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ON THE ELECTROMAGNETIC THEORY OF ANISOTROPIC GRATINGS

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Abstract

By "anisotropic grating" we mean a grating ruled on an anisotropic material, and possibly coated with anisotropic layers. We report briefly on the pioneering work carried out in our Laboratory over the past few years using essentialy integral and differential methods. We would like to acquaint our colleagues not only with our successes, but also with some of our disappointments ; a failure can be sometimes very instructive.

1. Notations

Using a time dependence in $\exp(-i\omega t)$, the time harmonic fields are represented by complex vectors $\vec{E}$ and $\vec{H}$. We denote by $\vec{e}_1$, $\vec{e}_2$, $\vec{e}_3$ the unit vectors of x, y, z axes (fig.1). The studied structure is z-invariant and the grating profile is the graph $y = f(x)$ of a periodic function f whose period d is the grating pitch. The permeability is μ_0 everywhere. The domain Ω^- $(y < f(x))$ is filled with an anisotropic material characterized by a matrix permittivity $[\varepsilon_2]$. The grating is illuminated under the incidence θ by a given plane wave propagating in the domain Ω^+ $(y > f(x))$ filled with an isotropic material (scalar and real relative permittivity ε_1). The incident wave vector is located in the (xy) plane, but the polarization is arbitrary. We look of course for the total electromagnetic field $(\vec{E}, \vec{H})$.

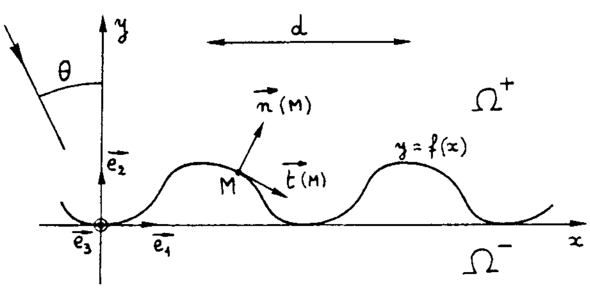

Fig.1. $\vec{t}$ and $\vec{n}$ are the unit vectors of the tangent and the normal.

Assuming existence and uniqueness, we know [1] that any field component $u(x,y)$ is pseudo-periodic and can be expanded in a generalized Fourier series :

$$u(x,y) = \sum_{n\in\mathbb{Z}} u_n(y)\ \psi_n(x)\ , \tag{1}$$

$$\psi_n(x) = \exp(i\alpha_n x)\ ,$$

$$\alpha_n = \sqrt{\varepsilon_1}\ k_0\ \sin\theta + n\ 2\pi/d \quad \text{and} \quad k_0 = \omega\sqrt{\varepsilon_0\mu_0}\ .$$

2. Integral method (I.M.)

A priori the unknowns must be the tangential components of the fields on the grating surface. We describe them by four functions $F_i(x)$, namely :

$$F_1(x) = \vec{E}(x,f(x)).\vec{e}_3\ ,\ F_2(x) = \vec{E}(x,f(x)).\vec{t} \tag{2}$$

$$F_3(x) = \vec{H}(x,f(x)).\vec{e}_3\ ,\ F_4(x) = \vec{H}(x,f(x)).\vec{t} \tag{2'}$$

First step is to determine a set of nine Green's functions $g_{ij}(x,y)$; g_{ij} being the j^{th} component of vector $\vec{g}_i$ which is solution of :

$$\text{curl curl}\ \vec{g}_i - k_0^2\ {}^t[\varepsilon_2]\ \vec{g}_i = \vec{e}_i \sum_{n\in\mathbb{Z}} \frac{1}{d}\,\delta(y)\ \bar{\psi}_n(x) \tag{3}$$

and satisfies the radiation condition for $y \to \pm\infty$. In (3), ${}^t[\varepsilon_2]$ denotes the transpose of $[\varepsilon_2]$ and δ the Dirac distribution. For an arbitrary $[\varepsilon_2]$ matrix, the obtaining of the g_{ij} shows itself a hard and very tedious task [2]. Up to now, we have obtained the g_{ij} in closed form, only in the case where $[\varepsilon_2]$ is diagonal in the x, y, z axes [2,3] (see appendix).

As a second step we express in each domain Ω^+ and Ω^- the diffracted field in term of the F_i with the help of the Green's functions (generalized Kirchhoff-Helmholtz formulas).

Finally a convenient and usual (but not trivial) limiting process leads to integral equations on the grating surface. It can be noted that of course several integral equations can be obtained ; they are not equivalent from both the theoretical and numerical point of view ; some of them are consequences of the other ones (for more or less obvious reasons).

As an example, we studied [4,5] in detail the case of a biaxial lossless material for which the xyz axes are the principal axes of the permittivity tensor. In other words, we assume $[\varepsilon_2]$ to be a diagonal matrix $\begin{bmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{bmatrix}$. In this case the set of integral equations can be split into two systems. One of them contains only F_1 and F_4, the other one F_2 and F_3. This means that the problems associated with TE and TM incident fields are independent ; if the incident field is TE (or TM) polarized, the total field is also TE (or TM). Moreover, in the TE case, the grating is equivalent to an isotropic grating of permittivity ε_z. On the contrary, in the TM case (except for uniaxial media for which the optical axis is parallel to $\vec{e}_3$ and therefore $\varepsilon_x = \varepsilon_y$) we are led to a system of two coupled integral equations for the unknowns F_2 and F_3. The kernels are given in [5], as well as some numerical recipes used to deal with the logarithmic singularities of some of them. Numerical reliable data have been obtained for sinusoidal or echelette profiles. An example is given in [6] for $\varepsilon_x = 6.31$, $\varepsilon_y = 6.81$, $\varepsilon_z = 7.34$.

We tried to use the I.M. for more general anisotropic media, i.e. when $[\varepsilon_2]$ is not diagonal in the coordinate system. But we have to confess that due to the cumbersomeness of the equations we finally abandoned. Then we understood that it was probably good, before to go on, to enter upon a structural analysis of the problem. This gave rise to rather academic and theoretical considerations [4] that we are going to summarize ; may be they can throw light on subsequent studies.

In order to describe the boundary value of a field $(\vec{E}, \vec{H})$, it is convenient to introduce the column matrix F whose elements are the four functions F_n. Such a matrix is said to belong to the vector space $\mathcal{V}_i^\sigma$ if it is associated with an outgoing field propagating in the domain Ω^σ (σ = + or −) filled with the material of permittivity ε_1 (if i = 1) or $[\varepsilon_2]$ (if i = 2). Denoting by F and F^{inc} the columns associated with the total and incident fields, the basic idea is that, for a given F^{inc}, the unknown F is characterized by the proposition :

$$(F - F^{inc}) \in \mathcal{V}_1^+ \qquad \text{and} \qquad F \in \mathcal{V}_2^- \tag{4}$$

Thus, from the mathematic point of view, the problem consists in finding the intersection of $\mathcal{V}_2^-$ and the manifold $(\mathcal{V}_1^+ + F^{inc})$ deduced from $\mathcal{V}_1^+$ by translation.

To this end, we can try to find adequate bases to describe $\mathcal{V}_1^+$ and $\mathcal{V}_2^-$. This natural idea is nothing other than the extension to anisotropic gratings of techniques developed for isotropic gratings by Yasuura and his collaborators [7]. In spite of all the recent improvements suggested by Okuno, the Yasuura type methods do not seem capable to compete with integral or differential methods. We think now that this is due to a bad choice of the total family used to represent the field on the profile ; fortunately, other choices are possible ... Promising work in this direction is now in progress in our Lab.

In our previous paper [4], we prefered to lay stress on four projection operators $\mathbb{P}_1^+$, $\mathbb{P}_1^-$, $\mathbb{P}_2^+$, $\mathbb{P}_2^-$ having the following properties :

$$F \in \mathcal{V}_i^+ \Leftrightarrow \mathbb{P}_i^+ F = F \Leftrightarrow \mathbb{P}_i^- F = 0 \tag{5}$$

$$F \in \mathcal{V}_i^- \Leftrightarrow \mathbb{P}_i^- F = F \Leftrightarrow \mathbb{P}_i^+ F = 0 \tag{5'}$$

$$\mathbb{P}_i^+ + \mathbb{P}_i^- = 1. \tag{5"}$$

As briefly explained in [4], these idempotent operators $\mathbb{P}_i^\sigma$ can be given explicitely from the knowing of the nine Green's functions g_{ij}. Proposition (4) is therefore equivalent to :

$$\mathbb{P}_1^-(F - F^{inc}) = 0 \quad (6) \qquad \text{and} \quad \mathbb{P}_2^+ F = 0. \qquad (6')$$

Moreover, it can be shown that any column F can be written as F = G + J, where $G \in \mathcal{V}_1^-$ and J is such that $J_1 = J_3 = 0$. Clearly, $\mathbb{P}_1^+ F = 0 + \mathbb{P}_1^+ J$, which from (6), (5'), (5") and because $F^{inc} \in \mathcal{V}_1^-$, yields :

$$F = \mathbb{P}_1^+ J + F^{inc}. \tag{7}$$

Then, from (6') and (7), we get :

$$\mathbb{P}_2^+ \mathbb{P}_1^+ J + \mathbb{P}_2^+ F^{inc} = 0. \tag{8}$$

This last equation represents a system of four integral equations for the two functions J_2 and J_4. Indeed, two of these equations are consequence of the other ones and, for an arbitrary polarization, the problem can be reduced to the solving of a system of two integral equations for the two principal unknowns J_2 and J_4. Finally, F is given by (7). This result can be considered as a generalization to anisotropic gratings of the method proposed by D. Maystre [1,8] for isotropic gratings (one integral equation for one unknown).

3. Differential method (D.M.)

In this method that we have already used in the sixties for isotropic gratings [1], we assume that one obtains a good approximate of a field component u(x,y) when keeping only N terms in expansion (1). The field is represented by a column matrix F_N with 4N components which are the $u_n(y)$ associated with E_x, E_z, H_x, H_z (E_y and H_y are easily deduced from these four functions). After some algebraic manipulations, it turns out [6] that the problem can be reduced to the numerical determination of $F_N(y)$ knowing that :

a) For 0 < y < a (a = max f(x)) :

$$\frac{dF_N}{dy} = A(y)\, F_N(y) \,, \tag{9}$$

A being a 4N × 4N matrix whose elements are given from the Fourier coefficients of the nine x-periodic elements $\varepsilon_{ij}(x,y)$ of the permittivity matrix.

b) $F_N(0)$ belongs to a certain 2N-dimensional subspace $\mathcal{E}_0$, which is a way to express the radiation condition for $y \longrightarrow -\infty$.

c) If we denote by F_N^{inc} the column associated with the incident field, then $F_N(a) - F_N^{inc}(a)$ belongs to another 2N-dimensional subspace $\mathcal{F}_a$; this is a way to say that the diffracted field is given by an outgoing plane wave expansion outside the groove region.

The method we use to solve this classical problem of mathematical physics has already been described [6]. Indeed, numerous numerical recipes are available to perform the numerical integration of (9) taking into account the associated boundary conditions b) and c). A computer code has been written which deals with a sinusoidal grating possibly coated with an anisotropic layer. The permittivity matrices can be "full matrices" ; they have not to be diagonal as assumed in section 2 (I.M.). This program gives reliable results for unlossy materials but unfortunately numerical experiments have shown that for lossy materials (such as gyrotropic cobalt) the case of deep gratings is much more difficult to solve especially in TM polarization [3,6]. Then, it appears that the convergence of the solution with respect to N is often very slow. Consequently two important numerical studies have been performed in our laboratory in order to try to improve the D.M. They have been described in the Hamburg S.P.I.E. meeting [6] but we have to confess that, in spite of our efforts, we did not achieve great triumphs ... In other terms, the game has not been worth the candle. We are now convinced that numerical difficulties will persist as long as the ψ_n basis will be used to describe the field according to (1). Probably some Gibbs phenomenons are responsible for our disappointments.

To conclude on a less pessimistic touch, it must be emphasized that whenever both I.M. and D.M. have been capable to solve a given anisotropic grating problem they have led to numerical results which are in good agreement [9]. This is of course a proof of the reliability of our computer codes.

4. Some further comments

Since 1980, a special attention has been devoted to the so-called slanted-grating (anisotropic or isotropic) by several authors, who claim that the methods they use avoid the numerical integration of a differential system. A slanted grating (Fig.2) is a grating for which the permittivity is a periodic function of $X = \vec{\ell}.\vec{r}$. In these circumstances, and putting $\sigma = (2\pi \, tg\alpha)/d$, it appears that :

$$G_N(y) \stackrel{\text{def}}{=} F_N(y)\exp(-in\sigma y)$$
satisfies :

$$\frac{dG_N(y)}{dy} = B\,G_N(y)\ , \qquad (9')$$

where the square matrix B no longer depends on y. As soon as the elements of A have been written down, this result is a straightforward generalization to anisotropic structures of what is explained in [10] in a simple situation (isotropic grating in TE polarization).

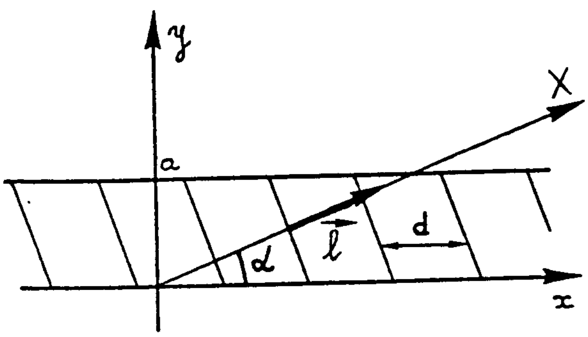

Fig.2. The slanted grating ; $\vec{\ell}$ is a unit vector, and the electromagnetic parameters only depend on X.

Then, the solution is obtainable in terms of the eigenvalues and the eigenvectors of B. This method, primally developed for isotropic gratings [11] has been extended to anisotropic gratings in Osaka Prefecture University [12]. Recently, the Japanese colleagues implemented the differential method on their computer. Because we have good relations with them, we know that, whatever the method they use, they also have to face serious numerical difficulties when dealing with lossy and deep gratings.

Conclusion

In this paper, we tried to summarize all our researches on gratings made with anisotropic materials. May be the reader will think that, in fact, we mainly advertize for several papers already published in optics litterature. But was it possible to do much better in only three pages ? ...

Appendix

Here are, from [2,3], the nine Green's functions $g_{ij}(x,y)$ when $[\varepsilon_2] = \begin{bmatrix}\varepsilon_x & 0 & 0\\ 0 & \varepsilon_y & 0\\ 0 & 0 & \varepsilon_z\end{bmatrix}$

$$g_{11} = \sum_{n\in\mathbb{Z}} \frac{i\beta_n}{2dk_0^2\varepsilon_x}\exp(-i\alpha_n x + i\beta_n|y|)$$

$$g_{12} = \sum_{n\in\mathbb{Z}} \frac{i\alpha_n}{2dk_0^2\varepsilon_y}\,\mathrm{sgn}(y)\exp(-i\alpha_n x + i\beta_n|y|)$$

$$g_{21} = g_{12}$$

$$g_{22} = \sum_{n\in\mathbb{Z}} \frac{1}{dk_0^2\varepsilon_y}\left[\frac{i\varepsilon_x\alpha_n^2}{2\varepsilon_y\beta_n} - \delta(y)\right]\exp(-i\alpha_n x + i\beta_n|y|)$$

$$g_{33} = \sum_{n\in\mathbb{Z}} \frac{i}{2d\beta'_n}\exp(-i\alpha_n x + i\beta'_n|y|)$$

$$g_{23} = g_{32} = g_{13} = g_{31} = 0$$

In these expressions :

$$\beta_n = \sqrt{(k_0^2\varepsilon_y - \alpha_n^2)\,\varepsilon_x/\varepsilon_y}$$

$$\beta'_n = \sqrt{(k_0^2\varepsilon_z - \alpha_n^2)}$$

The square roots are defined in the following way :

$$z \in \mathbb{C}, \qquad \mathrm{Im}(\sqrt{z}) > 0 \qquad \text{or} \qquad \sqrt{z} > 0.$$

The function sgn(y) is equal to 1 for y > 0 and −1 for y < 0.

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