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ANALYSIS OF SAW DIFFRACTION BY SURFACE-RELIEF GRATINGS WITH MULTI-WAVE COUPLED-WAVE THEORY

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Abstract: - In this paper, SAW propagation in surface-relief (corrugated) gratings is rigorously analyzed using multi-wave coupled-wave theory. Using this method of solution, it is possible to calculate the diffraction efficiencies of surface-relief gratings to an arbitrary level of accuracy. The analysis contains no restrictions with respect to grating profile, groove depth, angle of incidence, or wavelength.

Key-words: - surface-relief gratings, diffraction efficiencies, multi-wave coupled-wave theory

1 Introduction

Surface-relief (corrugated) gratings are of great technological importance. These surface-relief structures, like planar gratings, are also capable of very high diffraction efficiencies. Corrugated gratings can be rigorously analyzed using coupled-wave analysis [6]. This is done by dividing the surface-relief grating into a large number of thin (planar) layers. Each thin layer is then analyzed using the state variables method of solution of the rigorous coupled-wave equations for that grating.

By formulation the problem in a particular manner, it is shown that the grating layers may be treated one-at-a-time in sequence thus reducing the numerical calculations to an easily manageable size. There are no approximations in the analysis and results are obtainable to any arbitrary level of accuracy. The diffraction efficiencies of all orders of both the transmitted and reflected waves are determined in the process.

2 Problem formulation

Surface-relief (corrugated) grating with an arbitrary grating profile (dashed lines) is presented in Fig.1. Region 1 (the input region) is a homogeneous region with mass density ρ_I, and region 3 is homogeneous with density ρ_{III}.

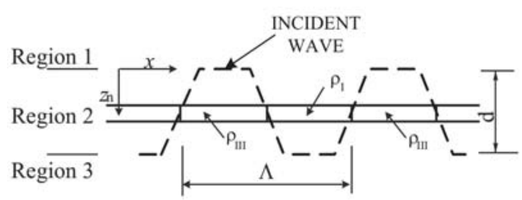

Fig.1. The *n*th planar grating resulting from the decomposition of a surface-relief grating into *N* thin planar gratings.

Region 2 (the grating region) consists of a periodic distribution of both types of materials. The boundary between the region ρ_I and the ρ_{III} in region 2 is given by

$$z = F(x)F(x+\Lambda) \tag{1}$$

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where Λ is the grating period. The function $F(x)$ thus represents the grating surface profile. Unlike most methods for analyzing surface-relief gratings, there are no restrictions on the form of $F(x)$ in this analysis. Curved lines, straight lines, shadow regions, hidden regions, etc., are all allowed. The total field in region 1 is the sum of the incident and backward-traveling waves in exactly the same manner as for planar grating [6]. The normalized total field in region 1 may thus be represented by

$$p_1 = e^{-jk_1 r} + \sum_{i=-\infty}^{+\infty} R_i e^{-jk_{1i} r} \tag{2}$$

where R_i is the normalized amplitude of the ith reflected wave in region 1 with wave vector k_{1i}. Likewise, the normalized total field in region 3 is

$$p_3 = \sum_{i=-\infty}^{+\infty} T_i e^{-jk_{3i}(r-dz)} \tag{3}$$

where T_i is the normalized amplitude of the ith transmitted wave in region 3 with wave vector k_{3i}, and d is the groove depth. Each ith field in region 1 and 3 must be phase matched to the ith space harmonic field (inhomogeneous plane wave) inside the grating.

In the present analysis, the grating region (region 2) is divided into N thin planar gratings slab perpendicular to the z axis as shown in Fig. 1. Then the rigorous coupled-wave analysis that has been developed for planar grating [4], is applied to each slab grating. If the individual planar gratings are sufficiently thin, any grating profile can be analyzed to an arbitrary level of accuracy. The nth slab within region 2 as shown in Fig. 1 will consist of a periodic distribution if ρ_{I} and ρ_{III} materials. The mass density for nth slab grating is periodic expressed as

$$\rho_n(x, z_n) = \rho_n(z + \Lambda, z_n) \tag{4}$$

and may be expanded in a Fourier series as

$$\rho_n(x, z_n) = \rho_{\mathrm{I}} + (\rho_{\mathrm{III}} - \rho_{\mathrm{I}}) \sum_{h=-\infty}^{\infty} \tilde{\rho}_{h,n} e^{jhKx} \tag{5}$$

where z_n is the z coordinate of the nth slab, h is the harmonic index, K is the magnitude of the grating vector ($K = 2\pi / \Lambda$), and $\tilde{\rho}_{h,n}$ are the normalized complex harmonic amplitude coefficients given by

$$\tilde{\rho}_{h,n} = \frac{1}{\Lambda} \int_0^{\Lambda} dx\, f(x, z_n) e^{-jhKx} \tag{6}$$

The function $f(x, z_n)$ is equal to either zero or unity depending whether, for a particular value of x, the grating density is ρ_{I} or ρ_{III}, respectively.

The total field in the slab may be expressed as

$$p_{2,n}(x, z) = \sum_{i=-\infty}^{\infty} S_{i,n}(z)\, e^{(k_{2,n} - iK) r} \tag{7}$$

Where $k_{2,n}$ is the wave vector of the zero-order (i=0) refracted wave having a magnitude of $k_{2,n}=2\pi(\rho_{0,n})^{1/2}/\lambda$, $\rho_{0,n}$ is the average density for the nth slab grating, and $S_i(z) \hat{=} \hat{S}_i(z) e^{-j(k_{2z} - iK\cos\phi) z}$.

Substituting $p_{2,n}(x,z)$ and $\varepsilon_n(x, z_n)$ into the wave equation

$$\nabla^2 p(x', z') + k^2 \rho(x') p(x', z') = 0 \tag{8}$$

and performing the indicated differentiations, and setting coefficient of each exponential term equal to zero for nontrivial solutions yields the rigorous coupled-wave equations for nth slab grating

$$\frac{d^2 S_{i,n}(z)}{dz^2} - jz\left(k_{2,n}^2 - k_1^2 \sin^2\theta'\right)^{1/2} \frac{d\,S_{i,n}(z)}{dz} + K^2 i(m-i) S_{i,n}(z) + k^2(\rho_{III} - \rho_I) \cdot \sum_{h=1}^{\infty} \left[\tilde{\rho}_{h,n} S_{i-h,n}(z) + \rho_{h,n}^{*} S_{i+h,n}(z)\right] = 0 \tag{9}$$

where θ' is the first Bragg angle. These coupled-wave equations can be solved for nth slab grating using state-variables method.

3 Problem Solution

The surface-relief grating diffraction problem as formulated in the previous section will be solved in a sequence steps. First, the rigorous coupled-wave equations will be solved for the *n*th slab grating using a state-variables method of solution. Second, boundary conditions (continuity of *p* and perpendicular velocity of particles *v*) will be applied between region 1 and the first slab grating, then between the first and second slab gratings, and so forth and finally between the *N*th slab grating and region 3. Third, the resulting arrays of boundary condition equations are solved for the reflected and transmitted diffracted amplitudes, T_i and R_i. From these amplitudes, the diffracted efficiencies are determined directly.

3.1 Calculational Procedure

Defining state variables as

$$S_{1,i}(z) = S_i(z)$$
$$S_{2,i}(z) = \frac{dS_i(z)}{dz} \qquad (10)$$

for *n*th slab grating, transforms the infinite set of second-order differential equations (5) into two infinite sets of first-order state equations

$$\frac{dS_{1,i,n}(z)}{dz} = S_{2,i,n}(z) \qquad (11)$$

$$\frac{dS_{2,i,n}(z)}{dz} = -k^2(\rho_{III}-\rho_I)\sum_{h=1}^{\infty}\tilde{\rho}_{h,n}S_{1,i-h,n}(z)$$
$$-K^2 i(m-i)S_{1,i,n}(z)$$
$$-k^2(\rho_{III}-\rho_I)\sum_{h=1}^{\infty}\tilde{\rho}^*_{h,n}S_{1,i+h,n}(z)$$
$$+2j\left(k_{2,n}^2-k_1^2\sin^2\theta'\right)S_{2,i,n}(z) \qquad (12)$$

In matrix form, the state equation for the *n*th slab grating may be written as

$$\begin{bmatrix} \vdots \\ \dot{\tilde{S}}_{1,p,n} \\ \vdots \\ \dot{\tilde{S}}_{2,p,n} \\ \vdots \end{bmatrix} = \left[\begin{array}{c|c} a_{p,q,n} & b_{p,q,n} \\ \hline c_{p,q,n} & d_{p,q,n} \end{array}\right] \begin{bmatrix} \vdots \\ \tilde{S}_{1,q,n} \\ \vdots \\ \tilde{S}_{2,q,n} \\ \vdots \end{bmatrix} \qquad (13)$$

where $\tilde{S}_{l,p,n} \equiv S_{l,i,n}$ (for l=1,2), $\dot{S} = \frac{dS}{dz}$, and the elements of the four submatrices (p=1 to s and q=1 to s) are specified by (11) and (12) for the *n*th slab grating. The integers p and q are the row and column indices of the four submatrices. The maximum value of these indices, s, is equal to the number of diffracted orders retained in the analysis. The value $p=1$ corresponds to most negative order (value of i) retained in the analysis and $p=s$ corresponds to the most positive order retained. For example, if an odd number of waves are retained symmetrically about $i=0$ (the undiffracted wave) in the analysis, then $p=i+(s+1)/2$. Equation (13) corresponds to an unforced state equation $\dot{\mathbf{S}} = \mathbf{AS}$. The solutions of (13) are

$$\tilde{S}_{p',n}(z) = \sum_{q'=1}^{2s} C_{q',n} w_{p',q',n} e^{\lambda_{q',n} z} \qquad (14)$$

where $\tilde{S}_{l,p,n}$ (for l=1,2) has been rewritten as $\tilde{S}_{p',n}$ with $p'=p+(l-1)s$. The quantities $\lambda_{q',n}$ and $w_{p',q',n}$ are the eigenvalues and eigenvectors of the matrix **A**. The integers p' and q' are the row and column indices of the eigenvector matrix [w] and p'=1 to 2s and q'=1 to 2s. The quantities $C_{q',n}$ are unknown constants to be determined by the boundary conditions. The desired diffracted wave amplitudes for the *n*th gratin layer are given by $S_{i,n}(z) = \tilde{S}_{p',n}(z)$ where p' is chosen to correspond to the *i*th diffracted wave.

Boundary conditions require that the pressure *p* and perpendicular component of velocity be continuous across the boundaries between the slabs. Velocity *v* of particles, however, must be obtained through equation $\nabla p = -\rho \frac{\partial v}{\partial t}$. The perpendicular component of v is in z direction and is given by $v = j \frac{1}{\rho\omega} \frac{\partial p}{\partial z}$. Therefore, for the boundary ($z = 0$) between region 1 (the input region) and the first slab grating, boundary conditions are

$$\delta_{i0} + R_i = \sum_{q'=1}^{2s} C_{q',1} w_{p',q',1} \qquad (15)$$

and

$$j(\bar{k}_{1,i} \cdot \hat{z})(R_i - \delta_{i0}) = \sum_{q'=1}^{2s} C_{q',1} w_{p',q',1} [\lambda_{q',1} - j(\bar{\sigma}_{i,1} \cdot \hat{z})] \qquad (16)$$

where the value of p' is chosen to correspond to the ith wave. For the boundary between nth and $n+1$th slab gratings ($z = nd/N$), the boundary conditions are

$$\sum_{q'=1}^{2s} C_{q',n} w_{p',q',n} e^{\left[\lambda_{q',n} - j\left(\bar{\sigma}_{i,n}\hat{z}\right)\right] nd/N} = \sum_{q'=1}^{2s} C_{q',n+1} w_{p',q',n+1} \cdot e^{\left[\lambda_{q',n+1} - j\left(\bar{\sigma}_{i,n+1}\hat{z}\right)\right] nd/N} \qquad (17)$$

and

$$\sum_{q'=1}^{2s} C_{q',n} w_{p',q',n} \left[\lambda_{q',n} - j\left(\bar{\sigma}_{i,n}\hat{z}\right)\right] \cdot e^{\left[\lambda_{q',n} - j\left(\bar{\sigma}_{i,n}\hat{z}\right)\right] nd/N} = \sum_{q'=1}^{2s} C_{q',n+1} w_{p',q',n+1} \left[\lambda_{q',n+1} - j\left(\bar{\sigma}_{i,n+1}\hat{z}\right)\right] \cdot e^{\left[\lambda_{q',n+1} - j\left(\bar{\sigma}_{i,n+1}\hat{z}\right)\right] nd/N} \qquad (18)$$

For the boundary between the Ntn slab grating and region 3 ($z = d$), the boundary conditions are

$$\sum_{q'=1}^{2s} C_{q',N} w_{p',q',N} e^{\left[\lambda_{q',N} - j\left(\bar{\sigma}_{i,N}.\hat{z}\right)\right] d} = T_i \qquad (19)$$

and

$$\sum_{q'=1}^{2s} C_{q',N} w_{p',q',N} \left[\lambda_{q',N} - j\left(\bar{\sigma}_{i,N}.\hat{z}\right)\right] \cdot e^{\left[\lambda_{q',N} - j\left(\bar{\sigma}_{i,N}.\hat{z}\right)\right] d} = -j(\bar{k}_{3i} \cdot \hat{z}) T_i \qquad (20)$$

Equations (15)-(20) represent a total of $2(N+1)s$ equations. There are s unknown values each of R_i and T_i and $2s$ unknown values of $C_{q',n}$ for each slab grating. Thus the total number of unknowns is $2(N+1)s$, the same as the number of boundary condition equations. If s values of i are retained in the analysis, then the calculations will yield s transmitted wave amplitudes (T_i) and s reflected wave amplitudes (R_i).

An efficient procedure to solve this large system of equations is to use a technique like Gauss elimination [7] applied successively to each boundary starting at the $z = 0$ input surface. By using this technique $N+1$ times in sequence, the s values of R_i and s values of T_i may be obtained in a single pass on the last step. As depicted in Fig.2, the boundary condition equations are written as a matrix equation. The matrix is $2(n+1)s$ by $2(n+1)s$ and consists of the coefficients $C_{q',n}$ (for $q' = 1$ to $2s$ and $n = 1$ to N), R_i, T_i (s values for both.)

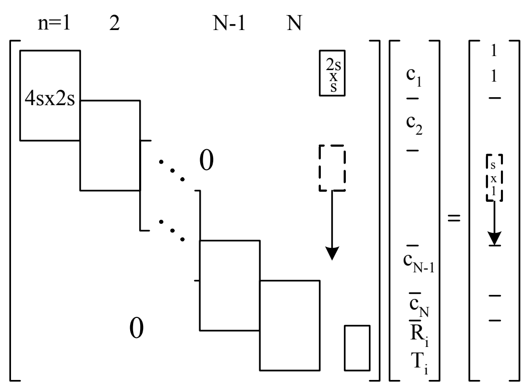

Fig.2 Matrix-equation representation of $2(N+1)s$ boundary-condition equations, where s is the total number of diffracted waves retained in the analysis.

For each slab grating, the boundary condition equation for its two boundaries produces $4s$x$4s$. Starting with the first ($n=1$) slab grating (represented by upper left submatrix), a technique like Gauss elimination is applied to make all of the elements of the lover half of the submatrix equal to zero. This reduces the system to $2Ns$ equations. Repeating this procedure on the next ($n=2$) $4s$ by $2s$ submatrix reduces the system to $2(N-1)s$ equations.

This process is continued until after N steps, only $2s$ equations in the diffracted amplitudes R_i and T_i remain. These are then solved for R_i and T_i. at each step in this sequential process, a new set of coefficients of R_i are produced as shown by the dashed box in Fig.2. After N steps, these coefficients have moved to the bottom of the matrix and the final set of $2s$ equations in R_i and T_i are formed. This sequential procedure enormously reduces the storage and computational requirements for this type of problem. At each step, only a small $4s$ by $2s$ matrix is being treated as opposed to the entire $2(N+1)s$ by $2(N+1)s$ matrix where N might typically be 50.

When amplitude R_i and T_i are known, then the diffraction efficiencies (ratio of diffracted intensity to output intensity) for the region 1 and region 3 may be determined respectively as

$$DE_{1i} = \mathrm{Re}\left[\frac{k_{1i}z}{k_{10}z}\right]R_iR_i^* = \mathrm{Re}\left\{\left\{\left[\sin\theta' - i\lambda\sin\phi/\left(\rho_1\right)^{1/2}\Lambda\right]^2\right\}^{1/2} / \cos\theta'\right\} R_iR_i^* \quad (21)$$

$$DE_{3i} = \mathrm{Re}\left[\frac{k_{3i}z}{k_{10}z}\right]T_iT_i^* = \mathrm{Re}\left\{\left\{\left(\rho_{III}/\rho_I\right) - \left[\sin\theta' - i\lambda\sin\phi/\left(\rho_1\right)^{1/2}\Lambda\right]^2\right\}^{1/2} / \cos\theta'\right\} T_iT_i^* \quad (22)$$

4 Conclusion

Using the method of solution described in the previous section, it is possible to calculate the diffraction efficiencies of surface-relief gratings to an arbitrary level of accuracy. The analysis contains no restrictions with respect to grating profile, groove depth, angle of incidence, or wavelength. The use of grating structure as the most fundamental element of SAW devices is very widespread in modern technology and directly affects many areas of digital communications.

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