Polarization conversion from diffraction gratings made of uniaxial crystals

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(Received 13 September 1995)

We study polarization conversion in the diffraction of light at the periodically corrugated boundary between an isotropic medium and a uniaxial crystal. To do so, we extend a rigorous method originally developed for diffraction gratings made of isotropic materials to include the case of anisotropic media. The theoretical formalism relies upon the use of easy coordinate transformations that map the periodic interface onto a plane. We consider a general configuration in which the incident beam is associated to waves coming either from the isotropic or from the uniaxial side, with any orientation with respect to the grooves of the grating for the plane of incidence (conical diffraction) and for the optical axis of the crystal. The analysis involves no restrictions on the surface relief profile. We apply the method to study conversion between polarization states upon reflection in two situations: (i) incidences from an isotropic, lossless dielectric onto a crystal near total reflection and (ii) from a crystal onto a metal near the resonant excitation of surface plasmons. Good results have been obtained for a groove height-to-period ratio up to 1. [S1063-651X(96)01507-3]

PACS number(s): 42.25.Fx, 42.79.Dj, 78.20.Fm, 73.20.Mf

I. INTRODUCTION

It is well known that conversion between s and p polarization states can occur upon reflection of light at the corrugated interface between isotropic materials when the direction of incidence is not perpendicular to the direction of the grooves (conical diffraction) [1,2]. Conversion between s and p polarization states can also take place at flat interfaces when anisotropic materials are involved. The effects of the simultaneous presence of anisotropy and corrugation on the rate of conversion between different polarization states was first studied in Ref. [3] in two cases: s to p conversion when the incidence is from the isotropic medium onto a crystal and conversion between ordinary and extraordinary modes when the incidence is from a uniaxial crystal onto a metal. The method used in Ref. [3] for calculating the diffracted fields was based on the Rayleigh hypothesis, an approximation that for gratings made of isotropic materials is known to be valid for shallow grooves. Due to this limitation, the results in Ref. [3] were concerned only with gratings with small values of the groove height to period ratio.

To explore the possibility of enhancing the conversion rate between polarization modes at a single anisotropic interface by means of surface reliefs with arbitrary profiles, methods based on the Rayleigh hypothesis cannot be used safely. A rigorous approach for calculating the fields diffracted at the corrugated surface of a uniaxial crystal has been presented in Refs. [4,5]. It is based on the use of coordinate transformations for the boundary conditions and although in principle it permits the surface relief to have an arbitrary profile, it has the disadvantage of requiring additional analytical or numerical effort to find the conformal mapping that transforms each grating profile into a plane. This difficulty is not present in a powerful method developed by Chandezon *et al.* for analyzing gratings made of isotropic materials [6]. It relies upon the use of very simple coordinate transformations (nonconformal) that simplify the treatment of the boundary conditions and that lead to the numerical solution of a system of differential equations with constant coefficients. This method, originally developed for configurations in which the plane of incidence is perpendicular to the grooves (classical diffraction), has been extended to include the case of conical diffraction [1,2,7] and recently it was improved through the use of the R-matrix algorithm [8]. Here we extend the method due to Chandezon *et al.* to the case of gratings ruled on the surface of an uniaxial crystal and use it to study the effects of the simultaneous presence of anisotropy and corrugation on the rate of conversion between different polarization states without being limited to gratings with shallow grooves as in Ref. [3].

II. FORMULATION OF THE PROBLEM

We consider a periodic corrugated boundary $y=a(x)$ (period d) that separates an isotropic medium (dielectric or metal with losses) from a uniaxial crystal with arbitrary orientation of its optic axis. The grooves of the grating are parallel to the z axis and the y axis points towards the isotropic medium (Fig. 1).

A. Constitutive relations

The isotropic medium is characterized by the following constitutive relations:

$$\vec{D}=\epsilon_1\vec{E}, \tag{2.1}$$

$$\vec{B}=\mu_1\vec{H}, \tag{2.2}$$

where ϵ_1 and μ_1 are the permittivity and the permeability of the medium, respectively. In the uniaxial medium the constitutive relations are given by

$$\vec{D}=\tilde{\epsilon}\cdot\vec{E}, \tag{2.3}$$

$$\vec{B}=\mu_2\vec{H}, \tag{2.4}$$

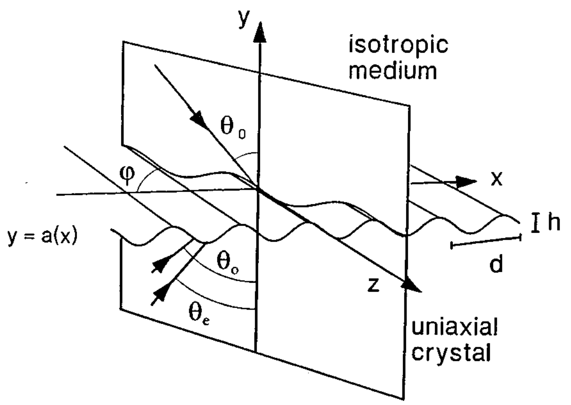

FIG. 1. View of the grating, showing the angles of incidence (θ_0, θ_o, and θ_e) corresponding to the three types of incident waves considered in this paper and the angle between the main section of the grating and the plane of incidence (φ).

where μ_2 is the permeability of the crystal and $\widetilde{\epsilon}$ is the dielectric tensor. This tensor can be written in dyadic form as

$$\widetilde{\epsilon}=\epsilon_{\perp}\widetilde{I}+(\epsilon_{\parallel}-\epsilon_{\perp})\hat{\hat{c}}_0\hat{\hat{c}}_0, \tag{2.5}$$

where $\epsilon_{\perp}$ and $\epsilon_{\parallel}$ are the eigenvalues of $\widetilde{\epsilon}$ and $\widetilde{I}$ is the unit dyadic. $\hat{\hat{c}}_0$ is a unit eigenvector (called optic axis) associated with the nonrepeated eigenvalue $\epsilon_{\parallel}$.

B. Propagation equations

Following the procedure presented in [1,6] we start from Maxwell's equations in each medium

$$\vec{\nabla}\times\vec{E}=-\frac{1}{c}\frac{\partial\vec{B}}{\partial t}, \tag{2.6}$$

$$\vec{\nabla}\times\vec{H}=\frac{1}{c}\frac{\partial\vec{D}}{\partial t}, \tag{2.7}$$

where c is the velocity of light in vacuum. In order to simplify the treatment of the boundary conditions at the interface $y=a(x)$, we use a coordinate transformation of the form

$$u=x, \tag{2.8}$$

$$v=y-a(x), \tag{2.9}$$

$$w=z, \tag{2.10}$$

where (x,y,z) and (u,v,w) are the original and the transformed coordinates, respectively. When we change from coordinates (x,y,z) to (u,v,w) the periodic interface is transformed into a plane and the coordinates x and z remain unchanged. The next step is to express the transformed Maxwell's equations in the isotropic and in the uniaxial zone.

1. Isotropic zone

Writing Maxwell's equations in the transformed frame we obtain a system of six equations with six unknowns (the $\vec{E}$-field and $\vec{H}$-field components). In matrix form this set of equations is written as (Appendix A)

$$\begin{bmatrix}\mathbf{C} & \mathbf{O}\\ \mathbf{O} & \mathbf{C}\end{bmatrix}\mathbf{G}=\frac{i\omega_0}{c}\begin{bmatrix}\mathbf{O} & \mu_1\mathbf{T}_1\\ -\epsilon_1\mathbf{T}_1 & \mathbf{O}\end{bmatrix}\mathbf{G}, \tag{2.11}$$

where $\mathbf{G}$ is a vector formed by the unknowns of the problem

$$\begin{bmatrix}E_u\\ E_v\\ E_w\\ H_u\\ H_v\\ H_w\end{bmatrix}.$$

The system (2.11) can be reduced to a four-variable system involving the components tangential to the grating surface in the $x-y$ plane and those in the z direction. The former are written in terms of the u and v component as

$$H_{\parallel}=[1+a'^2]H_u+a'H_v, \tag{2.12}$$

$$E_{\parallel}=[1+a'^2]E_u+a'E_v. \tag{2.13}$$

Writing Eq. (2.11) in terms of the $\parallel$ and w components of the fields, yields

$$\frac{\partial E_{\parallel}}{\partial v}=\frac{\partial}{\partial u}\left[\mathcal{Y}^2(u)E_{\parallel}-\frac{\mathcal{Y}^1(u)}{\epsilon_1}\left(\frac{c\gamma}{\omega_0}H_{\parallel}+\frac{ic}{\omega_0}\frac{\partial H_w}{\partial u}\right)\right]-\frac{i\omega_0\mu_1}{c}H_w, \tag{2.14}$$

$$\frac{\partial E_w}{\partial v}=\mathcal{Y}^1(u)\left[\left(\frac{i\omega_0\mu_1}{c}-\frac{i\gamma^2c}{\omega_0\epsilon_1}\right)H_{\parallel}+\frac{c\gamma}{\omega_0\epsilon_1}\frac{\partial H_w}{\partial u}\right]+\mathcal{Y}^2(u)\frac{\partial E_w}{\partial u}, \tag{2.15}$$

$$\frac{\partial H_{\parallel}}{\partial v}=\frac{\partial}{\partial u}\left[\mathcal{Y}^2(u)H_{\parallel}+\mathcal{Y}^1(u)\left(\frac{c\gamma}{\omega_0\mu_1}E_{\parallel}+\frac{ic}{\omega_0\mu_1}\frac{\partial E_w}{\partial u}\right)\right]+\frac{i\omega_0\epsilon_1}{c}E_w, \tag{2.16}$$

$$\frac{\partial H_w}{\partial v}=\mathcal{Y}^1(u)\left[\left(-\frac{i\omega_0\epsilon_1}{c}+\frac{ic\gamma^2}{\omega_0\mu_1}\right)E_{\parallel}-\frac{c\gamma}{\omega_0\mu_1}\frac{\partial E_w}{\partial u}\right]+\mathcal{Y}^2(u)\frac{\partial H_w}{\partial u}, \tag{2.17}$$

where we have considered the fact that each component of the fields F depends on the w coordinate in the form

$$F(u,v,w)=F(u,v)\exp(i\gamma w), \tag{2.18}$$

and the functions $\mathcal{Y}^1(u)$ and $\mathcal{Y}^2(u)$ are given by

$$\mathcal{Y}^1(u)=\frac{1}{1+a'^2},\quad \mathcal{Y}^2(u)=\frac{a'}{1+a'^2}.$$

2. Uniaxial zone

In the uniaxial zone, the transformed propagation equations are written in matrix form as (Appendix B)

$$\begin{bmatrix} \mathbf{C} & \mathbf{O} \\ \mathbf{O} & \mathbf{C} \end{bmatrix} \mathbf{G} = \frac{i\omega_0}{c} \begin{bmatrix} \mathbf{O} & \mu_2 \mathbf{T}_1 \\ -\mathbf{T}_2 & \mathbf{O} \end{bmatrix} \mathbf{G}. \tag{2.19}$$

Again, this system is reduced to a four-variable system involving the components $E_\parallel$, E_w, $H_\parallel$, and H_w,

$$\frac{\partial E_\parallel}{\partial v} = \frac{\partial}{\partial u}\left[\mathcal{X}^5(u)E_\parallel + \mathcal{X}^2(u)\left(-\frac{c\gamma}{\omega_0}H_\parallel - \frac{ic}{\omega_0}\frac{\partial H_w}{\partial u} - \epsilon_{vw}E_w \right)\right] - \frac{i\omega_0\mu_2}{c}H_w, \tag{2.20}$$

$$\frac{\partial E_w}{\partial v} = \left[\frac{i\omega_0\mu_2}{c}\mathcal{Y}^1(u) - \frac{i\gamma^2 c}{\omega_0}\mathcal{X}^2(u)\right]H_\parallel + i\gamma\mathcal{X}^3(u)E_\parallel + \frac{c\gamma}{\omega_0}\mathcal{X}^2(u)\frac{\partial H_w}{\partial u} - i\gamma\mathcal{X}^4(u)E_w + \mathcal{Y}^2(u)\frac{\partial E_w}{\partial u}, \tag{2.21}$$

$$\frac{\partial H_\parallel}{\partial v} = \frac{\partial}{\partial u}\left[\mathcal{Y}^2(u)H_\parallel + \mathcal{Y}^1(u)\left(\frac{c\gamma}{\omega_0\mu_2}E_\parallel + \frac{ic}{\omega_0\mu_2}\frac{\partial E_w}{\partial u}\right)\right] + \frac{i\omega_0}{c}\mathcal{X}^7(u)E_\parallel + i\gamma\mathcal{X}^8(u)H_\parallel - \mathcal{X}^8(u)\frac{\partial H_w}{\partial u} + \frac{i\omega_0}{c}\mathcal{X}^{10}(u)E_w, \tag{2.22}$$

$$\frac{\partial H_w}{\partial v} = \left[-\frac{i\omega_0}{c}\mathcal{X}^{11}(u) + \frac{ic\gamma^2}{\omega_0\mu_2}\mathcal{Y}^1(u)\right]E_\parallel + i\gamma[\mathcal{X}^{12}(u) + \mathcal{Y}^2(u)]H_\parallel - \mathcal{X}^{12}(u)\frac{\partial H_w}{\partial u} + \frac{i\omega_0}{c}\mathcal{X}^{13}(u)E_w - \frac{c\gamma}{\omega_0\mu_2}\mathcal{Y}^1(u)\frac{\partial E_w}{\partial u}, \tag{2.23}$$

where

$$\mathcal{X}^1(u) = 1 + a'^2 - a'\frac{\epsilon_{vu}}{\epsilon_{vv}},$$

$$\mathcal{X}^2(u) = \frac{1}{\epsilon_{vv}\mathcal{X}^1(u)},$$

$$\mathcal{X}^3(u) = \frac{\mathcal{X}^1(u) - (1+a'^2)}{(1+a'^2)a'\mathcal{X}^1(u)},$$

$$\mathcal{X}^4(u) = \epsilon_{vw}\mathcal{X}^2(u),$$

$$\mathcal{X}^5(u) = \frac{\mathcal{X}^1(u) - 1}{a'\mathcal{X}^1(u)},$$

$$\mathcal{X}^6(u) = \mathcal{X}^4(u),$$

$$\mathcal{X}^7(u) = \frac{\epsilon_{wu}}{\mathcal{X}^1(u)} + \epsilon_{wv}\left[\frac{\mathcal{X}^1(u) - (1+a'^2)}{a'\mathcal{X}^1(u)}\right],$$

$$\mathcal{X}^8(u) = \frac{a'\epsilon_{wu}}{\epsilon_{vv}\mathcal{X}^1(u)} - \frac{\epsilon_{wv}(1+a'^2)}{\epsilon_{vv}\mathcal{X}^1(u)},$$

$$\mathcal{X}^{10}(u) = \mathcal{X}^8(u)\epsilon_{vw} + \epsilon_{ww},$$

$$\mathcal{X}^{11}(u) = \frac{\epsilon_{uu}}{\mathcal{X}^1(u)} + \epsilon_{uv}\left[\frac{\mathcal{X}^1(u) - (1+a'^2)}{a'\mathcal{X}^1(u)}\right],$$

$$\mathcal{X}^{12}(u) = -\frac{a'\epsilon_{uu}}{\epsilon_{vv}\mathcal{X}^1(u)} + \frac{\epsilon_{uv}(1+a'^2)}{\epsilon_{vv}\mathcal{X}^1(u)},$$

$$\mathcal{X}^{13}(u) = \mathcal{X}^{12}(u)\epsilon_{vw} - \epsilon_{uw}.$$

To check these expressions, it is easy to demonstrate that Eqs. (2.20)–(2.23) reduce to (2.14)–(2.17) when $\epsilon_\parallel = \epsilon_\perp$ (isotropic medium).

C. Incident and diffracted fields

We consider that the grating may be illuminated from the isotropic (when it is a dielectric) or from the uniaxial side. In the dielectric medium the incident electric field $\vec{E}_1^i$ is written as

$$\vec{E}_1^i = \frac{1}{\eta}\left[\left(-\gamma\alpha_0 R + \frac{\omega_0}{c}\mu_1\beta_0 S\right)\hat{\vec{x}} + \left(-\frac{\omega_0}{c}\mu_1\alpha_0 S + \gamma\beta_0 R\right)\hat{\vec{y}} + R\hat{\vec{z}}\right]\exp(i\vec{k}_i\cdot\vec{r}). \tag{2.24}$$

and the incident magnetic field $\vec{H}_1^i$ is

$$\vec{H}_1^i = \frac{1}{\eta}\left[\left(-\gamma\alpha_0 S - \frac{\omega_0}{c}\epsilon_1\beta_0 R\right)\hat{\vec{x}} + \left(-\frac{\omega_0}{c}\epsilon_1\alpha_0 R + \gamma\beta_0 S\right)\hat{\vec{y}} + S\hat{\vec{z}}\right]\exp(i\vec{k}_i\cdot\vec{r}), \tag{2.25}$$

where

$$\eta = \frac{\omega_0^2\mu_1\epsilon_1}{c^2} - \gamma^2.$$

$\vec{k}_i$ is the incident wave vector and is given by

$$\vec{k}_i = \alpha_0\hat{\vec{x}} - \beta_0\hat{\vec{y}} + \gamma\hat{\vec{z}}, \tag{2.26}$$

where

$$\alpha_0 = \frac{\omega_0}{c}(\epsilon_1\mu_1)^{1/2}\sin\theta_0\cos\varphi, \tag{2.27}$$

$$\beta_0 = \frac{\omega_0}{c}(\epsilon_1\mu_1)^{1/2}\cos\theta_0, \tag{2.28}$$

$$\gamma = \frac{\omega_0}{c}(\epsilon_1\mu_1)^{1/2}\sin\theta_0\sin\varphi. \tag{2.29}$$

In these expressions θ_0 is the angle between the incident wave vector $\vec{k}_i$ and the y axis, and φ is the angle between the $x-y$ plane and the plane of incidence. R and S are the amplitudes of the z components of the incident electric and magnetic field, respectively. These amplitudes are expressed in terms of the s and p polarization amplitudes (A_s and A_p) of the incident electric field as

$$R = A_s\cos\varphi + A_p\cos\theta\sin\varphi, \tag{2.30}$$

$$S = \left(\frac{\epsilon_1}{\mu_1}\right)^{1/2}[-A_s\cos\theta\sin\varphi + A_p\cos\varphi]. \tag{2.31}$$

We now turn to incidence from the uniaxial side. Taking into account that waves of the ordinary or extraordinary type can propagate in the crystal we have to distinguish these two cases in the incident fields. The electric field associated with an ordinary incident wave is written as

$$\vec{E}_2^i = C_o\vec{e}_o\exp(i\vec{k}_o\cdot\vec{r}), \tag{2.32}$$

and the corresponding magnetic field is

$$\vec{H}_2^i = C_o\vec{h}_o\exp(i\vec{k}_o\cdot\vec{r}). \tag{2.33}$$

The vectors $\vec{e}_o$ and $\vec{h}_o$ specify the polarization of the incident electric and magnetic fields, respectively, and are given by

$$\vec{e}_o = \vec{k}_o\times\hat{\vec{c}}_0, \tag{2.34}$$

$$\vec{h}_o = \frac{c}{\omega_0\mu_2}(\vec{k}_o\times\vec{e}_o). \tag{2.35}$$

$\vec{k}_o$ is the wave vector associated with an ordinary incident wave and is written as

$$\vec{k}_o = \alpha_o\hat{\vec{x}} + \alpha_1\hat{\vec{y}} + \gamma\hat{\vec{z}}, \tag{2.36}$$

where

$$\alpha_o = \frac{\omega_0}{c}(\epsilon_\perp\mu_2)^{1/2}\sin\theta_o\cos\varphi, \tag{2.37}$$

$$\alpha_1 = \frac{\omega_0}{c}(\epsilon_\perp\mu_2)^{1/2}\cos\theta_o, \tag{2.38}$$

$$\gamma = \frac{\omega_0}{c}(\epsilon_\perp\mu_2)^{1/2}\sin\theta_o\sin\varphi, \tag{2.39}$$

θ_o being the angle between the incident wave vector and the y axis. For an incident wave of the extraordinary type with wave vector forming an angle θ_e with the y axis we have

$$\vec{E}_2^i = C_e\vec{e}_e\exp(i\vec{k}_e\cdot\vec{r}), \tag{2.40}$$

and the corresponding magnetic field is

$$\vec{H}_2^i = C_e\vec{h}_e\exp(i\vec{k}_e\cdot\vec{r}), \tag{2.41}$$

where C_e represents the incident amplitude. In this case, the polarizations of the fields are given by the vectors

$$\vec{e}_e = \frac{\omega_0^2}{c^2}\epsilon_\perp\mu_2\hat{\vec{c}}_0 - \vec{k}_e(\vec{k}_e\cdot\hat{\vec{c}}_0), \tag{2.42}$$

$$\vec{h}_e = \frac{c}{\omega_0\mu_2}(\vec{k}_e\times\vec{e}_e), \tag{2.43}$$

$\vec{k}_e$ being the wave vector associated with an extraordinary incident field. It can be expressed as

$$\vec{k}_e = \alpha_e\hat{\vec{x}} + \alpha_2\hat{\vec{y}} + \gamma\hat{\vec{z}}, \tag{2.44}$$

and

$$\alpha_e = \pm\Gamma(\theta_e)\sin\theta_e\cos\varphi, \tag{2.45}$$

$$\alpha_2 = \pm\Gamma(\theta_e)\cos\theta_e, \tag{2.46}$$

$$\gamma = \pm\Gamma(\theta_e)\sin\theta_e\sin\varphi, \tag{2.47}$$

with

$$\Gamma(\theta_e) = \frac{\omega_0}{c}\left[\frac{\mu_2\epsilon_\perp\epsilon_\|}{(\epsilon_\| - \epsilon_\perp)(c_{0x}\sin\theta_e\cos\varphi + c_{0y}\cos\theta_e + c_{0z}\sin\theta_e\sin\varphi)^2 + \epsilon_\perp}\right]^{1/2}. \tag{2.48}$$

The upper (lower) sign in expressions (2.45)–(2.47) corresponds to $\Psi \geqslant 0$ ($\Psi < 0$) where

$$\Psi = \epsilon_\perp\cos\theta_e + (\epsilon_\| - \epsilon_\perp)c_{0y}(c_{0x}\sin\theta_e\cos\varphi + c_{0y}\cos\theta_e + c_{0z}\sin\theta_e\sin\varphi). \tag{2.49}$$

We are now able to write the diffracted fields in both media. In the isotropic region (for a dielectric) the diffracted fields can be written as

$$\vec{E}_1^d = \sum_n \frac{1}{\eta}\left[\left(-\gamma\alpha_n R_n - \frac{\omega_0}{c}\mu_1\beta_n S_n\right)\hat{\vec{x}} + \left(\frac{\omega_0}{c}\mu_1\alpha_n S_n - \gamma\beta_n R_n\right)\hat{\vec{y}} + R_n\hat{\vec{z}}\right]\exp(i\vec{k}_{1n}\cdot\vec{r}), \tag{2.50}$$

$$\vec{H}_1^d = \sum_n \frac{1}{\eta}\left[\left(-\gamma\alpha_n S_n + \frac{\omega_0}{c}\epsilon_1\beta_n R_n\right)\hat{\vec{x}} + \left(-\frac{\omega_0}{c}\epsilon_1\alpha_n R_n - \gamma\beta_n S_n\right)\hat{\vec{y}} + S_n\hat{\vec{z}}\right]\exp(i\vec{k}_{1n}\cdot\vec{r}). \tag{2.51}$$

In these expressions R_n and S_n are unknown complex amplitudes and $\vec{k}_{1n}$ is the wave vector of the n diffracted order in the isotropic medium

$$\vec{k}_{1n}=\alpha_n\hat{\hat{x}}+\beta_n\hat{\hat{y}}+\gamma\hat{\hat{z}}, \tag{2.52}$$

where

$$\alpha_n=\alpha+\frac{2\pi n}{d}, \tag{2.53}$$

$$\beta_n=\left(\frac{\omega_0^2}{c^2}\epsilon_1\mu_1-\alpha_n^2-\gamma^2\right)^{1/2}. \tag{2.54}$$

The square root in expression (2.54) is selected so as to obtain $\mathrm{Im}(\beta_n)>0$ or $\beta_n>0$ if $\mathrm{Im}(\beta_n)=0$. α is the x component of the incident wave vector and is given by Eq. (2.27) for a wave incident from the isotropic side, by (2.37) for an ordinary incident wave and by (2.45) for an extraordinary one.

In the uniaxial medium the diffracted fields are written as

$$\vec{E}_2^d=\sum_n [C_{on}\vec{e}_{on}\exp(i\vec{k}_{on}\cdot\vec{r})+C_{en}\vec{e}_{en}\exp(i\vec{k}_{en}\cdot\vec{r})], \tag{2.55}$$

$$\vec{H}_2^d=\sum_n [C_{on}\vec{h}_{on}\exp(i\vec{k}_{on}\cdot\vec{r})+C_{en}\vec{h}_{en}\exp(i\vec{k}_{en}\cdot\vec{r})]. \tag{2.56}$$

In these expressions C_{on} and C_{en} are unknown complex amplitudes and $\vec{k}_{on}$ and $\vec{k}_{en}$ are wave vectors associated, respectively, with ordinary and extraordinary diffracted waves

$$\vec{k}_{on}=\alpha_n\hat{\hat{x}}+\alpha_{1n}\hat{\hat{y}}+\gamma\hat{\hat{z}}, \tag{2.57}$$

$$\alpha_{1n}=\begin{cases} -\left(\frac{\omega_0^2}{c^2}\epsilon_\perp\mu_2-\alpha_n^2-\gamma^2\right)^{1/2} & \text{for } \frac{\omega_0^2}{c^2}\epsilon_\perp\mu_2>\alpha_n^2+\gamma^2, \\ -i\left(\alpha_n^2+\gamma^2-\frac{\omega_0^2}{c^2}\epsilon_\perp\mu_2\right)^{1/2} & \text{for } \frac{\omega_0^2}{c^2}\epsilon_\perp\mu_2<\alpha_n^2+\gamma^2. \end{cases} \tag{2.58}$$

$$\vec{k}_{en}=\alpha_n\hat{\hat{x}}+\alpha_{2n}\hat{\hat{y}}+\gamma\hat{\hat{z}}, \tag{2.59}$$

$$\alpha_{2n}=\frac{-(\epsilon_\parallel-\epsilon_\perp)c_{0y}(\alpha_n c_{0x}+\gamma c_{0z})-(\Phi_n)^{1/2}}{\epsilon_\perp+(\epsilon_\parallel-\epsilon_\perp)c_{0y}^2}, \tag{2.60}$$

$$\Phi_n=c_{0y}^2(\epsilon_\parallel-\epsilon_\perp)^2(\alpha_n c_{0x}+\gamma c_{0z})^2-[\epsilon_\perp+(\epsilon_\parallel-\epsilon_\perp)c_{0y}^2]\Bigg[(\alpha_n^2+\gamma^2)\epsilon_\perp+(\epsilon_\parallel-\epsilon_\perp)(\alpha_n^2c_{0x}^2+\gamma^2c_{0z}^2)$$
$$+2\alpha_n\gamma(\epsilon_\parallel-\epsilon_\perp)c_{0x}c_{0z}-\frac{\omega_0^2}{c^2}\mu_2\epsilon_\perp\epsilon_\parallel\Bigg]. \tag{2.61}$$

The square root in expression (2.60) is selected so as to obtain $\mathrm{Im}(\Phi_n^{1/2})>0$. The fields associated with the ordinary diffracted orders are

$$\vec{e}_{on}=\vec{k}_{on}\times\hat{\vec{c}}_o, \tag{2.62}$$

$$\vec{h}_{on}=\frac{c}{\omega_0\mu_2}[\vec{k}_{on}\times\vec{e}_{on}], \tag{2.63}$$

whereas the fields associated with the extraordinary diffracted orders are given by

$$\vec{e}_{en}=\frac{\omega_0^2}{c^2}\epsilon_\perp\mu_2\hat{\vec{c}}_o-\vec{k}_{en}(\vec{k}_{en}\cdot\hat{\vec{c}}_o), \tag{2.64}$$

$$\vec{h}_{en}=\frac{\omega_0}{c}\epsilon_\perp(\vec{k}_{en}\times\hat{\vec{c}}_o). \tag{2.65}$$

Having found the expressions of the incident and diffracted fields in the dielectric medium and in the uniaxial one, we wish to write these expressions in the new coordinate system (u,v,w). We begin by transforming the fields in the isotropic region [1]. The w component of the incident electric field E_{1w}^i is written in the transformed space as

$$E_{1w}^i=R\exp(i\gamma w-i\beta_0 v)\exp[i\alpha_0 u-i\beta_0 a(u)], \tag{2.66}$$

and the w component of the magnetic field is

$$H_{1w}^i=S\exp(i\gamma w-i\beta_0 v)\exp[i\alpha_0 u-i\beta_0 a(u)]. \tag{2.67}$$

Performing a Fourier series expansion Eqs. (2.66) and (2.67) can be written as

$$E_{1w}^i=R\sum_m L_m(\beta_0)\exp[i(\alpha_m u-\beta_0 v+\gamma w)], \tag{2.68}$$

and

$$H^i_{1w}=S\sum_m L_m(\beta_0)\exp[i(\alpha_m u-\beta_0 v+\gamma w)], \quad (2.69)$$

where

$$L_m(s)=\frac{1}{d}\int_0^d \exp\{-i[a(u)s+mKu]\}du, \quad (2.70)$$

K being equal to $2\pi/d$. Next, we have to find the components $\parallel$ of the incident fields. Using Eqs. (2.15) and (2.17) we find that these components are written as

$$E^i_{1\parallel}=\frac{1}{f1}\sum_m \left[\left(\frac{\alpha_0}{\beta_0}mK-\beta_0\right)S+(\alpha_0+mK)\frac{\gamma c}{\omega_0\mu_1}R\right]\times L_m(\beta_0)\exp[i(\alpha_m u-\beta_0 v+\gamma w)], \quad (2.71)$$

$$H^i_{1\parallel}=\frac{1}{f2}\sum_m \left[\left(\frac{\alpha_0}{\beta_0}mK-\beta_0\right)R-(\alpha_0+mK)\frac{\gamma c}{\omega_0\epsilon_1}S\right]\times L_m(\beta_0)\exp[i(\alpha_m u-\beta_0 v+\gamma w)], \quad (2.72)$$

where

$$f1=\frac{c\gamma^2}{\omega_0\mu_1}-\frac{\omega_0\epsilon_1}{c},$$

$$f2=-\frac{c\gamma^2}{\omega_0\epsilon_1}+\frac{\omega_0\mu_1}{c}.$$

Using the same procedure, we obtain that the $\parallel$ components of the diffracted fields are given by

$$E^d_{1\parallel}=\frac{1}{f1}\sum_n\sum_m \left\{\left[-\frac{\alpha_n}{\beta_n}(m-n)K+\beta_n\right]S_n +[\alpha_n+(m-n)K]\frac{\gamma c}{\omega_0\mu_1}R_n\right\}L_{m-n}(-\beta_n)\times\exp[i(\alpha_m u+\beta_n v+\gamma w)], \quad (2.73)$$

$$H^d_{1\parallel}=\frac{1}{f2}\sum_n\sum_m \left\{\left[-\frac{\alpha_n}{\beta_n}(m-n)K+\beta_n\right]R_n -[\alpha_n+(m-n)K]\frac{\gamma c}{\omega_0\epsilon_1}S_n\right\}L_{m-n}(-\beta_n)\times\exp[i(\alpha_m u+\beta_n v+\gamma w)], \quad (2.74)$$

and the w components are written as

$$E^d_{1w}=\sum_n\sum_m R_n L_{m-n}(-\beta_n)\exp[i(\alpha_m u+\beta_n v+\gamma w)], \quad (2.75)$$

$$H^d_{1w}=\sum_n\sum_m S_n L_{m-n}(-\beta_n)\exp[i(\alpha_m u+\beta_n v+\gamma w)], \quad (2.76)$$

where R_n and S_n are unknowns of the problem and give the amplitudes of the diffracted orders in the dielectric zone.

We now write the transformed incident and diffracted fields in the uniaxial medium. By the same procedure followed in the isotropic zone the w components of the incident fields are written as

$$E^i_{2w}=C_{o,e}(\vec{e}_{o,e}\cdot\hat{\hat{z}})\sum_m [L_m(-\alpha_{1,2})\exp[i(\alpha_m u+\alpha_{1,2}v+\gamma w)], \quad (2.77)$$

$$H^i_{2w}=C_{o,e}(\vec{h}_{o,e}\cdot\hat{\hat{z}})\sum_m [L_m(-\alpha_{1,2})\exp[i(\alpha_m u+\alpha_{1,2}v+\gamma w)]. \quad (2.78)$$

Combining Eqs. (2.21) and (2.23) we find the $\parallel$ components of the incident fields

$$E^i_{2\parallel}=\sum_n\sum_m [(i\alpha_{1,2}J_{1n}+i\alpha_m J_{4n}+J_{5n})(\vec{e}_{o,e}\cdot\hat{\hat{z}}) +(i\alpha_{1,2}J_{2n}+i\alpha_m J_{3n})(\vec{h}_{o,e}\cdot\hat{\hat{z}})]C_{o,e}L_m(-\alpha_{1,2})\times\exp[i(\alpha_m u+\alpha_{1,2}v+\gamma w)], \quad (2.79)$$

$$H^i_{2\parallel}=\sum_n\sum_m [(i\alpha_{1,2}I_{1n}+i\alpha_m I_{4n}+I_{5n})(\vec{e}_{o,e}\cdot\hat{\hat{z}}) +(i\alpha_{1,2}I_{2n}+i\alpha_m I_{3n})(\vec{h}_{o,e}\cdot\hat{\hat{z}})]C_{o,e}L_m(-\alpha_{1,2})\times\exp[i(\alpha_m u+\alpha_{1,2}v+\gamma w)], \quad (2.80)$$

where the subscript 1 (2) corresponds to an ordinary (extraordinary) incident wave. The I's and the J's are the Fourier transforms of the following functions:

$$I_1(u)=\left[\frac{i\omega_0\mu_2}{c}\mathcal{Y}^1(u)-\frac{ic\gamma^2}{\omega_0}\mathcal{X}^2(u) +\frac{i\gamma^2\mathcal{X}^3(u)[\mathcal{X}^{12}(u)+\mathcal{Y}^2(u)]}{\frac{\omega_0}{c}\mathcal{X}^{11}(u)-\frac{c\gamma^2}{\omega_0\mu_2}\mathcal{Y}^1(u)}\right]^{-1},$$

$$I_2(u)=\frac{\gamma\mathcal{X}^3(u)I_1(u)}{\frac{\omega_0}{c}\mathcal{X}^{11}(u)-\frac{c\gamma^2}{\omega_0\mu_2}\mathcal{Y}^1(u)},$$

$$I_3(u)=I_2(u)\mathcal{X}^{12}(u)-\frac{c\gamma}{\omega_0}\mathcal{X}^2(u)I_1(u),$$

$$I_4(u)=\frac{c\gamma}{\omega_0\mu_2}\mathcal{Y}^1(u)I_2(u)-\mathcal{Y}^2(u)I_1(u),$$

$$I_5(u)=-\frac{i\omega_0}{c}\mathcal{X}^{13}(u)I_2(u)+i\gamma\mathcal{X}^4(u)I_1(u),$$

$$J(u) = -\frac{i\omega_0}{c}\mathcal{X}^{11}(u) + \frac{ic\gamma^2}{\omega_0\mu_2}\mathcal{Y}^1(u),$$

$$J_1(u) = -I_1(u)\gamma i[\mathcal{X}^{12}(u)+\mathcal{Y}^2(u)]/J,$$

$$J_2(u) = \{1 - I_2(u)\gamma i[\mathcal{X}^{12}(u)+\mathcal{Y}^2(u)]\}/J,$$

$$J_3(u) = \{\mathcal{X}^{12}(u) - I_3(u)\gamma i[\mathcal{X}^{12}(u)+\mathcal{Y}^2(u)]\}/J,$$

$$J_4(u) = \left\{\frac{c\gamma}{\omega_0\mu_2}\mathcal{Y}^1(u) - I_4(u)\gamma i[\mathcal{X}^{12}(u)+\mathcal{Y}^2(u)]\right\}\Big/ J,$$

$$J_5(u) = \left\{-I_5(u)\gamma i[\mathcal{X}^{12}(u)+\mathcal{Y}^2(u)] - \frac{i\omega_0}{c}\mathcal{X}^{13}(u)\right\}\Big/ J.$$

The $\|$ components of the diffracted fields in the uniaxial medium are given by

$$\begin{aligned} E^d_{2\|} = \sum_{n,m,p} &\{[i\alpha_{1n}(e_{onz}J_{1p}+h_{onz}J_{2p}) + i\alpha_m h_{onz}J_{3p} \\ &+(i\alpha_m J_{4p}+J_{5p})e_{onz}]C_{on}L_{m-n}(-\alpha_{1n})\exp(i\alpha_{1n}v) \\ &+[i\alpha_{2n}(e_{enz}J_{1p}+h_{enz}J_{2p}) + i\alpha_m h_{enz}J_{3p} \\ &+(i\alpha_m J_{4p}+J_{5p})e_{enz}]C_{en}L_{m-n}(-\alpha_{2n})\exp(i\alpha_{2n}v)\} \\ &\times\exp[i(\alpha_m u+\gamma w)], \end{aligned} \tag{2.81}$$

$$\begin{aligned} H^d_{2\|} = \sum_{n,m,p} &\{[i\alpha_{1n}(e_{onz}I_{1p}+h_{onz}I_{2p}) + i\alpha_m h_{onz}I_{3p} \\ &+(i\alpha_m I_{4p}+I_{5p})e_{onz}]C_{on}L_{m-n}(-\alpha_{1n})\exp(i\alpha_{1n}v) \\ &+[i\alpha_{2n}(e_{enz}I_{1p}+h_{enz}I_{2p}) + i\alpha_m h_{enz}I_{3p} \\ &+(i\alpha_m I_{4p}+I_{5p})e_{enz}]C_{en}L_{m-n}(-\alpha_{2n})\exp(i\alpha_{2n}v)\} \\ &\times\exp[i(\alpha_m u+\gamma w)], \end{aligned} \tag{2.82}$$

and the w components are

$$\begin{aligned} E^d_{2w} = \sum_{n,m} &[C_{on}e_{onz}L_{m-n}(-\alpha_{1n})\exp(i\alpha_{1n}v) \\ &+C_{en}e_{enz}L_{m-n}(-\alpha_{2n})\exp(i\alpha_{2n}v)] \\ &\times\exp[i(\alpha_m u+\gamma w)], \end{aligned} \tag{2.83}$$

$$\begin{aligned} H^d_{2w} = \sum_{n,m} &[C_{on}h_{onz}L_{m-n}(-\alpha_{1n})\exp(i\alpha_{1n}v) \\ &+C_{en}h_{enz}L_{m-n}(-\alpha_{2n})\exp(i\alpha_{2n}v)]\exp[i(\alpha_m u \\ &+\gamma w)], \end{aligned} \tag{2.84}$$

where e_{onz}, h_{onz}, e_{enz}, and h_{enz} are the z components of the vectors $\vec{e}_{on}$, $\vec{h}_{on}$, $\vec{e}_{en}$, and $\vec{h}_{en}$, respectively.

III. NUMERICAL SOLUTION

To solve the problem we have to find the solutions of Eqs. (2.14)–(2.17) in the isotropic medium and of Eqs. (2.20)–(2.23) in the uniaxial one. To do so, we expand all the functions of the grating profile in the Fourier series, i.e., each function $\mathcal{Y}$ in Eqs. (2.14)–(2.17) and $\mathcal{X}$ in Eqs. (2.20)–(2.23) can be written as

$$\mathcal{Y}(u) = \sum_q \mathcal{Y}_q\exp(iqKu), \tag{3.1}$$

and

$$\mathcal{X}(u) = \sum_q \mathcal{X}_q\exp(iqKu). \tag{3.2}$$

Analogously, each component of the fields F can be expressed as

$$F(u,v) = \sum_m F_m(v)\exp(i\alpha_m u). \tag{3.3}$$

Introducing these expansions in Eqs. (2.14)–(2.17) we obtain

$$\begin{aligned} -i\frac{\partial E^{\|}_j}{\partial v} = \sum_m &\alpha_j\mathcal{Y}^2_{j-m}E^{\|}_m - \frac{c\gamma}{\omega_0\epsilon_1}\alpha_j\mathcal{Y}^1_{j-m}H^{\|}_m \\ &+\left[\frac{c}{\omega_0\epsilon_1}\alpha_j\alpha_m\mathcal{Y}^1_{j-m} - \frac{\omega_0}{c}\mu_1\delta_{j,m}\right]H^w_m, \end{aligned} \tag{3.4}$$

$$\begin{aligned} -i\frac{\partial E^w_j}{\partial v} = \sum_m &\alpha_m\mathcal{Y}^2_{j-m}E^w_m + \left[\frac{\omega_0}{c}\mu_1 - \frac{\gamma^2 c}{\omega_0\epsilon_1}\right]\mathcal{Y}^1_{j-m}H^{\|}_m \\ &+\frac{c\gamma}{\omega_0\epsilon_1}\alpha_m\mathcal{Y}^1_{j-m}H^w_m, \end{aligned} \tag{3.5}$$

$$\begin{aligned} -i\frac{\partial H^{\|}_j}{\partial v} = \sum_m &\frac{c\gamma\alpha_j}{\omega_0\mu_1}\mathcal{Y}^1_{j-m}E^{\|}_m + \left[-\frac{c}{\omega_0\mu_1}\alpha_j\alpha_m\mathcal{Y}^1_{j-m}\right. \\ &\left.+\frac{\omega_0}{c}\epsilon_1\delta_{j,m}\right]E^w_m + \alpha_j\mathcal{Y}^2_{j-m}H^{\|}_m, \end{aligned} \tag{3.6}$$

$$\begin{aligned} -i\frac{\partial H^w_j}{\partial v} = \sum_m &\left[\frac{c\gamma^2}{\omega_0\mu_1} - \frac{\omega_0}{c}\epsilon_1\right]\mathcal{Y}^1_{j-m}E^{\|}_m - \frac{c\gamma}{\omega_0\mu_1}\alpha_m\mathcal{Y}^1_{j-m}E^w_m \\ &+\alpha_m\mathcal{Y}^2_{j-m}H^w_m. \end{aligned} \tag{3.7}$$

In order to solve these equations numerically, we truncate the series in such a way that the indices j and m have values between $-N$ and N. Defining a vector $\boldsymbol{\xi}$ [$(8N+4)$ elements] formed by the expansions of the components of the electric and magnetic field

$$\boldsymbol{\xi}(v) = \begin{bmatrix} E_\| \\ E_w \\ H_\| \\ H_w \end{bmatrix},$$

Eqs. (3.4)–(3.7) can be written in matrix notation as

$$-i\frac{d\boldsymbol{\xi}(v)}{dv} = \mathbf{Z}_1(v)\boldsymbol{\xi}(v), \tag{3.8}$$

where $\mathbf{Z}_1$ is a $(8N+4)\times(8N+4)$ matrix of the form

$$\mathbf{Z}_1 = \begin{bmatrix} \mathbf{A}_1 & \mathbf{O}_1 & \mathbf{C}_1 & \mathbf{D}_1 \\ \mathbf{O}_1 & \mathbf{F}_1 & \mathbf{G}_1 & \mathbf{H}_1 \\ \mathbf{I}_1 & \mathbf{J}_1 & \mathbf{A}_1 & \mathbf{O}_1 \\ \mathbf{M}_1 & \mathbf{N}_1 & \mathbf{O}_1 & \mathbf{F}_1 \end{bmatrix}, \tag{3.9}$$

and where we have followed the notation presented in [1] and

$$\mathbf{A}_1 = \alpha_j \mathcal{Y}^2_{j-m}, \tag{3.10}$$

$$\mathbf{C}_1 = -\frac{c\gamma}{\omega_0 \epsilon_1} \alpha_j \mathcal{Y}^1_{j-m}, \tag{3.11}$$

$$\mathbf{D}_1 = \frac{c}{\omega_0 \epsilon_1} \alpha_j \alpha_m \mathcal{Y}^1_{j-m} - \frac{\omega_0}{c} \mu_1 \delta_{j,m}, \tag{3.12}$$

$$\mathbf{F}_1 = \mathcal{Y}^2_{j-m} \alpha_m, \tag{3.13}$$

$$\mathbf{G}_1 = \left[\frac{\omega_0}{c} \mu_1 - \frac{\gamma^2 c}{\omega_0 \epsilon_1} \right] \mathcal{Y}^1_{j-m}, \tag{3.14}$$

$$\mathbf{H}_1 = \frac{c\gamma}{\omega_0 \epsilon_1} \alpha_m \mathcal{Y}^1_{j-m}, \tag{3.15}$$

$$\mathbf{I}_1 = \frac{c\gamma\alpha_j}{\omega_0 \mu_1} \mathcal{Y}^1_{j-m}, \tag{3.16}$$

$$\mathbf{J}_1 = -\frac{c}{\omega_0 \mu_1} \alpha_j \alpha_m \mathcal{Y}^1_{j-m} + \frac{\omega_0}{c} \epsilon_1 \delta_{j,m}, \tag{3.17}$$

$$\mathbf{M}_1 = \left[\frac{c\gamma^2}{\omega_0 \mu_1} - \frac{\omega_0}{c} \epsilon_1 \right] \mathcal{Y}^1_{j-m}, \tag{3.18}$$

$$\mathbf{N}_1 = -\frac{c\gamma}{\omega_0 \mu_1} \alpha_m \mathcal{Y}^1_{j-m}, \tag{3.19}$$

$$\mathbf{O}_1 = 0, \tag{3.20}$$

are matrices of $(2N+1)\times(2N+1)$ elements. Equations (2.20)–(2.23) are rewritten as

$$-i\frac{\partial E^{\parallel}_j}{\partial v} = \sum_m \alpha_j \mathcal{X}^5_{j-m} E^{\parallel}_m - \alpha_j \mathcal{X}^6_{j-m} E^w_m - \frac{c\gamma}{\omega_0} \alpha_j \mathcal{X}^2_{j-m} H^{\parallel}_m + \left[\frac{c}{\omega_0} \alpha_j \alpha_m \mathcal{X}^2_{j-m} - \frac{\omega_0}{c} \mu_2 \delta_{j,m} \right] H^w_m, \tag{3.21}$$

$$-i\frac{\partial E^w_j}{\partial v} = \sum_m \gamma \mathcal{X}^3_{j-m} E^{\parallel}_m + (\mathcal{Y}^2_{j-m}\alpha_m - \gamma \mathcal{X}^4_{j-m}) E^w_m + \left[\frac{\omega_0}{c} \mu_2 \mathcal{Y}^1_{j-m} - \frac{\gamma^2 c}{\omega_0} \mathcal{X}^2_{j-m} \right] H^{\parallel}_m + \frac{c\gamma}{\omega_0} \alpha_m \mathcal{X}^2_{j-m} H^w_m, \tag{3.22}$$

$$-i\frac{\partial H^{\parallel}_j}{\partial v} = \sum_m \left[\frac{c\gamma\alpha_j}{\omega_0 \mu_2} \mathcal{Y}^1_{j-m} + \frac{\omega_0}{c} \mathcal{X}^7_{j-m} \right] E^{\parallel}_m + \left[-\frac{c}{\omega_0 \mu_2} \alpha_j \alpha_m \mathcal{Y}^1_{j-m} + \frac{\omega_0}{c} \mathcal{X}^{10}_{j-m} \right] E^w_m + [\alpha_j \mathcal{Y}^2_{j-m} + \gamma \mathcal{X}^8_{j-m}] H^{\parallel}_m - \mathcal{X}^8_{j-m} \alpha_m H^w_m, \tag{3.23}$$

$$-i\frac{\partial H^w_j}{\partial v} = \sum_m \left[\frac{c\gamma^2}{\omega_0 \mu_2} \mathcal{Y}^1_{j-m} - \frac{\omega_0}{c} \mathcal{X}^{11}_{j-m} \right] E^{\parallel}_m + \left[\frac{\omega_0}{c} \mathcal{X}^{13}_{j-m} - \frac{c\gamma}{\omega_0 \mu_2} \alpha_m \mathcal{Y}^1_{j-m} \right] E^w_m + \gamma [\mathcal{X}^{12}_{j-m} + \mathcal{Y}^2_{j-m}] H^{\parallel}_m - \alpha_m \mathcal{X}^{12}_{j-m} H^w_m, \tag{3.24}$$

and this system of equations is expressed in matrix form as

$$-i\frac{d\boldsymbol{\xi}(v)}{dv} = \mathbf{Z}_2(v)\boldsymbol{\xi}(v), \tag{3.25}$$

where $\mathbf{Z}_2$ is a $(8N+4)\times(8N+4)$ matrix of the form

$$\mathbf{Z}_2 = \begin{bmatrix} \mathbf{A}_2 & \mathbf{B}_2 & \mathbf{C}_2 & \mathbf{D}_2 \\ \mathbf{E}_2 & \mathbf{F}_2 & \mathbf{G}_2 & \mathbf{H}_2 \\ \mathbf{I}_2 & \mathbf{J}_2 & \mathbf{K}_2 & \mathbf{L}_2 \\ \mathbf{M}_2 & \mathbf{N}_2 & \mathbf{O}_2 & \mathbf{P}_2 \end{bmatrix}, \tag{3.26}$$

and $\mathbf{A}_2 \ldots \mathbf{P}_2$ are matrices of $(2N+1)\times(2N+1)$ elements given by

$$\mathbf{A}_2 = \alpha_j \mathcal{X}^5_{j-m},$$

$$\mathbf{B}_2 = -\alpha_j \mathcal{X}^6_{j-m},$$

$$\mathbf{C}_2 = -\frac{c\gamma}{\omega_0} \alpha_j \mathcal{X}^2_{j-m},$$

$$\mathbf{D}_2 = \frac{c}{\omega_0} \alpha_j \alpha_m \mathcal{X}^2_{j-m} - \frac{\omega_0}{c} \mu_2 \delta_{j,m},$$

$$\mathbf{E}_2 = \gamma \mathcal{X}^3_{j-m},$$

$$\mathbf{F}_2 = (\mathcal{Y}^2_{j-m}\alpha_m - \gamma \mathcal{X}^4_{j-m}),$$

$$\mathbf{G}_2 = \frac{\omega_0}{c} \mu_2 \mathcal{Y}^1_{j-m} - \frac{\gamma^2 c}{\omega_0} \mathcal{X}^2_{j-m},$$

$$\mathbf{H}_2 = \frac{c\gamma}{\omega_0} \alpha_m \mathcal{X}^2_{j-m},$$

$$\mathbf{I}_2 = \frac{c\gamma\alpha_j}{\omega_0 \mu_2} \mathcal{Y}^1_{j-m} + \frac{\omega_0}{c} \mathcal{X}^7_{j-m},$$

$$\mathbf{J}_2 = -\frac{c}{\omega_0 \mu_2} \alpha_j \alpha_m \mathcal{Y}^1_{j-m} + \frac{\omega_0}{c} \mathcal{X}^{10}_{j-m},$$

$$\mathbf{K}_2=\alpha_j\mathcal{Y}^2_{j-m}+\gamma\mathcal{X}^8_{j-m},$$

$$\mathbf{L}_2=-\mathcal{X}^8_{j-m}\alpha_m,$$

$$\mathbf{M}_2=\frac{c\gamma^2}{\omega_0\mu_2}\mathcal{Y}^1_{j-m}-\frac{\omega_0}{c}\mathcal{X}^{11}_{j-m},$$

$$\mathbf{N}_2=\frac{\omega_0}{c}\mathcal{X}^{13}_{j-m}-\frac{c\gamma}{\omega_0\mu_2}\alpha_m\mathcal{Y}^1_{j-m},$$

$$\mathbf{O}_2=\gamma[\mathcal{X}^{12}_{j-m}+\mathcal{Y}^2_{j-m}],$$

$$\mathbf{P}_2=-\alpha_m\mathcal{X}^{12}_{j-m}.$$

Therefore, the scattering problem is reduced to find the solutions of the systems (3.8) and (3.25) with appropriate boundary conditions at the interface between the two media. Note that the first and second derivatives of the corrugation function $a(x)$ appear in the matrices $\mathbf{Z}_1$ and $\mathbf{Z}_2$. These derivatives are not defined if the grooves have abrupt corners. However, the method can also be applied to this kind of profile by replacing the function $a(x)$ by its series expansion.

As is shown in [1,6], the unknown vector $\boldsymbol{\xi}$ in Eqs. (3.8) and (3.25) can be expanded in terms of the eigenvalues and eigenvectors of the matrix $\mathbf{Z}_1$ and $\mathbf{Z}_2$, respectively. That is to say, in each medium the vector $\boldsymbol{\xi}$ is written as

$$\boldsymbol{\xi}(v)=\sum_q b^l_q\mathbf{V}^l_q\exp(ir^l_qv), \tag{3.27}$$

where $\mathbf{V}^l_q$ (r^l_q) indicates the q eigenvector (eigenvalue) in the medium l (l=1 isotropic and l= 2 uniaxial) and b^l_q are unknown complex amplitudes. Expansion (3.27) for the vector ξ in each medium will be used to impose the boundary conditions at the interface. It is easy to demonstrate that in the transformed space these conditions imply the continuity of ξ at the interface. When the isotropic medium is a dielectric, this is written as

$$\mathbf{T}^1\mathbf{b}^1+\mathbf{1}^1+\mathbf{U}^1\mathbf{B}^1=\mathbf{T}^2\mathbf{b}^2+\mathbf{1}^2+\mathbf{U}^2\mathbf{B}^2, \tag{3.28}$$

where the first term on the left (right) side of this equation gives the evanescent field, the second the incident field, and the third one the propagating field in the medium 1 (2), respectively. On the left hand side of this equation $\mathbf{T}^1$ is a $(8N+4)\times(4N+2-2P)$ matrix whose columns are the eigenvectors of the matrix $\mathbf{Z}_1$ associated with the $4N+2-2P$ eigenvalues r^1_q having positive imaginary part, P being the number of propagating modes in the dielectric zone. These eigenvalues are the ones that correspond to decaying waves as $y\to\infty$ (outgoing wave condition). $\mathbf{b}^1$ is an unknown vector of $(4N+2-2P)$ elements. The vector $\mathbf{1}^1$ gives the expansions defined in (2.68)–(2.72). Note that this vector is null for a wave incident from the uniaxial side. $\mathbf{U}^1$ is a matrix formed by the diffracted field expansions given by Eqs. (2.73)–(2.76) and $\mathbf{B}^1$ is a vector ($2P$ elements) formed by the unknowns R_n and S_n that give the amplitudes of the diffracted fields in the isotropic medium.

Analogously, on the right hand side we have the matrix $\mathbf{T}^2$ of $(8N+4)\times(4N+2-Po-Pe)$ elements. They are the eigenvectors of $\mathbf{Z}_2$ associated with the $4N+2-Po-Pe$ eigenvalues with a negative imaginary part (which correspond to the decaying waves as $y\to-\infty$). P_o (P_e) is the number of ordinary (extraordinary) propagating modes in the crystal. We should note that these modes are those which represent a flux of energy pointing towards $y<0$, i.e., the y component of their associated Poynting vector is less than zero. It can be demonstrated that this condition is satisfied only if the y components of the diffracted ordinary and extraordinary wave vectors (α_{1n} and α_{2n}) defined by Eqs. (2.58) and (2.60) are purely real. If they are complex, the Poynting vector has no component in the y direction and the wave is evanescent. In this case α_{1n} and α_{2n} have negative imaginary parts, as can be observed in Eqs. (2.58) and (2.60) (decaying waves as $y\to-\infty$). It can be seen that $\mathbf{b}^2$ is an unknown vector of $(4N+2-Po-Pe)$ elements. $\mathbf{1}^2$ is a vector giving the expansions (2.77)–(2.80). $\mathbf{U}^2$ is a matrix formed by the diffracted amplitudes defined in Eqs. (2.81)–(2.84) and $\mathbf{B}^2$ is an unknown vector formed by the amplitudes C_{on} and C_{en} of the ordinary and extraordinary propagating waves in the crystal. Thus, Eq. (3.28) represents a system of $8N+4$ equations with $8N+4$ unknowns: $4N+2-2P$ in $\mathbf{b}^1$, $2P$ in $\mathbf{B}^1$, $4N+2-P_o-P_e$ in $\mathbf{b}^2$ and P_o+P_e in $\mathbf{B}^2$. Therefore the solution of this system gives the unknown amplitudes R_n, S_n, C_{on}, and C_{en}.

Note that Eq. (3.28) is valid when the isotropic medium is a dielectric. For a metal it makes no sense to separate the field into evanescent and propagating orders and only incident waves from the uniaxial side are possible. In this case Eq. (3.28) is rewritten as

$$\mathbf{T}^1_m\mathbf{b}^1_m=\mathbf{T}^2\mathbf{b}^2+\mathbf{1}^2+\mathbf{U}^2\mathbf{B}^2, \tag{3.29}$$

where $\mathbf{T}^1_m$ has now $(8N+4)\times(4N+2)$ elements being the eigenvectors of the matriz $\mathbf{Z}_1$ which correspond to the $(4N+2)$ eigenvalues which are real and positive or have positive imaginary part and $\mathbf{b}^1_m$ is an unknown vector of $(8N+4)$ elements. The procedure to solve the problem is equal to the one explained above.

IV. RESULTS

In this section we use the formalism presented above to study polarization conversion from uniaxial gratings of sinusoidal profile in the configurations similar to those already considered in Refs. [3,9] but extending the range of corrugation strengths. Perfect agreement between the method based on the Rayleigh hypothesis and the formalism presented here was obtained for gratings with shallow grooves but discrepancies appear when the corrugation is increased. A detailed comparison between both methods, providing a way to check the validity of the Rayleigh hypothesis for anisotropic materials, will be reported elsewhere.

For values of h/d (groove height-to-period ratio) ranging between 0.1 and 0.5 energy conservation was required to hold within a tolerance of 10^{-6} and in the examples below this was usually achieved by retaining 11 terms ($N=5$) in the expansions of the fields. By increasing N from 5 to 6 the power carried by the specularly reflected and transmitted orders varies within the same tolerance. As the groove height-to-period ratio is increased, the convergence of the results is

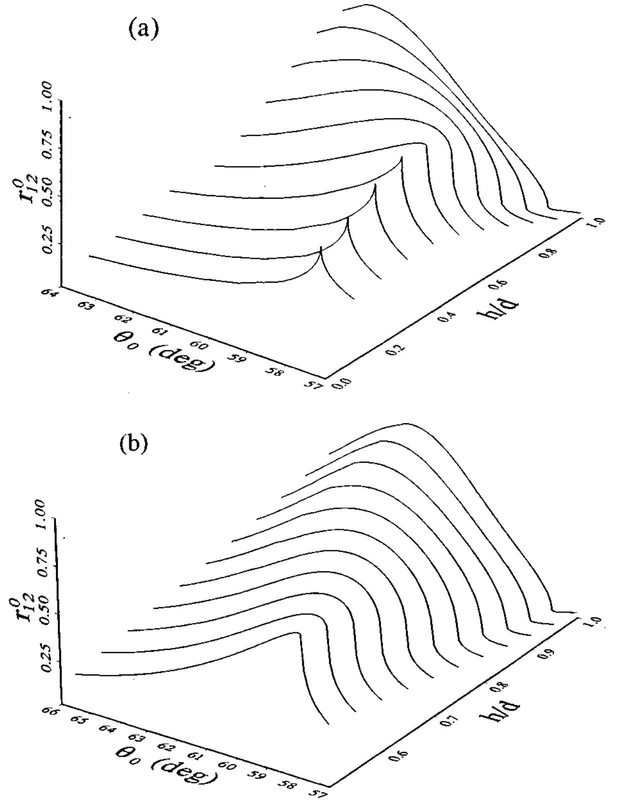

FIG. 2. (a) Efficiency of the cross-polarized component r^0_{12} of the zeroth reflected order by a sinusoidal grating as a function of the angle of incidence in the region of maximum *s*-*p* conversion (θ_0 between 57° and 64°) with h/d as a parameter (for h/d between 0.1 and 1). An *s* wave is incident from the isotropic medium with $\epsilon_1=3.5$ and $\mu_1=1$ into sodium nitrate with $\epsilon_\perp=2.58$, $\epsilon_\parallel=1.71$, and $\mu_2=1$. Other parameters are $\lambda_0/d=1$, $\varphi=0°$, and $\hat{\vec{c}}_0=(0,0.688,0.725)$. (b) Efficiency of the cross-polarized component r^0_{12} of the zeroth reflected order as a function of the angle of incidence in the region of *s*-*p* maximum conversion and for values of h/d greater than 0.5. Other parameters are the same as in (a).

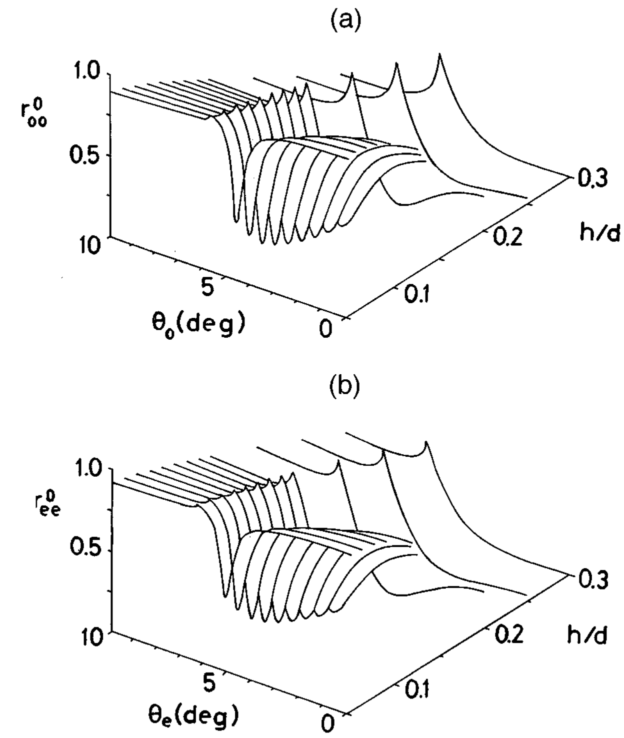

FIG. 3. (a) Efficiency of the ordinary-to-ordinary r^0_{oo} zeroth reflected order as a function of the angle of incidence θ_o for $0°<\theta_o<10°$ and with h/d as a parameter. An ordinary wave is incident from sodium nitrate $\epsilon_\perp=2.58$, $\epsilon_\parallel=1.71$, and $\mu_2=1$ into a metal with $\epsilon_1=-21.6+1.4i$ and $\mu_1=1$. Other parameters are $\lambda_0/d=0.7424$, $\varphi=0°$, and $\hat{\vec{c}}_0=(0.57,0.57,0.57)$. (b) Efficiency of the extraordinary-to-extraordinary r^0_{ee} zeroth reflected order as a function of the angle of incidence θ_e for $0°<\theta_e<10°$ and for different values of h/d. Other parameters are the same as in (a).

also obtained for $N=5$, but the error in the power conservation is of the order of 10^{-3}.

Next, we consider a sinusoidal boundary between a nonlossy isotropic medium ($\epsilon_1=3.5$ and $\mu_1=1$) and sodium nitrate ($\epsilon_\perp=2.58$, $\epsilon_\parallel=1.71$ and $\mu_2=1$) illuminated from the isotropic medium by an *s* wave. The optic axis is $\hat{\vec{c}}_0=0.688\hat{\vec{y}}+0.725\hat{\vec{z}}$, a value that gives a maximum *s*-*p* conversion for $h/d=0$. The wavelength-to-period ratio (free space) was set to 1 and $\varphi=0$ (classical mounting). In Fig. 2(a) we show the efficiency of the cross-polarized component in the zeroth reflected order (r^0_{12}) as a function of the angle of incidence (for θ_0 between 57° and 64°) and for values of h/d varying from 0.1 to 1, the step of variation being 0.1. For a flat interface, maximum conversion is observed at that angle of incidence where both transmitted waves (ordinary and extraordinary) become evanescent (total reflection). For the parameters chosen in Fig. 2(a), this angle is $\theta_0=57.85°$ (the zeroth ordinary and extraordinary transmitted waves disappear at $\theta_0=57.85°$ and $\theta_0=45.57°$, respectively). As pointed out in [3], one may think that introducing a corrugation to the boundary, the power reflected in the zeroth reflected order would decrease due to the presence of other orders that propagate into the crystal. However in the example presented there it was shown that the efficiency of conversion in the specularly reflected order is not reduced at least for weak corrugations [with the same parameters as in Fig. 2(a) but for $\lambda_0/d=0.5$] and that the peaks are present at exactly the same angles of incidence for which maximum conversion is observed when h/d is equal to zero ($\theta_0=57.85°$). In our example, we also observe that the efficiency of the cross-polarized zeroth reflected order increases as the value of h/d increases. Moreover, the peaks of conversion appear at the same angle at which maximum conversion takes place in a flat interface for h/d lower than 0.4, approximately. For higher values of h/d the angles of incidence at which the maximum conversion occurs do not coincide with the disappearance of the zeroth transmitted orders and the values of the cross-polarized efficiency are even higher than the ones observed for h/d varying from 0.1 to 0.4, reaching a value of 0.837 at $\theta_0=62.67°$ for $h/d=1$. This can be observed in Fig. 2(b) where we plot the efficiency of the cross-polarized zeroth reflected order as a function of the angle of incidence ($57°\leqslant\theta_0\leqslant 66°$) for h/d between 0.5 and 1, in steps of 0.05. In this example we have shown data for values of h/d up to 1. For values of h/d ranging between 0.1 and 0.5 power conservation is verified with an error of 10^{-6}. As the groove height-to-period ratio increases this error also increases, being 10^{-2} for h/d equal

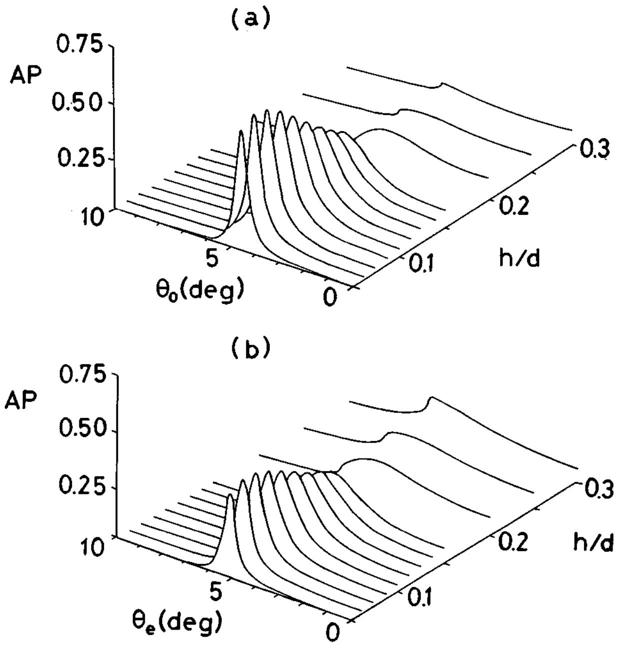

FIG. 4. (a) Absorbed power normalized to the incident power AP for the same parameters considered in 3(a). (b) Absorbed power normalized to the incident power AP for the same parameters considered in 3(b).

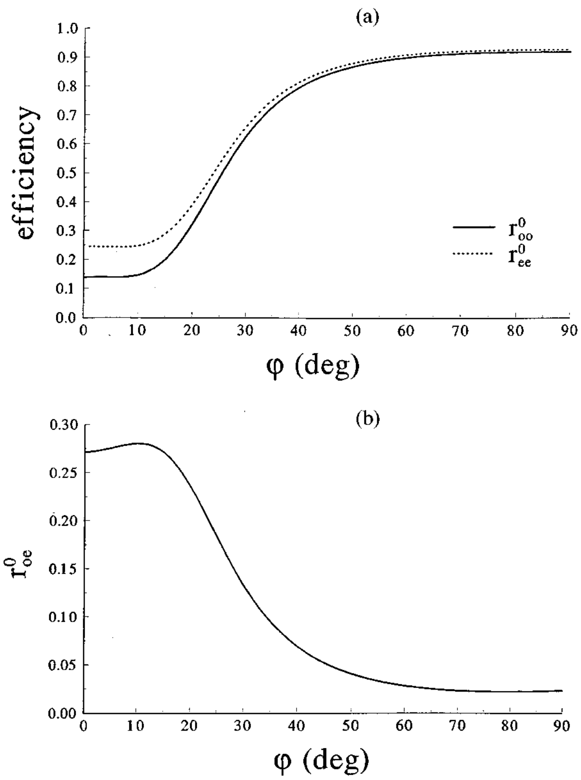

FIG. 5. (a) Efficiency of the ordinary-to-ordinary and extraordinary-to-extraordinary zeroth reflected order (r^0_{oo} and r^0_{ee}) as a function of φ. $h/d=0.075$ and $\theta_o=4.53°$ for the curve r_{oo} or $\theta_e=5.06°$ for the curve r_{ee}. Other parameters are the same as Fig. 4(a). (b) Efficiency of the cross-polarized zeroth reflected order r^0_{oe} as a function of φ. The incident wave is ordinary. $\theta_0=4.53°$ and $h/d=0.075$. Other parameters are the same as Fig. 4(a).

to 1. Gratings with higher values of h/d could be considered if this error were reduced. We are working in overcoming this restriction by using a numerical technique based on the R-matrix propagation algorithm [8].

Next, we consider a grating illuminated from the uniaxial side in a region where resonant excitation of surface plasmons is expected. We use a sinusoidal boundary between a metal (gold at a wavelength of 800 nm with $\epsilon_1=-21.6+1.4i$ and $\mu_1=1$) and sodium nitrate ($\epsilon_\perp=2.58$, $\epsilon_\parallel=1.71$, and $\mu_2=1$). Other parameters are $\hat{c}_0=(0.577,0.577,0.577)$, $\lambda_0/d=1.7424$, and $\varphi=0$. The effects produced by the excitation of surface plasmons are shown in Fig. 3 where we plot the ordinary-to-ordinary (r^0_{oo}) and extraodinary-to-extraordinary (r^0_{ee}) efficiencies in the zeroth reflected orders [Figs. 3(a) and 3(b), respectively] as a function of the angle of incidence and for values of h/d varying from 0.05 to 0.3, the step of variation being 0.05. In Fig. 3(a) we observe a narrow minima in the region $4°<\theta_o<4.6°$ for h/d between 0.05 and 0.15. When the polarization of the incident wave is extraordinary [Fig. 3(b)], a similar behavior is observed and the peaks appear at angles of incidence between 4.5° and 5.2°.

In Figs. 4(a) and 4(b) we plot the absorbed power normalized to the incident power (AP) as a function of the angle of incidence with h/d as a parameter for the same gratings considered in Figs. 3(a) and 3(b), respectively. Both figures show absorption peaks at approximately the same angles where the minimum in r^0_{oo} and r^0_{ee} occurs. These peaks become higher for h/d up to 0.075, approximately. For this value of h/d the maximum absorbed power is 0.59 for an ordinary incident wave [Fig. 4(a)] or 0.434 for an incident wave of the extraordinary type [Fig. 4(b)]. For greater values of the groove height-to-period ratio the peaks become lower and disappear when h/d is approximately equal to 0.3. The presence of minima in Figs. 3(a) and 3(b) and of absorption peaks in Figs. 4(a) and 4(b) is associated with the excitation of surface plasmons at the interface. For shallow gratings the position of these peaks can be predicted in an approximated way by an equation similar to (2.53) where α is the real part of the complex pole of the determinant of the reflection matrix for a plane interface.

In Fig. 5(a) we plot the ordinary-to-ordinary and the extraordinary-to-extraordinary efficiencies of the zeroth reflected order as a function of φ for the same gratings considered in Figs. 3(a) and 3(b). The angle of incidence and the groove height-to-period ratio were selected from Figs. 3(a) and 3(b) as the ones that minimize the quantities r^0_{oo} ($\theta_o=4.53°$, $h/d=0.075$) and r^0_{ee} ($\theta_e=5.06°$, $h/d=0.075$), respectively. The other parameters are the same as in the previous figures. We observe that r^0_{oo} and r^0_{ee} are strongly dependent on the value of φ. When $\varphi=0°$, r^0_{oo} and r^0_{ee} have their minimum value (0.138 for r^0_{oo} and 0.244 for r^0_{ee}). If we increase the value of φ these quantities also increase reaching a maximum ($r^0_{oo}=0.919$ and $r^0_{ee}=0.927$) when $\varphi=90°$. In Fig. 5(b) we show the efficiency of the zeroth extraordinary reflected order (r^0_{oe}) as a function of φ. The polarization of the incident wave is ordinary and the angle of incidence is $\theta_o=4.53°$. Other parameters are the same as Fig. 5(a). In this case, we observe that the efficiency decreases when the value of φ is increased, being r^0_{oe} lower than 0.025 for φ greater than 70° approximately.

V. CONCLUSION

Surface relief gratings with birefringent properties are of interest in communication technology and many other applications in which we are interested in mechanisms that provide means of switching information flow from one channel to another. In this paper we explored the possibility of enhancing the conversion rate between polarization modes at a single anisotropic interface by means of surface reliefs with arbitrary profiles. To do so, we extended to the anisotropic media a versatile rigorous method originally developed by Chandezon *et al.* [6] for the diffraction gratings made of isotropic materials. Whereas previous studies on the subject were valid only for weak corrugations, our analysis has no restriction on the surface relief profile. Furthermore, it can handle general configurations in which the incident beam is associated to waves coming either from the isotropic or from the uniaxial side and any orientations with respect to the grooves of the grating for the plane of incidence and for the optical axis of the crystal.

ACKNOWLEDGMENTS

This work was supported by grants from CONICET, Fundación Antorchas, and UBA.

APPENDIX A

In the new coordinate system, Eq. (2.6) is written as [1]

$$\left[\vec{v}^{\,1}\frac{\partial}{\partial u}+\vec{v}^{\,2}\frac{\partial}{\partial v}+\vec{v}^{\,3}\frac{\partial}{\partial w}\right](E_u\vec{v}_1+E_v\vec{v}_2+E_w\vec{v}_3) = \frac{i\omega_0}{c}\mu_1(H_u\vec{v}_1+H_v\vec{v}_2+H_w\vec{v}_3), \tag{A1}$$

where we have assumed a harmonic time dependence of the form $\exp(-i\omega_0 t)$, ω_0 being the frequency of the incident radiation. The $\vec{v}$'s are the contravariant and covariant vectors and for this system are given by

$$\vec{v}^{\,1}=\hat{\vec{x}},\quad \vec{v}^{\,2}=\hat{\vec{y}}-a'\hat{\vec{x}},\quad \vec{v}^{\,3}=\hat{\vec{z}},$$

$$\vec{v}_1=\hat{\vec{x}}+a',\hat{\vec{y}}\quad \vec{v}_2=\hat{\vec{y}},\quad \vec{v}_3=\hat{\vec{z}},$$

where $\hat{\vec{x}},\hat{\vec{y}},\hat{\vec{z}}$ are the unit vectors in the original space and a' is the derivative of $a(u)$ with respect to u.

Analogously, Eq. (2.7) is transformed into

$$\left[\vec{v}^{\,1}\frac{\partial}{\partial u}+\vec{v}^{\,2}\frac{\partial}{\partial v}+\vec{v}^{\,3}\frac{\partial}{\partial w}\right](H_u\vec{v}_1+H_v\vec{v}_2+H_w\vec{v}_3) = -\frac{i\omega_0}{c}\epsilon_1(E_u\vec{v}_1+E_v\vec{v}_2+E_w\vec{v}_3). \tag{A2}$$

Expansion of Eqs. (A1) and (A2) leads to a system of six equations with six unknowns (E_u, E_v, E_w, H_u, H_v, and H_w). Following the notation presented in [1] this system can be written in matrix form as

$$\begin{bmatrix}\mathbf{C} & \mathbf{O}\\ \mathbf{O} & \mathbf{C}\end{bmatrix}\mathbf{G}=\frac{i\omega_0}{c}\begin{bmatrix}\mathbf{O} & \mu_1\mathbf{T}_1\\ -\epsilon_1\mathbf{T}_1 & \mathbf{O}\end{bmatrix}\mathbf{G}, \tag{A3}$$

where $\mathbf{O}$ is a matrix of zeros (3×3). The matrices $\mathbf{C}$ and $\mathbf{T}_1$ are given by

$$\mathbf{C}=\begin{bmatrix} -a'\frac{\partial}{\partial w} & \frac{-\partial}{\partial w} & \frac{\partial}{\partial v}\\ \frac{\partial}{\partial w} & 0 & \frac{-\partial}{\partial u}+a'\frac{\partial}{\partial v}\\ a'\frac{\partial}{\partial u}+a''-[1+a'^2]\frac{\partial}{\partial v} & \frac{\partial}{\partial u}-a'\frac{\partial}{\partial v} & 0\end{bmatrix}, \tag{A4}$$

$$\mathbf{T}_1=\begin{bmatrix}1 & 0 & 0\\ a' & 1 & 0\\ 0 & 0 & 1\end{bmatrix}, \tag{A5}$$

and $\mathbf{G}$ is a vector formed by the unknowns of the problem

$$\begin{bmatrix}E_u\\ E_v\\ E_w\\ H_u\\ H_v\\ H_w\end{bmatrix}.$$

APPENDIX B

As in the isotropic medium, in the uniaxial zone Eq. (2.6) is transformed into an expression of the form (A1)

$$\left[\vec{v}^{\,1}\frac{\partial}{\partial u}+\vec{v}^{\,2}\frac{\partial}{\partial v}+\vec{v}^{\,3}\frac{\partial}{\partial w}\right](E_u\vec{v}_1+E_v\vec{v}_2+E_w\vec{v}_3)$$

$$=\frac{i\omega_0}{c}\mu_2(H_u\vec{v}_1+H_v\vec{v}_2+H_w\vec{v}_3), \tag{B1}$$

where we have only changed μ_1 by μ_2.

By a similar procedure Eq. (2.7) is written as

$$\left[\vec{v}^{\,1}\frac{\partial}{\partial u}+\vec{v}^{\,2}\frac{\partial}{\partial v}+\vec{v}^{\,3}\frac{\partial}{\partial w}\right](H_u\vec{v}_1+H_v\vec{v}_2+H_w\vec{v}_3)$$

$$=-\frac{i\omega_0}{c}(D_u\vec{v}_1+D_v\vec{v}_2+D_w\vec{v}_3). \tag{B2}$$

Taking into account Eq. (2.3), the components D_u, D_v, and D_w are written in terms of E_u, E_v, and E_w, as follows:

$$D_u=\epsilon_{uu}E_u+\epsilon_{uv}E_v+\epsilon_{uw}E_w, \tag{B3}$$

$$D_v=\epsilon_{vu}E_u+\epsilon_{vv}E_v+\epsilon_{vw}E_w, \tag{B4}$$

$$D_w=\epsilon_{wu}E_u+\epsilon_{wv}E_v+\epsilon_{ww}E_w, \tag{B5}$$

where $\epsilon_{i,j}$ are the elements of the tensor $\tilde{\epsilon}$ in the transformed frame and are given by

$$\epsilon_{uu}=\epsilon_\perp+(\epsilon_\parallel-\epsilon_\perp)(c_{0x}^2+a'c_{0x}c_{0y}), \tag{B6}$$

$$\epsilon_{uv}=(\epsilon_\parallel-\epsilon_\perp)c_{0x}c_{0y}, \tag{B7}$$

$$\epsilon_{uw}=(\epsilon_\parallel-\epsilon_\perp)c_{0x}c_{0z}, \tag{B8}$$

$$\epsilon_{vu}=(\epsilon_\parallel-\epsilon_\perp)[a'(c_{0y}^2-c_{0x}^2)+(1-a'^2)c_{0x}c_{0y}], \tag{B9}$$

$$\epsilon_{vv}=\epsilon_\perp+(\epsilon_\parallel-\epsilon_\perp)(c_{0y}^2-a'c_{0x}c_{0y}), \tag{B10}$$

$$\epsilon_{vw}=(\epsilon_\parallel-\epsilon_\perp)c_{0z}(-a'c_{0x}+c_{0y}), \tag{B11}$$

$$\epsilon_{wu}=(\epsilon_\parallel-\epsilon_\perp)c_{0z}(a'c_{0y}+c_{0x}), \tag{B12}$$

$$\epsilon_{wv}=(\epsilon_\parallel-\epsilon_\perp)c_{0y}c_{0z}, \tag{B13}$$

$$\epsilon_{ww}=\epsilon_\perp+(\epsilon_\parallel-\epsilon_\perp)c_{0z}^2, \tag{B14}$$

where c_{0x}, c_{0y}, and c_{0z} are the rectangular components of the optic axis $\hat{\vec{c}}_0$.

Expressing the components D_u, D_v and D_w in Eq. (B2) in terms of E_u, E_v and E_w, Eqs. (B1) and (B2) represent a system of six equations with six unknowns which can be express in matrix notation as

$$\begin{bmatrix}\mathbf{C} & \mathbf{O}\\ \mathbf{O} & \mathbf{C}\end{bmatrix}\mathbf{G}=\frac{i\omega_0}{c}\begin{bmatrix}\mathbf{O} & \mu_2\mathbf{T}_1\\ -\mathbf{T}_2 & \mathbf{O}\end{bmatrix}\mathbf{G}, \tag{B15}$$

where the $\mathbf{C}$, $\mathbf{O}$, $\mathbf{T}_1$, and $\mathbf{G}$ have been defined before and

$$\mathbf{T}_2=\begin{bmatrix}\epsilon_{uu} & \epsilon_{uv} & \epsilon_{uw}\\ a'\epsilon_{uu}+\epsilon_{vu} & a'\epsilon_{uv}+\epsilon_{vv} & a'\epsilon_{uw}+\epsilon_{vw}\\ \epsilon_{wu} & \epsilon_{wv} & \epsilon_{ww}\end{bmatrix}. \tag{B16}$$

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