About the electromagnetic theory of gratings made with anisotropic materials

R. Petit and G. Tayeb

Laboratoire d'Optique Electromagnétique, U.A. CNRS n° 843, Faculté des Sciences, Centre de St-Jérôme, 13397 Marseille Cedex 13, France

ABSTRACT

As far as we know, only a few studies have been, up to now, devoted to anisotropic gratings. We only have heard of the paper by our Japanese colleagues of Osaka Prefecture University.[1] We are also working in this field, in view of potential applications. Although some partial and unpublished results have been obtained some years ago in the framework of a contract with a private company (P.A. Technology, Cambridge), we think that we have to face a difficult problem which is far from being wholly resolved. We would like to report briefly on our theoretical work in order to inform "practical people" and, should the occasion arise, to initiate new collaborations.

Throughout the paper we use a rectangular coordinate system Oxyz and we denote by $\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$ the unit vectors of axes Ox, Oy, Oz. We deal with time-harmonic fields represented by complex vectors $\vec{E}$ and $\vec{H}$, using a time dependence in $\exp(-i\omega t)$. The permeability is equal to μ_0 everywhere and the relative permittivity is described by a 3 x 3 matrix $[\varepsilon]$:

$$[\varepsilon] = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} .$$

We denote by ε_0 the vacuum permittivity, and we put $k_0 = \omega\sqrt{\varepsilon_0\mu_0} = 2\pi/\lambda_0$. We say that the fields are TE (or TM) polarized when $\vec{E}$ (or $\vec{H}$) is parallel to Oz.

1. MULTILAYERED MEDIA

This problem, with which we started our own investigations on anisotropic structures, has been studied by many authors[2,3,4,5] (fig.1). It can be solved by matrix techniques, each layer being represented by a 4 x 4 matrix. The computer code which has been written in our Laboratory can deal with lossy and anisotropic materials described by matrices $[\varepsilon]$ whose all the elements are a priori different from zero. Of course this program has been extensively used in our preliminary studies on coated gratings. We also used it to try to well understand (from the electromagnetic theory) the curious phenomenon of conical refraction as described in optics text-books.[6] When a linearly polarized plane wave illuminates under a well chosen incidence angle θ_0 the plane interface (y = 0) between vacuum and a biaxial crystal, the direction of the Poynting vector $\vec{\mathcal{P}}$ associated with the refracted wave depends on the direction of the incident field $\vec{E}^i$. In other words, when $\vec{E}^i$ rotates 360° about the incident wave vector, the point P defined as $\vec{OP} = \vec{\mathcal{P}}$ moves on a cone (may be some practical applications are possible). This cone cuts the plane $y = -y_0$ along a circle of radius R, as we have verified in good agreement with the computations we have performed for aragonite ($[\varepsilon]$ is diagonal in the substrate, with $\varepsilon_{xx} = 2.843$, $\varepsilon_{yy} = 2.341$, $\varepsilon_{zz} = 2.829$; $\theta_0 = 14.52°$; $R/y_0 = 0.016$).

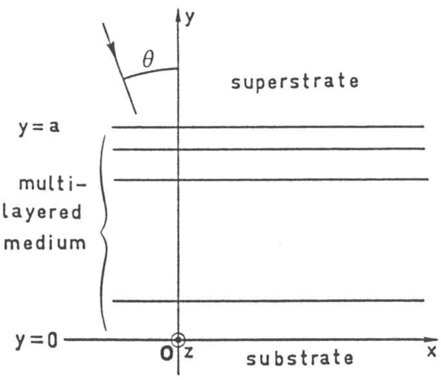

Figure 1. Multilayered media. The layers (0 < y < a) and the substrate are made of anisotropic materials.

2. THE COATED GRATING STUDIED BY THE DIFFERENTIAL METHOD

The structure we study is described in figure 2 ; space is divided into three regions : two homogeneous regions (the superstrate (y > a) and the substrate (y < 0)) and an inhomogeneous region (0 < y < a) in which $[\varepsilon]$ is a function of x and y which is periodic with

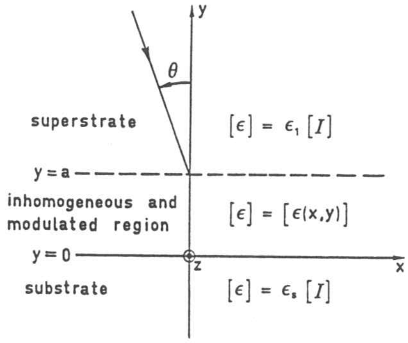

Figure 2. The structure we study in the differential method. The region $y < a$ may be filled with lossy materials

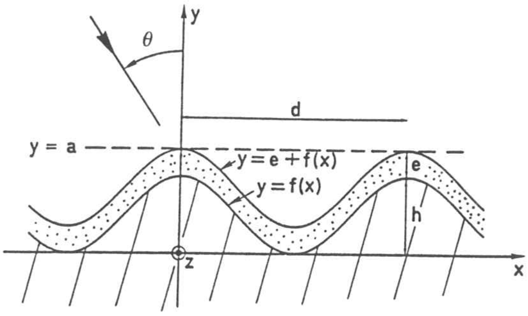

Figure 3. A particular case of fig.2 : a coated grating

respect to x (period $d = 2\pi/K$). As for the superstrate and the substrate, they are assumed to be isotropic* media, with permittivities $\varepsilon_1.[I]$ and $\varepsilon_s.[I]$ ($[I]$ denotes the unit 3 x 3 matrix). Numbers ε_1 and ε_s are respectively real and complex. This formulation allows us to deal with rather complicated structures. However, up to now, our computations have been limited to the structure of fig.3, i.e. a sinusoidal grating coated with one anisotropic layer. The grating is illuminated by a plane wave under the incidence θ, and we look for the total field. We assume for the sake of simplicity that the incident wave vector lies in the xy plane and that consequently the fields are z independent. This hypothesis can be abandoned without any particular new theoretical difficulty, but of course the equations are then more cumbersome. Assuming existence and uniqueness of the solution, any field-component $u(x,y)$ is known to be "pseudo-periodic",[7] which means that

$$u(x + d, y) = \exp(i \sqrt{\varepsilon_1}\, k_0\, d \sin\theta)\, u(x,y) .$$

Consequently, $u(x,y)$ can be expanded in a generalized Fourier series according to :

$$u(x,y) = \sum_{n=-\infty}^{+\infty} u_n(y)\, \psi_n(x) ;$$

$$\psi_n(x) \overset{\text{def}}{=} \exp\,[i\,(\sqrt{\varepsilon_1}\, k_0 \sin\theta + nK)\, x] = \exp(i\, \alpha_n\, x) .$$

In the differential method that we have already used some years ago for isotropic gratings,[7] it is assumed that one obtains a good approximation of $u(x,y)$ when keeping only N components on the ψ_n basis. The field is represented by a vector $\vec{\mathcal{F}}_N(y)$ (column matrix) with 4N components which are the $u_n(y)$ associated with E_x, E_z, H_x, H_z (E_y and H_y can be easily deduced from this 4 components). After boring manipulations, it turns out that the problem can be reduced to the numerical integration of a differential system on a bounded interval :

$$\text{for} \quad 0 < y < a , \qquad \frac{d\, \vec{\mathcal{F}}_N(y)}{dy} = A(y)\, \vec{\mathcal{F}}_N(y) ,$$

A being a known matrix depending on the structure. The system must be integrated taking into account some boundary conditions (at $y = 0$ and $y = a$) which can be deduced from the following physical remarks : for $y > a$, the field is the sum of the incident plane wave and of an outgoing plane waves Rayleigh expansion, and for $y \to -\infty$ it must verify certain radiation conditions. In conclusion, we are led to a classical problem of mathematical physics, and many "numerical recipes" are available to perform the integration.

As a first step and to solve a practical problem in the framework of our contract with P.A., we wrote a computer code allowing us to deal with isotropic substrates coated by an anisotropic layer described by a matrix $[\varepsilon_\ell]$. It must be emphasized that $[\varepsilon_\ell]$ has the most general form : all its elements can be different from zero. This program gives reliable results (for which the efficiencies stabilize quickly when N increases) for lossless dielectric materials (table 1). Unfortunately, it must be said that numerical difficulties have been encountered when dealing

* The generalization to anisotropic substrates is not a difficult matter.

with metallic or dielectric gratings coated with gyrotropic layers, except for sufficiently shallow grooves. An example is given in table 2, which corresponds to the case of an unlossy dielectric grating coated with a gyrotropic cobalt layer. As the ratio (e + h)/d increases, the efficiencies stabilize slower and slower. Anyway, in this example, the expected effect (here the enhancement of the change in polarization when replacing a plane interface by a grating) is not observed. Because the differential method is very flexible and easy to implement, we made an important effort to remove these numerical difficulties.[8] Unfortunately the game is not worth the candle ; whatever the tricks we have tried, it always appeared that any small improvement always entails a large increasing of the computation time. We decided therefore to investigate the possibilities of integral methods for the study of periodic anisotropic structures.

	Order	Reflected			Transmitted		
		Angle (degrees)	TM → TM	TM → TE	Angle	TM → TM	TM → TE
N=15	- 2				-66.48	0.5719 E-2	0.1656 E-3
	- 1	-30.03	0.2305 E-1	0.5374 E-4	-19.49	0.8689 E-2	0.1063 E-3
150	0	22.00	0.4364 E-1	0.4088 E-3	14.46	0.8490	0.1137 E-1
steps	1				56.42	0.5614 E-1	0.1610 E-2
N=9	- 2				-66.48	0.5548 E-2	0.1626 E-3
	- 1	-30.03	0.2301 E-1	0.5155 E-4	-19.49	0.8508 E-2	0.1055 E-3
80	0	22.00	0.4361 E-1	0.4040 E-3	14.46	0.8502	0.1137 E-1
steps	1				56.42	0.5557 E-1	0.1591 E-2

Table 1. Structure is the same as in fig. 3. Superstrate is vacuum. Anisotropic layer is a TiO_2 deposit, with

$$[\varepsilon_\ell] = \begin{bmatrix} 4.4800 & -0.1174 & 0.0923 \\ -0.1174 & 4.7975 & 0.0985 \\ 0.0923 & 0.0985 & 4.5125 \end{bmatrix}$$

Substrate : dielectric, $\varepsilon_s = 2.25$; $d = 0.8$ µm, $e = 0.495$ µm, $h = 0.1$ µm, $\lambda_0 = 0.7$ µm, $\theta = 22°$. The incident field is TM polarized. The table gives the efficiencies in the different orders. First results are obtained when truncating with N = 15, and using 150 steps for the integration. These parameters are not critical as shown by the following results performed with N = 9 and 80 steps.

h	N	Incident TE wave		Incident TM wave	
		TE → TE	TE → TM	TM → TE	TM → TM
0.06 µm	11	0.466660	0.208 E-4	0.208 E-4	0.2066
	15	0.466629	0.201 E-4	0.201 E-4	0.1999
	19	0.466634	0.198 E-4	0.198 E-4	0.1973
	23	0.466634	0.195 E-4	0.195 E-4	0.1944
0.02 µm	7	0.478795	0.2881 E-4	0.2881 E-4	0.4367
	11	0.478793	0.2870 E-4	0.2870 E-4	0.4354
	15	0.478793	0.2866 E-4	0.2866 E-4	0.4348
	19	0.478793	0.2863 E-4	0.2863 E-4	0.4345

Table 2. Structure is the same as in fig.3. Superstrate is vacuum. Gyrotropic cobalt layer :

$$[\varepsilon_\ell] = \begin{bmatrix} \varepsilon_c & 0 & \varepsilon_{xz} \\ 0 & \varepsilon_c & 0 \\ -\varepsilon_{xz} & 0 & \varepsilon_c \end{bmatrix}, \qquad \begin{aligned} \varepsilon_c &= (-8.19 + i\,16.38)\,, \\ \varepsilon_{xz} &= (-0.495 - i\,0.106)\,. \end{aligned}$$

Substrate : dielectric, $\varepsilon_s = 2.25$; $d = 0.617$ µm, $e = 0.02$ µm, $\lambda_0 = 0.6328$ µm, $\theta = 0°$. The table gives the zero order reflected efficiencies. 40 steps have been used for the integration. N is the number of terms retained in the developments of the fields in generalized Fourier series.

3. THE COATED GRATING STUDIED BY THE INTEGRAL METHOD

For the sake of simplicity, let us explain the principle of this method in the case of an anisotropic grating without coating. The unknowns are now the tangential components of $\vec{E}$ and $\vec{H}$ on the grating profile $\mathcal{P}$, which, as well known, are continuous. These components can be described by 4 functions ($\vec{E}.\vec{e}_z$, $\vec{E}.\vec{t}$, $\vec{H}.\vec{e}_z$, $\vec{H}.\vec{t}$) that we consider as the components of a column matrix F(x). The "key idea" consists in expressing the two following facts :

a) $(F - F^i)$ is the boundary value* on $\mathcal{P}$ of an outgoing field propagating in Ω_1 ; we will refer to this property saying that $(F - F^i)$ belongs to a certain vector space called $\mathcal{V}_1^+$.

b) F is the boundary value on $\mathcal{P}$ of an outgoing field propagating in Ω_2 $(F \in \mathcal{V}_2^-)$.

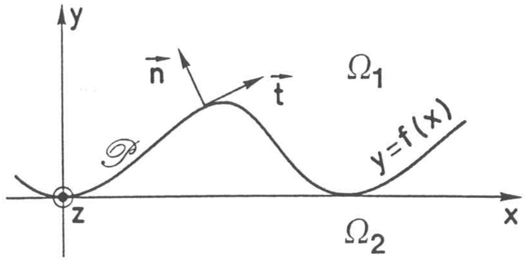

Figure 4. The domain Ω_1 $(y > f(x)$, medium 1) is filled with an isotropic material. The domain Ω_2 $(y < f(x)$, medium 2) is filled with an anisotropic material.

Anyone who has been working in mathematical physics as applied in the electromagnetic theory of gratings will understand that to do that we need a set of nine Green's functions g_{ij}. Putting :

$$\vec{g}_i = \sum_{j=1}^{3} g_{ij}\, \vec{e}_j\,, \qquad i = 1,\, 2,\, 3\,, \tag{1}$$

the g_{ij} are solution of :

$$\text{curl curl}\, \vec{g}_i - k_0^2\, {}^t[\varepsilon]\, \vec{g}_i = \vec{e}_i \sum_n \frac{1}{d}\, \delta(y)\, \overline{\psi}_n(x)\,, \tag{2}$$

where ${}^t[\varepsilon]$ is the transpose of $[\varepsilon]$, $\overline{\psi}_n$ the complex conjugate of ψ_n and δ the Dirac distribution. Indeed, the determination of the Green's functions is not a trivial matter. Nevertheless, we have been able to find the $g_{ij}(x,y)$ in the special case where $[\varepsilon]$ is a diagonal matrix. The interested reader can find more details (including considerations on the Green's functions for infinite space in the case of anisotropic media) in reference 9. We give here the results without proof :

When $[\varepsilon]$ is diagonal, the solutions of (2), which verify an outgoing wave condition when $y \to \pm\infty$, have components which take the form :

$$g_{11}(x,y) = \sum_n \frac{i\,\beta_n}{2d\, k_0^2\, \varepsilon_{xx}} \exp\left(-\, i\, \alpha_n\, x + i\, \beta_n\, |y|\right)$$

$$g_{12}(x,y) = g_{21}(x,y) = \sum_n \frac{i\,\alpha_n}{2d\, k_0^2\, \varepsilon_{yy}}\, \text{sgn}(y)\, \exp\left(-\, i\, \alpha_n\, x + i\, \beta_n\, |y|\right)$$

$$g_{22}(x,y) = \sum_n \frac{1}{d\, k_0^2\, \varepsilon_{yy}} \left[\frac{i\, \varepsilon_{xx}\, \alpha_n^2}{2\, \varepsilon_{yy}\, \beta_n} - \delta(y)\right] \exp\left(-\, i\, \alpha_n\, x + i\, \beta_n\, |y|\right)$$

$$g_{33}(x,y) = \sum_n \frac{i}{2d\, \beta'_n} \exp\left(-\, i\, \alpha_n\, x + i\, \beta'_n\, |y|\right),$$

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

---

* F^i corresponds to the incident field.

In these expressions, sgn(y) denotes the function equal to 1 when y > 0 and to -1 when y < 0. Coefficients β_n and β'_n are defined by :

$$\beta_n = \sqrt{(k_0^2\ \varepsilon_{yy} - \alpha_n^2)\ \varepsilon_{xx}/\varepsilon_{yy}} \quad ; \qquad \beta'_n = \sqrt{k_0^2\ \varepsilon_{zz} - \alpha_n^2}$$

and the square roots (possibly complex if the ε_{ij} are complex) are determined in the following way :

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

With the help of these Green's functions, and after a convenient limiting process (again a non trivial matter!), it turns out that the two propositions a) and b) of the "key idea" can be written in a more explicit manner :

$$\begin{cases} F - F^i \in \vartheta_1^+ \text{ is equivalent to } F - F^i = A_1^+\,(F - F^i)\ , & (3) \\ F \in \vartheta_2^- \text{ is equivalent to } F = A_2^-\,F\ , & (4) \end{cases}$$

where A_1^+ (resp. A_2^-) are integral operators whose kernels depend only on the g_{ij} of medium 1 (resp. medium 2) and their first and second derivatives. Equations (3) and (4) form a system of 8 integral equations for the 4 unknowns. This system S will be called hereafter the "fundamental system". Clearly, many other systems S_i of integral equations can be deduced from the fundamental system. For example, among the 8 equations of S, there are 4 which do not contain the second derivatives of the Green's functions. Let us call S_1 the system that they form. If we assume uniqueness of the solution for both S and S_1, and existence for S, then S and S_1 are equivalent (here they have the same solution). We can wonder which of the systems S_i is the most convenient. Of course the answer to this question can not be given before the world "convenient" had been clearly defined. This problem gave us food for thought during the last months. At the present time we think that S_1 is a good one (if not the best) because the kernels it contains are those to which we have been accustomed when dealing with isotropic gratings (unbounded kernels with a logarithmic singularity).

In conclusion, we are now ready to begin the numerical study of the anisotropic grating when [ε] is a diagonal matrix in the coordinate system we use. Taking into account the experience of our Laboratory in the field of integral equations, we tackle this new task with optimism. On the contrary, it is to be feared that the case of an arbitrary matrix [ε] would give rise to a formidable problem.

ACKNOWLEDGMENTS

Thanks are due to Professor M. Cadilhac for valuable discussions and advices.

We also would like to thank our colleague D. Maystre. He has been working with us when we had the contract with P.A. Technology, and he wrote the first version of our program for anisotropic layers.

The computing facilities used in this paper have been given by the Scientific Council of the "Centre de Calcul Vectoriel pour la Recherche".

REFERENCES

1. Rokushima and Yamakita, "Analysis of anisotropic dielectric gratings", J. Opt. Soc. Am., Vol. 73, n° 7, 901-908, (1983).
2. D.W. Berreman, "Optics in stratified and anisotropic media : 4 x 4 matrix formulation" J. Opt. Soc. Am, Vol. 62, n° 4, 502-510 (1972).
3. P. Yeh, "Electromagnetic propagation in birefringent layered media", J. Opt. Soc. Am., Vol. 69, n° 5, 742-755, (1979).
4. Lin-Chung and Teitler, "4 x 4 matrix formalism for optics in stratified anisotropic media", J. Opt. Soc. Am. A, Vol. 1, n° 7, 703-705, (1984).
5. O. Schwelb, "Stratified lossy anisotropic media : general characteristics", J. Opt. Soc. Am. A, Vol. 3, n° 2, 188-193, (1986).
6. Principles of Optics, Born and Wolf, Pergamon Press, (1965).
7. Electromagnetic Theory of Gratings, Ed. : R. Petit, Topics in Current Physics, Vol. 22, Springer Verlag, (1980).
8. G. Tayeb, R. Petit, M. Cadilhac, "On the theoretical and numerical study of diffraction gratings coated with anisotropic layers." Proceedings of the 14th Congress of the ICO, Québec, August 1987.

9. G. Tayeb, "Sur la résolution de l'équation rot rot $\vec{E}$ - $[A]\vec{E} = \vec{S}$ en théorie des réseaux anisotropes". Proceedings of the 9th Meeting on Hertzian Optics and Dielectrics, Pisa (Italy), September 1987.