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Researches on gratings made with anisotropic materials: how is the work progressing in our Laboratory.

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ABSTRACT

We report on our work about the electromagnetic theory of gratings made with anisotropic materials. We describe briefly and give the fields of application of both differential and integral methods.

At the present time, a computer program based on the integral method works for an arbitrary uncoated dielectric anisotropic grating, the surface of which is given by $y=f(x)$, provided that the principal axes of the permittivity matrix be the ones used to describe the geometry of the structure.

The differential method, which is very flexible and easy to implement, allows us to deal with a great variety of problems. A computer program has been written which treats the problem of an anisotropic substrate covered with an anisotropic layer, and does not require any restrictive condition on the permittivity matrices. Unfortunately, the numerical difficulties which appear especially for deep and lossy gratings are not yet completely removed.

1. DEFINITION OF THE PROBLEM

Using a time dependence in $\exp(-i\omega t)$, the time harmonic fields are represented by complex vectors $\vec{E}$ and $\vec{H}$. We use a rectangular coordinate system and denote by $\vec{e}_1$, $\vec{e}_2$, $\vec{e}_3$ the unit vectors of x, y, z axes (fig.1). The permeability is μ_0 everywhere; ϵ_0 denotes the vacuum permittivity. The grating is illuminated with the incidence θ by a plane wave of arbitrary polarization propagating in the superstrate (wavelength λ). In the case where the electric incident field vector $\vec{E}$ (resp. the magnetic incident field vector $\vec{H}$) is parallel to $\vec{e}_3$, we will speak of TE (resp. TM) polarization case.

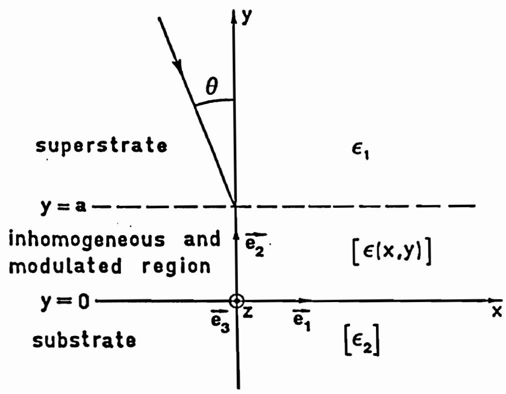


Figure 1.

In the superstrate the relative permittivity is a real number ϵ_1. The region $0<y<a$ is filled by anisotropic materials and its relative permittivity is a 3×3 matrix $[\epsilon(x,y)]$, whose elements are periodic functions of x (period d). The substrate is filled by an homogeneous anisotropic material of relative permittivity $[\epsilon_2]$. Because the wave vector of the incident plane wave is assumed to lie in the xy plane and the structure is z-invariant, all the fields are z-independent. Assuming existence and uniqueness of the solution, it is known [1] that any field-component $u(x,y)$ is pseudo-periodic and can be expanded in a generalized Fourier series development:

$$u(x,y) = \sum_{n\in Z} u_n(y)\ \psi_n(x)\ ,\ \text{where}\ \psi_n(x) = \exp(i\alpha_n x)\ , \qquad (1)$$

$\alpha_n = \sqrt{\epsilon_1}\ k_0 \sin\theta + n\ 2\pi/d$ and $k_0 = \omega\sqrt{\epsilon_0\mu_0}$. The $u_n(y)$ will be called the generalized Fourier coefficients of the function $u(x,y)$. We look for the total electromagnetic field with a special care to the efficiencies in the different reflected and (in the case of a lossless substrate) transmitted orders.

2. THE CLASSICAL DIFFERENTIAL METHOD (C.D.M.)

This method has been already used some years ago in the case of isotropic gratings [1]. It is easy to implement and is able to deal with the more general problems of anisotropic gratings: anisotropic substrate covered with an (or several) anisotropic layers (fig.2), "slanted" anisotropic gratings (fig.3), gratings in which the permittivity is continuously modulated, etc...In fact,the method can be applied to the general problem described in section 1, with matrices $[\epsilon(x,y)]$ and $[\epsilon_2]$ of the most general form (i.e. complex matrices with all elements a priori different from zero). Unfortunately, some numerical difficulties occur, particularly for deep gratings in the case where the region $0<y<a$ contains lossy materials. These difficulties have already been encountered in the Laboratory for isotropic gratings, and are probably inherent in the C.D.M..

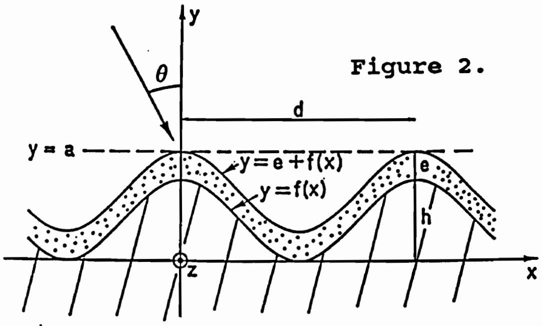


Figure 2.

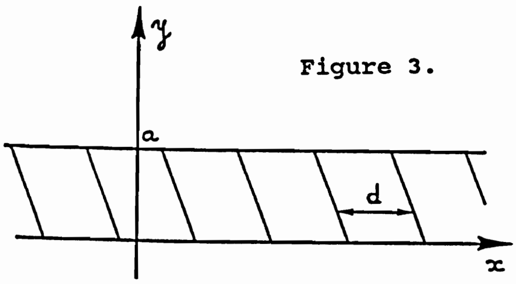


Figure 3.

Let us now expose the principle of the C.D.M.. We suppose that the field components are well described by their N components on the ψ_n basis (i.e. we use truncated developments (1), where n goes from -P to +P, and N=2P+1). It is easy to show that the electromagnetic field can be described by a column $\vec{\mathcal{F}}_N(y)$ with 4N components which are the generalized Fourier coefficients of E_x, E_z, H_x, H_z (the other components E_y and H_y are easily deduced from these four components). The problem is finally reduced to the determination of $\vec{\mathcal{F}}_N(y)$ knowing that:

a) For $0<y<a$, $\dfrac{d\vec{\mathcal{F}}_N(y)}{dy} = A(y)\,\vec{\mathcal{F}}_N(y)$, A being a 4N×4N known matrix containing the Fourier coefficients of the nine x-periodic functions $\epsilon_{ij}(x,y)$ composing the matrix $[\epsilon(x,y)]$ and the parameters k_0, ω , μ_0, α_n.

b) $\vec{\mathcal{F}}_N(0)$ belongs to a certain 2N-dimensional subspace E_0 for which we know an orthonormal basis $\vec{v}_n(0)$. This is a way to express the radiation condition for $y \to -\infty$. In the case of isotropic substrates the determination of this basis is straightforward remembering that for $y<0$ the field can be expressed as an outgoing plane waves Rayleigh expansion. In the case of anisotropic substrates, we can write for $y<0$ that $\dfrac{d\vec{\mathcal{F}}_N(y)}{dy} = A\,\vec{\mathcal{F}}_N(y)$, where A no longer depends on y. For $i=1,2,...4N$, we call λ_i and $\vec{x}_i$ the eigenvalues and the associated eigenvectors of A. It comes:

$$\text{for } y<0\ ,\ \vec{\mathcal{F}}_N(y) = \sum_{i=1,..4N} C_i \exp(\lambda_i y)\,\vec{x}_i\ ,$$

where the C_i are complex constants. Only 2N values of the λ_i are convenient to fulfil the radiation condition. Denoting by $\mathcal{J}$ the set of the associated indices, $\vec{\mathcal{F}}_N(y)$ takes the form:

$$\text{for } y<0\ ,\ \vec{\mathcal{F}}_N(y) = \sum_{i\in\mathcal{J}} C_i \exp(\lambda_i y)\,\vec{x}_i\ ,$$

which shows that the $\vec{x}_i$, $i\in\mathcal{J}$, form a basis of E_0.

c) $\vec{\mathcal{F}}_N^{inc}$ representing the incident field, $\vec{\mathcal{F}}_N(a) - \vec{\mathcal{F}}_N^{inc}(a)$ belongs to another 2N-dimensional subspace F_a for which we know an orthonormal basis. This expresses that for $y>a$, the diffracted field is given by an outgoing plane waves Rayleigh expansion.

To solve the problem we proceed as follows. For $0<y<a$ and for each n, we determine $\vec{v}_n(y)$ from the initial value $\vec{v}_n(0)$ and the numerical integration of

$$\frac{d\vec{v}_n(y)}{dy} = A(y)\ \vec{v}_n(y)$$. Obviously, whatever the constants a_n,

$\vec{\mathcal{F}}_N(y) = \sum a_n \ \vec{v}_n(y)$ satisfies a) and b) . The a_n associated with the solution must be determined in order to fulfil c) , i.e.

$\sum a_n \ \vec{v}_n(a) - \vec{\mathcal{F}}_N^{inc}(a) \in F_a$. We are led to a classical problem of linear analysis.

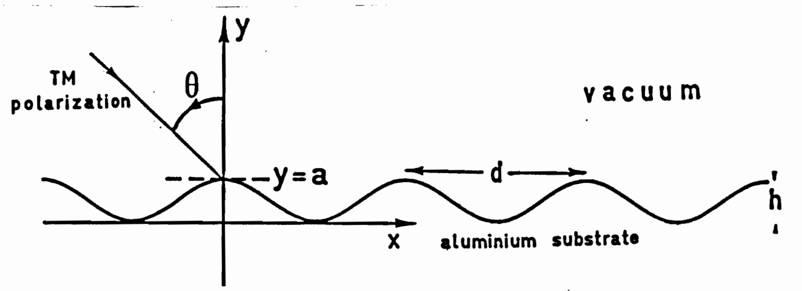
At the present time, a computer code has been written which deals with the structure depicted fig.2 , i.e. an anisotropic substrate with a sinusoidal surface, covered by an anisotropic layer. Their permittivities are complex matrices and have the most general form. Some numerical results have already been published in the case of dielectric anisotropic layers and gyrotropic metallic layers [2] . Let us give an idea of the possibilities of this program when the wavelength of the light is about the grating spacing d. In the case of unlossy materials, reliable results are obtained when the ratio a/d is less than about 0.5. For lossy materials, this ratio depends on various parameters, and in particular the polarization of the incident light and the permittivities of the media. No practical rule can be given, but some calculations have shown that in the most difficult case (aluminium substrate, TM polarization) the relative accuracy on all efficiencies is about 10% (resp. 20%) when a/d is near 0.1 (resp. 0.2). Some other data obtained with a gyrotropic cobalt layer deposed on a dielectric substrate show that reliable results are obtained when a/d is about 0.1.

Let us emphasize that when using the C.D.M. for unlossy media, the energy balance criterion can not be used as a check of validity of the numerical results, which has been shown in a preceding paper [3] . Indeed, it is automatically verified by the truncated solution, whatever the order of truncature N. The only ways to test the reliability of the results is to observe the convergence of the solution when N increases, or to make comparisons with results obtained through the implementation of others methods (integral method for instance). Such a comparison is made in another paper presented at the same session by the same authors [4].

3. ATTEMPTS IN ORDER TO IMPROVE THE DIFFERENTIAL METHOD

Two studies have been achieved in order to get rid of the numerical difficulties which limit the field of application of the C.D.M.. These studies have been developed in a simplified case which leads to the same troubles as the general anisotropic grating, i.e. an isotropic aluminium grating illuminated by a TM polarized plane wave (fig. 4).

Figure 4.



3.1. Reorthonormalizations

The method has briefly been described in a preceding paper [5]. With sufficiently deep gratings, we observe with the C.D.M. that the computed efficiencies have not stabilized before N reaches a reasonable value (say some tens) and suddenly become greater than 1! By performing reorthonormalizations in the course of the integration of the basis $\vec{v}_n(y)$ between $y=0$ and $y=a$, it is possible to use greater values of N than with the C.D.M.. Unfortunately, the convergence of the solution with respect to N is slow and we are led to very long computation times.

3.2. Integration of the "impedance matrix"

We still consider the simplified case depicted fig.4. Here we put $u_1(x,y) = H_z(x,y) = \sum_n u_{1n}(y)\ \psi_n(x)$ and $u_2(x,y) = E_x(x,y) = \sum_n u_{2n}(y)\ \psi_n(x)$. These developments are truncated keeping N terms on the ψ_n basis; let us denote by $\vec{U}_1(y)$ the column with N elements which are the $u_{1n}(y)$, by $\vec{U}_2(y)$ the column with N elements which are the $u_{2n}(y)$ and by $\vec{U}(y)$ the column with 2N elements which is: $\vec{U}(y) = \begin{pmatrix}\vec{U}_1(y)\\ \vec{U}_2(y)\end{pmatrix}$.

The problem to solve can be written in the following manner:

a) for $0<y<a$, $\dfrac{d\vec{U}(y)}{dy} = A(y)\ \vec{U}(y)$, $A(y)$ being a 2N×2N known matrix of the same kind that the one defined in section 2, and which here takes the form: $A = \begin{pmatrix}0 & A_2\\ A_1 & 0\end{pmatrix}$, where A_1 and A_2 are N×N matrices. In other words, for $0<y<a$, it is equivalent to say that:

$$\left\{\begin{aligned}\frac{d\vec{U}_1(y)}{dy} &= A_2(y)\ \vec{U}_2(y)\\ \frac{d\vec{U}_2(y)}{dy} &= A_1(y)\ \vec{U}_1(y)\end{aligned}\right. . \qquad (2)$$

Let us introduce another N×N matrix $Z(y)$ such as:

$$\vec{U}_2(y) = Z(y)\ \vec{U}_1(y) \quad . \qquad (3)$$

This matrix has the dimensions of an impedance and will be called the impedance matrix. From (2) and (3) it is easy to get:

$$\frac{dZ(y)}{dy} = A_1(y) - Z(y)\ A_2(y)\ Z(y) \quad . \qquad (4)$$

b) expressing the radiation condition for $y \to -\infty$, we obtain easily $Z(0)$.

c) $\vec{U}^{inc}$ representing the incident field, $\vec{U} - \vec{U}^{inc}$ must verify another radiation condition for $y \to +\infty$. It is not a difficult matter to show that this property can take the form (Z_a being a known N×N matrix):

$$\vec{U}_2(a) = Z_a\ \vec{U}_1(a) - 2\ Z_a\ \vec{U}_1^{inc}(a) \quad . \qquad (5)$$

The problem is solved in the following way. From the value of $Z(0)$ and through the integration of (4) we obtain $Z(y)$ for $0<y<a$. Equations (3) and (5) give the linear system $Z(a)\ \vec{U}_1(a) = Z_a\ \vec{U}_1(a) - 2\ Z_a\ \vec{U}_1^{inc}(a)$, which allows us to determine the reflected field. In order to get the transmitted field, we can write from the first equality of (2):

$$\frac{d\vec{U}_1(y)}{dy} = A_2(y)\ Z(y)\ \vec{U}_1(y) \quad . \qquad (6)$$

As $Z(y)$ and $\vec{U}_1(a)$ are known, the integration of (6) from $y=a$ to $y=0$ gives $\vec{U}_1(0)$. Clearly, this impedance matrix method (I.M.M.) is quite different from the C.D.M.. From the numerical point of view, and in this case (isotropic materials), the C.D.M. leads to the integration of N vectors with 2N components, whereas the I.M.M. needs to determine the reflected field the integration of N^2 matrix elements and to determine the transmitted field the integration of the N components of $\vec{U}_1$.

Our computations have shown instabilities in the integration of (4), which has been performed using Adam's 5th order formulae with prediction and correction, starting with Runge-Kutta's 4th order algorithm. For example, let us consider the problem: d = 0.833 μm, h = a = 0.1 μm, λ = 0.6 μm, normal incidence; we take for the aluminium the refractive index 1.3 + i 7.1 and represent the fields with N=33 Fourier coefficients. If the number of steps of integration J is less than about 100, the integration process diverges. Then, when J is taken greater (200 for example), we obtain the same solution as with the C.D.M.. As for the C.D.M., it is much less sensitive to the value of J, and in this example, J = 50 is sufficient.

Confronted with these troubles, we have tried some modifications of the I.M.M.. Instead of the impedance matrix, we can consider the "admittance matrix" defined by $\vec{U}_1(y) = \mathcal{A}(y)\,\vec{U}_2(y)$. We are led to a similar problem, i.e. the integration of $\frac{d\mathcal{A}(y)}{dy} = A_2 - \mathcal{A}\,A_1\,\mathcal{A}$ knowing $\mathcal{A}(0)$. The main difference between the methods is that Z(y) is (before the truncature of the Fourier series) an unbounded operator whereas $\mathcal{A}(y)$ is bounded. But the numerical studies have shown that this last method leads to greater instabilities in the integration process that the I.M.M., and must be used with a higher number of integration steps. Consequently, it has been forsaken.

In conclusion, we can say that, all the differential methods which have been implemented give, for a given value of N and convenient value of J, the same results. In the difficult cases (deep gratings, lossy media, TM polarization case), the convergence of the solution towards N can be slow, and great computation times are necessary to get valuable results. We are now convinced that this problem will persist as long as the ψ_n basis will be used to describe the fields according to (1)

4. INTEGRAL METHOD (I.M.)

4.1. Presentation of the I.M.

Because of the difficulties encountered with the differential methods, we have investigated during the last two years the possibilities of integral methods for the study of periodic anisotropic structures. At the present time, a computer program based on the I.M. works for an arbitrary uncoated dielectric anisotropic grating, the surface of which is given by y=f(x), provided that the principal axes of the permittivity matrix be the ones used to describe the geometry of the structure (fig. 5). In other words, $[\epsilon_2]$ is here a diagonal matrix $\begin{bmatrix}\epsilon_x & 0 & 0\\ 0 & \epsilon_y & 0\\ 0 & 0 & \epsilon_z\end{bmatrix}$. This method has been recently described in two papers [6,7] in which the interested reader will find more detailed explanations.

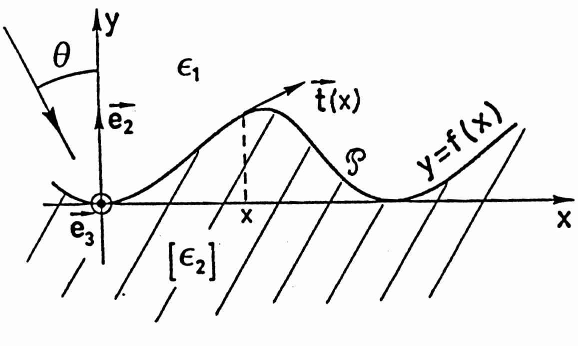


Figure 5.

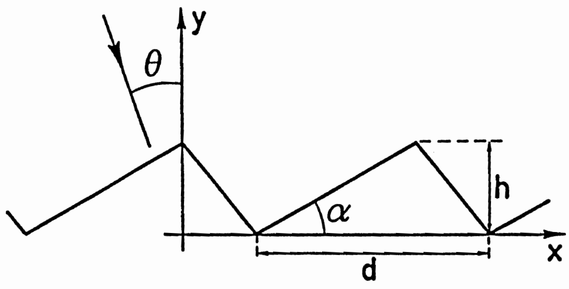


Figure 6.
h = 0.2 μm, α = 30°, d = 0.5 μm.

In this paper, we will only summarize the main lines of our study, which is an adaptation to the case of anisotropic gratings of a well known three steps process. The unknowns are now the tangential components of the electromagnetic field on the grating profile $\mathcal{P}$, and they can be described by four functions: $\vec{E}(x,f(x)).\vec{e}_3$, $\vec{E}(x,f(x)).\vec{t}(x)$, $\vec{H}(x,f(x)).\vec{e}_3$, $\vec{H}(x,f(x)).\vec{t}(x)$ (fig. 5).

First step is to determine a set of nine "Green's functions" $g_{ij}(x,y)$ which are defined as $\vec{g}_i = \sum_{j=1}^{3} g_{ij}\, \vec{e}_j$ where the $\vec{g}_i$ are solution of:

$$\text{curl curl } \vec{g}_i - k_0^2 \; {}^t[\epsilon_2]\, \vec{g}_i = \vec{e}_i \sum_{n\in Z} \frac{1}{d}\, \delta(y)\, \bar{\psi}_n(x) \; , \quad i=1,2,3, \qquad (7)$$

and must satisfy a radiation condition for $y \to \mp\infty$. In equation (7), ${}^t[\epsilon_2]$ is the transpose of $[\epsilon_2]$, $\bar{\psi}_n$ the complex conjugate of ψ_n and δ the Dirac distribution. This determination has been performed in the case where $[\epsilon_2]$ is diagonal [8]. For more general matrices, the determination of the g_{ij} seems to be a very hard and tedious task, which has not been carried out.

Second step is to express the diffracted field in terms of the four unknowns defined on $\mathcal{P}$ (generalized Kirchhof-Helmholtz formulae) and with the help of the Greens's functions.

Third step is to get integral equations for the unknowns by the mean of a convenient limiting process. The different integral equations we can obtain are not equivalent from both the theoretical and numerical point of view. Finally, we have retained those which contain the less singular kernels (unbounded kernels with a logarithmic singularity). They are similar to those already encountered in the case of isotropic gratings. Putting $\beta_n = \sqrt{\frac{\epsilon_x}{\epsilon_y}\,(k_0^2\,\epsilon_y - \alpha_n^2)}$, with the determination $\mathrm{Im}(\beta_n) > 0$ or $\beta_n > 0$, and denoting by sgn(y) the function equal to +1 if y>0 and to -1 if y<0, we have to deal with the kernels:

$$K(x,x') = \frac{1}{\sqrt{1+f'(x)^2}} \sum_n \frac{\epsilon_x k_0^2}{\beta_n}\, \Phi_n(x,x') \quad ,$$

$$K'(x,x') = \frac{1}{\sqrt{1+f'(x)^2}} \sum_n \left[\frac{\epsilon_x \alpha_n}{\epsilon_y \beta_n} f'(x') + \mathrm{sgn}(f(x')-f(x)) \right] \Phi_n(x,x') \; ,$$

with $\Phi_n(x,x') = \exp(i\alpha_n(x-x') + i\beta_n|f(x)-f(x')|)$.

From the numerical point of view, a slight change of unknowns permits us to get integral equations in which kernels and unknowns are periodic, and we therefore represent them by their Fourier series. The Fourier coefficients of the kernels are obtained via a discrete Fourier transform, and the problem is finally reduced to the solving of a linear system.

4.2. Consequences of the diagonal form of the permittivity matrix

Expressing the Maxwell's equations $\mathrm{curl}\vec{E} = i\omega\mu_0\vec{H}$ and $\mathrm{curl}\vec{H} = -i\omega\epsilon_0[\epsilon_2]\vec{E}$ in a medium of diagonal permittivity matrix, it appears that the six obtained equations can be split in two systems of three equations. Each of them contains only three field components: (E_z,H_x,H_y) or (H_z,E_x,E_y). The incident field can also be split in two parts: one (we call it the TE part) contains the components E_z^{inc}, H_x^{inc}, H_y^{inc}; the other (TM part) contains the components H_z^{inc} , E_x^{inc} , E_y^{inc} . The problems associated to a TE or to a TM incident wave are therefore independent. In other words, <u>if the incident field is TE (resp. TM) polarized, the total field will be everywhere TE (resp. TM) polarized.</u> From Maxwell's equations again, one can persuade himself of the following results. <u>In the TE case, the grating is equivalent to an isotropic grating of permittivity ϵ_z. In the TM case, and when ϵ_x and ϵ_y have a common value ϵ, the grating is equivalent to an isotropic grating of permittivity ϵ.</u> Thus the case of an uniaxial medium disposed with its optical axis parallel to the grating's grooves can be solved with the help of computer programs made for isotropic gratings.

4.3. Numerical results

From the preceding section, it is clear that the numerical study must concern the TM polarization case, when $\epsilon_x \neq \epsilon_y$. We deal with a substrate which has three plainly different permittivities: $\epsilon_x = 6.31$, $\epsilon_y = 6.81$, $\epsilon_z = 7.34$, which, according to reference 9, corresponds to the lithargite. It is therefore a very academic example... Superstrate is vacuum ($\epsilon_1 = 1$). The grating is illuminated by a TM incident plane wave (λ = 0.6 μm) under the incidence θ = 20°. The grating period is d = 0.5 μm. The groove depth is h = max(f(x))-min(f(x)). In these conditions, we get two reflected orders: orders -1 and 0 propagating under the angles -59.09° and 20°, and four transmitted orders (-2, -1, 0 and 1). These orders have wave vectors which make with vector $-\vec{e}_2$ the angles -53.11°, -18.88°, 7.82° and 37.27° whereas their Poynting vectors make with $-\vec{e}_2$ the angles -50.99°, -18.53°, 7.25° and 35.19°. We denote by (see section 4.1.):

NSOM the number of terms retained for the summation of the series giving the kernels (summation is performed from -NSOM to +NSOM),

N the number of Fourier coefficients retained in the developments of the kernels and unknowns in Fourier series (summation is performed from -(N-1)/2 to +(N-1)/2),

ND the number of sampling points (for one grating period) used for the integrations via the discrete Fourier transform.

The numerical tests show (table 1) a fast convergence of the solution when N, ND and NSOM increase. We also see that the energy balance gives an estimation of the accuracy of the computed efficiencies. We have also reported in table 1 the computation times on CRAY 2 (they are about the same as those obtained on IBM 3090, which is probably a more "common" computer).

Table 2 shows the results obtained for the echelette grating depicted figure 6. As the I.M. deals with profiles described by functions of class C^2, the function f is represented by a Fourier series truncated to the harmonic NH. One will notice the fast convergence of the solution when NH increases.

Table 1. Sinusoidal profile; h = 0.2 μm.

	order	N=7,ND=15 NSOM=10	N=11,ND=25 NSOM=20	N=25,ND=45 NSOM=30
reflected efficiencies	-1	0.0914	0.0923	0.0923
	0	0.0003	0.0003	0.0003
transmitted efficiencies	-2	0.0082	0.0078	0.0078
	-1	0.2608	0.2530	0.2530
	0	0.2185	0.2230	0.2231
	1	0.4275	0.4238	0.4235
sum of efficiencies		1.0067	1.0002	1.0000
computation time		1 s	3 s	11 s

Table 2. Echelette grating (fig. 6); N=25, ND=45, NSOM=30.

	order	NH = 3	NH = 5	NH = 10
reflected efficiencies	-1	0.1226	0.1167	0.1166
	0	0.0126	0.0142	0.0143
transmitted efficiencies	-2	0.0119	0.0126	0.0128
	-1	0.1339	0.1363	0.1365
	0	0.4782	0.4766	0.4758
	1	0.2408	0.2436	0.2439

In conclusion, let us say that the I.M. , which leads to reliable results, seems quite difficult to extend to more general anisotropic media (i.e. when the permittivity matrix is not diagonal in the coordinate system we use).

5. ACKNOWLEDGMENTS

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