## General polarized ray-tracing method for inhomogeneous uniaxially anisotropic media

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Uniaxial optical anisotropy in the geometrical-optics approach is a classical problem, and most of the theory has been known for at least fifty years. Although the subject appears frequently in the literature, wave propagation through inhomogeneous anisotropic media is rarely addressed. The rapid advances in liquid-crystal lenses call for a good overview of the theory on wave propagation via anisotropic media. Therefore, we present a novel polarized ray-tracing method, which can be applied to anisotropic optical systems that contain inhomogeneous liquid crystals. We describe the propagation of rays in the bulk material of inhomogeneous anisotropic media in three dimensions. In addition, we discuss ray refraction, ray reflection, and energy transfer at, in general, curved anisotropic interfaces with arbitrary orientation and/or arbitrary anisotropic properties. The method presented is a clear outline of how to assess the optical properties of uniaxially anisotropic media. © 2008 Optical Society of America

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### 1. INTRODUCTION

The optical properties of uniaxially anisotropic media are essential for many applications such as liquid-crystal displays [1], switchable lenticulars for autostereoscopic 2D/3D displays [2,3], anisotropic gradient-index lenses [4], or liquid-crystal spatial light modulators for beam steering [5]. Therefore, it is desired to understand and predict the propagation of light in optical systems containing optically anisotropic elements. The problem of optical anisotropy in the geometrical-optics approach is classical, and most of the theory has been known for more than fifty years. During the past few decades, optical anisotropy has often been studied in the literature [6-30]. However, the literature is nearly silent about wave propagation through inhomogeneous anisotropic media. At the same time, the rapid advances in liquid-crystal applications call for a good exposition of the theory on wave propagation via anisotropic media. Therefore, we present a general polarized ray-tracing method for inhomogeneous uniaxially anisotropic media in three dimensions. In addition, we describe how to assess the optical properties of anisotropic interfaces with arbitrary orientation and/or anisotropic properties. In order to support a general approach, we apply vector notation. We will derive vector equations that are compact and simple. Hence, the method presented in this article is also a clear overview of how (and under which conditions) to apply the classical theory to anisotropic optical systems that can be found in the type of applications mentioned above.

A general approach would be to model biaxial aniso-

tropy. Unfortunately, biaxial anisotropy is more complex to model than uniaxial anisotropy. As a result, the step from uniaxial to biaxial anisotropy is not a trivial one. In addition, uniaxial anisotropy is more frequently applied in practice than biaxial anisotropy, and biaxial anisotropy can often be neglected.

In general, the optical properties of an anisotropic medium are defined by two regions. These are the boundary, which forms the interface between the anisotropic medium and the surrounding medium, and the bulk material. Locally, the interface region has homogeneous anisotropic properties. In general, the bulk region has inhomogeneous anisotropic properties. Similarly, the theory presented in this article is divided into two parts. One part applies to the interface, and one part applies to the bulk region.

In the definition of the electromagnetic wave field, we apply the quasi-plane-wave approximation [31–33]. For inhomogeneous media, the quasi-plane-wave approximation applies in the case where the optical properties of the medium change slowly with respect to the wavelength. If the properties of the medium change rapidly with respect to the wavelength, we need to take into account the wave character of light. In that case, we leave the domain of validity of geometrical optics, which is beyond the scope of this article.

When polarized ray tracing is applied to an optical system, we are interested mainly in the energy flux, represented by the Poynting vector. In anisotropic media, the Poynting vector and wave vector are not parallel in general, since the electric field vector  $\mathbf{E}$  and the electric flux density vector  $\mathbf{D}$  are not parallel. For this reason, we define a ray as the trajectory of the Poynting vector rather than the orthogonal trajectory of the wavefront (i.e., the trajectory of the wave vector).

This article is set up in the following way. We begin with a summary of the classical theory on geometrical optics in Section 2 [32]. In Section 3, we derive the equation for the optical indicatrix [34], also known as Fresnel's surface of wave normals or the normal surface [35]. This surface determines the mutual orientation of an individual wave vector and its corresponding Poynting vector. In addition, each Poynting vector has corresponding electric and magnetic field vectors. In Section 4, we derive vector equations for the directions of these electric and magnetic field vectors in terms of the corresponding wave vector. The concise notation presented here cannot be found in the literature.

Next, we discuss the optical properties of the bulk material of anisotropic media. Here we describe a powerful method for the calculation of a ray path through an inhomogeneous anisotropic medium. We call this method the Hamiltonian method. An important conclusion is that the Hamiltonian method incorporates the fact that ray paths inside inhomogeneous media are curved. The Hamiltonian method is based on the theory introduced by Kline and Kay [30]. In Kraan et al. [4], this theory is worked out for a two-dimensional liquid-crystal profile in a gradientindex lens. In Section 5 of this article, we derive the Hamiltonian method for arbitrary liquid-crystal profiles in three dimensions. In particular, we introduce novel ray equations in terms of the position-dependent optical axis (the director) and the position-dependent index of refraction.

Then we focus on the optical properties of an interface between two (an)isotropic media. In Section 6, we derive an expression for the wave vector as a function of the Poynting vector for arbitrary indices of refraction. In addition, we derive vector equations for reflected and refracted wave vectors at anisotropic interfaces. In Section 7, we discuss the energy transfer of reflected and refracted rays when light crosses the interface between two anisotropic transparent media with different orientation and/or anisotropic properties. The Fresnel coefficients are calculated with the help of the Fresnel equations [17,18] and the vector equations from Sections 4 and 6. The energy transfer is described in terms of intensity transmittance and reflectance factors T and R, respectively. Although this procedure is known in the literature, it is significantly simplified by the use of the vector equations derived in Sections 4 and 6.

In Section 8, we summarize the polarized ray-tracing method. To this end, we apply the method to an anisotropic medium and discuss the procedure for the calculation of the optical properties. In Subsection 8.A, we discuss the procedure at an anisotropic interface, and in Subsection 8.B, we discuss the procedure for an anisotropic bulk material. These procedures form a clear outline of how to apply our method in practice.

Finally, as a demonstration, we apply the model to an air-calcite interface in Subsection 9.A and to an artificial inhomogeneous anisotropic structure in Subsection 9.B.

# 2. QUASI-PLANE WAVES AND GEOMETRICAL OPTICS

The macroscopic Maxwell equations for the electric field  $\mathbf{E}$  combined with the macroscopic material equations for isotropic media without dispersion can be transformed into

$$\nabla^{2}\mathbf{E} - \frac{\varepsilon\mu}{c^{2}}\frac{\partial^{2}\mathbf{E}}{\partial t^{2}} + (\nabla\ln\mu) \times \nabla \times \mathbf{E} + \nabla(\mathbf{E}\cdot\nabla\ln\varepsilon) = 0,$$
(1)

with a similar expression for the magnetic field **H** (cf. [32], p. 10). If the medium is homogeneous,  $\nabla \ln \mu = 0$  and  $\nabla \ln \varepsilon = 0$ . Hence, Eq. (1) reduces to the Helmholtz equation

$$\nabla^2 \mathbf{E} - \frac{\varepsilon \mu}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0.$$
 (2)

Equation (2) is a standard equation of wave motion and suggests the existence of electromagnetic waves propagating with a velocity  $v = \frac{c}{\sqrt{e\mu}}$ . One of the solutions of Eq. (2) is the time-harmonic plane wave. In regions far away from light sources, we may define a more general type of wave field. Here the wave field may locally be represented by a time-harmonic quasi-plane wave (cf. [32], p. 111) given by

$$\mathbf{E}(\mathbf{r},t) = \widetilde{\mathbf{E}}(\mathbf{r})e^{i(k_0\psi(\mathbf{r})-\omega t)},\tag{3}$$

with  $\mathbf{\tilde{E}}(\mathbf{r})$  a complex vector and  $\psi(\mathbf{r})$  the optical pathlength function, which is also called the eikonal function. For anisotropic media, we are looking for solutions of the wave field of the form given by Eq. (3). In general, the complex amplitude vector can be written as

$$\widetilde{\mathbf{E}}(\mathbf{r}) = A(\mathbf{r})e^{i\,\delta(\mathbf{r})}\widehat{\mathbf{E}},\tag{4}$$

where  $\hat{\mathbf{E}}$  is a unit vector, the amplitude  $A(\mathbf{r})$  is real, and the phase term  $\delta(\mathbf{r})$  is real. We assume that there is no absorption and no scattering of the wave field inside a medium. Therefore, we can say that the amplitude A and phase  $\delta$  are constant throughout the medium. Only when a wave is refracted or reflected at an interface are the amplitude and phase terms changed. For this reason, we calculate the entire wave field only at an (an)isotropic interface. In the bulk material of an (an)isotropic medium, it is sufficient to calculate the light path of the propagating wave.

The type of wave field given by Eq. (3) is suggested by Sommerfeld and Runge (cf. [33], p. 291) and is also referred to as the Sommerfeld-Runge ansatz. Assuming that Eq. (2) yields, as a solution, a quasi-plane wave, we imply that the local amplitude  $|\tilde{\mathbf{E}}|$  and wave vector  $|\mathbf{k}| = k_0 |\nabla \psi|$  vary insignificantly over the distance of one wavelength, i.e.,

$$\frac{1}{k_0} \frac{\boldsymbol{\nabla} |\mathbf{\hat{E}}|}{|\mathbf{\tilde{E}}|} \ll 1, \quad \frac{1}{k_0} \frac{\boldsymbol{\nabla} |\mathbf{k}|}{|\mathbf{k}|} \ll 1.$$
(5)

The optical properties of the interface and bulk material of a medium with electrical anisotropy are determined by the Maxwell equations. When we substitute the quasi-plane wave of Eq. (3) into the Maxwell equations, we obtain (we consider only nonmagnetic media:  $\mu = 1$ )

$$\nabla \psi \times \widetilde{\mathbf{H}} + c \varepsilon_{0} \underline{\underline{\varepsilon}} \widetilde{\mathbf{E}} = -\frac{1}{ik_{0}} \nabla \times \widetilde{\mathbf{H}},$$

$$\nabla \psi \times \widetilde{\mathbf{E}} - c \mu_{0} \widetilde{\mathbf{H}} = -\frac{1}{ik_{0}} \nabla \times \widetilde{\mathbf{E}},$$

$$\nabla \psi \cdot \underline{\underline{\varepsilon}} \widetilde{\mathbf{E}} = -\frac{1}{ik_{0}} \nabla \cdot \underline{\underline{\varepsilon}} \widetilde{\mathbf{E}},$$

$$\nabla \psi \cdot \widetilde{\mathbf{H}} = -\frac{1}{ik_{0}} \nabla \cdot \widetilde{\mathbf{H}}.$$
(6)

In the geometrical-optics approach, we are interested in solutions of the wave field for large values of  $k_0$ . As long as the right-hand side terms in Eq. (6) are small with respect to one, they may be neglected. However, rapid changes in the optical properties of the medium could lead to large values of the divergence of  $\underline{\varepsilon} \mathbf{\tilde{E}}$ . Hence, we demand that

$$\frac{|\nabla \cdot \underline{\underline{\varepsilon}} \underline{\mathbf{E}}|}{k_0} \ll 1. \tag{7}$$

This condition implies that the elements of the dielectric tensor (i.e., the material properties) should change very slowly over the distance of a wavelength. In addition, the wave amplitude should change very slowly over the distance of a wavelength, as we concluded earlier.

#### **3. UNIAXIAL OPTICAL INDICATRIX**

In Eq. (6), we can confine our attention to the first two equations, since the last two follow from them on scalar multiplication with  $\nabla \psi$ . By introducing the vector  $\mathbf{p} = \nabla \psi$  (wave normal) and eliminating  $\tilde{\mathbf{H}}$  from Eq. (6), we obtain the "eikonal equation" for media with electrical anisotropy

$$\mathbf{p} \times (\mathbf{p} \times \widetilde{\mathbf{E}}) + \underline{\varepsilon} \widetilde{\mathbf{E}} = \mathbf{0}. \tag{8}$$

The wave normal **p** is equivalent to the wave vector **k** scaled by a factor  $k_0$ . The elements of the dielectric tensor are constants of the medium determined by the choice of our Cartesian coordinate system. Since  $\underline{\varepsilon}$  is a real symmetric matrix, it is always possible to find a coordinate system in which the off-diagonal elements of the dielectric tensor are zero. The dielectric tensor can then be written as

$$\underline{\varepsilon} = \begin{pmatrix} \varepsilon_x & 0 & 0\\ 0 & \varepsilon_y & 0\\ 0 & 0 & \varepsilon_z \end{pmatrix}, \tag{9}$$

where  $\varepsilon_x$ ,  $\varepsilon_y$ , and  $\varepsilon_z$  are the relative principal dielectric constants and the *x*, *y*, and *z* axes are the principal dielectric axes of the medium. These axes form the principal coordinate system. The relative principal dielectric con-



Fig. 1. Octant of the uniaxial optical indicatrix in the principal coordinate system. The two surfaces, sphere and ellipsoid, touch each other in their common points of intersection with the z axis. Here we assumed positive birefringence, i.e.,  $n_e > n_o$ .

stants are related to the principal indices of refraction  $n_x$ ,  $n_y$ , and  $n_z$  by  $\varepsilon_i = n_i^2$ , with i = x, y, z. A medium is called uniaxially anisotropic if two of the principal indices of refraction are defined as  $n_x = n_y = n_o$  and  $n_z = n_e$ , where  $n_o$  is the ordinary and  $n_e$  is the extraordinary index of refraction. If we solve Eq. (8) for the eigenvectors  $\tilde{\mathbf{E}}$  and the corresponding eigenvalues n, we obtain the electromagnetic eigenmodes: the ordinary and extraordinary waves.

We can write Eq. (8) as a matrix equation according to

$$\mathbf{A}(\mathbf{p})\widetilde{\mathbf{E}} = \mathbf{0},\tag{10}$$

with **A** a  $3 \times 3$  matrix. Equation (10) has only nontrivial solutions for the eigenvector  $\tilde{\mathbf{E}}$  if the determinant of the matrix **A** vanishes. This demand leads to a quadratic equation  $\mathcal{H}(p_x^2, p_y^2, p_z^2) = 0$ , and its solution represents a three-dimensional surface in **p** space. This surface is called the optical indicatrix (cf. [34], p. 20) and, in the principal coordinate system, is given by

$$\mathcal{H} = \left(\frac{p_x^2 + p_y^2}{n_e^2} + \frac{p_z^2}{n_o^2} - 1\right) \left(\frac{|\mathbf{p}|^2}{n_o^2} - 1\right) = 0.$$
(11)

The uniaxial optical indicatrix consists of two concentric shells: a sphere with radius  $n_o$  and an ellipsoid with semiaxes  $n_o$  and  $n_e$ . The ordinary wave is represented by the sphere  $(\mathcal{H}_o)$ , and the extraordinary wave is represented by the ellipsoid  $(\mathcal{H}_e)$ . The two shells have two points in common, namely,  $\mathbf{p} = (0, 0, \pm n_o)$ . The line that goes through the origin and these points is the *z* axis and is called the optical axis. Figure 1 shows one octant of the optical indicatrix in the principal coordinate system. In the principal coordinate system, the optical axis is in the *z* direction.

### 4. GEOMETRICAL ANALYSIS OF POLARIZATION VECTORS

As discussed in Section 2, the electric field vector can be written as  $\tilde{\mathbf{E}} = a\hat{\mathbf{E}}$ , with  $\hat{\mathbf{E}}$  a unit vector and *a* the complex amplitude. The unit vector  $\hat{\mathbf{E}}$  is called the electric polar-

ization vector. In anisotropic media, the polarization vectors depend on the direction of propagation, the optical axis, and the direction of the Poynting vector. In this section, we derive concise expressions for the electric and magnetic polarization vectors. The complex amplitude aof an electric or magnetic field vector is discussed in Section 7.

The polarization vectors for the ordinary and extraordinary waves can be obtained from Eq. (10). In addition, it is convenient to use the geometrical properties of the optical indicatrix to derive the expressions for the polarization vectors: For ordinary waves, the wave normal is defined  $\mathbf{p}_o = n_o \hat{\mathbf{p}}$ , with  $\hat{\mathbf{p}}$  a unit vector. Then Eq. (10) yields

$$\begin{pmatrix} \hat{p}_{x}^{2} & \hat{p}_{x}\hat{p}_{y} & \hat{p}_{x}\hat{p}_{z} \\ \hat{p}_{y}\hat{p}_{x} & \hat{p}_{y}^{2} & \hat{p}_{y}\hat{p}_{z} \\ \hat{p}_{z}\hat{p}_{x} & \hat{p}_{z}\hat{p}_{y} & \frac{n_{e}^{2}}{n_{o}^{2}} - \hat{p}_{x}^{2} - \hat{p}_{y}^{2} \end{pmatrix} \mathbf{E}_{o} = 0, \qquad (12)$$

with  $\mathbf{E}_o$  the direction of the ordinary electric field vector. Equation (12) implies that  $\mathbf{E}_o$  is given by

$$\mathbf{E}_{o} = \begin{pmatrix} \hat{p}_{y} \\ -\hat{p}_{x} \\ 0 \end{pmatrix}.$$
 (13)

Apparently, in the principal coordinate system,  $\mathbf{E}_o$  is perpendicular to the optical axis  $\hat{\mathbf{o}} = (0,0,1)$  and the direction of propagation  $\mathbf{p}_o$ . These properties of  $\mathbf{E}_o$  are generalized, since they are independent of the choice of the coordinate system. As a result, the ordinary electric polarization vector can be written as the unit vector

$$\hat{\mathbf{E}}_{o} = \frac{\mathbf{p}_{o} \times \hat{\mathbf{o}}}{|\mathbf{p}_{o} \times \hat{\mathbf{o}}|}.$$
(14)

According to the Maxwell equations, the corresponding magnetic polarization vector is (apart from a factor  $c\mu_0$ )  $\mathbf{H}_o = \mathbf{p}_o \times \hat{\mathbf{E}}_o$ . Hence, the magnetic polarization vector is by definition not a unit vector.

The electric polarization vector of the extraordinary wave can be written as

$$\hat{\mathbf{E}}_{e} = \frac{(\mathbf{p}_{e} \times \hat{\mathbf{o}}) \times \nabla_{p} \mathcal{H}_{e}}{|(\mathbf{p}_{e} \times \hat{\mathbf{o}}) \times \nabla_{p} \mathcal{H}_{e}|},\tag{15}$$

where  $\mathbf{p}_e$  is the extraordinary wave normal,  $\nabla_p = (\partial/\partial p_x, \partial/\partial p_y, \partial/\partial p_z)$ , and  $\mathcal{H}_e$  represents the ellipsoid surface (not necessarily in the principal coordinate system). In addition, the corresponding magnetic polarization vector is defined as  $\mathbf{H}_e = \mathbf{p}_e \times \hat{\mathbf{E}}_e$ . Apparently, the electric polarization vector  $\hat{\mathbf{E}}_e$  is perpendicular to both  $\mathbf{p}_e \times \hat{\mathbf{0}}$  and  $\nabla_p \mathcal{H}_e$ . In what follows, we will prove this.

By using the vector identity  $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$ , Eq. (8) can be transformed into  $\underline{\mathbf{s}} \mathbf{\tilde{E}} - (|\mathbf{p}|^2 \mathbf{\tilde{E}} - (\mathbf{\tilde{E}} \cdot \mathbf{p})\mathbf{p}) = 0$ . Hence, the vector components of  $\mathbf{\tilde{E}}$  can be written as

$$\tilde{E}_i = \frac{(\mathbf{E} \cdot \mathbf{p})p_i}{|\mathbf{p}|^2 - \varepsilon_i}, \quad i = x, y, z.$$
(16)

Obviously, Eq. (16) applies only if  $|\mathbf{p}|^2 \neq \varepsilon_i$ . For ordinary waves, Eq. (14) requires that  $\mathbf{\tilde{E}}_o \cdot \mathbf{p}_o = 0$ . Then Eq. (16) yields  $\mathbf{\tilde{E}}_o = 0$ . However, we are not interested in trivial solutions. For extraordinary waves, the inner product  $\mathbf{\tilde{E}}_e \cdot \mathbf{p}_e$  does not necessarily vanish. In this case, we can conclude from Eq. (16) that  $(\mathbf{p}_e \times \mathbf{\hat{o}}) \cdot \mathbf{\tilde{E}}_e = 0$ , since, in the principal coordinate system,  $\mathbf{p}_e \times \mathbf{\hat{o}} = (p_{ey}, -p_{ex}, 0)$ . When  $(\mathbf{p}_e \times \mathbf{\hat{o}}) \cdot \mathbf{\tilde{E}}_e$  vanishes in the principal coordinate system, it also vanishes in another coordinate system.

Next, we show that  $\nabla_p \mathcal{H}_e \cdot \hat{\mathbf{E}}_e = 0$ . When we expand the inner product with the help of Eqs. (11) and (16), we obtain

$$\boldsymbol{\nabla}_{p} \mathcal{H}_{e} \cdot \widetilde{\mathbf{E}}_{e} = \frac{2(\widetilde{\mathbf{E}}_{e} \cdot \mathbf{p}_{e})|\mathbf{p}_{e}|^{2}}{(|\mathbf{p}_{e}|^{2} - n_{o}^{2})(|\mathbf{p}_{e}|^{2} - n_{e}^{2})} \mathcal{H}_{e},$$
(17)

with  $\mathcal{H}_e$  defined in the principal coordinate system. For extraordinary waves,  $\mathcal{H}_e=0$ . As a result, the inner product of Eq. (17) vanishes. If  $|\mathbf{p}_e|=n_o$  or  $|\mathbf{p}_e|=n_e$ , we apply l'Hôpital's rule to Eq. (17) and still conclude that the inner product  $\nabla_p \mathcal{H}_e \cdot \tilde{\mathbf{E}}_e$  vanishes. Similar to the conclusions mentioned above, we conclude that  $\nabla_p \mathcal{H}_e \cdot \tilde{\mathbf{E}}_e=0$  in any arbitrary coordinate system.

We conclude that  $\tilde{\mathbf{E}}_e$  is perpendicular to both  $\mathbf{p}_e \times \hat{\mathbf{o}}$  and  $\nabla_p \mathcal{H}_e$ , and therefore Eq. (15) is proved.

The optical indicatrix is depicted again in Fig. 2, but now with the electric polarization vectors of the ordinary waves and the extraordinary waves indicated. Apparently, both the magnetic and electric polarization vectors are tangent to the optical indicatrix. As a result, the timeaveraged Poynting vector, given by



Fig. 2. Octant of the optical indicatrix in the principal coordinate system. The electric polarization vectors of the ordinary waves are indicated by the arrows on the sphere surface. The electric polarization vectors of the extraordinary waves are indicated by the arrows on the ellipsoid surface. The polarization vectors of both the ordinary and extraordinary waves are tangent to the optical indicatrix.

$$\langle \mathbf{S} \rangle = \frac{1}{2} \operatorname{Re}(\mathbf{E} \times \mathbf{H}^*), \qquad (18)$$

where  $\mathbf{H}^*$  is the complex conjugate of  $\mathbf{H}$ , is perpendicular to the optical indicatrix. Consequently, the direction of  $\langle \mathbf{S} \rangle$  is the same as the direction of  $\nabla_{p} \mathcal{H}$ , yielding

$$\langle \mathbf{S} \rangle \propto \nabla_p \mathcal{H}.$$
 (19)

### 5. HAMILTONIAN METHOD FOR INHOMOGENEOUS MEDIA

We define a ray as the trajectory of the Poynting vector, given by the integral curve of the Poynting vector field in terms of the parameter  $\tau$  according to

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}\tau} = C \langle \mathbf{S}(\mathbf{r}(\tau)) \rangle, \qquad (20)$$

where C is a proportionality constant. In a homogeneous medium, the light rays will propagate along a straight line. However, light rays are curved in the bulk of an inhomogeneous medium, due to a gradient in the refractive index. In what follows, we describe a method to calculate the curved trajectory of the Poynting vector in the bulk of an anisotropic medium. Inside an inhomogeneous uniaxial anisotropic medium, the direction of the optical axis depends on position. We call the position-dependent optical axis the director. The director is indicated by a unit vector  $\hat{\mathbf{d}} = (\hat{d}_x, \hat{d}_y, \hat{d}_z)$  and is parallel to the local optical axis  $\hat{\mathbf{o}}$ . The component of the electric field in the direction of the director is  $(\mathbf{E} \cdot \hat{\mathbf{d}})\hat{\mathbf{d}}$ , and the dielectric permittivity in this direction is  $\varepsilon_0 \varepsilon_{\parallel}$ , with  $\varepsilon_{\parallel} = n_e^2$ . The component perpendicular to the director is  $\mathbf{E} - (\mathbf{E} \cdot \hat{\mathbf{d}})\hat{\mathbf{d}}$ , and the dielectric permittivity in this direction is  $\varepsilon_0 \varepsilon_{\perp}$ , with  $\varepsilon_{\perp} = n_o^2$ . The product of the dielectric permittivities and the electric field vector components yields the electric flux density vector  $\mathbf{D}$  according to

$$\mathbf{D} = \varepsilon_0 \varepsilon_{\parallel} (\mathbf{E} \cdot \hat{\mathbf{d}}) \hat{\mathbf{d}} + \varepsilon_0 \varepsilon_{\perp} (\mathbf{E} - (\mathbf{E} \cdot \hat{\mathbf{d}}) \hat{\mathbf{d}}).$$
(21)

This is the macroscopic material equation in terms of the director  $\hat{\mathbf{d}}$ . With  $\triangle \varepsilon = \varepsilon_{\parallel} - \varepsilon_{\perp}$ , Eq. (21) reads

$$\mathbf{D} = \varepsilon_0 \varepsilon_{\perp} \mathbf{E} + \varepsilon_0 \bigtriangleup \varepsilon (\mathbf{E} \cdot \hat{\mathbf{d}}) \hat{\mathbf{d}}.$$
(22)

On the Cartesian basis (x, y, z), the components of **D** read  $D_i = \varepsilon_0 \varepsilon_{ij} E_j$ , where

$$\varepsilon_{ij} = \varepsilon_{\perp} \delta_{ij} + \bigtriangleup \varepsilon \hat{d}_i \hat{d}_j, \quad i, j = x, y, z,$$
(23)

with  $\delta_{ij}$  the Kronecker delta. Given the dielectric tensor of Eq. (23), Eq. (8) can be written in terms of the director vector components according to the matrix equation

$$\begin{pmatrix} \varepsilon_{\perp} + \bigtriangleup \varepsilon \hat{d}_{x}^{2} + p_{x}^{2} - |\mathbf{p}|^{2} & \bigtriangleup \varepsilon \hat{d}_{x} \hat{d}_{y} + p_{x} p_{y} & \bigtriangleup \varepsilon \hat{d}_{x} \hat{d}_{z} + p_{x} p_{z} \\ \bigtriangleup \varepsilon \hat{d}_{y} \hat{d}_{x} + p_{y} p_{x} & \varepsilon_{\perp} + \bigtriangleup \varepsilon \hat{d}_{y}^{2} + p_{y}^{2} - |\mathbf{p}|^{2} & \bigtriangleup \varepsilon \hat{d}_{y} \hat{d}_{z} + p_{y} p_{z} \\ \bigtriangleup \varepsilon \hat{d}_{z} \hat{d}_{x} + p_{z} p_{x} & \bigtriangleup \varepsilon \hat{d}_{z} \hat{d}_{y} + p_{z} p_{y} & \varepsilon_{\perp} + \bigtriangleup \varepsilon \hat{d}_{z}^{2} + p_{z}^{2} - |\mathbf{p}|^{2} \end{pmatrix} \mathbf{E} = 0.$$

$$(24)$$

Like Eq. (10), this equation has nontrivial solutions if the determinant of the matrix vanishes. The determinant reads

$$\begin{aligned} \mathcal{H}(x,y,z,p_x,p_y,p_z) \\ = (\varepsilon_{\perp}|\mathbf{p}|^2 + \bigtriangleup \varepsilon(\mathbf{p} \cdot \mathbf{\hat{d}})^2 - \varepsilon_{\perp}(\varepsilon_{\perp} + \bigtriangleup \varepsilon))(|\mathbf{p}|^2 - \varepsilon_{\perp}) = 0 \end{aligned}$$

(25) the vector components of 
$$\hat{d}$$
 depend on the second

where the vector components of **d** depend on the coordinates x, y, and z. If we take  $\hat{\mathbf{d}} = (0,0,1)$ , we obtain the optical indicatrix in the principal coordinate system as defined in Eq. (11). In addition, Eq. (25) can be written as  $\mathcal{H} = \mathcal{H}_e \mathcal{H}_o = 0$ , where  $\mathcal{H}_e$  corresponds to extraordinary waves and  $\mathcal{H}_o$  corresponds to ordinary waves.

In order to find an expression for the ray path of a light ray, we will use Eq. (25). A light ray can be denoted by the parametric equations  $x=x(\tau)$ ,  $y=y(\tau)$ , and  $z=z(\tau)$ , where the parameter  $\tau$  can be considered as time. Since we are interested primarily in the energy transfer of a light ray, we define a ray to be the trajectory of the Poynting vector, given by Eq. (20). According to Eq. (19), the direction of the Poynting vector  $\langle \mathbf{S} \rangle$  is the same as the direction of  $\nabla_{p}\mathcal{H}$ . Hence, we can write a set of equations for the ray path given by

$$\frac{\mathrm{d}i}{\mathrm{d}\tau} = \alpha \frac{\partial \mathcal{H}}{\partial p_i}, \quad i = x, y, z, \tag{26}$$

where the factor  $\alpha$  is an arbitrary function of  $\tau$  and influences only the parametric presentation of the ray position. As we move along the ray, the wave normal also changes. Hence, the vector components of the wave normal are also functions of  $\tau$ . Likewise, we can derive a set of equations for the wave normal (cf. [30], p. 110) reading

$$\frac{\mathrm{d}p_i}{\mathrm{d}\tau} = -\alpha \frac{\partial \mathcal{H}}{\partial i}, \quad i = x, y, z.$$
(27)

The next step is crucial, since we apply a classicalmechanical interpretation to the light rays: A mathematical light ray is considered a particle with coordinates  $\mathbf{r}=(x,y,z)$  and generalized momentum  $\mathbf{p}=(p_x,p_y,p_z)$ (cf. [30], p. 115), which satisfy Eqs. (26) and (27), respectively. Moreover, this particle has the energy  $\mathcal{H}(x,y,z,p_x,p_y,p_z)=0$ . With this mechanical interpretation of a light ray, Eq. (25) represents a Hamiltonian system with canonical equations given by

$$\frac{\mathrm{d}(x,y,z)}{\mathrm{d}\tau} = \alpha \nabla_p \mathcal{H}, \qquad (28)$$

$$\frac{\mathrm{d}(p_x, p_y, p_z)}{\mathrm{d}\tau} = -\alpha \nabla_r \mathcal{H}, \qquad (29)$$

where the ray position  $\mathbf{r}(\tau)$  and momentum  $\mathbf{p}(\tau)$  are functions of the parameter  $\tau$ . Equations (28) and (29) are also called the Hamilton equations. Equation (28) describes the ray path of the Poynting vector. For each position  $\mathbf{r}(\tau)$ , there is a corresponding momentum  $\mathbf{p}(\tau)$ , determined by Eq. (29).

The gradients with respect to the wave normal and the position of the Hamiltonian in Eq. (25) can be written as

$$\boldsymbol{\nabla}_{p}\mathcal{H} = \mathcal{H}_{o}\boldsymbol{\nabla}_{p}\mathcal{H}_{e} + \mathcal{H}_{e}\boldsymbol{\nabla}_{p}\mathcal{H}_{o}, \qquad (30)$$

$$\boldsymbol{\nabla}_{r} \mathcal{H} = \mathcal{H}_{o} \boldsymbol{\nabla}_{r} \mathcal{H}_{e} + \mathcal{H}_{e} \boldsymbol{\nabla}_{r} \mathcal{H}_{o}. \tag{31}$$

For ordinary waves,  $\mathcal{H}_o=0$ . As a result, the Hamilton equations for ordinary waves reduce to

$$\frac{\mathrm{d}(x,y,z)}{\mathrm{d}\tau} = \alpha \nabla_p \mathcal{H}_o, \qquad (32)$$

$$\frac{\mathrm{d}(p_{ox}, p_{oy}, p_{oz})}{\mathrm{d}\tau} = -\alpha \nabla_r \mathcal{H}_o, \qquad (33)$$

where the term  $\mathcal{H}_e$  is incorporated in the factor  $\alpha$ . For extraordinary waves, we obtain the same set of equations, except that the index o is replaced with the index e. By using Eq. (25), we will introduce novel expressions for the gradients of Eqs. (28) and (29) in terms of the director  $\hat{\mathbf{d}}$ .

In general, the Hamiltonian allows inhomogeneous dielectric constants. When the dielectric constants are inhomogeneous, their values are position dependent. Then the partial derivatives of  $\mathcal{H}_o$  read

$$\frac{\partial \mathcal{H}_o}{\partial i} = -\frac{\partial \varepsilon_{\perp}}{\partial i}, \quad \frac{\partial \mathcal{H}_o}{\partial p_{oi}} = 2p_{oi}, \quad i = x, y, z.$$
(34)

The partial derivatives of  $\mathcal{H}_e$  are less trivial and yield

$$\begin{split} \frac{\partial \mathcal{H}_e}{\partial i} &= 2(\varepsilon_{\parallel} - \varepsilon_{\perp})(\mathbf{p}_e \cdot \mathbf{\hat{d}}) \left( p_{ex} \frac{\partial \hat{d}_x}{\partial i} + p_{ey} \frac{\partial \hat{d}_y}{\partial i} + p_{ez} \frac{\partial \hat{d}_z}{\partial i} \right) + \varepsilon_{\perp} \frac{\partial \varepsilon_{\parallel}}{\partial i} \\ &+ (\varepsilon_{\parallel} + |\mathbf{p}_e|^2) \frac{\partial \varepsilon_{\perp}}{\partial i}, \end{split}$$

$$\frac{\partial \mathcal{H}_e}{\partial p_{ei}} = 2\varepsilon_{\perp} p_{ei} + 2(\varepsilon_{\parallel} - \varepsilon_{\perp})(\mathbf{p}_e \cdot \hat{\mathbf{d}})\hat{d}_i, \quad i = x, y, z.$$
(35)

However, for many liquid-crystal applications,  $\varepsilon_{\perp}$  and  $\varepsilon_{\parallel}$  are position-independent. Only the director  $\hat{\mathbf{d}}$  depends on position. Then  $\mathcal{H}_o$  is independent of position and the partial derivatives of  $\mathcal{H}_o$  read

$$\frac{\partial \mathcal{H}_o}{\partial i} = 0, \quad \frac{\partial \mathcal{H}_o}{\partial p_{oi}} = 2p_{oi}, \quad i = x, y, z.$$
(36)

As a result,  $\mathbf{p}_{o}$  is constant [see Eq. (33)] and  $x(\tau)$ ,  $y(\tau)$ , and  $z(\tau)$  represent a straight line. Likewise, the partial derivatives of  $\mathcal{H}_{e}$  reduce to

$$\begin{split} &\frac{\partial \mathcal{H}_{e}}{\partial i} = 2(\varepsilon_{\parallel} - \varepsilon_{\perp})(\mathbf{p}_{e} \cdot \mathbf{\hat{d}}) \left( p_{ex} \frac{\partial \hat{d}_{x}}{\partial i} + p_{ey} \frac{\partial \hat{d}_{y}}{\partial i} + p_{ez} \frac{\partial \hat{d}_{z}}{\partial i} \right), \\ &\frac{\partial \mathcal{H}_{e}}{\partial p_{ei}} = 2\varepsilon_{\perp} p_{ei} + 2(\varepsilon_{\parallel} - \varepsilon_{\perp})(\mathbf{p}_{e} \cdot \mathbf{\hat{d}}) \hat{d}_{i}, \quad i = x, y, z. \end{split}$$
(37)

We conclude that, in contrast with ordinary waves, the ray paths of extraordinary waves are curved.

For a homogeneous isotropic medium, i.e.,  $\varepsilon_{\perp} = \varepsilon_{\parallel}$ , the Hamilton equations reduce to

$$\frac{\mathrm{d}(x,y,z)}{\mathrm{d}\tau} = \alpha(p_x,p_y,p_z), \quad \frac{\mathrm{d}(p_x,p_y,p_z)}{\mathrm{d}\tau} = 0, \quad (38)$$

where  $\alpha$  incorporates any residual terms. Hence, for homogeneous isotropic media, the ray paths are straight lines.

Although the properties of the medium are allowed to change slowly over the wavelength, we conclude that the ray paths of the ordinary wave are straight lines. Apparently, the director may change along the ray path while the wave remains ordinary. Effectively, the ordinary wave behaves as if it is a wave in an isotropic medium with index of refraction  $n = n_o$ .

The equations of this section suggest that inside an inhomogeneous uniaxial anisotropic medium, the ordinary wave and extraordinary wave remain ordinary and extraordinary, respectively. In other words, the light is not scattered and propagates "adiabatically." Moreover, Eq. (25) suggests that the ordinary and extraordinary waves are mutually independent, since  $\mathcal{H} = \mathcal{H}_e \mathcal{H}_o = 0$ . This result is also known as mode independency. However, the mode independency is valid only to some approximation. Imagine that  $\Delta n = |n_e - n_o| \rightarrow 0$ . Under these circumstances, the ordinary and extraordinary waves can interact after being refracted at an anisotropic interface. In this case, the anisotropy can be considered as a weak disturbance of the isotropic properties of the medium. The latter is called a quasi-isotropic approximation [31]. However, we will assume the ordinary waves and extraordinary waves propagate independently.

# 6. GEOMETRICAL ANALYSIS OF THE WAVE NORMALS AT THE INTERFACE

In the bulk material of an inhomogeneous medium, we are now able to calculate the ray paths of light rays by using the Hamiltonian method. In order to calculate the optical properties at an anisotropic interface, it is necessary to calculate the wave field at an interface, according to Eq. (3). In Section 4, we have already derived the vector equations for the electric and magnetic polarization vectors. In order to calculate the polarization vectors of the electric and magnetic field vectors at an anisotropic interface, we must know the corresponding wave normals. In this section, we derive the vector equations for reflected and refracted wave normals at an anisotropic interface. In Section 7, we will calculate the complex amplitudes aof the field vectors  $\tilde{\mathbf{E}}$  and  $\tilde{\mathbf{H}}$  with the help of the results obtained in the current section.

First, we consider a normalized incident Poynting vector  $\langle \hat{\mathbf{S}}_i \rangle$  of an incident extraordinary wave. This vector defines the direction of the energy transfer of a wave incident at an interface between two anisotropic media. By using the properties of the ellipsoid surface  $\mathcal{H}_e$  and the unit vector  $\langle \hat{\mathbf{S}}_i \rangle$ , we will derive an expression for the corresponding incident extraordinary wave normal  $\mathbf{p}_{ie}$ . According to Eq. (19),  $\langle \hat{\mathbf{S}}_i \rangle$  has the same direction as  $\nabla_p \mathcal{H}_e$ . Therefore, we obtain

$$\langle \hat{\mathbf{S}}_i \rangle = \frac{\nabla_p \mathcal{H}_e}{|\nabla_p \mathcal{H}_e|}.$$
(39)

Together with the condition that  $\mathcal{H}_e=0$ , Eq. (39) results in four equations with three unknowns: the three vector components of  $\mathbf{p}_{ie}$ . This set of equations is solvable. As a result, we obtain an expression for the incident extraordinary wave normal in terms of the vector components of  $\langle \hat{\mathbf{S}}_i \rangle$  and, in the principle coordinate system, it reads

$$\mathbf{p}_{ie} = \frac{(n_e^2 \langle \hat{S}_{ix} \rangle, n_e^2 \langle \hat{S}_{iy} \rangle, n_o^2 \langle \hat{S}_{iz} \rangle)}{\sqrt{n_e^2 + (n_o^2 - n_e^2) \langle \hat{S}_{iz} \rangle^2}}.$$
(40)

If  $n_e = n_o = n$ , Eq. (40) reduces to  $\mathbf{p}_i = n \langle \hat{\mathbf{S}}_i \rangle$ , which applies for ordinary waves and waves in isotropic media. Hence, for arbitrary values of  $n_o$  and  $n_e$ , we can apply Eq. (40) to both isotropic and anisotropic media in the principal coordinate system.

For a proper determination of the reflected and refracted wave normals at the interface, we apply Snell's law in vector notation given by

$$\mathbf{p}_i \times \mathbf{\hat{n}} = \mathbf{p} \times \mathbf{\hat{n}},\tag{41}$$

where  $\hat{\mathbf{n}}$  is the local normal vector to the boundary,  $\mathbf{p}_i$  is an incident wave normal, and  $\mathbf{p}$  is the corresponding transmitted or reflected wave normal. Snell's law demands that the tangential component of the wave normal  $(\mathbf{p}_{tn})$  be continuous across the boundary. Given the incident wave normal  $\mathbf{p}_i$ , the tangential wave normal  $\mathbf{p}_{tn}$  can be calculated by subtracting the normal component from the incident wave normal, yielding

$$\mathbf{p}_{tn} = \mathbf{p}_i - (\mathbf{p}_i \cdot \hat{\mathbf{n}}) \hat{\mathbf{n}}. \tag{42}$$

At this point, the waves can be either reflected or refracted. In the case of reflection, we define the  $n_o$  and  $n_e$  of the incident medium. In the case of refraction, we define the  $n_o$  and  $n_e$  of the second medium. In what follows, we derive general expressions for the reflected and refracted wave normals for which  $n_o$  and  $n_e$  can be chosen arbitrarily.

For ordinary waves, the wave normal is determined by the intersection of the vector  $\mathbf{p}_o = \mathbf{p}_{tn} + \xi \hat{\mathbf{n}}$  with the surface  $\mathcal{H}_o = 0$ , where  $\xi$  is a variable. Since  $\mathcal{H}_o = 0$  represents a sphere with radius  $n_o$ ,  $\xi$  must satisfy the condition  $|\mathbf{p}_{tn}|^2 + \xi^2 = n_o^2$ . Therefore, we conclude that the transmitted or reflected ordinary wave normal reads

$$\mathbf{p}_o = \mathbf{p}_{tn} \pm \sqrt{n_o^2 - |\mathbf{p}_{tn}|^2} \mathbf{\hat{n}}, \qquad (43)$$

where the plus sign applies to transmitted waves and the minus sign applies to reflected waves. In isotropic media, we can apply Eq. (43) if  $n_o$  is replaced with n.

Similarly, the extraordinary wave normal is given by

$$\mathbf{p}_e = \mathbf{p}_{tn} + \xi \mathbf{\hat{n}}. \tag{44}$$

The constant  $\xi$  is determined by the condition that the end point of the wave normal  $\mathbf{p}_e$  lies on the ellipsoid surface  $\mathcal{H}_e=0$ . Therefore, in the principal coordinate system,  $\xi$  is now given by

$$\xi = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A},$$

$$A = \frac{\hat{n}_z^2}{n_o^2} + \frac{\hat{n}_x^2 + \hat{n}_y^2}{n_e^2},$$

$$B = \frac{2p_{tnz}\hat{n}_z}{n_o^2} + \frac{2p_{tnx}\hat{n}_x + 2p_{tny}\hat{n}_y}{n_e^2},$$

$$C = \frac{p_{tnz}^2}{n_o^2} + \frac{p_{tnx}^2 + p_{tny}^2}{n_e^2} - 1.$$
(45)

Again, the plus sign applies to transmitted waves, and the minus sign applies to reflected waves. If  $n_e = n_o = n$ ,  $A = 1/n^2$ ,  $B = 2/n^2 (\mathbf{p}_{tn} \cdot \hat{\mathbf{n}}) = 0$ , and  $C = |\mathbf{p}_{tn}|^2/n^2 - 1$ . Then  $\xi = \pm \sqrt{n^2 - |\mathbf{p}_{tn}|^2}$ , which applies for isotropic media and ordinary waves (see Eq. (43)).

In this section, we have derived concise vector equations in order to calculate the incident, reflected, and refracted wave normals of both ordinary and extraordinary waves at an anisotropic interface. These equations apply to arbitrary values of  $n_o$  and  $n_e$ . The reflected and refracted normalized Poynting vectors are defined in Eq. (39). The vector equations derived in this section apply only in the principal coordinate system. In addition, it can be concluded that all wave normals, together with  $\hat{\mathbf{n}}$ , are in the same plane: the plane of incidence.

# 7. FRESNEL COEFFICIENTS AT THE INTERFACE

Since we now can calculate the polarization vectors with the corresponding wave propagation vectors, we are left with the calculation of the complex amplitudes a of the electric and magnetic field vectors  $\tilde{\mathbf{E}}$  and  $\tilde{\mathbf{H}}$ , respectively.

Consider a plane boundary that forms the interface between two different transparent media. Locally, these media either have homogeneous isotropic or homogeneous uniaxially anisotropic properties. This gives rise to four different kinds of interfaces, namely, isotropic–isotropic, isotropic–anisotropic, anisotropic–isotropic, and anisotropic–anisotropic. In order to calculate the electromagnetic fields at both sides of an interface, we apply boundary conditions. The boundary conditions (derived from Maxwell's equations) demand that across the boundary, the tangential components of the field vectors  $\tilde{\mathbf{E}}$  and  $\tilde{\mathbf{H}}$  should be continuous (cf. [36], p. 18). In an isotropic medium, these boundary conditions are applied to two independent modes. One mode is *s* polarized, with the electric polarization vector component perpendicular to the plane of incidence. The other mode is *p* polarized, which means that the electric polarization vector component is in the plane of incidence. In anisotropic media, the boundary conditions are applied to the ordinary wave and the extraordinary wave separately.

For a general approach, we consider the case for an anisotropic–anisotropic interface. Figure 3 shows the refracted and reflected waves at an anisotropic–anisotropic interface. In general, there are two reflected waves, namely, an ordinary wave and an extraordinary wave, indicated by  $R_o$  and  $R_e$ , respectively. Similarly, there is a transmitted ordinary wave and a transmitted extraordinary wave, indicated by  $T_o$  and  $T_e$ , respectively.

In order to apply the boundary conditions, we define two orthogonal vectors  $\mathbf{t}_s$  and  $\mathbf{t}_p$  tangential to the interface given by

$$\mathbf{t}_s = \mathbf{p}_i \times \hat{\mathbf{n}}, \quad \mathbf{t}_p = \hat{\mathbf{n}} \times \mathbf{t}_s. \tag{46}$$

The boundary conditions are applied to both the *s* components and the *p* components of the electromagnetic field vectors. Application of the boundary conditions yields four linear equations given by (cf. [18], p. 2391)

$$\mathbf{t}_{s} \cdot (a_{to}\hat{\mathbf{E}}_{to} + a_{te}\hat{\mathbf{E}}_{te}) = \mathbf{t}_{s} \cdot (\widetilde{\mathbf{E}}_{i} + a_{ro}\hat{\mathbf{E}}_{ro} + a_{re}\hat{\mathbf{E}}_{re}),$$

$$\mathbf{t}_{p} \cdot (a_{to}\hat{\mathbf{E}}_{to} + a_{te}\hat{\mathbf{E}}_{te}) = \mathbf{t}_{p} \cdot (\widetilde{\mathbf{E}}_{i} + a_{ro}\hat{\mathbf{E}}_{ro} + a_{re}\hat{\mathbf{E}}_{re}),$$

$$\mathbf{t}_{s} \cdot (a_{to}\mathbf{H}_{to} + a_{te}\mathbf{H}_{te}) = \mathbf{t}_{s} \cdot (\widetilde{\mathbf{H}}_{i} + a_{ro}\mathbf{H}_{ro} + a_{re}\mathbf{H}_{re}),$$

$$\mathbf{t}_{p} \cdot (a_{to}\mathbf{H}_{to} + a_{te}\mathbf{H}_{te}) = \mathbf{t}_{p} \cdot (\widetilde{\mathbf{H}}_{i} + a_{ro}\mathbf{H}_{ro} + a_{re}\mathbf{H}_{re}), \quad (47)$$

where  $\tilde{\mathbf{E}}_i$  and  $\tilde{\mathbf{H}}_i$  are the incident electric and magnetic field vectors, respectively. The vectors  $\hat{\mathbf{E}}$  and  $\mathbf{H}$  are the electric and magnetic polarization vectors defined in Eqs. (14) and (15), respectively. The indices r and t denote re-

Fig. 3. Refraction and reflection at an anisotropic–anisotropic interface. The transmitted ordinary wave and extraordinary wave are indicated by  $T_o$  and  $T_e$ , respectively. The reflected ordinary wave and extraordinary wave are indicated by  $R_o$  and  $R_e$ , respectively.

flected and transmitted waves, respectively. The indices o and e denote ordinary and extraordinary waves, respectively. These equations are the Fresnel equations and can be written as a linear matrix equation given by

$$\begin{pmatrix} \mathbf{t}_{s} \cdot \hat{\mathbf{E}}_{to} & \mathbf{t}_{s} \cdot \hat{\mathbf{E}}_{te} & -\mathbf{t}_{s} \cdot \hat{\mathbf{E}}_{ro} & -\mathbf{t}_{s} \cdot \hat{\mathbf{E}}_{re} \\ \mathbf{t}_{p} \cdot \hat{\mathbf{E}}_{to} & \mathbf{t}_{p} \cdot \hat{\mathbf{E}}_{te} & -\mathbf{t}_{p} \cdot \hat{\mathbf{E}}_{ro} & -\mathbf{t}_{p} \cdot \hat{\mathbf{E}}_{re} \\ \mathbf{t}_{s} \cdot \mathbf{H}_{to} & \mathbf{t}_{s} \cdot \mathbf{H}_{te} & -\mathbf{t}_{s} \cdot \mathbf{H}_{ro} & -\mathbf{t}_{s} \cdot \mathbf{H}_{re} \\ \mathbf{t}_{p} \cdot \mathbf{H}_{to} & \mathbf{t}_{p} \cdot \mathbf{H}_{te} & -\mathbf{t}_{p} \cdot \mathbf{H}_{ro} & -\mathbf{t}_{p} \cdot \mathbf{H}_{re} \\ \end{pmatrix} \begin{vmatrix} a_{to} \\ a_{te} \\ a_{ro} \\ a_{re} \end{vmatrix} \\ = \begin{pmatrix} \mathbf{t}_{s} \cdot \tilde{\mathbf{E}}_{i} \\ \mathbf{t}_{p} \cdot \tilde{\mathbf{E}}_{i} \\ \mathbf{t}_{s} \cdot \tilde{\mathbf{H}}_{i} \\ \mathbf{t}_{p} \cdot \tilde{\mathbf{H}}_{i} \end{pmatrix}.$$
(48)

The only unknowns in this matrix equation are the complex amplitudes  $a_{to}$ ,  $a_{te}$ ,  $a_{ro}$ , and  $a_{re}$ . These complex amplitudes are the Fresnel coefficients. The matrix equation can be solved analytically and by any of the standard methods as, e.g., described in [37]. Note that  $\tilde{\mathbf{E}}_i$  should represent a polarization eigenmode of the incident medium. For this type of interface, this means that  $\tilde{\mathbf{E}}_i$  represents either an ordinary wave or an extraordinary wave. In an isotropic medium,  $\tilde{\mathbf{E}}_i$  is always a polarization eigenmode of the medium so that  $\tilde{\mathbf{E}}_i$  can be chosen arbitrarily.

The advantage of Eq. (48) is that it is also applicable to the remaining types of interfaces. Consider for example an isotropic–anisotropic interface. For this type of interface,  $a_{ro}$  and  $a_{re}$  need to be replaced with  $a_{rs}$  and  $a_{rp}$ , respectively. In addition,  $\hat{\mathbf{E}}_{ro}$ ,  $\hat{\mathbf{E}}_{re}$ ,  $\mathbf{H}_{ro}$ , and  $\mathbf{H}_{re}$  are replaced with  $\hat{\mathbf{E}}_{rs}$ ,  $\hat{\mathbf{E}}_{rp}$ ,  $\mathbf{H}_{rs}$ , and  $\mathbf{H}_{rp}$ , respectively. Of course, Eqs. (14) and (15) no longer apply for the reflected waves. Instead, we define the electric polarization vector of the *s*-polarized wave component

$$\hat{\mathbf{E}}_{rs} = \frac{\mathbf{p}_r \times \hat{\mathbf{n}}}{|\mathbf{p}_r \times \hat{\mathbf{n}}|},\tag{49}$$

and the electric polarization vector of the p-polarized wave component is defined as

$$\hat{\mathbf{E}}_{rp} = \frac{\hat{\mathbf{E}}_{rs} \times \mathbf{p}_r}{|\hat{\mathbf{E}}_{rs} \times \mathbf{p}_r|}.$$
(50)

For an anisotropic–isotropic interface, Eqs. (49) and (50) apply as well, provided that the index r is replaced with the index t, resulting in the set of Fresnel coefficients  $a_{ts}$ ,  $a_{tp}$ ,  $a_{ro}$ , and  $a_{re}$ . For isotropic–isotropic interfaces, Eqs. (49) and (50) apply for both the index r and the index t, yielding  $a_{ts}$ ,  $a_{tp}$ ,  $a_{rs}$ , and  $a_{rp}$ .

As a result, the electromagnetic field of, e.g., a reflected wave in an isotropic medium is given by



$$\mathbf{E}_{r} = (a_{rs}\mathbf{\hat{E}}_{rs} + a_{rp}\mathbf{\hat{E}}_{rp})e^{i(k_{0}\psi_{r}-\omega t)},$$
$$\mathbf{H}_{r} = \frac{1}{c\,\mu_{0}}(a_{rs}\mathbf{H}_{rs} + a_{rp}\mathbf{H}_{rp})e^{i(k_{0}\psi_{r}-\omega t)},$$
(51)

while the electromagnetic field of a transmitted extraordinary wave is given by

$$\mathbf{E}_{te} = a_{te} \hat{\mathbf{E}}_{te} e^{i(k_0 \psi_{te} - \omega t)}, \quad \mathbf{H}_{te} = \frac{1}{c \mu_0} a_{te} \mathbf{H}_{te} e^{i(k_0 \psi_{te} - \omega t)}.$$
(52)

From the electromagnetic field, we can calculate the timeaveraged Poynting vector using Eq. (18). Moreover, we can determine the phase and the polarization state.

Finally, for an arbitrary type of interface, we can apply the law of conservation of energy flow in the direction of the normal vector  $\hat{\mathbf{n}}$ . For an anisotropic–anisotropic interface, this yields

$$\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{to} \rangle + \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{te} \rangle - \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{ro} \rangle - \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{re} \rangle = \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle.$$
(53)

The minus sign appears since, for reflected waves,  $\hat{\mathbf{n}} \cdot \langle \mathbf{S}_r \rangle \leq 0$ . By dividing both sides of Eq. (53) by  $\hat{\mathbf{n}} \cdot \langle \mathbf{S}_i \rangle$ , we obtain

$$\frac{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{to} \rangle}{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle} + \frac{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{te} \rangle}{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle} - \frac{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{ro} \rangle}{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle} - \frac{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{re} \rangle}{\hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle} = 1.$$
(54)

The electromagnetic field at an anisotropic-anisotropic interface has to satisfy Eq. (54). Each term on the left-hand side of Eq. (54) represents either an intensity transmittance factor T or an intensity reflectance factor R. Consequently, Eq. (54) can be written as

$$T_o + T_e + R_o + R_e = 1, (55)$$

with

$$T_{o} = \begin{vmatrix} \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{to} \rangle \\ \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle \end{vmatrix}, \quad T_{e} = \begin{vmatrix} \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{te} \rangle \\ \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle \end{vmatrix},$$
$$R_{o} = \begin{vmatrix} \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{ro} \rangle \\ \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle \end{vmatrix}, \quad R_{e} = \begin{vmatrix} \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{re} \rangle \\ \hat{\mathbf{n}} \cdot \langle \mathbf{S}_{i} \rangle \end{vmatrix}. \tag{56}$$

For the remaining types of interfaces, we obtain similar results. The difference is that for an isotropic–anisotropic interface, we obtain  $T_o$ ,  $T_e$ , and R. For an anisotropic–isotropic interface, we obtain  $R_o$ ,  $R_e$ , and T. For isotropic–isotropic interfaces, we simply obtain R and T.

The procedure described in this section is known in the literature. However, the main conclusion of this section is that the calculation of the Fresnel coefficients is significantly simplified with the help of the vector equations derived in Sections 4 and 6.

#### 8. GENERAL PROCEDURE FOR SLOWLY VARYING ANISOTROPIC MEDIA

In this section, we will discuss a general procedure that can be applied when we are interested in the optical properties of the interface and the bulk of an anisotropic medium. In practice, one usually begins the process of ray tracing outside an anisotropic medium. Hence, we first discuss the optical properties of an anisotropic interface. Then we describe how to proceed in the anisotropic bulk material.

#### A. Optical Properties of an Anisotropic Interface

In general, an anisotropic interface is locally defined by the surface normal  $\hat{\mathbf{n}}$  and the optical properties of the incident medium (medium 1) and the second medium (medium 2). In order to maintain a general approach, we will assume that both medium 1 and medium 2 are anisotropic. The optical properties of medium 1 are defined by the local optical axis at the interface  $\hat{\mathbf{o}}_1$  and the local indices of refraction  $n_{o1}$  and  $n_{e1}$ . Likewise, the optical properties of medium 2 are defined by  $\hat{\mathbf{o}}_2$ ,  $n_{o2}$ , and  $n_{e2}$ . With this information, the configuration is specified.

Then we need to define an incident wave field with normalized Poynting vector  $\langle \hat{\mathbf{S}}_i \rangle$  and electric polarization vector  $\hat{\mathbf{E}}_i$ . This electric polarization vector should be a polarization eigenmode of the medium. For anisotropic media, this means that  $\hat{\mathbf{E}}_i$  either represents an ordinary wave or an extraordinary wave. For the moment, we assume an extraordinary wave.

With Eqs. (40) and (42), we calculate the incident extraordinary wave normal  $\mathbf{p}_{ie}$  and the tangential wave normal  $\mathbf{p}_{tn}$ . However, Eq. (40) applies only in the principal coordinate system. Therefore, the optical axis  $\hat{\mathbf{o}}_1$ , the surface normal  $\hat{\mathbf{n}}$ , and the incident Poynting vector  $\langle \hat{\mathbf{S}}_i \rangle$ should be transformed to a local coordinate system in which the optical axis  $\hat{\mathbf{o}}_1 = (0, 0, 1)$ . Consider a matrix  $\mathcal{A}_1$ that represents a linear orthogonal transformation that transforms the optical axis  $\hat{\mathbf{o}}_1$  to  $\mathcal{A}_1 \hat{\mathbf{o}}_1 = (0,0,1)$ . Then the "new input" is given by  $\langle \hat{\mathbf{S}}_i^p \rangle = \mathcal{A}_1 \langle \hat{\mathbf{S}}_i \rangle$  and  $\hat{\mathbf{n}}^p = \mathcal{A}_1 \hat{\mathbf{n}}$ , where the index p denotes the principal coordinate system. These vectors can be applied to Eqs. (40) and (42). As a result, we know  $\mathbf{p}_{ie}^{p}$  and  $\mathbf{p}_{tn}^{p}$  in the local principal coordinate system of medium 1. In addition, we can calculate the reflected wave normals  $\mathbf{p}_{ro}^{p}$  and  $\mathbf{p}_{re}^{p}$  in the principal coordinate system of medium 1 by applying Eqs. (43)-(45). Obviously, we apply the minus sign in Eq. (45).

Subsequently, we need to transform the calculated wave normals  $\mathbf{p}_{ie}^{p}$ ,  $\mathbf{p}_{in}^{p}$ ,  $\mathbf{p}_{ro}^{p}$ , and  $\mathbf{p}_{re}^{p}$  and the vectors  $\langle \hat{\mathbf{S}}_{i}^{p} \rangle$ ,  $\hat{\mathbf{n}}^{p}$ , and  $\hat{\mathbf{o}}_{1}^{p}$  back to the original coordinate system of medium 1. To this end, we apply the inverse of the matrix  $\mathcal{A}_{1}$ , denoted by  $\mathcal{A}_{1}^{-1}$ .

Next, we calculate the refracted wave normals  $\mathbf{p}_{to}$  and  $\mathbf{p}_{te}$  by using Eqs. (43)–(45). Since Eq. (45) applies only in the principal coordinate system,  $\hat{\mathbf{n}}$  and  $\mathbf{p}_{tn}$  need to be transformed to the principal coordinate system of medium 2. Similar to the considerations mentioned above, we define a matrix  $\mathcal{A}_2$  that transforms the optical axis  $\hat{\mathbf{o}}_2$  to  $\mathcal{A}_2\hat{\mathbf{o}}_2=(0,0,1)$ . In this case, the new vectors in the principal coordinate system of medium 2 are defined as  $\hat{\mathbf{n}}^p$  and  $\mathbf{p}_{tn}^p$ . These vectors are applied to Eqs. (43)–(45). This time, we apply the plus sign in Eq. (45). Finally, the vectors  $\hat{\mathbf{n}}^p$ ,  $\mathbf{p}_{tn}^p$ ,  $\hat{\mathbf{o}}_2^p$ ,  $\mathbf{p}_{to}^p$ , and  $\mathbf{p}_{te}^p$  are transformed back to the original coordinate system of medium 2 by applying the inverse matrix  $\mathcal{A}_2^{-1}$ .

The transformation matrices  $\mathcal{A}$  denote rotation matrices. The rotation matrices used here are  $3 \times 3$  matrices that represent a geometric rotation about a fixed origin in

three-dimensional space. The exact definition of these matrices depends on the definition of the optical axis  $\hat{\mathbf{o}}$ . The procedure for finding the right rotation matrices entails straightforward linear algebra. Hence, we will not discuss this procedure here.

For the calculation of the Fresnel coefficients, we first need to calculate the electric and magnetic polarization vectors of the incident, refracted, and reflected waves. By applying Eqs. (14) and (15), we obtain

$$\hat{\mathbf{E}}_{to} = \frac{\mathbf{p}_{to} \times \hat{\mathbf{o}}_2}{|\mathbf{p}_{to} \times \hat{\mathbf{o}}_2|},$$

$$\hat{\mathbf{E}}_{te} = \frac{(\mathbf{p}_{te} \times \hat{\mathbf{o}}_2) \times \nabla_p \mathcal{H}_e |_{\mathbf{p} = \mathbf{p}_{te}}}{|(\mathbf{p}_{te} \times \hat{\mathbf{o}}_2) \times \nabla_p \mathcal{H}_e |_{\mathbf{p} = \mathbf{p}_{te}}|},$$

$$\hat{\mathbf{E}}_{ro} = \frac{\mathbf{p}_{ro} \times \hat{\mathbf{o}}_1}{|\mathbf{p}_{ro} \times \hat{\mathbf{o}}_1|},$$

$$\hat{\mathbf{E}}_{re} = \frac{(\mathbf{p}_{re} \times \hat{\mathbf{o}}_1) \times \nabla_p \mathcal{H}_e |_{\mathbf{p} = \mathbf{p}_{re}}}{|(\mathbf{p}_{re} \times \hat{\mathbf{o}}_1) \times \nabla_p \mathcal{H}_e |_{\mathbf{p} = \mathbf{p}_{re}}|}.$$
(57)

Take note of the fact that before  $\nabla_{p}\mathcal{H}_{e}$  can be applied to Eq. (57), it needs to be calculated in the principal coordinate system and the resulting vector products on the right-hand sides of Eqs. (57) must than be transformed back to the original coordinate system. As mentioned before, the electric polarization vector  $\hat{\mathbf{E}}_{i}$  of the incident wave is an input vector. In addition, the incident magnetic polarization vector is given by  $\mathbf{H}_{i}=\mathbf{p}_{ie}\times\hat{\mathbf{E}}_{i}$ . Likewise, we can calculate the magnetic polarization vectors of the refracted and reflected waves  $\mathbf{H}_{to}$ ,  $\mathbf{H}_{te}$ ,  $\mathbf{H}_{ro}$ , and  $\mathbf{H}_{re}$ . Finally, the orthogonal vectors  $\mathbf{t}_{s}$  and  $\mathbf{t}_{p}$  are given by Eq. (46).

In general, it is convenient to define the incident electric field vector  $\tilde{\mathbf{E}}_i = \hat{\mathbf{E}}_i$ . Then the Fresnel coefficients can be obtained from the matrix equation given by Eq. (48). This matrix equation can be solved analytically or by any of the standard procedures described in Numerical Recipes (cf. [37], Chapter 2). As a result, the electromagnetic fields of the incident and refracted waves are given by

$$\begin{split} \mathbf{E}_{i} &= \hat{\mathbf{E}}_{i} e^{i(k_{0}\psi_{i}-\omega t)}, \quad \mathbf{H}_{i} = \frac{1}{c\mu_{0}} \mathbf{H}_{i} e^{i(k_{0}\psi_{i}-\omega t)}, \\ \mathbf{E}_{to} &= a_{to} \hat{\mathbf{E}}_{to} e^{i(k_{0}\psi_{to}-\omega t)}, \quad \mathbf{H}_{to} = \frac{1}{c\mu_{0}} a_{to} \mathbf{H}_{to} e^{i(k_{0}\psi_{to}-\omega t)}, \\ \mathbf{E}_{te} &= a_{te} \hat{\mathbf{E}}_{te} e^{i(k_{0}\psi_{te}-\omega t)}, \quad \mathbf{H}_{te} = \frac{1}{c\mu_{0}} a_{te} \mathbf{H}_{te} e^{i(k_{0}\psi_{te}-\omega t)}. \end{split}$$
(58)

The reflected electromagnetic fields are similar, provided that the index t is replaced with the index r. When we apply Eq. (18), the phase terms of the corresponding electric and magnetic fields in Eq. (58) cancel out. Finally, we apply Eqs. (55) and (56) in order to calculate the intensity transmittance and reflectance factors  $T_o$ ,  $T_e$ ,  $R_o$ , and  $R_e$ .

#### **B.** Optical Properties of an Anisotropic Bulk Material

At this point, we can continue with the calculation of the ray paths  $\mathbf{r}(\tau)$  in the bulk of medium 1 and medium 2. The ray paths can be calculated if the director  $\hat{\mathbf{d}} = (\hat{d}_x, \hat{d}_y, \hat{d}_z)$  is known as a function of position inside the medium. In other words, we assume that the normalized vector field  $\hat{\mathbf{d}}(x,y,z)$  is given. In addition, we assume position-independent refractive indices  $n_o$  and  $n_e$ .

As an example, we can determine the ray path of the refracted extraordinary wave. If we redefine  $\tau$  such that  $\alpha=1$ , the corresponding Hamilton equations are

$$\frac{\mathrm{d}\mathbf{r}(\tau)}{\mathrm{d}\tau} = \nabla_p \mathcal{H}_e(\hat{\mathbf{d}}),$$
$$\frac{\mathrm{d}\mathbf{p}_e(\tau)}{\mathrm{d}\tau} = -\nabla_r \mathcal{H}_e(\hat{\mathbf{d}}), \tag{59}$$

with  $\nabla_p \mathcal{H}_e$  and  $\nabla_r \mathcal{H}_e$  as defined in Eq. (37):

$$\begin{aligned} \frac{\partial \mathcal{H}_e}{\partial i} &= 2(\varepsilon_{\parallel} - \varepsilon_{\perp})(\mathbf{p}_e \cdot \mathbf{\hat{d}}) \left( p_{ex} \frac{\partial \hat{d}_x}{\partial i} + p_{ey} \frac{\partial \hat{d}_y}{\partial i} + p_{ez} \frac{\partial \hat{d}_z}{\partial i} \right), \\ \frac{\partial \mathcal{H}_e}{\partial p_{ei}} &= 2\varepsilon_{\perp} p_{ei} + 2(\varepsilon_{\parallel} - \varepsilon_{\perp})(\mathbf{p}_e \cdot \mathbf{\hat{d}}) \hat{d}_i, \quad i = x, y, z. \end{aligned}$$
(60)

These equations of Eq. (59) are a set of six coupled firstorder differential equations for the vector components of  $\mathbf{r}(\tau)$  and  $\mathbf{p}_e(\tau)$ . These differential equations can be solved with, e.g., the first-order Runge–Kutta method, also known as the Euler method (cf., [37], p. 704). If we start at the anisotropic interface at "time"  $\tau = \tau_0$ , the initial conditions for the set of first-order differential equations are given by

$$\mathbf{r}(\tau_0) = (x_0, y_0, z_0),$$
  
$$\mathbf{p}_e(\tau_0) = \mathbf{p}_{te}.$$
 (61)

By taking steps  $\Delta \tau$  in the time  $\tau$ , the Runge–Kutta method solves the ray path  $\mathbf{r}(\tau_0+N\Delta \tau)$  and the corresponding wave normal  $\mathbf{p}_e(\tau_0+N\Delta \tau)$ , with  $N \in \mathbb{N}$ . In this way, we obtain the ray path of the extraordinary wave in the bulk material of medium 2. Likewise, we can calculate the ray paths of the refracted ordinary wave in medium 2 and the reflected waves in medium 1.

We always need to define a director profile before we can apply the model. This director profile may be specified by an explicit mathematical formula. This means that the director is known at all points in space. Then we say that the director profile is continuous. On the other hand, numerical director profiles define the director only at discrete points in space. Numerical director profiles are produced by optical analysis software programs, like LCD Master [38] or 2dimMOS [39]. In that case, the director profile can be interpolated and the order of the interpolation must be the order of the Runge–Kutta method. Our model can be applied to both mathematical and numerical director profiles.

In this section, the vector equations for the polarized ray tracing of an extraordinary wave are clearly displayed. Altogether, the procedure described here is a clear outline of how to apply the polarized ray-tracing method derived in Sections 4–7 in practice.

# 9. SOME MODELING RESULTS FOR PRACTICAL GEOMETRIES

In order to establish a link with the real world of anisotropic phenomena, we present two cases to which our model is applied. First, we apply the model to an aircalcite interface. Second, we apply the model to an inhomogeneous anisotropic director profile in three dimensions.

# A. Transmission and Reflection at an Air–Calcite Interface

The model described in Sections 3-7 can be used to determine the optical properties of an anisotropic medium at an interface. As an example, we apply the model to a plane isotropic-anisotropic interface. We define the isotropic and anisotropic medium to be air and calcite, respectively. We use calcite with an ordinary index of refraction  $n_0 = 1.655$  and an extraordinary index of refraction  $n_e = 1.485$  (negative birefringence) [16]. These values for the refractive indices are valid for light with a wavelength of 633 nm. The plane of incidence is the *xz* plane, and the optical axis  $\hat{\mathbf{o}}$  is at 45° with the xz plane. The incident light has a linear polarization in the plane of incidence (p polarization). As a function of the angle of incidence  $\theta_i$ , we calculate the transmittance factor  $T_o$  for the ordinary wave. Similarly, we calculate  $T_e$ ,  $R_s$ , and  $R_p$ . The results are depicted in Fig. 4. The sum of  $T_o$ ,  $T_e$ ,  $R_s$ , and  $R_p$  is indicated by  $T_t$  and should result in 1 for any value of  $\theta_i$ .

It appears that the tilted optical axis generates both extraordinary and ordinary waves. In addition, the reflected light is mainly p polarized. The Brewster angle  $\theta_B$  is defined as the angle where  $R_p$  vanishes. From Fig. 4, we can read a Brewster angle of 59.76°. In Lekner, the Brewster angle is calculated analytically [22]. There the reflection



Fig. 4. Transmittance and reflectance factors as a function of the angle of incidence  $\theta_i$  for an air-calcite interface. The optical axis is at 45° with the plane of incidence;  $T_o$  and  $T_e$  are the ordinary and extraordinary transmittance factors, respectively;  $R_s$  and  $R_p$  are the reflectance factors for *s*- and *p*-polarized light, respectively;  $T_i$  is the sum of these factors and should result in 1 for any value of  $\theta_i$ . The Brewster angle  $\theta_B$  is the angle where  $R_p$  vanishes and reads 59.76°.



Fig. 5. Brewster angle  $\theta_B$  for an air-calcite interface as a function of  $\gamma^2$ . The optical axis is in the plane of incidence. The parameter  $\gamma$  is the cosine of the angle  $\Gamma$  between the optical axis  $\hat{\mathbf{o}}$  and the surface normal  $\hat{\mathbf{n}}$ .

amplitudes result in a quartic equation of which one of the physical roots determines the Brewster angle. Lekner predicts a Brewster angle of 59.75° (cf. [22], Table 1, p. 2766). Lekner also calculates the Brewster angle  $\theta_B$  as a function of the angle  $\Gamma$  that the optical axis makes with the normal  $\hat{\mathbf{n}}$  [16]. In this case, the optical axis is defined in the plane of incidence. Figure 5 shows the Brewster angle as a function of the square of the cosine of the angle  $\Gamma$ , denoted by  $\gamma^2$ . We can conclude that Lekner's results are well reproduced (cf. [16], Fig. 1, p. 2061).

#### **B.** Artificial Gradient-Index Lens

In this section, we apply the model to light rays incident on an artificial three-dimensional inhomogeneous director profile. With this artificial director profile, we aim to demonstrate the capacity of our method to provide insight into the optical behavior of such configurations.

Consider a Cartesian coordinate system in which the plane z=0 is defined as a grounded conducting plate with electric potential  $\Phi=0$ . Let there be a point charge in (0,0,a), for some a>0, with positive charge q (see Fig. 6). Using the method of images [36], we can write the electric potential due to the charge q for  $z \ge 0$  as

$$\Phi(x,y,z) = \frac{q}{4\pi\varepsilon_0} \frac{1}{\sqrt{x^2 + y^2 + (z-a)^2}} - \frac{q}{4\pi\varepsilon_0} \frac{1}{\sqrt{x^2 + y^2 + (z+a)^2}}.$$
 (62)



Fig. 6. Point charge q at a distance a above the origin. The plane z=0 is defined as a grounded conducting plate. As a result, there is an electric field in the half-space  $z \ge 0$ .

The corresponding electric field is then given by  $\mathbf{E}(x,y,z) = -\nabla \Phi(x,y,z)$ . Let the space  $z \ge 0$  be filled with an anisotropic medium with the material properties of liquid crystal. We will assume that the field is so high that all directors follow the field direction. In other words, the electric energy is considered to be much higher than the elastic energy between the directors. Hence, the director profile due to the electric field of the point charge q is

$$\hat{\mathbf{d}}(x,y,z) = \frac{\mathbf{E}(x,y,z)}{|\mathbf{E}(x,y,z)|}, \quad z \ge 0.$$
(63)

Figure 7 shows the director profile in the *xz* plane for *a* =50,  $x \in [-50, 50]$ , and  $z \in [0, 100]$ . The anisotropic medium in the upper half-space  $z \ge 0$  has an ordinary index of refraction  $n_o = 1.5$  and an extraordinary index of refraction  $n_e = 1.7$ . The lower half-space z < 0 is assumed to be glass with an index of refraction  $n_{glass} = 1.5$ .

We will use the Hamilton equations to calculate the ray paths of waves propagating from the glass into the anisotropic medium. In particular, we calculate the ray paths of extraordinary waves by using Eqs. (59) and (60). By taking small steps in the "time"  $\tau$ , the position  $\mathbf{r}(\tau)$  and momentum  $\mathbf{p}(\tau)$  are calculated using the first-order Runge–Kutta method.

Figure 8 shows several ray paths of extraordinary waves at normal incidence to the plane z=0. The plane of incidence is the xz plane. Apparently, light is absent in the region above the point charge q, and the ray paths seem to form a "curtainlike" appearance.

At z = 100, a matrix of intervals in x and y is defined, which is used to bin the x and y coordinates of ray paths. The number of rays collected by each interval is a measure for the intensity. Then the spatial intensity distribution at z = 100 should give us an idea of the optical behavior.

We define rays of light propagating in the z direction incident on the (transparent) conducting plate. The initial



Fig. 7. Director profile (i.e., the normalized electric field due to the point charge q) in the xz plane for a=50,  $x \in [-50, 50]$ , and  $z \in [0,100]$ . The profile has azimuthal symmetry.



Fig. 8. Ray paths of several extraordinary waves at normal incidence to the plane z=0, where the xz plane is the plane of incidence. Note the "curtainlike" behavior, allowing no light in the region above the point charge.

positions of the rays  $(x_0, y_0, z_0)$  randomly lie inside a square defined by  $x_0 \in [-10, 10]$  and  $y_0 \in [-10, 10]$ . These rays are refracted at the conducting plate at z=0, where  $\hat{\mathbf{d}} = (0, 0, -1)$ . Propagating along the *z* direction, the rays would result in ordinary waves after being refracted. Hence, according to the Hamilton equations, the rays would not be curved. To overcome this effect, we perturb the incident angle of the rays to  $10^{-6}$  deg in the *xz* plane. In addition, we define a linear polarization parallel to the *xz* plane. As a result, the refracted waves are extraordinary waves.

Figure 9(a) shows the intensity distribution I at z = 100. The number of rays that is traced is 30.000. The white square indicates the boundary in which the initial positions (at z=0) of the incident rays lie. In Figs. 9(b)-9(f), this square is moved along the line x=y. It is clear that the intensity distribution changes with the position of the square.

In Fig. 9(f), the distortion of the square light source is only little, since the square is far away from the point charge. However, in Fig. 9(a), the square light source at z=0 is transformed into a circularlike light distribution at z=100. This is the case when the center of the square is exactly below the point charge.

Although the anisotropic structure examined here is fictitious, it brings the application of liquid-crystal material in anisotropic gradient-index lenses to mind.

## **10. CONCLUSIONS**

In this article, we have developed a general and complete ray-tracing method in the geometrical-optics approach. We can use the model to calculate ray paths with polarized ray tracing in the bulk material of inhomogeneous anisotropic media in three dimensions, provided the properties of the medium change slowly over one wavelength. In addition, this model enables one to calculate the optical properties of, in general, curved interfaces with arbitrary orientation and/or anisotropic properties. Finally, we have derived vector equations that are general, concise, and easy to apply. In combination with these vector equations, the ray-tracing method presented in this article becomes a clear outline of how to apply the classical theory in practice.



Fig. 9. (Color online) Intensity distribution *I* at z = 100 for  $x \in [-50, 50]$  and  $y \in [-50, 50]$ . The square (white) indicates the boundary in which the initial positions of the incident rays lie. This boundary is moved along the line x=y.

We have shown that computations to anisotropic interfaces in existing literature can be well reproduced by the model. In addition, the model is applied to an artificial anisotropic gradient-index profile in three dimensions. It has been shown that, given an arbitrary director profile within defined boundaries, our method can be applied in order to assess the optical properties of the anisotropic optical system.

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