical instabilities in TM polarization when dealing with deep gratings and highly reflecting materials. These instabilities are cumulative and of two types. The first type, contamination by growing exponential terms during numerical integration, was recently solved by use of the S-matrix propagation algorithm.[2] In this Letter a solution for the second type of error, caused by the bad convergence rate of the Fourier series of discontinuous field components, is proposed.

Let us consider a grating lying in the $x-z$ plane with grooves parallel to the z axis and y axis perpendicular to the mean plane of the grating. The cladding is air. In TM polarization, the continuous-in-y electromagnetic field component is the z component H_z of the magnetic field, and the x and y components (E_x and E_y) of the electric field are generally discontinuous. The differential method integrates the following equations in TM polarization:

$$\frac{\mathrm{d}}{\mathrm{d}y}[H_z(x, y)]_n = -i[k^2(x, y)E_x(x, y)]_n ,$$

$$\frac{\mathrm{d}}{\mathrm{d}y}[E_x(x, y)]_n = -i[H_z(x, y)]_n + i\alpha_n[E_y(x, y)]_n , \quad (1)$$

with $E_y(x, y) = -ik^{-2}(x, y)\partial H_z/\partial x$. In Eqs. (1), $[\,]_n$ denotes the Fourier components of the functions in brackets with respect to x, $k^2(x, y) = {k_0}^2 n^2(x, y)$, $n(x, y)$ is the refractive index, k_0 is the wave number, $\alpha_m = k_0 \sin\theta_i + mK$, K is the grating wave number ($K = 2\pi/d$, where d is the grating period), and θ_i is the angle of incidence with respect to the y axis. For convenience, H_z is substituted with $\omega\mu_0 H_z$. The classical formulation of the differential method uses a direct representation of the Fourier decomposition of a product of two functions,

$$[k^2E_x]_n = \sum_m [k^2]_{n-m}[E_x]_m ,$$

$$[E_y]_n = \sum_m [k^{-2}]_{n-m}\alpha_m[H_z]_m . \quad (2)$$

The summations in Eqs. (2) involve infinite numbers of terms. However, computer implementation of this method requires truncation of the Fourier series and the summation index. Whereas in TE polarization this truncation does not raise problems, in TM polarization it is necessary to represent the Fourier component of a product of discontinuous functions with shared discontinuity points. As was pointed out by Li,[3] this requirement leads to valid mathematical operations in only two cases: (A) if the two functions have no common discontinuities, in particular, if one of them is continuous and the other one is discontinuous, and (B) if, at the points where the two functions are both discontinuous, their product is continuous, particularly if their product is continuous everywhere. For case (B), it was established in the research reported in Ref. 3 that the product can be factorized by use of an inverse rule. For example, for lamellar gratings, where E_x is discontinuous when crossing the lamella sides but the product k^2E_x is continuous, the Fourier components after truncation are correctly given as $[k^{-2}]^{-1}[E_x]$, where $[k^{-2}]^{-1}$ is a matrix that is the inverse of the Toeplitz matrix $[k^{-2}]$ and, in general, is not equal to $[k^2]$. The resulting equations for lamellar gratings, obtained in the research reported in Ref. 4 (and analyzed in detail in Ref. 5) are

$$[k^2E_x]_n = \sum_m ([k^{-2}]^{-1})_{n-m}[E_x]_m ,$$

$$[E_y]_n = \sum_m ([k^2]^{-1})_{n-m}\alpha_m[H_z]_m . \quad (3)$$

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However, for an arbitrary grating profile, neither E_x nor k^2E_x is continuous when it is crossing the profile, and thus neither of the two rules (direct or inverse) applies. This is why neither Eqs. (2) nor Eqs. (3) give numerical results with acceptable convergence rates. Figure 1 presents a comparison, made for a metallic sinusoidal grating, of the convergence rates with respect to the number of diffraction orders taken into account in the calculations (equal to $2N + 1$). As can be observed from the figure, the convergence in the TE polarization is rapid, leading to results with a relative error of less than 1% for $N = 10$, whereas in TM polarization the error remains greater than 50% even for $N = 30$. In fact, it is necessary to increase N to as much as 150 to reduce this error.

We have been able to obtain a new formulation of the Fourier transformation of the products in Eq. (1), using products of classes (A) and (B) only. This formulation is obtained by decomposition of E_x and E_y into components that are locally tangential (E_T) and normal (E_N) to the profile by use of the x and y components of the unit vector tangential to the profile, t_x and t_y, respectively. t_x and t_y are defined only on the grating profile, but to calculate their Fourier components it is necessary to define them for each x. There are several possible ways of doing this, depending on the profile function $y = f(x)$. The simplest way is to use

$$t_x = 1 \Big/ \sqrt{1 + (f')^2}\,,$$

$$t_y = f' \Big/ \sqrt{1 + (f')^2}\,,$$

where f' is the derivative of $f(x)$, when the derivative exists. If the derivative does not exist, one can use different definitions for t_x and t_y by introducing, for example, a curvilinear parameter of the profile.

By use of the fact that E_T and k^2E_N are continuous, the final result can be obtained (written in matrix form) after several simple operations:

$$[k^2E_x] = ([k^{-2}]^{-1} + [{t_x}^2]\Delta)[E_x] + [t_xt_y]\Delta[E_y], \qquad (4)$$

$$[E_y] = ([k^2] - [{t_x}^2]\Delta)^{-1}(\alpha[H_z] - [t_xt_y]\Delta[E_x]). \qquad (5)$$

Δ is a matrix,

$$\Delta = [k^2] - [k^{-2}]^{-1}, \qquad (6)$$

and α is a diagonal matrix with elements equal to α_m. It is important to note that $[E_y]$ is obtained not by a direct Fourier transform but by use of several matrix operations in Eq. (5).

When $t_y = 0$, i.e., for profiles with infinitely small modulation, Eqs. (4)–(6) take the same form as Eq. (2), the classical formulation of the differential method. For lamellar profiles, $t_x = 0$, and Eqs. (4)–(6) take the same form as in Eqs. (3) proposed in Ref. 4. However, very deep sinusoidal profiles, i.e., gratings with ~100% modulation, and cylindrical rod gratings are difficult to treat from the point of view that the tangential to the profile vector changes its direction from parallel to the x axis [for which the classical formulation in Eqs. (2) holds] to parallel to the y axis [for which Eqs. (3) converge better than Eqs. (2)] through all intermediate cases. Equations (4)–(6) are quite general, because they are valid for slanted or curved profiles, too. This is shown by the open triangles in Fig. 1. The convergence in TM polarization by use of Eqs. (4)–(6) instead of (2) or (3) approaches the convergence rate in the TE case. The same conclusion is also valid for a dielectric grating with high contrast of the refractive index (equal to 1 in the cladding and 2.5 in the substrate; see Fig. 2).

It is interesting to compare the calculation times of the new and the classical differential methods, because of the many Fourier transformations and matrix multiplications and inversions required at each integration step. For a metallic sinusoidal grating the number of integration steps (I) required is approximately $\lambda/150$, and the number of slices M that are necessary for decomposition of the grating height when one is applying the S-matrix algorithm depends on the truncation parameter N. For example, for $N = 10$, it is sufficient to take $M = 4$ and $I = 240$. With this choice of technical parameters, the computation time on a Pentium II 300-MHz PC for TE polarization is 1.6 s, increasing to 3.9 s for TM polarization for the classical formulation and 7.6 s for the new formulation, Eqs. (4)–(6). If, for better precision, N is increased to 20, it is necessary to increase M to 8 and I to 320. Then, computation in the TE case takes 11 s, the classical TM formulation

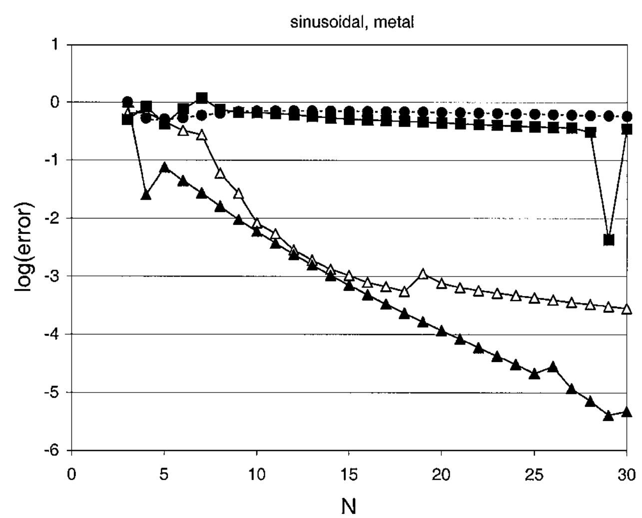

Fig. 1. Logarithm of the relative error in the propagating diffraction orders as a function of truncation parameter N (the total number of diffraction orders taken into account is $2N + 1$). Filled squares, results obtained with Eqs. (2); filled circles, Eqs. (3); open triangles, Eqs. (4)–(6). For comparison, the filled triangles show the convergence for TE polarization. The parameters of the sinusoidal metallic grating used are period $d = 1\ \mu$m; depth $h = 1\ \mu$m; complex refractive index, $1.3 + i7.6$; incidence from air at a 30° angle; and wavelength, 0.6328 μm. The error is calculated as the difference between the numerical results and the results of the integral method.[6] The reference efficiencies are order −2, 0.2120; order −1, 0.1598; and order 0, 0.2638.

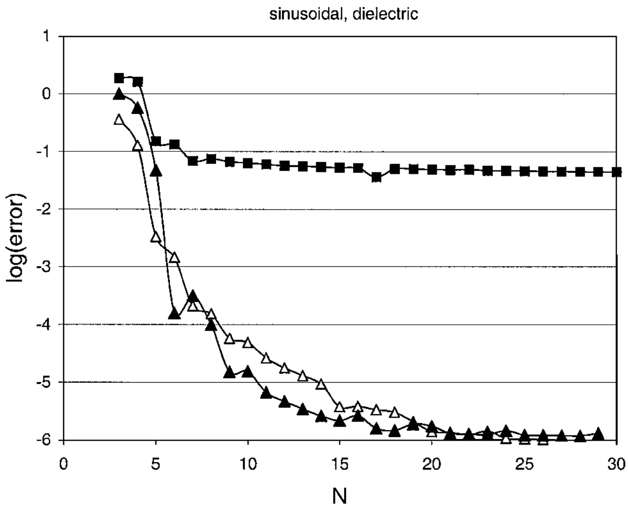

Fig. 2. Same as in Fig. 1, except that the grating material is dielectric, with refractive index 2.5. The results for Eqs. (3) are not presented. The reference efficiencies in transmission are order −3, 0.1472; order −2, 0.2261; order −1, 0.2830; and order +2, 0.2205.

[Eqs. (2)] requires 25 s, and the new formulation requires 45 s. The same ratio (approximately 1:2:4) is preserved when N, M, and I vary over a large range. This result indicates that the new version of the differential method does not lead to a drastic increase in computation time (it is only twice the time for the old version). On the other hand, the faster convergence helps one to gain time, because fixing the number of slices M in the S-matrix algorithm results in a computation time that is roughly proportional to N^3. Moreover, the increase of N requires a larger number of slices M, owing to the exponential terms, which grow faster for greater N.

We have removed the limitation that has plagued the differential theory of gratings over the last quarter of a century. The approach presented here opens a wide range of applications not only for TM polarization but also for conical diffraction, crossed gratings, and three-dimensional problems in linear and nonlinear optics.

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References

1. P. Vincent, in *Electromagnetic Theory on Gratings*, R. Petit, ed. (Springer-Verlag, Berlin, 1980), Chap. 4.
2. L. Li, J. Opt. Soc. Am. A **13,** 1024 (1996).
3. L. Li, J. Opt. Soc. Am. A **13,** 1870 (1996).
4. P. Lalanne and G. Morris, J. Opt. Soc. Am. A **13,** 779 (1996).
5. P. Lalanne, J. Opt. Soc. Am. A **14,** 1583 (1997).
6. D. Maystre, in *Electromagnetic Theory of Gratings*, R. Petit, ed. (Springer-Verlag, Berlin, 1980), Chap. 3.