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CONICAL DIFFRACTION MOUNTING GENERALIZATION OF A RIGOROUS DIFFERENTIAL METHOD

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MOTS CLÉS :
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Réseaux

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SUMMARY : A generalization of the method of Chandezon *et al.* is presented for conical diffraction mounting. The applicability of the invariance theorem for real metal and dielectric gratings is discussed and the existence of some polarization effects is demonstrated. A formulation of the reciprocity theorem in conical diffraction mounting is proposed, valid not only for the diffracted orders efficiencies but for the amplitudes, too.

Montage de diffraction conique. Généralisation d'une méthode différentielle rigoureuse

RÉSUMÉ : Nous présentons une généralisation de la méthode de Chandezon *et al.* pour le montage de diffraction conique. La validité du théorème de l'invariance pour un métal réel et un réseau diélectrique est discutée et l'existence des effets de polarisation est démontrée. Une formulation du théorème de réciprocité dans un montage de diffraction conique valable non seulement pour l'efficacité des ordres de diffraction, mais aussi pour les amplitudes est présentée.

I. — *INTRODUCTION*

In the *x*-ray and *xuv* region the efficiency of the diffraction gratings is very small due to the low reflectivity of metals [1]. Both experimental measurements [2, 3] and theoretical calculations [4-6] show that the efficiency can be improved if the grating is used in the so-called conical diffraction mounting when the incident wave vector lies out of the plane normal to the grooves. As it has been pointed out by Spencer and Murty [7] in this case the diffracted orders directions lie on a cone with axis parallel to the grooves and whose half-angle is closed between the zeroth order and the ruling direction.

One of the strongest tools to treat the conical diffraction mount is the invariance theorem established by Maystre and Petit [8, 9]. It allows to predict the efficiency of perfectly conducting gratings from the grating efficiencies of in-plane *TE* and *TM* polarizations. However, the invariance theorem is not valid for real metal and dielectric gratings.

On the other hand during the last decade a great interest has been shown to the different coupling phenomena in corrugated waveguides in normal and oblique with respect to the grooves incidence.

The difficulties follow from the fact that in the conical case neither the Maxwell equations nor the boundary conditions can be devided into two independent fundamental cases of polarization. Furthermore, a linearly polarized incident wave generates, in general, elliptically polarized diffracted waves. For the treatment of all these problems rigorous electromagnetic theories have to be used. Generalization of different rigorous electromagnetic methods based on the integral [10] and differential [5] formalisms have been reported. In particular it has been shown numerically that the diffraction efficiency larger than 40 % for wavelengths less than 500 Å can be achieved for holographic gratings [10].

In this paper we present a generalization of the rigorous differential formalism of Chandezon *et al.* [11] for the case of conical diffraction mounting. We have chosen this method because it is applicable for a large spectral region and for many types of gratings — perfectly conducting, real metal, dielectric and (multi) coated gratings [11, 12]. The domain of application and the advantages of the method in comparison with the Rayleigh-Fourier formalism for the in-plane case have been discussed in [12].

2. — MATHEMATICAL PRESENTATION OF THE CONICAL DIFFRACTION PROBLEM

Since our study deals with a generalization of the differential formalism of Chandezon *et al.* it seems natural to follow the presentation of the problem in [11].

A cylindrically corrugated medium with a complex refractive index n_1 and a corrugation period d is coated with a system of M layers with complex refractive indices n_j and thicknesses t_j, $j = 2, ..., M$ (*fig. 1*). The interfaces between the layers are defined by equations

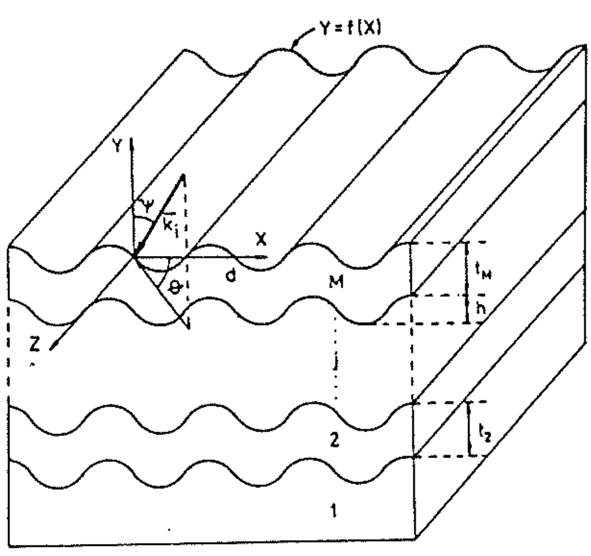

FIG. 1. — *Geometry of the grating structure and the incident wave vector* $\mathbf{k}^i$.

$y = f(x) + l_j$ and the origin of the coordinate system is chosen so that $l_M = 0$. From air ($n_{M+1} = 1$) a linearly polarized vector wave with a wavevector $\mathbf{k}^i = (\alpha_0, h_0, \beta_0)$, $\alpha_0^2 + h_0^2 + \beta_0^2 = k^2 n_{M+1}^2$, illuminates the structure, where $k = 2\pi/\lambda$ and λ is the wavelength of the incident wave. A time dependent factor $\exp(i\omega t)$ is omitted throughout the paper. The polarization direction and the wave amplitudes are given through the z-components of the electric $\mathbf{E}^i$ and magnetic $\mathbf{H}^i$ vectors :

$$E_z^i = \mathcal{E}^i \exp(i\mathbf{k}^i \cdot \mathbf{r})$$
$$-\omega\mu_0 H_z^i = k n_{M+1} \mathcal{H}^i \exp(i\mathbf{k}^i \cdot \mathbf{r}) \, . \quad (1)$$

where $\mathbf{r} = (x, y, z)$ and μ_0 is a vacuum permittivity.

The propagating diffraction orders are, in general, elliptically polarized vector waves with wavevectors $\mathbf{k}_m^d = (\alpha_m, h_m, \beta_0)$, where

$$\alpha_m = \alpha_0 + mK$$
$$K = 2\pi/d \quad (2)$$
$$h_m = (k^2 n_{M+1}^2 - \alpha_m^2 - \beta_0^2)^{1/2}$$

and $m = 0, \pm 1, \pm 2, ...$, so that h_m is real.

Above the grating surface ($y > f(x)$) the propagating diffraction orders can be represented in the form of Rayleigh expansion :

$$E_{z,m}^d = \mathcal{E}_m \exp(i\mathbf{k}_m^d \cdot \mathbf{r}) \quad (3)$$
$$-\omega\mu_0 H_{z,m}^d = k n_{M+1} \mathcal{H}_m \exp(i\mathbf{k}_m^d \cdot \mathbf{r}) \, .$$

We have to emphasize on the statement in [11] that this formalism should not be confused with the Rayleigh hypothesis because the expansion (3) is taken only for the propagating orders and not for the whole diffracted field.

Similar to Eqs. (2) and (3) expressions can be written for the propagating orders in the lower medium. However, for the sake of clearness further on we shall deal only with the propagating orders in air.

From (1) and (3) the diffraction efficiency of the m-th order can be expressed in a simple and convenient form :

$$\eta_m = \frac{|\mathcal{E}_m|^2 + |\mathcal{H}_m|^2}{|\mathcal{E}^i|^2 + |\mathcal{H}^i|^2} \frac{h_m}{h_0} \, . \quad (4)$$

To be able to obtain the unknown coefficients $\mathcal{E}_m$ and $\mathcal{H}_m$ we need an electromagnetic field representation, satisfying the Maxwell equations, the boundary conditioned at the corrugated interfaces and the outgoing wave conditions. Following [11] a transformation of the coordinate system is introduced, defined by :

$$u = x$$
$$v = y - f(x) \quad (5)$$
$$w = z \, .$$

The boundary conditions in the new Ouvw coordinate system are applied on plane interfaces $v = l_j$, but the Maxwell equations become much more complicated. After tedious routine calculations the Maxwell equations in each medium j can be written in the following form :

$$
\begin{aligned}
\frac{\partial E_w}{\partial v} &= \mathcal{D}(u)\frac{\partial E_w}{\partial u} + \mathrm{i}\omega\mu_0\, \mathcal{C}(u)\left[H_u + \frac{1}{k^2 n_j^2}\frac{\partial}{\partial w}\left(\frac{\partial H_u}{\partial w} - \frac{\partial H_w}{\partial u}\right)\right],\\
\omega\mu_0\frac{\partial H_u}{\partial v} &= \omega\mu_0\frac{\partial}{\partial u}\left[\mathcal{D}(u)\, H_u\right] + \mathrm{i}k^2 n_j^2\left\{E_w - \frac{1}{k^2 n_j^2}\frac{\partial}{\partial u}\left[\mathcal{C}(u)\left(\frac{\partial E_u}{\partial w} - \frac{\partial E_w}{\partial u}\right)\right]\right\},\\
\omega\mu_0\frac{\partial H_w}{\partial v} &= \omega\mu_0\, \mathcal{D}(u)\frac{\partial H_w}{\partial u} - \mathrm{i}k^2 n_j^2\, \mathcal{C}(u)\left[E_u + \frac{1}{k^2 n_j^2}\frac{\partial}{\partial w}\left(\frac{\partial E_u}{\partial w} - \frac{\partial E_w}{\partial u}\right)\right],\\
\frac{\partial E_u}{\partial v} &= \frac{\partial}{\partial u}\left[\mathcal{D}(u)\, E_u\right] - \mathrm{i}\omega\mu_0\left\{H_w - \frac{1}{k^2 n_j^2}\frac{\partial}{\partial u}\left[\mathcal{C}(u)\left(\frac{\partial H_u}{\partial w} - \frac{\partial H_w}{\partial u}\right)\right]\right\},
\end{aligned}
\tag{6}
$$

where

$$\mathcal{C}(u) = \frac{1}{1 + [f'(u)]^2}, \qquad \mathcal{D}(u) = f'(u)\, \mathcal{C}(u).$$

Introducing the column vector

$$F = \begin{bmatrix} F^1 \\ F^2 \\ F^3 \\ F^4 \end{bmatrix} = \begin{bmatrix} E_w \\ \omega\mu_0\, H_u \\ -\omega\mu_0\, H_w \\ E_u \end{bmatrix} \tag{7}$$

and taking into account the periodicity in u, the solution of (6) can be expressed in the form :

$$F^k(u, v, w) = \sum_m F_m^k(v) \exp[\mathrm{i}(\alpha_m u + \beta_0 w)], \qquad k = 1, \dots, 4. \tag{8}$$

In this equation $m \in (-\infty, \infty)$. However, for numerical treatment a truncation of m is necessary : $m \in [-N, N]$. Denoting by G_j a column vector

$$G_j^k = \begin{bmatrix} G_j^1 \\ G_j^2 \\ G_j^3 \\ G_j^4 \end{bmatrix},$$

where

$$G_j^k = \begin{bmatrix} F_{-N}^k \\ \vdots \\ F_N^k \end{bmatrix},$$

we derive the Maxwell equations in a matrix form :

$$-\mathrm{i}\frac{\mathrm{d}G_j}{\mathrm{d}v} = R^j G_j, \tag{9}$$

where

$$R^j = \begin{bmatrix} A^j & B^j & -\frac{P^j}{kn_j} & 0 \\ C^j & D^j & 0 & kn_j\, Q^j \\ kn_j\, P^j & 0 & A^j & k^2 n_j^2\, B^j \\ 0 & -\frac{Q^j}{kn_j} & \frac{C^j}{k^2 n_j^2} & D^j \end{bmatrix} \tag{10}$$

The elements of the submatrices of R^j are :

$$
\begin{aligned}
A_{m,p}^j &= \alpha_p\, \mathcal{D}_{m-p},\\
B_{m,p}^j &= (k^2 n_j^2 - \beta_0^2)\, \mathcal{C}_{m-p}/k^2 n_j^2,\\
C_{m,p}^j &= \delta_{mp}\, k^2 n_j^2 - \alpha_m \alpha_p\, \mathcal{C}_{m-p},\\
D_{m,p}^j &= \alpha_m\, \mathcal{D}_{m-p},\\
P_{m,p}^j &= \beta_0\, \alpha_p\, \mathcal{C}_{m-p}/kn_j,\\
Q_{m,p}^j &= \beta_0\, \alpha_m\, \mathcal{C}_{m-p}/kn_j,
\end{aligned}
\tag{11}
$$

where

$$
\begin{aligned}
\mathcal{C}_m &= 1/d \int_0^d \mathcal{C}(x) \exp(\mathrm{i}mKx)\, \mathrm{d}x,\\
\mathcal{D}_m &= 1/d \int_0^d \mathcal{D}(x) \exp(\mathrm{i}mKx)\, \mathrm{d}x,
\end{aligned}
\tag{12}
$$

δ_{mp} is a Kronecker symbol and $j = 1, \dots, M + 1$.

The solution of (9) is searched for in the form :

$$G_j = T^j\, \phi^j(v)\, a^j,$$

where

$$\phi_{mp}^j(v) = \exp(\mathrm{i}r_m^j v)\, \delta_{mp}.$$

Here T^j is a square matrix of size $(8N + 4) \times (8N + 4)$ whose columns are the eigenvectors of R^j, r_m^j are the corresponding eigenvalues of R^j and a^j is a column vector of unknown amplitudes a_m^j.

The components of G_j represent the tangential components of electric and magnetic field. The boundary conditions applied to the each of the interfaces (which are flat surfaces in Ouvw coordinate system) yield

$$T^j\, \phi^j(l_j)\, a^j = T^{j+1}\, \phi^{j+1}(l_j)\, a^{j+1}. \tag{13}$$

From (13) we derive a connection between the field amplitudes in the upper and the lower media :

$$T^{M+1}\, a^{M+1} = T T^1\, \phi^1(l_1)\, a^1, \tag{14}$$

where

$$T = T^M\, \phi^M(l_M)\, (T^M)^{-1} \dots T^2\, \phi^2(l_2)\, (T^2)^{-1}.$$

In the lower medium only the orders whose amplitudes vanish in infinity or are propagating downwards must be taken into consideration, i.e. in the right hand side of (14) the terms with $\mathrm{Im}\,(r_m^1) < 0$ or $\mathrm{Im}\,(r_m^1) = 0$

and $\mathrm{Re}(r_m^1) < 0$ must be kept. Since the propagating orders in air are given by expansion (3) in the left hand side of (14) only the terms with $\mathrm{Im}(r_m^{M+1}) > 0$ should remain. The incident and the propagating orders terms $\tilde{G}_{M+1}$ given by (1) and (3) must be added in (14) expressed in the Ouvw coordinate system : $\tilde{G}_{M+1} = \tilde{T}^{M+1}\tilde{F}$, where :

$$\tilde{F} = \begin{bmatrix} \mathcal{E}_{-N} \\ \vdots \\ \mathcal{E}_N \\ \mathcal{K}_{-N} \\ \vdots \\ \mathcal{K}_N \end{bmatrix}, \quad \tilde{T}^{M+1} = \begin{bmatrix} R^{\mathrm{I}} & 0 \\ kn_{M+1}\, R^{\mathrm{II}} & kn_{M+1}\, R^{\mathrm{III}} \\ 0 & kn_{M+1}\, R^{\mathrm{I}} \\ -R^{\mathrm{III}} & R^{\mathrm{II}} \end{bmatrix}, \tag{15}$$

with

$$R^{\mathrm{I}}_{m,p} = \mathcal{L}_{m-p}(h_p)$$
$$R^{\mathrm{II}}_{m,p} = \frac{kn_{M+1}}{k^2 n^2_{M+1} - \beta_0^2}\left[h_p\, \mathcal{L}_{m-p}(h_p) - \alpha_p\, \mathcal{K}_{m-p}(h_p)\right],$$
$$R^{\mathrm{III}}_{m,p} = \frac{\beta_0}{k^2 n^2_{M+1} - \beta_0^2}\left[\alpha_p\, \mathcal{L}_{m-p}(h_p) + h_p\, \mathcal{K}_{m-p}(h_p)\right], \tag{16}$$

and

$$\mathcal{L}_m(y) = 1/d \int_0^d \exp\{\,\mathrm{i}[f(x)\, y + mKx]\,\}\, \mathrm{d}x\,,$$

$$\mathcal{K}_m(y) = 1/d \int_0^d f'(x) \exp\{\,\mathrm{i}[f(x)\, y + mKx]\,\}\, \mathrm{d}x\,.$$

The inhomogeneous part of the linear algebraic system of Eqs. (14)-(16) represents the incident wave field whose amplitudes can be obtained from (15) replacing all of the elements of $\tilde{F}$ with zero except for $\mathcal{E}_0 = \mathcal{E}^i$ and $\mathcal{K}_0 = \mathcal{K}^i$. As can be expected this formalism coincides with the method of Chandezon *et al.* [11] if $\beta_0 = 0$.

In order to obtain the unknown amplitudes $\mathcal{E}_m$, $\mathcal{K}_m$, a_m^{M+1} and a_m^1, a computer code was performed to solve the system of Eqs. (14)-(16). The eigenvalue and the eigenvector problems were treated by a standard *QR* method for complex non-symmetrical matrices, using EISPACK. The matrix inversion was performed by Gauss-Jordan scheme. Numerical tests, such as energy preservation law (in lossless media), reciprocity theorem and invariance theorem (for perfectly conducting gratings), as well as a comparison with the results obtained by other numerical codes [12] for in-plane diffraction were carried out. The main difference between the presented here formalism and that of Chandezon *et al.* [11] for in-plane case is that the solution of conical diffraction problem needs four times greater memory requirements, but on the other hand, applied to the in-plane case the generalized code gives the diffraction orders efficiencies for *TE* and *TM* polarization simultaneously. One of the greatest advantages for both in-plane and conical methods is that the computer codes work fairly well for both lossless and lossy dielectric, perfectly conducting and real metallic gratings and coated gratings with very large ratio $h/d > 1$. Moreover they are not so sophisticated from a mathematical point of view. Another merit is that the convergence rate with respect to truncation parameter *N* in the case of conical diffraction mounting remains the same as in the in-plane diffraction.

As an example, in *figure 2* the dependence of the convergence rate on the angle between the incident beam and the plane perpendicular to the grooves is given. For different values of the angle the convergence is achieved for practically one and the same truncation parameter *N*. In the calculation the projection of the incident wave vector on the plane perpendicular to the grooves is kept constant, thus λ is varied, and in addition the incident electric field vector remains perpendicular to the grooves.

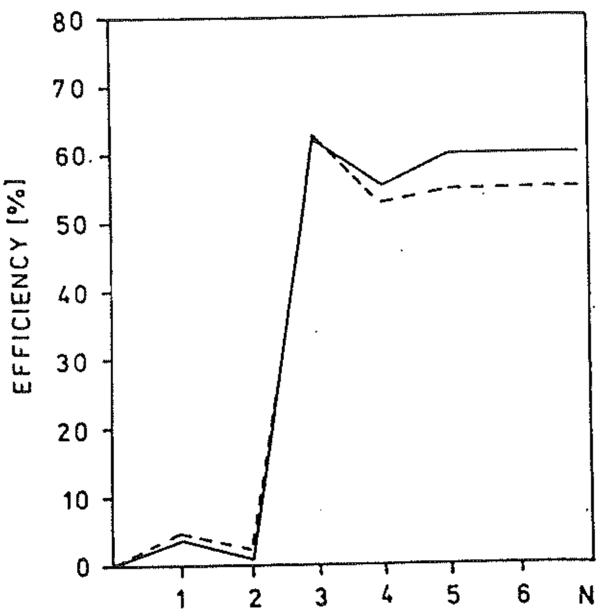

FIG. 2. — *Convergence rate for $\theta = 0°$ (solid curve) and $\theta = 60°$ (dashed curve). The grating parameters are $d = 0.6$ µm, $h = 0.6$ µm. For $\theta = 30°$ the results coincide with the curve for $\theta = 0°$. For the in-plane case $\lambda = 0.6$ µm.*

3. — RECIPROCITY THEOREM

Let us consider an incident wave with a wavevector $\mathbf{k}_1^i$ and an electric field vector $\mathbf{E}_1^i$ which illuminates a grating and generates a diffracted wave with a wavevector $\mathbf{k}_1^d$ and an electric field vector $\mathbf{E}_1^d$. The reciprocical case is when an incident wave has a wavevector $\mathbf{k}_2^i = -\mathbf{k}_2^d$ and $\mathbf{k}_2^d = -\mathbf{k}_1^i$. The invariant formulation of the reciprocity theorem is given by [13] :

$$h_i^1\, \mathbf{E}_1^{i*} \cdot \mathbf{E}_2^d = h_i^2\, \mathbf{E}_2^{i*} \cdot \mathbf{E}_1^d\,, \tag{17}$$

where the asterisks means complex conjugation.

For each of the waves we introduce a plane of propagation L which is parallel to the corresponding wavevector and is perpendicular to the grating plane. Each one of the electric field vectors can be represented as a sum of a component $\mathbf{E}_\perp$ perpendicular to the corresponding plane of propagation, and a component $\mathbf{E}_\parallel$ parallel to this plane.

The introduction of this decomposition seems quite convenient because :

(i) In the classical optics the polarization parameters of the electromagnetic vector wave are usually defined in the coordinate system connected with the plane of reflection and transmission and the two fundamental *TE* and *TM* polarizations are defined with respect to this plane.

(ii) The invariance theorem is valid not only for the total diffracted in the given order energy [13], but for the amplitudes $\mathcal{E}_\perp$ and $\mathcal{E}_\parallel$ of $\mathbf{E}_\perp$ and $\mathbf{E}_\parallel$ respectively.

Taking into account that the longitudinal field components are equal to zero and that $\mathbf{k}_1^i = -\mathbf{k}_2^d$ and $\mathbf{k}_2^i = -\mathbf{k}_1^d$ ($L_1^i \equiv L_2^d$, $L_2^i \equiv L_1^d$) Eq. (17) can be represented as

$$h_i^1(\mathcal{E}_{1\parallel}^{i*}\,\mathcal{E}_{2\parallel}^d + \mathcal{E}_{1\perp}^{i*}\,\mathcal{E}_{2\perp}^d) = h_i^2(\mathcal{E}_{2\parallel}^{i*}\,\mathcal{E}_{1\parallel}^d + \mathcal{E}_{2\perp}^{i*}\,\mathcal{E}_{1\perp}^d)\,. \quad (18)$$

The connection between the different fundamental cases (// and $\perp$) are shown in *table* 1.

TABLE I

Reciprocity theorem relations for $\perp$ and // cases.

Reciprocal case \ Direct case	$\mathcal{E}_{1\parallel}^i = 0$	$\mathcal{E}_{1\perp}^i = 0$
$\mathcal{E}_{2\parallel}^i = 0$	$h_i^1\,\mathcal{E}_{2\perp}^d = h_i^2\,\mathcal{E}_{1\perp}^d$	$h_i^1\,\mathcal{E}_{2\parallel}^d = h_i^2\,\mathcal{E}_{1\perp}^d$
$\mathcal{E}_{2\perp}^i = 0$	$h_i^1\,\mathcal{E}_{2\perp}^d = h_i^2\,\mathcal{E}_{1\parallel}^d$	$h_i^1\,\mathcal{E}_{2\perp}^d = h_i^2\,\mathcal{E}_{1\perp}^d$

4. — NUMERICAL RESULTS

As it has been pointed out in [14] the invariance theorem can be used, within some limits, even for real metal gratings. Its application, however, must be performed most carefully. Let us define an angle γ between the electric field vector $\mathbf{E}^i$ and the vector $\mathbf{u}$ lying in the Oxy plane and perpendicular to $\mathbf{k}^i$. According to the invariance theorem if the projection of $\mathbf{k}^i$ on Oxy plane and γ are kept constant the diffracted efficiency remains one and the same varying θ. The dependence of the diffracted energy in 1st order on the groovedepth is given in *figure 3* for an aluminium grating. The parameters $\theta = 30°$, $\lambda = 0.5765\ \mu$m, $\psi = 35.2°$ and $\gamma = 0°$ correspond to the *TM* Littrow in-plane mount with $\lambda = 0.6\ \mu$m. The difference between the numerical results for $\theta = 0°$ and $\theta = 30°$ is less than 1 %. For larger angles, however, this difference is enlarged and reaches a value of 5 % for $\theta = 60°$ and $h/d = 1$ *(fig. 2)*. Even when the efficiency is approximately constant with θ, some polarization effects may occur that can not be predicted by

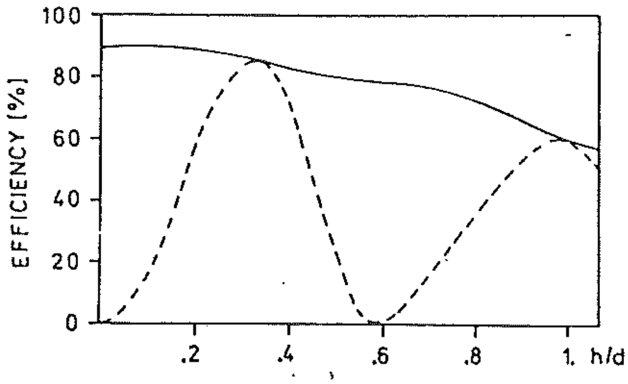

FIG. 3. — *The first order diffraction efficiency (dashed curve) and total diffracted energy (solid curve) of an aluminium grating with the same parameters as in figure 2. θ = 30°.*

the invariance theorem. For infinite conducting gratings and $\gamma = 0°$ or $\gamma = 90°$ a linearly polarized incident wave is diffracted into a linearly polarized wave, too. This is no more true when the finite conductivity of the metal is taken into account. The calculated phase shift between $\mathcal{E}_\parallel$ and $\mathcal{E}_\perp$ *(fig. 4)* is not a multiple of π therefore the diffracted wave is elliptically pola-

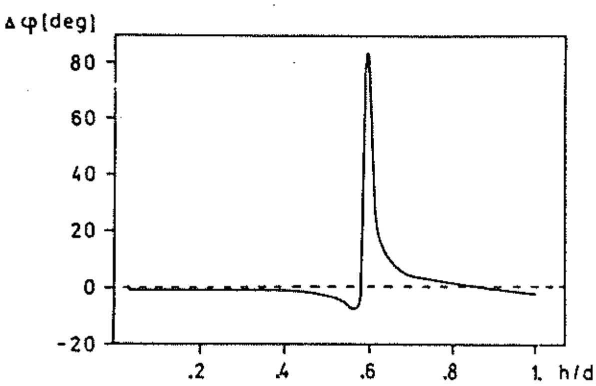

FIG. 4. — *Phase shift between $\mathcal{E}_\parallel$ and $\mathcal{E}_\perp$ for the case of figure 3.*

rized. The variation of the diffraction efficiency with θ is stronger for dielectric gratings. The angular dependence of the 1st transmitted order efficiency is given in *figure 5*. Like in the previous calculations, the projection of the wavevector $\mathbf{k}^i$ on Oxy plane and the angle γ are corresponding to the in-plane *TM* Littrow mount with $\lambda = 0.6\ \mu$m. Increasing θ up to 50° the efficiency grows up with more than 25 %. For greater angles Wood anomalies exist due to the appearance of new diffracted orders in the substrate. Although the projections on the Oxy plane of the incident and diffracted in air wave vectors are constant, the projection of the diffracted in the substrate wave vectors are changing with θ, thus new transmitted orders can appear.

Therefore, for non-perfectly conducting gratings

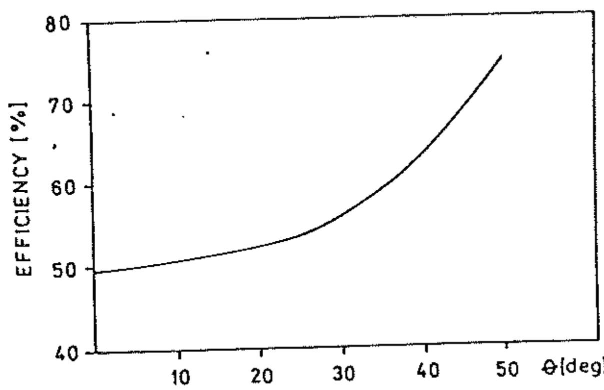

FIG. 5. — *First order efficiency as a function of θ of a transmission grating with parameters* $n_1 = 1.66$, $n_2 = 1$, $d = 0.4$ μm *and* $h/d = 1$.

in conical diffraction mounting rigorous electromagnetic methods have to be used in the calculation of the diffraction efficiency behaviour.

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