On the Convergence of the Coupled-Wave Approach for
Lamellar Diffraction Gratings

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I. INTRODUCTION

Among the many existing rigorous methods for analyzing diffraction of electromagnetic waves by diffraction gratings, the coupled-wave approach[1] stands out because of its versatility and simplicity. It can be applied to volume gratings and surface relief gratings, and its numerical implementation is much simpler than others. In addition, its predictions have been experimentally validated in several cases[2-4]. These facts explain the popularity of the coupled-wave approach among many optical engineers in the field of diffractive optics. However, a comprehensive analysis of the convergence of the model predictions has never been presented, although several authors[5,6] have recently reported convergence difficulties with the model when it is used for metallic gratings in TM polarization.

In this short paper, we will make three points: *(1) In the TM case, the coupled-wave approach converges much slower than the modal approach of Botten et al.[7,8]. (2) The slow convergence is caused by the use of Fourier expansions for the permittivity and the fields in the grating region, and (3) is manifested by the slow convergence of the eigenvalues and the associated modal fields.* The reader is assumed to be familiar with the mathematical formulations of the coupled-wave approach and the modal approach.

II. ANALYSIS

a. Two Types of Modal Approaches

There are two types of modal approaches: Modal Approach using a Scalar (characteristic) Equation[7,8] (MASE) and Modal Approach using a Matrix (characteristic) Equation[9] (MAME). *The coupled-wave approach (CWA) is equivalent to a MAME.* In the MASE, the eigenvalues and modal fields in the grating region are solved one at a time from a scalar characteristic equation. Each modal field thus found satisfies Maxwell's equations and the boundary conditions exactly. In the MAME, however, N eigenvalues and modal fields are solved simultaneously from a matrix characteristic equation. Unless $N = \infty$, none of these modes satisfies Maxwell's equation exactly.

b. Two Kinds of Infinities

When solving grating problems by any method, one always has to deal with two kinds of infinities: the infinity of the discrete set Z (the set of all integers), and the infinity of the continuum [0,d), where d is the grating period. The first infinity is due to the periodicity of the grating, which generates an infinite number of diffraction orders. The second infinity is related to the continuous nature of Maxwell's equations. In any method, one has to solve Maxwell's equations on [0,d), with the pseudo-periodic boundary condition. In the MASE, the infinity of [0,d) is handled analytically. The infinity of Z is not truncated until the matching of boundary conditions at the interfaces between uniform regions and corrugated region is completed. In the MAME, the infinity of Z is handled similarly. However, the infinity of [0,d) is transformed into that of the coefficients of the Fourier expansions, which happens to be degenerate with the infinity of the diffraction orders. *It is this tempering of the infinity of [0,d) that leads to the slow convergence of the CWA.*

c. Two Convergence Processes

In the CWA, the permittivity of the periodic medium in the grating region is represented by its Fourier expansion. When this infinite expansion is truncated, *the physical problem is changed* (the original discontinuous permittivity is changed to a smooth-varying one). Hence, both the electromagnetic field and the grating profile are approximated as a result of the truncation. This means that the convergence of the diffraction efficiency and phase values relies on the convergence

of both the modal fields and the permittivity representation.

d. *The Convergence Rates of Related Fourier Series*

The analysis above indicates that the CWA, or the MAME in general, should be expected to converge slower than the MASE. This point is reinforced by the following asymptotic analysis of the Fourier coefficients for the permittivity and the fields. Let the permittivity be $\epsilon(x+d) = \epsilon(x)$, $\epsilon(x) = \epsilon_1$, $|x| < a$, and $\epsilon(x) = \epsilon_2$, $a < |x| < d/2$. It is easy to check that $c_n = O(n^{-1})$ as $n \to \infty$, where c_n is a Fourier coefficient of $\epsilon(x)$. Evidently, the convergence of the permittivity expansion is very slow.

We now consider the Fourier expansion coefficient, f_n, of the fields. For TE polarization, the boundary conditions demand that both the electric field and its derivative be continuous at the permittivity discontinuity. Consequently, $f_n = O(n^{-3})$, as $n \to \infty$. For TM polarization, the magnetic field is continuous, but its derivative is not. Instead, we have $\epsilon_1^{-1}(dH/dx)|_{x=a=0}=\epsilon_2^{-1}(dH/dx)|_{x=a=0}$; therefore, $f_n = O(n^{-2})$, as $n \to \infty$. Hence the Fourier expansion for a TM field converges slower than that for a TE field. Next, suppose $\epsilon_1 = 1$, and the polarization is TM. For a lossless dielectric grating, ϵ_1 and ϵ_2 are both positive; while for a metallic grating, ϵ_1 and ϵ_2 have different signs, if the small imaginary part of ϵ_2 is neglected. Accordingly, the H-field at the permittivity discontinuity in a dielectric grating is "smoother" than it is in a metallic grating. In other words, the H-field has weaker high frequency components in a dielectric grating than it has in a metallic grating. The analysis above rationalizes why the CWA converges slower for TM polarization than for TE polarization, and why it converges slower for metallic gratings than for dielectric gratings.

e. *Eigenvalues and Modal fields*

The difficulty in the analysis of gratings lies in the accurate characterization of the fields in the grating region. For modal approaches of both types (including the CWA), this means that *it is imperative to determine the eigenvalues accurately* because it is trivial to determine the modal fields once the eigenvalues are known. In the CWA approach, the eigenvalues are solved from the characteristic matrix equation, which is obtained from the truncated and slowly converging Fourier expansions of the permittivity and the fields. Thus, the convergence of the eigenvalues is slow, as numerically demonstrated in the next section.

III. NUMERICAL EXAMPLES

Let us arbitrarily choose a fixed groove depth to wavelength ratio, say $d/\lambda=1$, from Fig. 3 of Ref. 5 (a gold lamellar grating). We examine how the diffraction efficiencies and the eigenvalues converge with the CWA and with the MASE. Our numerical implementation of the CWA is based on the third paper in Ref. 1. The truncated matrix ϵ_{mn}^{-1} is obtained by numerically taking the inverse of ϵ_{mn}, as recommended by Moharam and Gaylord[10]. Our numerical implementation of the MASE is based on Refs. 7 and 8. Both computer programs have been thoroughly checked against the available results in the literature and against each other. In the following, N denotes the total number of space-harmonics retained in the computations. For the results of the MASE, the number of modal fields is set to equal N.

Figs. 1a and 1b show the convergence of diffraction efficiencies as N increases for TE and TM polarizations. For both polarizations, the MASE converges extremely fast. For TE polarization, the CWA converges reasonably fast toward the MASE. For TM polarization, however, the CWA converges very slowly toward the MASE; in fact, it does not begin converging until N > 40.

Figs. 2a and 2b show the convergence of the real and imaginary parts of the square of the tenth TE eigenvalue and the ninth TM eigenvalue, respectively. Similar to the convergence of diffraction efficiencies, the TE eigenvalue computed with CWA converges reasonably fast toward that computed with the MASE (dashed-lines), but the TM eigenvalue converges very slowly. We should mention that all the TE eigenvalues computed with CWA converge at a rate similar to that in Fig. 2a, and some of the TM eigenvalues do converge faster than the one shown in Fig. 2b.
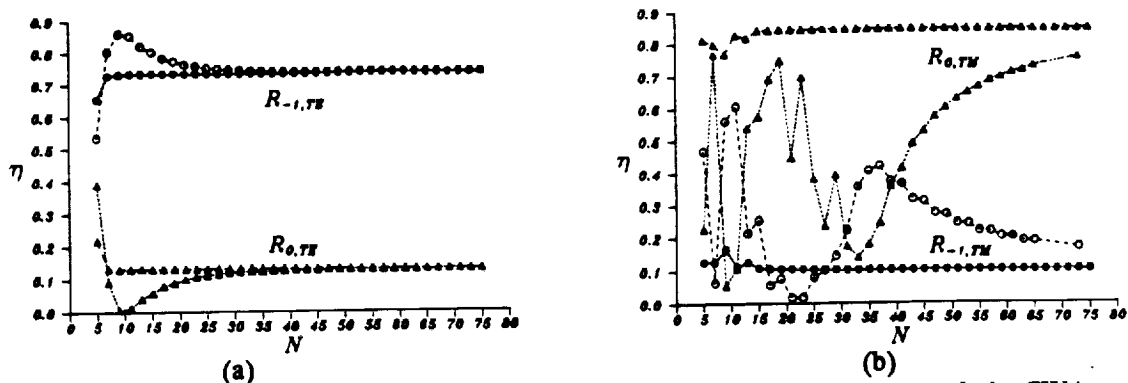
Fig. 1. Convergence of diffraction efficiencies. Solid symbols, MASE. Open symbols, CWA.
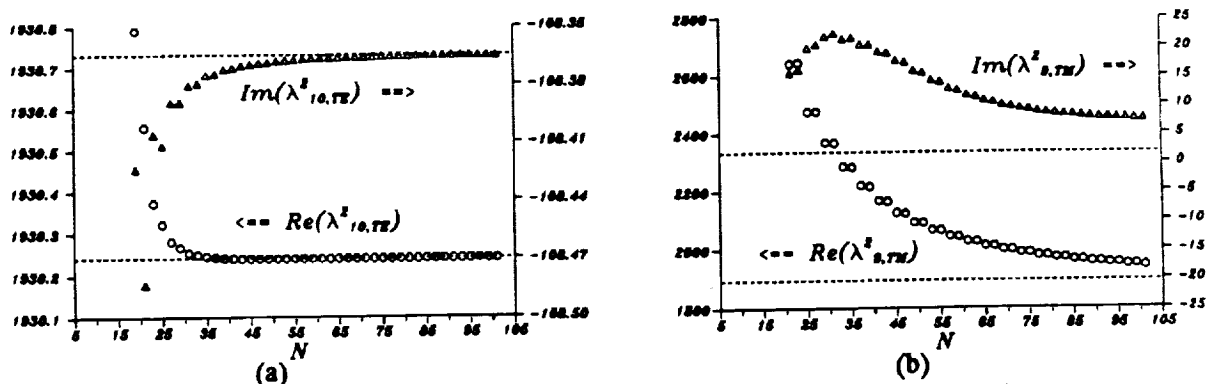

Fig. 2. Convergence of eigenvalues computed with coupled-wave approach.

IV. CONCLUSIONS

We have demonstrated with numerical examples that the predictions of the CWA converge slowly toward those of the MASE of Botten et al. for metallic gratings in TM polarization. We have shown that the slow convergence is caused by the use of slowly convergent Fourier expansions for the permittivity and the fields in the grating region. *Despite its popularity, versatility, and simplicity, the coupled-wave approach should be used with caution for metallic surface relief gratings in TM polarization.* Although we have only compared the CWA with the MASE, much of the analysis applies to the MAME and differential methods utilizing Fourier expansions in general.

V. REFERENCES

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