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A NEW THEORETICAL METHOD FOR DIFFRACTION GRATINGS AND ITS NUMERICAL APPLICATION

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Une nouvelle méthode d'étude théorique des réseaux de diffraction et son application numérique

RÉSUMÉ : Nous présentons un nouveau formalisme de la diffraction par un réseau, très différent de ceux actuellement utilisés. Il se caractérise par l'utilisation d'un système de *coordonnées de translation* qui permet, après emploi des équations de Maxwell en coordonnées curvilignes, d'aboutir à un système d'équations différentielles à coefficients constants. L'application numérique est fondée sur le calcul matriciel élémentaire. Le programme est testé à l'aide de critères numériques et par comparaison des résultats avec ceux issus de la méthode intégrale.

SUMMARY : We are going to describe a new formalism for the study of diffraction by a grating, quite different from those used nowadays. It is characterized by a *translation coordinate system* which allows us to write a system of linear partial differential equations with constant coefficients, after using the Maxwell equations in curvilinear coordinates. The numerical application is based on elementary matrix calculus. The program has been tested through classical numerical criteria and also by comparisons with results given by the integral method.

INTRODUCTION

In the last fifteen years, the theoretical problem of diffraction of light by gratings has been investigated by many authors. A detailed review of this field has been recently published [1]. Roughly, the rigorous theories which have been implemented and verified on a computer can be classified in two categories : the integral and the differential methods. The integral approach leads one to the resolution of an integral equation (and sometimes of coupled integral equations). On the other hand, the differential formalism requires the resolution of an infinite system of coupled differential equations. Owing to the fact that the coefficients of the differential equations are constant, our theory, although being differential in nature, differs strongly from the previous ones.

This feature has a fundamental importance in the numerical application of the theory, because it makes it possible to be content with classical calculations which result in the finding of eigenvalues and eigenvectors of a matrix whose coefficients are known in a closed form. Another advantage of the analytic form of our differential equations is the possibility to achieve easily a perturbation treatment on the groove depth of the grating. This has allowed us to obtain simple formulae able to express the efficiencies of shallow gratings in terms of grating parameters, and in the resonance domain. This last study will be presented in a future paper.

The basic characteristic of our method is the use of a new system of coordinate axes which maps the grating surface onto a plane. For numerical reasons, we have been led to separate the field associated with the evanescent waves from that associated with the *ingoing* and *outgoing* waves. Only the first part of the field is expressed after using the new system of non orthogonal coordinate axes, called *translation coordinates system*. To this aim, it is convenient to use the covariant form of the Maxwell equations [2]. On the other hand, the second part of the field is described by plane waves, even in the grooves. This must not be confused with the hypothesis of the Rayleigh expansion method which states that the total field can be represented by a plane wave expansion. The theoretical calculation results in a classical problem of finding eigenvalues and eigenvectors, which can be solved numerically. Finally, the efficiencies are obtained by solving a set of linear equations.

The numerical application has been achieved for perfectly conducting gratings. We will show that our numerical program is able to compute the efficiencies of blazed or holographic gratings.

I. — DESCRIPTION OF THE PROBLEM AND NOTATIONS

Let us consider *(figure 1)* a rectangular coordinate system $Oxyz$ and a cylindrical periodic surface of arbitrary shape and period d. Let us call $y = a(x)$ its equation. Throughout the paper, the metal of the grating, filling the region $y < a(x)$, is assumed to be perfectly conducting, but without doubt our theory can be generalized to the more general case of finite conductivity. In vacuum, an electromagnetic monochromatic plane wave strikes the grating under

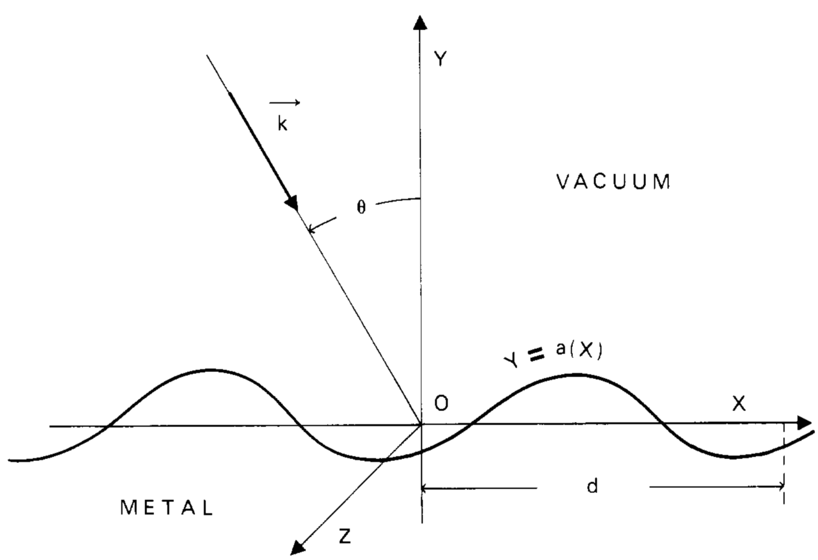

FIG. 1. — *Reference coordinate system.*

the incidence θ and with wavevector $\mathbf{k}$ which lies in the Oxy plane ($|\mathbf{k}| = k = 2\pi/\lambda$, λ being the wavelength in vacuum).

Since the problem is unchanged after a translation on the Oz axis, it can be considered as a two dimensional one. We thus shall study the two fundamental cases of polarization called $E_{\parallel}$ (electric field parallel to Oz axis) and $H_{\parallel}$ (magnetic field parallel to Oz axis). By using a time dependence in $\exp(i\omega t)$, we define the complex amplitudes E_x, E_y, E_z, H_x, H_y, H_z, of the projections of the electric and magnetic fields on the coordinate axis. Then in the two fundamental cases of polarization, the incident field with unit amplitude is given by :

$$\text{(1)} \qquad \left.\begin{array}{l}\text{in } E_{\parallel} \text{ case : } E_z^i \\ \text{in } H_{\parallel} \text{ case : } ZH_z^i\end{array}\right\} = F^i = \exp(-\,ikx\sin\theta + iky\cos\theta)\,,$$

with $Z = \sqrt{\mu_0/\varepsilon_0}$.

The diffracted field F^d is the difference between the total field F and the incident field F^i. It is well known that it can be described, outside the grooves, by a plane wave expansion [1] :

$$\text{(2)} \qquad \left.\begin{array}{l}\text{in } E_{\parallel} \text{ case : } E_z^d \\ \text{in } H_{\parallel} \text{ case : } ZH_z^d\end{array}\right\} = F^d = \sum_n B_n \exp(-\,ik\alpha_n\, x - ik\beta_n\, y)\,,$$

where

$$\alpha_n = \sin\theta + n\lambda/d\,, \tag{3}$$

$$\beta_n = \sqrt{1-\alpha_n^2} \quad \text{or} \quad \beta_n = -\,i\sqrt{\alpha_n^2 - 1}\,, \tag{3'}$$

the symbol $\sum_n$ denoting a sum from $n = -\infty$ to $n = +\infty$.

It must be noted that the more general form of the field outside the grooves, including all the possible incident waves, is given by :

$$F = F^i + F^d = \sum_n A_n \exp(-\,\mathrm{i}k\alpha_n x + \mathrm{i}k\beta_n y) + \sum_n D_n \exp(-\,\mathrm{i}k\alpha_n x - \mathrm{i}k\beta_n y)\,. \tag{4}$$

It is worth noting that the right hand side of Eq. (2) contains two parts very different in nature from a physical point of view. The first part, which we call asymptotic diffracted field F^{ad} is equal to the sum of the finite number of terms for which β_n is real. This part represents the asymptotic value of the field when $y \to \infty$. The sum of the remaining terms of the series defines the evanescent diffracted field F^{ed}, which tends towards zero when $y \to \infty$. In order to distinguish these two fields, we define U, the set of values of n for which β_n is real. When $n \in U$, $|\alpha_n|$ is less than one and defining θ_n by $\alpha_n = \sin\theta_n$, allows us to derive from (3) the classical formula of gratings :

$$\sin\theta_n = \sin\theta + n\lambda/d\,.$$

Furthermore, if $n \in U$, we can define the efficiency $\mathcal{E}_n$ in the order n, as the energy diffracted in the order n over the incident energy ratio. Bearing in mind that the incident wave has a unit amplitude, it yields :

$$\mathcal{E}_n = B_n \overline{B}_n \cos\theta_n/\cos\theta\,. \tag{5}$$

In practice, for opticists, the problem reduces to the determination of these efficiencies.

II. — GENERAL FORMULATION

To determine the values of the efficiencies $\mathcal{E}_n$ (for $n \in U$) one must know the values of the fields at infinity. This needs the resolution of a boundary problem ; in our case, this condition occurs on the surface $y = a(x)$, we thus have to determine the fields everywhere above this surface using the following conditions :

— if $y > a(x)$ all the components of the fields satisfy a Helmholtz equation

— if $y = a(x)$ the tangential component of the electric field vanishes

— if $y \to \infty$ the diffracted field remains finite and must go away from the grating (out-going wave condition OWC).

The most important feature of our method, consists in writing the Maxwell equations in a coordinate system such that one of the coordinate surfaces is nothing else than the grating surface. We have chosen the most simple of these systems which we call *translation coordinate system*. In this new system, the coordinates x and z are unchanged ; on the other hand, y is replaced by u :

$$u = y - a(x)\,. \tag{6}$$

For the sake of simplicity, we shall not describe here the tensorial calculus which enables us to know the fields equations in this new system (one can find its summary in annex 1). It allows us to derive the equation of propagation for the covariant component E_z (or H_z) :

$$\left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial u^2} + k^2 + \dot{a}^2 \frac{\partial^2}{\partial u^2} - 2\dot{a}\frac{\partial}{\partial u\,\partial x} - \ddot{a}\frac{\partial}{\partial u} \right\}_{H_z}^{E_z} = 0 \tag{7}$$

where $\dot{a}$ and $\ddot{a}$ denote respectively $\mathrm{d}a/\mathrm{d}x$ and $\mathrm{d}^2a/\mathrm{d}x^2$.

Because of the presence of $\ddot{a}$, in (7), difficulties occur when the surface of the grating contains edges. This is the case for ruled gratings. As we shall see later on, one can get over this difficulty ; however, for the time being, we suppose that $\dot{a}$ is continuous.

The boundary condition can be expressed in the following form :

if $u = 0$,

$$\forall x,\ E_z = 0 \text{ in the } E_{\parallel} \text{ case}$$

or

$$E_x = 0 \text{ in the } H_{\parallel} \text{ case}\,.$$

We could solve the problem for both fundamental cases of polarization but beforehand, it is interesting to note that in the $H_{\parallel}$ case, the boundary condition applies to the electric field. We could look for the specific equation concerning E_x, but this would lead us to the resolution of two different equations in this particular case. We have overcome this difficulty by writing a system of two partial differential equations of the first order in u, valid for the two polarizations. To this aim, we introduce a new function G, such that :

$$\begin{cases} F = E_z & \text{and} \quad G = ZH_x \quad \text{in} \quad E_{\parallel} \text{ case} \\ F = ZH_z & \text{and} \quad G = -E_x \quad \text{in} \quad H_{\parallel} \text{ case}\,. \end{cases} \tag{8}$$

Using these new notations, one gets the following equations :

$$\frac{\partial F}{\partial u} = \frac{-\,i}{1+\dot{a}^2}\,kG + \frac{\dot{a}}{1+\dot{a}^2}\,\frac{\partial F}{\partial x}\,, \tag{9}$$

(10)

$$\frac{\partial kG}{\partial u} = -i\frac{\partial}{\partial x}\left(\frac{1}{1+\dot{a}^2}\frac{\partial F}{\partial x}\right) - ik^2 F + \frac{\partial}{\partial x}\left(\frac{\dot{a}}{1+\dot{a}^2}kG\right),$$

the boundary conditions being now expressed for $u = 0$ by :

(11) $F(x, u = 0) = E_z = 0$ in $E_{\|}$ case

(12) $G(x, u = 0) = -E_x = 0$ in $H_{\|}$ case.

We notice that the function $a(x)$ appears only in the two following functions :

$$c(x) = \frac{1}{1+\dot{a}^2} \quad \text{and} \quad e(x) = \frac{\dot{a}}{1+\dot{a}^2}.$$

These two periodic functions can be developed in Fourier series :

(13) $$c(x) = \sum_p c_p \exp(-\,i\,2\,\pi px/d)$$

(14) $$e(x) = \sum_p e_p \exp(-\,i\,2\,\pi px/d).$$

The theorem of Floquet-Bloch leads us to look for a solution of the form :

(15) $$F = \sum_m F_m(u) \exp(-\,ik\alpha_m x)$$

(16) $$G = \sum_m G_m(u) \exp(-\,ik\alpha_m x).$$

Introducing the right hand member of (15) and (16) in (9) and (10), we derive an infinite set of differential equations of the first order with constant coefficients :

(9′)

$$\frac{i}{k}\frac{dF_m}{du} = \sum_p (\alpha_p e_{m-p} F_p + c_{m-p} G_p)$$

(10′)

$$\frac{i}{k}\frac{dG_m}{du} = \sum_p (\delta_{mp} - \alpha_p \alpha_m c_{m-p}) F_p + \alpha_m e_{m-p} G_p),$$

δ_{mp} being the Kronecker symbol.

The unknowns are the double set of functions F_m and G_m. In order to solve these equations, we use the classical method where $F_m(u)$ and $G_m(u)$ are developed in series of elementary exponential solutions :

(17) $$F_m(u) = \sum_{n=1}^{\infty} F_{mn} \exp(-\,ikr_n u)$$

(18) $$G_m(u) = \sum_{n=1}^{\infty} G_{mn} \exp(-\,ikr_n u).$$

In order to simplify (17) and (18), it is convenient to define the infinite vectors $f(u)$, $g(u)$, f_n and g_n having respectively for components the Fourier coefficients $F_m(u)$, $G_m(u)$, F_{mn} and G_{mn}, in such a way that :

(17′) $$f(u) = \sum_{n=1}^{\infty} f_n \exp(-\,ikr_n u),$$

(18′) $$g(u) = \sum_{n=1}^{\infty} g_n \exp(-\,ikr_n u).$$

III. — RESOLUTION

We have now to determine the vectors f and g. To this aim, we first must ensure that the expressions of $F_m(u)$ and $G_m(u)$ given by (17) and (18) satisfy (9′) and (10′). Denoting by the symbol $\begin{pmatrix} f_n \\ g_n \end{pmatrix}$ the infinite generalized vector whose components are successively those of f_n and those of g_n, it yields :

(19) $$\begin{pmatrix} f_n \\ g_n \end{pmatrix} = C_n \begin{pmatrix} \tilde{f}_n \\ \tilde{g}_n \end{pmatrix},$$

where $\begin{pmatrix} \tilde{f}_n \\ \tilde{g}_n \end{pmatrix}$ is the n-th eigenvector, associated to the eigenvalue r_n, of a generalized matrix M which is obtained by juxtaposing four infinite matrices M_1, M_2, M_3, M_4 :

(20) $$M\begin{pmatrix} \tilde{f}_n \\ \tilde{g}_n \end{pmatrix} = r_n \begin{pmatrix} \tilde{f}_n \\ \tilde{g}_n \end{pmatrix},$$

with $$M = \begin{pmatrix} M_1 & M_2 \\ M_3 & M_4 \end{pmatrix},$$

$$M_{1,m,p} = \alpha_p e_{m-p}, \quad M_{2,m,p} = c_{m-p},$$

$$M_{3,m,p} = \delta_{m,p} - \alpha_p \alpha_m c_{m-p}, \quad M_{4,m,p} = \alpha_m e_{m-p}.$$

After resolution of (20), the eigenvectors and eigenvalues $\begin{pmatrix} \tilde{f}_n \\ \tilde{g}_n \end{pmatrix}$ and r_n are known, the boundary condition in $u = 0$ and the OWC permit to determine the unknown coefficients C_n linking the vector $\begin{pmatrix} f_n \\ g_n \end{pmatrix}$ to the eigenvector $\begin{pmatrix} \tilde{f}_n \\ \tilde{g}_n \end{pmatrix}$ of M. However, it is first necessary to make same remarks on the solution of Eq. (20).

Comparing Eqs. (4) and (17) and taking into account (6) and (15) we see easily by identification that the set of r_n (values of r_n when matrix M is infinite) is the set of $+\beta_n$ and $-\beta_n$, the values of r_n corresponding to the $-\beta_n$ being associated to incident waves.

In the same manner, one could give the analytic expression of $\tilde{f}_n$ and $\tilde{g}_n$. To express the incident field in the xOy plane, we must know the index q of r_q such that $r_q = -\beta_0$: the eigenvector which corresponds to r_q gives the representation of the incident wave :

(21) $$F^i(x, u) = s \sum_m \tilde{F}_{mq} \exp(-\,ik\alpha_m x + ikr_q u),$$

where the quantity s is calculated through identification between (21) and (1) and by using (6). If we call V_∞^+ the infinite set of the values of p such that $r_p = +\beta_n$, we can represent the diffracted wave in the system $Oxuz$ by the equation :

$$F^d(x, u) = \sum_{p \in V_\infty^+} \sum_m C_p \tilde{F}_{mp} \exp(-ik\alpha_m x - ikr_p u) .$$

The diffracted field given above obeys the OWC. The determination of the unknown coefficient C_p may be achieved by writing the boundary condition (for $u = 0$) and for example, in $E_{\|}$, we obtain the following equation :

$$(22) \quad \sum_{p \in V_\infty^+} \sum_m C_p \tilde{F}_{mp} \exp(-ik\alpha_m x) = = s \sum_m \tilde{F}_{mq} \exp(-ik\alpha_m x) .$$

Through identification between the coefficients of the two Fourier series obtained after multiplying (22) by $\exp(ikx \sin\theta)$ we finally deduce an infinite linear system :

$$(23) \qquad \forall m, \sum_{p \in V_\infty^+} \tilde{F}_{mp} C_p = s\tilde{F}_{mq} .$$

IV. — REFLEXIONS ON THE TRUNCATION

The numerical resolution on a computer requires a limitation of the values of m and p. If we denote by V_P^+ the set of the $2P + 1$ values of p belonging to V_∞^+, and with r_p of least modulus, we can write Eq. (23) under the reduced form (23') :

$$(23') \quad \forall m \in (-P, +P), \sum_{p \in V_P^+} \tilde{F}_{mp} C_p = s\tilde{F}_{mq} .$$

On the other hand, it may seem advantageous to use the analytic solution of the problem of the eigenvalues and eigenvectors of (20), if we operate in such a way, we can show that this method is equivalent to the well known Rayleigh expansion method, which leads to a numerical failure. In particular, it is not able to satisfy the boundary condition on the grating.

This leads us to the following conclusion. The failure of the Rayleigh expansion method has been interpreted as a consequence of theoretical defects. Since it does not seem to be the case for our theory, we may think that our failure lies in the choice of the above truncated eigenvectors and corresponding eigenvalues, which are related to the infinite matrix M.

We could on the other hand define r_n and $\tilde{f}_n$ as the eigenvalues and eigenvectors of the matrix M truncated to the order $4P + 2$, each of the matrices M_1, M_2, M_3, M_4 being truncated to order $2P + 1$. If this solution is more difficult to adopt, one can show that, after resolution of (23'), the boundary condition in $u = 0$ is perfectly satisfied.

So, if the problem defined by (20) and (23) has mathematically the same formulation as the Rayleigh expansion method, the simultaneous truncation of these equations leads us to quite different results from those which would have been obtained by truncation of the Rayleigh expansion. This remark can be compared to the conclusion of recent works on this last method [5].

Table I fully confirms this assumption. One can see that the numerically obtained r_p are different from the $\pm\beta_n$ given by (3') especially when n is increased. Therefore, a new difficulty appears : if the r_p are different from the $\pm\beta_n$, it may be difficult to associate these two sets of values. This dramatically occurs in the vicinity of the Littrow mounting where the β_n are pratically equal two by two. Thus, it becomes impossible to associate an order of diffraction to an eigenvector $\tilde{f}_n$ as we did for exemple, in (21) and the calculation cannot then be achieved.

In order to overcome this difficulty, we have modified Eq. (23) to describe the incident field E^i and the asymptotic diffracted fields E^{ad} by a plane wave representation in the xOy plane. This second originality of our theoretical approach has been numerically very efficient. We write F^{ad} everywhere (even inside the grooves of the grating) as a finite set of plane waves :

$$(24) \quad \forall y > a(x), \; F^{ad} = \sum_{n \in U} B_n \exp(-ik\alpha_n x - ik\beta_n y) .$$

This must not be confused with the inexact considerations of the *Rayleigh expansion method*, which suppose that the whole diffracted field can be described by a sum of plane waves for $y > a(x)$. On the contrary, our method do not need any assumption on the form of F^{ed} inside the grooves of the grating. In fact Eq. (24) must be considered as a definition of F^{ad} and

$$F^{ed} = F^d - F^{ad} ,$$

and this is quite correct from a mathematical point of view : it is always possible to consider that an unknown function is the sum of a given function and an other unknown one ! When y is replaced by $u + a(x)$ in (1) and (2), (23) and (25) yields :

$$(25) \quad \sum_{p \in W_P^+} \sum_m C_p \tilde{F}_{mp} \exp(-ik\alpha_n x) + \sum_{n \in U} B_n \exp(-ik\alpha_n x - ik\beta_n a(x)) + \exp(-ikx \sin\theta + ika(x)\cos\theta) = 0$$

where W_P^+ is the set of values of p belonging to V_P^+ and such that r_p has a negative imaginary part different from zero (the associated waves thus being evanescent).

If we note that the total number of unknowns C_p and B_n is equal to $2P + 1$ (because there exist as many values of $n \in U$ as elements of V_P^+ with imaginary part equal to zero) we just need to project (25) on the $2P + 1$ first terms of the Fourier basis to obtain $2P + 1$ linear equations with $2P + 1$ unknowns. We then calculate directly the values of B_n and the efficiencies $\mathcal{E}_n$ can be readily deduced.

This last method, implemented on a CDC 7600, is more powerful than the previous one. The value of P needed is generally about 10 and, in these conditions, the computation time is a fraction of a second.

V. — CHECKING OF THE RESULTS

We have compared our results with those obtained from the integral method [6]. The later has been successfully tested against numerous numerical criteria and has also thoroughly been verified by experiments, so its results can be considered as rigorous with an accuracy better than 10^{-4}.

The comparisons are shown in tables 1 and 2. The results have been computed successively for a sinusoïdal grating ($a(x) = h \cos 2\pi x/d$) in normal incidence with several values of h, and for a ruled grating having perpendicular faces) with some blaze angles b. Since $\ddot{a}(x)$ is not defined on the edge of a ruled grating, we have described this type of profile by its truncated Fourier series. We know that the new grating so defined, which has no edges, gives practically the same efficiency as the echelete one, as soon as the number of Fourier coefficients exceeds about 10 [7].

Looking at these tables show, for the sinusoidal grating, an excellent agreement between the two methods. For the ruled grating, the mismatch generally does not exceed 10^{-2} in relative value. This precision could be enhanced by increasing the order of the matrix M which here is equal to 42 ($P = 10$).

One can also see the relevance of the energy balance criterion which readily gives a good indication on the accuracy of the results.

TABLE 1

Comparison of our results with those obtained from the integral method, for sinusoidal grating ($a(x) = h \cos 2\pi x/d$), $P = 9$, $\theta = 0$, $\lambda/d = 0{,}436\,8$.

	h/d	$\mathcal{E}_{-2} = \mathcal{E}_2$	$\mathcal{E}_{-1} = \mathcal{E}_1$	$\mathcal{E}_0$	$\sum_{n \in U} \mathcal{E}_n$	$\mathcal{E}_1$ (integral method)
$E_{\parallel}$	$1/5\,\pi$	0.048 8	0.385 2	0.132 1	1.000 1	0.385 1
	$2/5\,\pi$	0.261 6	0.095 2	0.286 4	1.000 0	0.095 2
	$3/5\,\pi$	0.184 9	0.133 5	0.363 3	0.999 8	0.133 5
	$4/5\,\pi$	0.172 1	0.147 8	0.360 3	1.000 1	0.147 5
	$1/\pi$	0.244 2	0.127 3	0.256 9	0.999 9	0.127 8
	h/d	$\mathcal{E}_{-2} = \mathcal{E}_2$	$\mathcal{E}_{-1} = \mathcal{E}_1$	$\mathcal{E}_0$	$\sum_{n \in U} \mathcal{E}_n$	$\mathcal{E}_1$ (integral method)
$H_{\parallel}$	$1/5\,\pi$	0.110 7	0.347 9	0.082 9	1.000 1	0.347 9
	$2/5\,\pi$	0.477 3	0.000 05	0.045 3	1.000 0	0.000 05
	$3/5\,\pi$	0.111 8	0.129 2	0.517 2	0.999 2	0.129 3
	$4/5\,\pi$	0.056 17	0.185 9	0.515 8	0.999 9	0.185 8
	$1/\pi$	0.012 99	0.264 1	0.445 8	1.000 0	0.264 3

VI. — NOTE ON THE CALCULATION OF THE EFFICIENCIES

It is possible to give to the diffraction by a grating an interpretation in terms of quantum mechanics. For a photon impinging on the grating with angle θ, the efficiency $\mathcal{E}_n$ can be considered as the presence probability of the photon after diffraction in the direction θ_n, this direction being the analogue of an energy level.

This leads us to think that efficiencies could be calculated from the knowledge of the eigenvectors, following a scheme usual in quantum mechanics for the calculation of the presence probability. In the first method we proposed, (23) allowed us to compute the values of the C_n. The efficiencies can be derived from these coefficients.

This requires us to apply the Poynting theorem to a well chosen rectangular parallelepiped in the xuz coordinates. The sides of this parallelepiped are parallel to the axis, with length respectively equal to 1 and d on Oz and Ox. Moreover, the top and the bottom must be located as both sides of the xOz plane. After rather tedious calculation, we derive the efficiency $\mathcal{E}_n$ in the order n :

$$n \in V_P^+ \,, \quad \mathcal{E}_n = \frac{C_p\, C_p^* \sum_m \tilde{F}_{mp}^* \,\tilde{G}_{mp}}{ss^* \sum_m \tilde{F}_{mq}^* \,\tilde{G}_{mq}} \,,$$

p being the integer such that r_p is associated to β_n.

This last expression is independent of the polarization and of the shape of the grating. Moreover, as it is the faithful application of Poyting's theorem, it includes the energy balance criterion. One can verify that, for any value of P, the sum of the efficiencies is always equal to one.

One can also verify, which is most surprising,

TABLE 2

Comparison of our results with those obtained from the integral method, for ruled gratings with perpendicular facets : $P = 10$, $\lambda/d = 1$, $\sin\theta = 1/4$.

b	$E_{\parallel}$: $\mathcal{E}_{-1}$ (integral method)	$E_{\parallel}$: $\mathcal{E}_{-1}$	$E_{\parallel}$: $\mathcal{E}_0$	$E_{\parallel}$: $\mathcal{E}_0 + \mathcal{E}_{-1}$	$H_{\parallel}$: $\mathcal{E}_{-1}$ (integral method)	$H_{\parallel}$: $\mathcal{E}_{-1}$	$H_{\parallel}$: $\mathcal{E}_0$	$H_{\parallel}$: $\mathcal{E}_{-1} + \mathcal{E}_0$
5°	0.019 8	0.020 4	0.980 4	1.000 8	0.072 8	0.073 0	0.927 6	1.000 6
10°	0.080 0	0.087 0	0.923 4	1.000 4	0.316 7	0.313 8	0.690 1	1.003 9
15°	0.170 0	0.176 8	0.843 0	1.019 8	0.645 1	0.634 6	0.373 0	1.007 6
20°	0.280 3	0.280 9	0.720 9	1.001 8	0.864 8	0.864 7	0.136 0	1.000 7
25°	0.400 2	0.400 1	0.601 2	1.001 3	0.966 3	0.961 8	0.034 4	0.996 2
30°	0.507 3	0.507 1	0.491 1	0.998 2	0.978 5	0.966 1	0.021 4	0.987 5
35°	0.585 9	0.586 7	0.413 3	1.000 0	0.902 0	0.901 7	0.098 0	0.999 7
40°	0.632 3	0.632 7	0.367 4	1.000 1	0.767 0	0.767 1	0.232 5	0.999 6
45°	0.647 4	0.647 1	0.352 4	0.999 5	0.693 1	0.693 5	0.306 1	0.999 6

that for any value of P the very stringent theorem of reciprocity [6] is always satisfied.

Thus, in order to test the accuracy of our numerical results, we need another criterion which can, for instance be the convergence of the results when P is in creased.

This method for calculating the efficiencies, which is very elegant from a theoretical point of view, is not numerically used because the direct calculation of the B_n from (25) is more efficient.

CONCLUSION

We have developed here an original formalism which allows us, by very classical numerical methods, to solve most of the problems of infinitely conducting gratings. We plan to extend this formalism to the study of gratings with finite conductivity, on which most of the work is carried out nowadays.

We have been able to show why this new formalism is fundamentally different from the previous ones, and how the two cases of polarization can be handled at the same time.

Another advantage of this formalism consists in its analyticity which has led us to a perturbation treatment, to obtain simple formulas in closed form giving the efficiencies of any grating with shallow grooves. This last work, which could be valuable for grating users, will be described in a future paper.

* * *

ANNEX 1

THE EQUATIONS OF MAXWELL UNDER COVARIANT FORM

In curvilinear coordinates, and in the absence of true currents and space charges, the Maxwell equations can be written in the form :

$$\varepsilon^{ijk}\,\partial_j E_k = -\frac{\partial B^i}{\partial t}\,;\quad \varepsilon^{ijk}\,\partial_j H_k = \frac{\partial D^i}{\partial t}$$

where ε^{ijk} is the Levi Civita indicator [2] and where the indices 1, 2, 3 denot the components of the fields (depending on time) on the three coordinate axes.

The affine equations thus written are called « invariant » or better « covariant », because the components E_i and H_i of the vectors **E** and **H**, and the contravariant components B^i and D^i of the pseudovectors **B** and **D** transform themselves, when the coordinates are changed, according to the tensorial laws. Thus to a system $x^{i'}$ from a system x^i, we can write :

$$E_{i'} = A^i_{i'}\,E_i \qquad B^{i'} = |\Delta|^{-1}\,A^{i'}_i\,B^i$$

$$H_{i'} = A^i_{i'}\,H_i \qquad D^{i'} = |\Delta|^{-1}\,A^{i'}_i\,D^i$$

with

$$A^i_{i'} = \frac{\partial x^i}{\partial x^{i'}}\,,\quad A^{i'}_i = \frac{\partial x^{i'}}{\partial x^i}\,,\quad \Delta = \det(A^{i'}_i)\,.$$

In this formalism, the system of coordinates takes place explicitly only in the medium relation ships, and through the metric tensor g^{ij}. In the case of vacuum, with permittivity ε_0 and permeability μ_0, we can write :

$$B_i = \mu_0\sqrt{g}g^{ij}\,H_j \quad D^i = \varepsilon_0\sqrt{g}g^{ij}\,E_j$$

with $\qquad g = \det(g^{ij})\,.$

and setting these relations in the above Maxwell equation yields :

$$\varepsilon^{ijk}\,\partial_j E_k = -\,\mu_0\sqrt{g}g^{ij}\frac{\partial H_i}{\partial t} = -\,\mathrm{j}\omega\mu_0\sqrt{g}g^{ij}\,H_j$$

$$\varepsilon^{ijk}\,\partial_j H_k = \varepsilon_0\sqrt{g}g^{ij}\frac{\partial E_j}{\partial E} = \mathrm{j}\omega\varepsilon_0\sqrt{g}g^{ij}\,E_j\,.$$

Using these last equations, we derive the equations of the covariant components E_i or H_i, which are the propagation equations of these fields.

$$\left\{\varepsilon^{ijk}\,\varepsilon^{lmn}\,\partial_j\frac{g_{kl}}{\sqrt{g}}\,\partial_m\right\}^{E_n}_{H_n} + \left\{\frac{\omega^2}{c^2}\sqrt{g}g^{ij}\right\}^{E_j}_{H_j} = 0$$

where $\varepsilon_0\,\mu_0\,c^2 = 1$.

* * *

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