ELECTROMAGNETIC DIFFRACTION EFFICIENCIES FOR PLANE REFLECTION DIFFRACTION GRATINGS

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Final Report
Prepared for the
National Aeronautics and
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Under Contract NAS5-11456

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Introduction

This is the final report for NASA contract No. NAS5-11456. The contract period began on 15 July 1973 and ended 15 January 1974. A three-month, no-cost extension of this contract ended on 15 April 1974.

During the contracted time we developed the theory and computer programs, based on rigorous electromagnetic theory, required for the analysis and design of echelle gratings. These gratings are designed for instruments that operate in the ultraviolet portion of the spectrum. The theory has been developed so that the resulting computer programs will be able to analyze deep (up to 30 wavelengths) gratings by including as many as 100 real or homogeneous diffraction orders. The program calculates the complex amplitude coefficient for each of the diffracted orders. Also, a check on the numerical method used to solve the integral equations is provided by a conservation of energy calculation.

Theory

For our work we adopted the rigorous vector diffraction theory first described by Zaki[1] and Kalhor.[2] The essentials of this theory are contained in our second-year final report dated July 1973.[3] Below we describe the equations resulting from this theory and how they are used to obtain the desired amplitude coefficients. Some of the equations are reproduced here for ease of reference.

For the E-parallel state of polarization the incident electric field vector is parallel to the grooves of the reflection grating. Application of the boundary conditions for this polarization state yields the following equations:

$$E_i(x',y') = \int_0^a \sqrt{1+[f'(x)]^2}\; G'(x,y;x',y') \frac{\partial E(x,y)}{\partial n}\, dx \qquad (1)$$

$$A_m = \frac{1}{i2a\gamma_m} \int_0^a \sqrt{1+[f'(x)]^2}\; e^{-i(\beta_m x + \gamma_m y)} \frac{\partial E(x,y)}{\partial n}\, dx \qquad (2)$$

where the integrals are to be evaluated on the grating surface so that

$y = f(x)$ and $y' = f(x')$, where $f(x)$ is the function that describes the grating profile. Also,

E_i is the incident field

$E_i + E_d$ is the total electric field (incident + diffracted)

$\partial E/\partial n$ is the derivative of the total electric field with respect to the grating surface normal

A_m is the desired amplitude coefficient for the m^{th} diffraction order

$G'(x,y;x',y')$ is the Green's function of the problem and in the plane wave representation assumes the form

$$G(x,y;x',y') = -\frac{e^{-ikx\sin\theta_i}}{2ia}\sum_{m=-\infty}^{\infty}\frac{e^{-i2\pi m(x-x')/a}\, e^{+ik\cos\theta_m|y-y'|}}{k\cos\theta_m} \qquad (3)$$

The various diffraction angles, for a given set of operating conditions, are given by the well known grating equation

$$\sin\theta_i + \sin\theta_m = -m\lambda/a$$

where a is the grating period and λ is the wavelength.

In Eq. (1) the quantity $\partial E/\partial n$ describes the induced current distribution on the surface of the grating and is the only unknown. Therefore Eq. (1) can be solved for $\partial E/\partial n$ and the answer can be inserted into Eq. (2) so that the unknown amplitude coefficients A_m can be determined. Below we briefly describe the method that we have chosen to perform these calculations.

We first note that in order to evaluate the continuous functions of Eqs. (1) and (2) they must be cast into a discrete form suitable for digital computation. This can be done by first noticing that the integrals in Eqs. (1) and (2) are over a finite interval (0,a) with respect to the variable of integration x. A discrete representation of the quantities appearing in Eqs. (1) and (2) can be obtained by expanding each function in terms of its complex Fourier series expansion with a period of a. In this manner we may define the following:

$$E_i(x',f(x')) \equiv \sum_{j=-\infty}^{\infty} h_j e^{+i2\pi jx'/a} \tag{4}$$

$$G'(x,f(x);x',f(x')) \equiv \sum_{j=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} K_{j,n}\, e^{+i2\pi jx'/z}\, e^{-i2\pi nx/a} \tag{5}$$

$$\{1+[f'(x)]^2\}^{\frac{1}{2}} \frac{\partial E(x,f(x))}{\partial n} \equiv \sum_{\infty}^{\infty} g_n\, e^{+i2\pi nx/a} \tag{6}$$

$$e^{-i\beta_m x}\, e^{+i\gamma_m f(x)} \equiv \sum_{n=-\infty}^{\infty} e_{m,n}\, e^{+i2\pi nx/a} \tag{7}$$

and we have used the definitions

$$\begin{aligned} \beta_m &\equiv (2\pi/\lambda)\sin\theta_m \\ \gamma_m &\equiv (2\pi/\lambda)\cos\theta_m. \end{aligned} \tag{8}$$

The complex-valued Fourier expansion coefficients h_j, $K_{j,n}$, g_n, and $e_{m,n}$ are calculated by making use of the orthogonality of the complex exponentials appearing on the right-hand sides of Eqs. (4) through (8). Their determination in this way assures the faithful representation of the continuous functions in the interval (0,a). Substitution of Eqs. (4) through (8) into Eqs. (1) and (2) casts the continuous integral equations into a set of equivalent matrix equations

$$h_j = a \sum_{n=-\infty}^{\infty} K_{j,n}\, g_n \tag{9}$$

$$A_m = \frac{1}{2\gamma_m} \sum_{n=-\infty}^{\infty} e_{m,n}\, g_n. \tag{10}$$

Equations (9) and (10) each represent an infinite set of simultaneous equations. The unknown coefficients g_n must be determined from Eq. (9)

once the coefficients h_j and $k_{j,n}$ have been calculated with sufficient accuracy. The values for g_n so obtained are then used in Eq. (10) to calculate the unknown amplitude coefficients A_m by simple matrix multiplication.

Computer Program

We now consider the discrete equations (9) and (10). Although the sums involved are over all possible positive and negative integers, the actual computer calculation must be limited to a finite number of integers. The set of integers chosen depends on the operating conditions and the particular grating that is being considered. The set of integers must include all of the real orders that are present and a sufficient number of evanescent orders that reliable results are obtained.

Despite the mathematical complexity of the analytical calculation, Eqs. (9) and (10) for the digital computation are remarkably simple. It is this simplicity that lends this program to be more versatile than the Berkeley programs.

We now discuss some of the features that must be considered when calculating the required matrix elements. We begin with the matrix K composed of elements $K_{j,n}$. Each element must be calculated accurately and the dimensionality of K must be properly chosen if the corresponding values for g_n are to be accurate. In order to calculate the elements $K_{j,n}$ the grating profile f(x) must be specified. A simple profile is shown in Fig. 1.

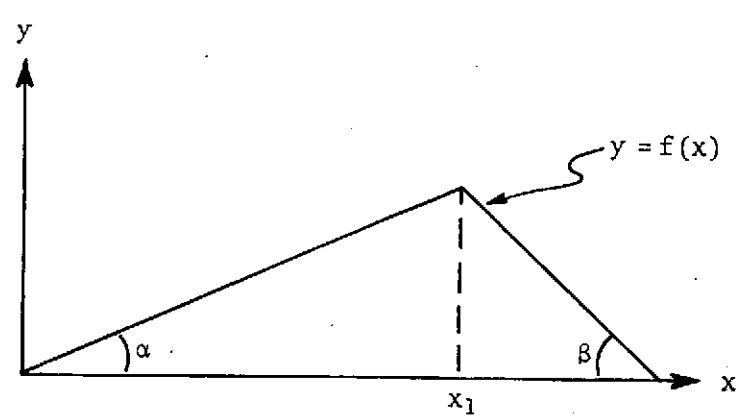

Fig. 1. Grating profile f(x).

For this profile the corresponding expression for the matrix elements $K_{j,n}$ is given by Eq. (11) (next page). The parameters appearing in Eq. (11) are defined as follows:

$$A = \tan\alpha$$
$$B = \tan\beta$$
$$q_{mn}^{(1)} = \beta_m a - Aa\gamma_m - 2\pi n$$
$$q_{mn}^{(2)} = \beta_m a + Aa\gamma_m - 2\pi n$$

The expressions for $p_{mn}^{(1)}$ and $p_{mn}^{(2)}$ are the same as for $q_{mn}^{(1)}$ and $q_{mn}^{(2)}$, respectively, except that the slope A is replaced by the slope B. The parameter $\bar{x}_1$ is the normalized apex location of the profile

$$\bar{x}_1 \equiv x_1/a.$$

Note that the expression for $K_{j,n}$ involves a sum over m. In order to obtain an accurate value of $K_{j,n}$ it will be necessary to perform this infinite sum unless the terms $K_{jn}(m)$ converge rapidly. Let M be the maximum value of the integer m and define the corresponding value for $K_{j,n}$ obtained by using this M as

$$K_{j,n}^{M} \equiv \sum_{m=-M}^{M} K_{j,n}(m),$$

where $K_{j,n}(m)$ is the m^{th} term in the sum. Let ε be a small number. It is possible to find a value for M such that

$$|K_{j,n}^{M} - K_{j,n}^{M-1}| < \varepsilon. \qquad (12)$$

When this condition is satisfied, the sum over m is truncated, and it is assumed that the resulting value for $K_{j,n}$ is the acceptable true value.

In the computer program we have written, we set M = 50 and $\varepsilon = 10^{-6}$. This means that m can assume 101 values (including zero). We have found that under these conditions a stable solution for $K_{j,n}$ that satisfies Eq. (12) is obtained before m assumes the maximum number of allowed values.

$$K_{j,n} = \sum_{m=-\infty}^{\infty} C_m \Bigg[e^{-i q^{(1)}_{mn} \bar{x}_1} \left\{ \frac{e^{+i\beta_m a}\sqrt{1+A^2}}{P^{(1)}_{mj}\, q^{(1)}_{mn}} - \frac{\sqrt{1+A^2}}{q^{(1)}_{mj}\, q^{(1)}_{mn}} + \frac{\sqrt{1+B^2}}{q^{(1)}_{mj}\, P^{(1)}_{mn}} - \frac{e^{+i\beta_m a}\sqrt{1+B^2}}{P^{(1)}_{mj}\, P^{(1)}_{mn}} \right\}$$

$$+ e^{+i2\pi(n-j)\bar{x}_1} \left\{ \frac{\sqrt{1+A^2}}{q^{(2)}_{mj}\, q^{(2)}_{mn}} - \frac{\sqrt{1+A^2}}{2\pi(n-j)} \left(\frac{1}{q^{(1)}_{mj}} - \frac{1}{q^{(2)}_{mj}} \right) + \frac{\sqrt{1+A^2}}{P^{(2)}_{mj}\left(q^{(2)}_{mn} - \frac{A}{B} P^{(2)}_{mj}\right)} - \frac{\sqrt{1+A^2}}{P^{(2)}_{mj}\, q^{(2)}_{mn}} - \frac{\sqrt{1+A^2}}{P^{(1)}_{mj}\left(q^{(1)}_{mn} - \frac{A}{B} P^{(1)}_{mj}\right)} \right.$$

$$\left. + \frac{\sqrt{1+B^2}}{q^{(1)}_{mj}\left(\frac{B}{A} q^{(1)}_{mj} - P^{(1)}_{mn}\right)} - \frac{\sqrt{1+B^2}}{q^{(2)}_{mj}\, P^{(2)}_{mn}} + \frac{\sqrt{1+B^2}}{q^{(2)}_{mj}\left(P^{(2)}_{mn} - \frac{B}{A} q^{(2)}_{mj}\right)} + \frac{\sqrt{1+B^2}}{P^{(2)}_{mj}\, P^{(2)}_{mn}} - \frac{\sqrt{1+B^2}}{2\pi(n-j)} \left(\frac{1}{P^{(1)}_{mj}} - \frac{1}{P^{(2)}_{mj}} \right) \right\}$$

$$+ e^{+i q^{(2)}_{mj} \bar{x}_1} \left\{ \frac{\sqrt{1+A^2}}{P^{(2)}_{mj}\, q^{(2)}_{mn}} - \frac{\sqrt{1+A^2}}{q^{(2)}_{mj}\, q^{(2)}_{mn}} + \frac{e^{-i\beta_m a}\sqrt{1+B^2}}{q^{(2)}_{mj}\, P^{(2)}_{mn}} - \frac{e^{-i\beta_m a}\sqrt{1+B^2}}{P^{(2)}_{mj}\, P^{(2)}_{mn}} \right\}$$

$$+ e^{+i\beta_m a} \left\{ \frac{-\sqrt{1+A^2}}{P^{(2)}_{mj}\left(q^{(2)}_{mn} - \frac{A}{B} P^{(2)}_{mj}\right)} - \frac{\sqrt{1+A^2}}{P^{(1)}_{mj}\, q^{(1)}_{mn}} + \frac{\sqrt{1+A^2}}{P^{(1)}_{mj}\left(q^{(1)}_{mn} - \frac{A}{B} P^{(1)}_{mj}\right)} \right\}$$

$$+ e^{-i\beta_m a} \left\{ \frac{-\sqrt{1+B^2}}{q^{(1)}_{mj}\left(\frac{B}{A} q^{(1)}_{mj} - P^{(1)}_{mn}\right)} - \frac{\sqrt{1+B^2}}{q^{(1)}_{mj}\, P^{(1)}_{mn}} - \frac{\sqrt{1+B^2}}{q^{(2)}_{mj}\left(P^{(2)}_{mj} - \frac{B}{A} q^{(2)}_{mj}\right)} \right\}$$

$$+ \sqrt{1+A^2} \left\{ \frac{1}{q^{(1)}_{mj}\, q^{(1)}_{mn}} + \left(\frac{1}{2\pi(n-j)} \right) \left(\frac{1}{q^{(1)}_{mj}} - \frac{1}{q^{(2)}_{mj}} \right) \right\} + \sqrt{1+B^2} \left\{ \frac{1}{P^{(1)}_{mj}\, P^{(1)}_{mn}} + \left(\frac{1}{2\pi(n-j)} \right) \left(\frac{1}{P^{(1)}_{mj}} - \frac{1}{P^{(2)}_{mj}} \right) \right\} \Bigg] \qquad (11)$$

Despite the length of the expression for $K_{j,n}$ (Eq. 11) and the realization that the calculation must be performed many times for each value of j and n, we have found the program to be very efficient. For example, the program for the E-parallel polarization requires less than 3 sec execution time for 10 diffraction orders in most cases. The execution times required to analyze coarse echelle gratings will, of course, be considerably longer. However, because the program is efficient, the required execution times will be reduced considerably.

Currently we are in the final stages of debugging the computer program for the E-parallel polarization. The complexity of the program has hampered this effort to some extent, but we have demonstrated that our method is indeed workable and that the program is much more efficient, simpler to run, and capable of analyzing four times as many diffraction orders as any known existing programs.

Outlook

The program for the H-parallel state of polarization has not been written even though the theory has been derived. We are awaiting the opportunity to completely test the E-parallel polarization before proceeding to the H-parallel case. The final combination of the two programs will allow complete efficiency evaluations as well as polarization studies to be continued.

The special profile shown below in Fig. 2 has unique properties when used in autocollimation.

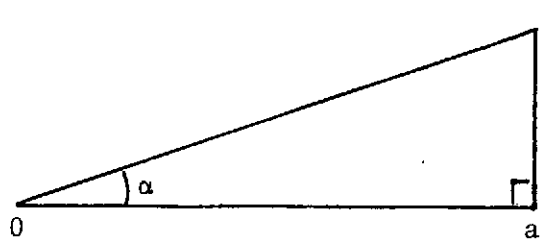

Fig. 2. Special grating profile.

This profile should be evaluated to verify our previous findings, which were based on an approximate theory. We were not able to verify these findings by using the Berkeley programs. The following results should be established: (a) whether the amplitude coefficients vary as a function of groove depth, (b) whether all the energy is found in one order and zero or negligible energy is present in all the other orders, and (c) the wavelength interval for which the grating displays a high blaze.

References

1. Zaki, K. A. E. H., "Numerical methods for the analysis of scattering from nonplanar periodic structures," Dissertation, University of California at Berkeley, 1969.

2. Kalhor, H. A., "Numerical integral-equation analysis at scattering from diffraction gratings," Dissertation, University of California at Berkeley, 1970.

3. Marathay, A. S., and T. E. Shrode, "Electromagnetic Diffraction Efficiencies for Plane Reflection Diffraction Gratings," Final Report for NASA Contract NAS5-11456, July 1973.