Ray-optics analysis of inhomogeneous biaxially anisotropic media

Maarten Sluijter,1,* Dick K. G. de Boer,1 and H. Paul Urbach2

1Philips Research Europe, High Tech Campus 34, MS 31, 5656 AE Eindhoven, The Netherlands
2Optics Research Group, Department of Imaging Science and Technology, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands
*Corresponding author: Maarten.Sluijter@philips.com

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Firm evidence of the biaxial nematic phase in liquid crystals, not induced by a magnetic or electric field, has been established recently. The discovery of these biaxially anisotropic liquid crystals has opened up new areas of both fundamental and applied research. The advances in biaxial liquid-crystal-related topics call for a good overview on the propagation of waves through biaxially anisotropic media. Although the literature sporadically discusses biaxial interfaces, the propagation of waves through inhomogeneous biaxially anisotropic bulk materials has never been fully addressed. For this reason, we present a novel ray-tracing method for inhomogeneous biaxially anisotropic media. In the geometrical-optics approach, we clearly show how to assess the optical properties of inhomogeneous biaxially anisotropic media in three dimensions. © 2009 Optical Society of America


1. INTRODUCTION

Optical anisotropy in the geometrical-optics approach is a classical problem, and most of the theory has been known for more than a century. In particular, uniaxial anisotropy is frequently discussed in the literature due to the rapid advances in nematic liquid-crystal applications [1–12]. Firm evidence of the biaxial nematic phase in liquid crystals, not induced by a magnetic or electric field, has only been established recently. The first reports of a nematic biaxial liquid crystal appeared in 2004 [13–15]. The discovery of this new type of nematic liquid crystals has opened up new areas of both fundamental and applied research. It is predicted that the application of biaxial nematic liquid crystals in, for example, displays will increase response times and result in improved performance and efficiency; see, e.g., [16]. The optical properties of these types of applications can be calculated with, for example, the Berreman 4 × 4 matrix method [17]. On the other hand, other possible future applications, such as biaxial liquid-crystal lenses, require a different approach. At the same time, the literature is nearly silent about biaxial anisotropy. Sporadically, the optical properties of biaxially anisotropic interfaces are discussed [18–24]. However, a full discussion on ray-optics analysis of inhomogeneous bulk materials of biaxially anisotropic media cannot be found in the literature. Therefore, we present a novel polarized ray-tracing method for inhomogeneous biaxially anisotropic media.

In earlier work, we have developed a ray-tracing method for inhomogeneous uniaxially anisotropic media, in which we apply the so-called Hamiltonian method for the ray-tracing process [12]. In this paper, we will apply the same Hamiltonian principle to inhomogeneous biaxially anisotropic media. However, the theory presented in this paper is not trivial and requires more than the Hamiltonian principle for the ray-tracing process alone. The derivation of these formulas involves a more complicated process than for uniaxial anisotropy. Furthermore, in our way of presenting the theory, the formulas are ready for use and easy to implement in a ray-tracing simulation program. To the best of our knowledge, this cannot be found in the literature.

When polarized ray tracing is applied to an optical system, we are mainly interested in the energy flux, represented by the Poynting vector. In anisotropic media, either uniaxial or biaxial, the Poynting and wave vectors are not parallel in general, since the electric field vector E and the electric flux density vector D are not parallel. For this reason, we define a ray as an integral curve to which the Poynting vector is tangential rather than a curve that is everywhere orthogonal to the wavefront.

This paper is organized as follows. In Sections 2–4 we briefly discuss the classical theory of geometrical optics. In Section 2, we propose the quasi-plane-wave as a solution of the optical wave field [25–27]. Then, in Section 3, we derive an equation for the biaxial optical indicatrix [28–31], a formula that relates the directions of propagation with their corresponding effective indices of refraction. In Section 4, we derive expressions for the directions of the electric and magnetic field vectors with respect to the biaxial optical indicatrix. At this point, we have a theoretical basis at our disposal that we will need in the derivation of a new ray-tracing method.

In Section 5, the Hamiltonian formulation of the ray-tracing process for inhomogeneous biaxially anisotropic media is presented in a unique way. The content of this section exceeds the state of the art. In contrast with uniaxial anisotropy, biaxial anisotropy is characterized by
two optical axes. In inhomogeneous media, the direction of these optical axes depends on position. Before we apply the Hamiltonian principle, we derive an expression for the position-dependent optical indicatrix in terms of the two (position-dependent) optical axes. The result is new and plays a crucial role in the derivation of the ray-tracing process for inhomogeneous biaxially anisotropic media. With the help of the position-dependent biaxial optical indicatrix, we work out the Hamiltonian principle for biaxial anisotropy. In this paper we present concise formulas in vector notation for the ray-tracing process. In the end, we are able to calculate the curved ray paths of light waves through inhomogeneous biaxially anisotropic media in three dimensions.

One usually begins the process of ray tracing outside an anisotropic medium. Hence, it is necessary to calculate the wave field at an anisotropic interface. Since we aim for a general approach of the theory we cannot ignore biaxially anisotropic interfaces, despite the fact that this subject is already known in the literature [18–24]. The optical properties of a uniaxially anisotropic interface are extensively discussed in [12]. For biaxially anisotropic interfaces the procedure is largely the same. For the sake of clarity, we discuss the procedure for the interface between an isotropic and a biaxially anisotropic medium with arbitrary orientation and/or anisotropic properties in Section 6. In addition, we briefly discuss the case for propagation along one of the optical axes. For these directions of propagation, the biaxial optical indicatrix has a singularity, which corresponds to a phenomenon known as conical refraction [32–35]. Conical refraction contains both ray- and wave-optics effects. For this reason, conical refraction is often termed conical diffraction. However, a full discussion on the wave optics of this special phenomenon is beyond the scope of this paper.

Finally, in Section 7, we show simulations of an inhomogeneous biaxially anisotropic optical system. In [12], we investigated the optical properties of the director profile of a nematic liquid crystal due to the electric field of a point charge. In this paper we investigate the same optical system, but now with a biaxial nematic liquid crystal with different orientations of the optical axes.

2. QUASI-PLANE-WAVES AND GEOMETRICAL OPTICS

In this paper we are looking for solutions of the wave field of the form given by

\[
\mathbf{E}(\mathbf{r}, t) = \tilde{\mathbf{E}}(\mathbf{r}) e^{i(k_0 \psi(\mathbf{r}) - \omega t)},
\]

\[
\mathbf{H}(\mathbf{r}, t) = \tilde{\mathbf{H}}(\mathbf{r}) e^{i(k_0 \psi(\mathbf{r}) - \omega t)},
\]

with \(\tilde{\mathbf{E}}(\mathbf{r})\) and \(\tilde{\mathbf{H}}(\mathbf{r})\) being complex vectors for the electric and magnetic fields and \(\psi(\mathbf{r})\) being the optical path length function, which is also called the eikonal function. This type of wave field is a time-harmonic quasi-plane-wave (cf. [25], p. 111) and applies in particular to regions far away from light sources. The quasi-plane-wave was suggested by Sommerfeld and Runge (cf. [26], p. 291) and is also referred to as the Sommerfeld–Runge ansatz.

In general, the complex amplitude vector can be written as

\[
\mathbf{E}(\mathbf{r}) = A(\mathbf{r}) e^{i(\delta(\mathbf{r}) - \omega t)} \tilde{\mathbf{E}}(\mathbf{r}),
\]

where \(\tilde{\mathbf{E}}(\mathbf{r})\) is a complex unit vector, i.e., \(|\tilde{E}_x(\mathbf{r})|^2 + |\tilde{E}_y(\mathbf{r})|^2 + |\tilde{E}_z(\mathbf{r})|^2 = 1\), the amplitude \(A(\mathbf{r})\) is real and positive 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, in the approximation that we use in this paper, which is the lowest order in \(1/k_0\), we can say that the amplitude \(A\) and phase \(\delta\) are independent of position throughout the medium. Only when a wave is refracted or reflected at an interface do the amplitude and phase terms change. For this reason, it is only necessary to calculate the entire wave field 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 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. (1) into the Maxwell equations, we obtain (we consider only nonmagnetic media: \(\mu = 1\))

\[
\nabla \psi \times \mathbf{H} + c\varepsilon_0 \varepsilon \tilde{\mathbf{E}} = -\frac{1}{ik_0} \nabla \times \mathbf{H},
\]

\[
\nabla \psi \times \varepsilon \tilde{\mathbf{E}} - c\mu_0 \tilde{\mathbf{H}} = -\frac{1}{ik_0} \nabla \times \varepsilon \tilde{\mathbf{E}},
\]

\[
\nabla \psi \cdot g \tilde{\mathbf{E}} = -\frac{1}{ik_0} \nabla \cdot g \tilde{\mathbf{E}},
\]

\[
\nabla \psi \cdot \tilde{\mathbf{H}} = -\frac{1}{ik_0} \nabla \cdot \tilde{\mathbf{H}}.
\]

(3)

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. (3) 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 \(g \tilde{\mathbf{E}}\). Hence, we demand that

\[
\frac{|\nabla \cdot g \tilde{\mathbf{E}}|}{k_0} \ll 1.
\]

(4)

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. At an interface when \(g\) is discontinuous, condition (4) is violated. Therefore the analysis presented in Sections 3–5 does not apply. This case is treated separately in Section 6.

If the right-hand side terms in Eq. (3) vanish, we can express the magnetic amplitude vector \(\tilde{\mathbf{H}}\) in terms of the electric amplitude vector \(\tilde{\mathbf{E}}\): \(\tilde{\mathbf{H}} = (1/c\mu_0) \nabla \psi \times \tilde{\mathbf{E}}\). Therefore, when we know the electric amplitude vector \(\tilde{\mathbf{E}}\), we also
know the magnetic amplitude vector $\vec{H}$. Hence, for the rest of this paper, it is sufficient to discuss the electric amplitude vector $\vec{E}$.

We conclude that in the geometrical-optics approach the optical properties of an inhomogeneous medium should 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 paper.

3. BIAXIAL OPTICAL INDICATRIX

In Eq. (3), we can confine 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 $\vec{H}$ from Eq. (3) we obtain the “eikonal equation” for media with electrical anisotropy:

$$\mathbf{p} \times (\mathbf{p} \times \vec{E}) + \varphi \vec{E} = 0.$$  

By definition, the wave normal $\mathbf{p}$ is equivalent to the wave vector $\mathbf{k}$ scaled by the wavenumber in vacuum $k_0$. The elements of the dielectric tensor are determined by the choice of our Cartesian coordinate system. Since $\varepsilon$ is a real symmetric matrix, it is always possible to find a local orthonormal coordinate system in which the off-diagonal elements of the dielectric tensor are zero. This local coordinate system is defined by the local orthonormal basis $\{\hat{u}(\mathbf{r}), \hat{v}(\mathbf{r}), \hat{w}(\mathbf{r})\}$. The dielectric tensor is then represented by

$$\varepsilon(\mathbf{r}) = \begin{pmatrix} \varepsilon_u(\mathbf{r}) & 0 & 0 \\ 0 & \varepsilon_v(\mathbf{r}) & 0 \\ 0 & 0 & \varepsilon_w(\mathbf{r}) \end{pmatrix},$$

where $\varepsilon_u(\mathbf{r})$, $\varepsilon_v(\mathbf{r})$, and $\varepsilon_w(\mathbf{r})$ are the relative principal dielectric constants and the $u$, $v$, and $w$ axes are the principal axes of the medium. These axes form the principal coordinate system. From now on, for convenience, we will assume that $\varepsilon_u < \varepsilon_v < \varepsilon_w$. The principal indices of refraction $n_u$, $n_v$, and $n_w$ are defined by $n_i = \sqrt{\varepsilon_i}$, with $i = u, v, w$. A medium is called biaxially anisotropic when the principal indices of refraction are all different.

We can write Eq. (5) as a matrix equation,

$$\mathbf{A}(\mathbf{p})\vec{E} = 0,$$

with $\mathbf{A}$ being the $3 \times 3$ matrix. The solutions $\vec{E}$ define the null space of the matrix $\mathbf{A}$ according to

$$\text{Null}(\mathbf{A}) = \{\vec{E} \in \mathbb{C}^3 | \mathbf{A}\vec{E} = 0\}.$$  

Equation (7) has only nontrivial solutions for the eigen-modes $\vec{E}$ if the determinant of the matrix $\mathbf{A}$ vanishes. This demand leads to a quadratic equation $\mathcal{H}(p_u^2, p_v^2, p_w^2) = 0$ and its solutions are on two three-dimensional surfaces in $\mathbf{p}$ space. This surface is called the biaxial optical indicatrix (cf. [29], p. 20) and, in the principal coordinate system, is given by

$$\mathcal{H} = (\varepsilon_u p_u^2 + \varepsilon_v p_v^2 + \varepsilon_w p_w^2)(p_u^2 + p_v^2 + p_w^2) - \varepsilon_u p_u^2(\varepsilon_v + \varepsilon_w) - \varepsilon_v p_v^2(\varepsilon_u + \varepsilon_w) + \varepsilon_w p_w^2(\varepsilon_u + \varepsilon_v) + \varepsilon_u \varepsilon_v \varepsilon_w = 0.$$  

Given Eq. (9), it is convenient to write the wave normal $\mathbf{p}$ in terms of its magnitude and direction,

$$\mathbf{p} = |\mathbf{p}|\hat{\mathbf{p}},$$

where $\hat{\mathbf{p}}$ is a unit vector and $|\mathbf{p}| = n$ is the index of refraction. When we substitute Eq. (10) into Eq. (9), we obtain

$$\mathcal{H} = (\varepsilon_u \hat{p}_u^2 + \varepsilon_v \hat{p}_v^2 + \varepsilon_w \hat{p}_w^2)|\mathbf{p}|^4 - (\varepsilon_u \hat{p}_u^2(\varepsilon_v + \varepsilon_w) + \varepsilon_v \hat{p}_v^2(\varepsilon_u + \varepsilon_w) + \varepsilon_w \hat{p}_w^2(\varepsilon_u + \varepsilon_v) + \varepsilon_u \varepsilon_v \varepsilon_w)|\mathbf{p}|^2 + \varepsilon_u \varepsilon_v \varepsilon_w = 0.$$  

Equation (11) implies that, for any arbitrary direction of propagation $\hat{\mathbf{p}}$, there are two solutions for $|\mathbf{p}|^2$. As a result, the three-dimensional surface represented by Eq. (11) consists of two concentric shells: an inner and an outer shell. These two shells have four points in common (cf. [36], p. 93). The two lines that go through these points and the origin are called the optical axes. Note that these optical axes vary with position since the principal coordinate system depends on position. In case $\hat{\mathbf{p}}$ is parallel to one of the optical axes, the two solutions for the refractive index $|\mathbf{p}|$ are identical. Figure 1 shows one octant of the optical indicatrix in the principal coordinate system and the intersections of the optical indicatrix with the principal $uv$, $uw$, and $uv$ planes. Recall that we have assumed that $\varepsilon_w > \varepsilon_v > \varepsilon_u$. Then the optical axes lie in the $uw$ plane. The angle $\vartheta$ between the $w$ axis and the optical axis is the same for both optical axes [see Fig. 1(d)]. This angle is de-
terminated by the material properties and satisfies [cf. [22], p. 3127, Eq. (115)]
\[
\tan(\theta) = \sqrt{\frac{e_u(e_v - e_u)}{e_u(e_v - e_u)}}.
\]  
(12)

For propagation along an optical axis, we have \(|\mathbf{p}| = e_v\) and the four corresponding directions of propagation are given by
\[
\hat{\mathbf{p}} = \pm \sqrt{\frac{e_u(e_v - e_u)}{e_v(e_v - e_u)}} \hat{\mathbf{u}} + 0 \hat{\mathbf{v}} \pm \sqrt{\frac{e_u(e_v - e_u)}{e_u(e_v - e_u)}} \hat{\mathbf{w}},
\]  
(13)

with all quantities depending on position \(\mathbf{r}\). For this particular direction of propagation, the surfaces of the biaxial optical indicatrix have a singularity. This special case is addressed in Section 6.

4. ANALYSIS OF THE POLARIZATION VECTORS

As discussed in Section 2, the electric field vector can be written as \(\hat{\mathbf{E}} = \mathbf{A}(\mathbf{r})e^{i\mathbf{r}\cdot\mathbf{E}}\mathbf{E}(\mathbf{r})\) with \(\hat{\mathbf{E}}(\mathbf{r})\) being a complex unit vector. The unit vector \(\hat{\mathbf{E}}(\mathbf{r})\) is called the electric polarization vector. In anisotropic media, the electric (and magnetic) polarization vectors depend on the direction of propagation and the orientation of the optical indicatrix with respect to a reference coordinate system. In this section, we first derive concise expressions for the electric and magnetic polarization vectors. Second, we derive the orientation of the polarization vectors and the Poynting vector with respect to the optical indicatrix.

On the local principal basis \(\{\hat{\mathbf{u}}(\mathbf{r}), \hat{\mathbf{v}}(\mathbf{r}), \hat{\mathbf{w}}(\mathbf{r})\}\), \(\xi(\mathbf{r})\) is diagonal. Then, 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. (5) can be written as
\[
|\mathbf{p}|^2 \hat{\mathbf{E}}_u - e_v \hat{\mathbf{E}}_u = (\hat{\mathbf{E}} \cdot \mathbf{p})p_u,
\]  
(14)
\[
|\mathbf{p}|^2 \hat{\mathbf{E}}_v - e_v \hat{\mathbf{E}}_v = (\hat{\mathbf{E}} \cdot \mathbf{p})p_v,
\]  
(15)
\[
|\mathbf{p}|^2 \hat{\mathbf{E}}_w - e_u \hat{\mathbf{E}}_w = (\hat{\mathbf{E}} \cdot \mathbf{p})p_w.
\]  
(16)

Hence, in the principal coordinate system, the vector components of \(\hat{\mathbf{E}}\) can be written as
\[
\hat{\mathbf{E}} = C \frac{(\hat{\mathbf{E}} \cdot \mathbf{p})p_i}{|\mathbf{p}|^2 - e_i}, \quad i = u, v, w,
\]  
(17)

where \(C\) is a complex normalization constant and \(|\mathbf{p}|^2 \neq e_i\). Equation (17) is proportional to a real vector and therefore corresponds to a linear polarization state. Now consider the case for which \(|\mathbf{p}|^2 = e_u\). Then, from Eq. (14), we deduce that either \(\hat{\mathbf{E}} \cdot \mathbf{p} = 0\) or \(p_u = 0\). In case \(\hat{\mathbf{E}} \cdot \mathbf{p} = 0\), Eqs. (15) and (16) tell us that \(\hat{\mathbf{E}}_v = \hat{\mathbf{E}}_w = 0\), and the value of \(\hat{\mathbf{E}}_u\) is arbitrary. Hence we conclude that \(\hat{\mathbf{E}} = (\pm 1, 0, 0)\). In case \(p_u = 0\), the wave normal \(\mathbf{p}\) lies in the \(uv\) plane [see also Fig. 1(b)]. Equations (15) and (16) do not depend on \(\hat{\mathbf{E}}_u\) and are a homogeneous system for \(\hat{\mathbf{E}}_v\) and \(\hat{\mathbf{E}}_w\). The determinant of this homogeneous system can be shown to be nonzero, hence \(\hat{\mathbf{E}}_v = \hat{\mathbf{E}}_w = 0\) and the value for \(\hat{\mathbf{E}}_u\) is arbitrary. We can conclude that if \(|\mathbf{p}|^2 = e_u\), then the polarization vector is given by
\[
\hat{\mathbf{E}} = (\pm 1, 0, 0).
\]  
(18)

Similarly, if \(|\mathbf{p}|^2 = e_v\), we obtain \(\hat{\mathbf{E}} = (0, \pm 1, 0)\) and if \(|\mathbf{p}|^2 = e_w, \hat{\mathbf{E}} = (0, 0, \pm 1)\). The magnetic polarization vector is defined as \(\mathbf{H} = \mathbf{p} \times \hat{\mathbf{E}}\). Hence, the magnetic polarization vectors are by definition not unit vectors. Note that the equations for the polarization vectors only apply in the principal coordinate system.

With the help of Eq. (17), we shall now show that the vector \(\nabla_p \hat{\mathbf{r}}(\mathbf{r}, \mathbf{p})\) is perpendicular to both \(\hat{\mathbf{E}}(\mathbf{r})\) and \(\mathbf{H}(\mathbf{r})\) (at the same point \(\mathbf{r}\)). From this result, we will derive that the Poynting vector is always perpendicular to the optical indicatrix.

We consider the optical indicatrix \(\mathcal{H}(\mathbf{r}, \mathbf{p})\) in a fixed point \(\mathbf{r}\) of space. Let \(\{\hat{\mathbf{u}}(\mathbf{r}), \hat{\mathbf{v}}(\mathbf{r}), \hat{\mathbf{w}}(\mathbf{r})\}\) be the orthonormal principal basis on which \(\xi(\mathbf{r})\) is diagonal at the given point \(\mathbf{r}\). Since this basis is orthonormal, the gradient of \(\mathbf{p} \rightarrow \mathcal{H}(\mathbf{r}, \mathbf{p})\) is given by
\[
\nabla_p \mathcal{H}(\mathbf{r}, \mathbf{p}) = \frac{\partial \mathcal{H}(\mathbf{r}, \mathbf{p})}{\partial p_u} \hat{\mathbf{u}}(\mathbf{r}) + \frac{\partial \mathcal{H}(\mathbf{r}, \mathbf{p})}{\partial p_v} \hat{\mathbf{v}}(\mathbf{r}) + \frac{\partial \mathcal{H}(\mathbf{r}, \mathbf{p})}{\partial p_w} \hat{\mathbf{w}}(\mathbf{r}).
\]  
(19)

First, we will investigate the inner product \(\nabla_p \mathcal{H} \cdot \hat{\mathbf{E}} = 0\). When we expand the inner product \(\nabla_p \mathcal{H} \cdot \hat{\mathbf{E}}\) with the help of Eqs. (9) and (17), we obtain
\[
\nabla_p \mathcal{H} \cdot \hat{\mathbf{E}} = \frac{C(\hat{\mathbf{E}} \cdot \mathbf{p})p_i}{(|\mathbf{p}|^2 - e_i)} - \frac{C(\hat{\mathbf{E}} \cdot \mathbf{p})p_i}{(|\mathbf{p}|^2 - e_u)(|\mathbf{p}|^2 - e_v)} \mathcal{H},
\]  
(20)

with \(f(p_u, p_v, p_w)\) being a polynomial of degree four, given by
\[
f(p_u, p_v, p_w) = 2|\mathbf{p}|^4 - p_u^2(e_v + e_w) - p_v^2(e_v + e_u) - p_w^2(e_u + e_v).
\]  
(21)

By definition, \(\mathcal{H} = 0\) and as a result the inner product of Eq. (20) vanishes, provided that \(|\mathbf{p}|^2 \neq e_i\). It can be shown that in case \(|\mathbf{p}|^2 = e_i\), the inner product between \(\nabla_p \mathcal{H}\) and \(\hat{\mathbf{E}}\) also vanishes. Similarly, it can be shown that \(\nabla_p \mathcal{H} \cdot \mathbf{H} = \nabla_p \mathcal{H} \cdot (\mathbf{p} \times \mathbf{E}) = 0\) and \(\nabla_p \mathcal{H} \cdot \mathbf{H}^* = (\nabla_p \mathcal{H} \cdot \mathbf{H})^* = 0\), where \(\mathbf{H}^*\) is the complex conjugate of \(\mathbf{H}\).

Figure 2 shows the biaxial optical indicatrix again, but now with the electric polarization vectors indicated (see also [31], p. 91). The properties of the polarization vectors are general, since they are independent of the choice of the coordinate system. Altogether, we conclude that both the electric and magnetic polarization vectors are tangent to the biaxial optical indicatrix. As a result, the time-averaged Poynting vector, given by
\[
\mathbf{S} = \frac{1}{2} \text{Re}(\mathbf{E} \times \mathbf{H}^*),
\]  
(22)

is perpendicular to the optical indicatrix. Then, the vector \(\mathbf{S}\) is proportional to the vector \(\nabla_p \mathcal{H}\).
where \( \mathbf{H} \) is a parameter that can be considered as time. In the derivation of a novel ray-tracing method for inhomogeneous biaxially anisotropic bulk materials in three dimensions.

Since \( (\mathbf{S} \cdot \mathbf{p}) = C_2 |\mathbf{p}|^2 \mathbf{E}^2 - (\mathbf{p} \cdot \mathbf{E})^2 \geq 0 \), with \( C_2 \) being a positive constant, and \( \nabla_j \mathbf{H} \cdot \mathbf{p} \geq 0 \), \( (\mathbf{S}) \) and \( \nabla_j \mathbf{H} \) are always parallel and never antiparallel. In Section 5 we will use Eq. (23) in the derivation of the Poynting vector in the bulk of an inhomogeneous medium.

5. HAMILTONIAN METHOD FOR INHOMOGENEOUS MEDIA

We define a ray as an integral curve of the Poynting vector field,

\[
\frac{d\mathbf{r}}{d\tau} = (\mathbf{S}(\mathbf{r}(\tau)))
\]

where \( \tau \) is a parameter that can be considered as time. In a homogeneous medium light rays are straight. However, inside an inhomogeneous medium light rays are curved due to a gradient in the permittivity. The inhomogeneous properties of an anisotropic medium can be ascribed to two effects: the position dependency of the principal dielectric constants \( \varepsilon_{\mu}, \varepsilon_{\upsilon}, \) and \( \varepsilon_{\omega} \) and the position dependency of the direction of the optical axes. For the moment, we will assume that both effects are relevant. In what follows we describe a method to calculate the curved trajectory of the Poynting vector in the bulk of an inhomogeneous biaxially anisotropic medium.

Inside an inhomogeneous biaxially anisotropic medium the optical indicatrix is a function of position. Therefore, the directions of the two optical axes also depend on position. We call the position-dependent optical axes the directors. Let \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \) be the unit vectors that are parallel to the two local optical axes. The directors \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \) then satisfy [see Eq. (13)]

Figure 3 shows two local directors and the local Cartesian coordinate system, defined by the unit vectors \( \hat{\mathbf{u}}, \hat{\mathbf{v}}, \) and \( \hat{\mathbf{w}} \). These unit vectors can be expressed in terms of the directors \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \), according to

\[
\hat{\mathbf{u}} = \frac{\mathbf{d}_1 - \mathbf{d}_2}{|\mathbf{d}_1 - \mathbf{d}_2|},
\]

\[
\hat{\mathbf{v}} = \frac{\mathbf{d}_2 \times \mathbf{d}_1}{|\mathbf{d}_2 \times \mathbf{d}_1|},
\]

\[
\hat{\mathbf{w}} = \frac{\mathbf{d}_1 + \mathbf{d}_2}{|\mathbf{d}_1 + \mathbf{d}_2|}.
\]

In conclusion, if we know the unit vectors \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \), we also know the local principal basis \( \{\hat{\mathbf{u}}, \hat{\mathbf{v}}, \hat{\mathbf{w}}\} \) and vice versa. On the principal basis \( \{\hat{\mathbf{u}}, \hat{\mathbf{v}}, \hat{\mathbf{w}}\} \), the macroscopic material equation reads [25]

\[
\mathbf{D} = \varepsilon_0 \varepsilon_{\mu} \mathbf{E} \hat{\mathbf{u}} + \varepsilon_0 \varepsilon_{\upsilon} \mathbf{E} \cdot \hat{\mathbf{v}} + \varepsilon_0 \varepsilon_{\omega} (\mathbf{E} \cdot \hat{\mathbf{w}}) \hat{\mathbf{w}}.
\]
Like Eq. (7), this equation only has nontrivial solutions if the determinant of the matrix vanishes. Accordingly, the determinant reads

$$\mathcal{H}(x,y,z,p_x,p_y,p_z) = [e_{uu}(p \cdot \hat{u})^2 + e_{uv}(p \cdot \hat{v})^2 + e_{uw}(p \cdot \hat{w})^2] |p|^2$$

$$+ e_u e_v \hat{u} \cdot (p \times \hat{u})^2 - |p|^2$$

$$+ e_v e_w \hat{v} \cdot (p \times \hat{v})^2 - |p|^2$$

$$+ e_u e_w \hat{w} \cdot (p \times \hat{w})^2 - |p|^2$$

$$+ e_u e_v e_w = 0,$$  \hspace{1cm} (29)

where the unit vectors \(\hat{u}, \hat{v},\) and \(\hat{w}\) are given by Eq. (26). If we substitute \(\hat{u}=(1,0,0), \hat{v}=(0,1,0),\) and \(\hat{w}=(0,0,1),\) we obtain the biaxial optical indicatrix in the principal coordinate system as defined in Eq. (9). In addition to this, if we set \(e_u=e_o n_u^2\) and \(e_v=e_o n_v^2,\) where the indices \(o\) and \(e\) denote ordinary and extraordinary waves, we obtain the optical indicatrix in the principal coordinate system for uniaxial anisotropy [cf. [12], Eq. (11)]. The position-dependent biaxial optical indicatrix of Eq. (29) plays a crucial role in the derivation of the ray-tracing process for inhomogeneous biaxially anisotropic media.

In what follows, we will derive a ray-tracing method that is based on the Hamiltonian principle. The Hamiltonian method for the ray-tracing process of inhomogeneous uniaxially anisotropic media has already been introduced in [12]. However, in the remainder of this section we work out the successive steps in the derivation of the Hamiltonian method for biaxial anisotropy with the help of Eq. (29). To the best of our knowledge, the formulas produced by this paper cannot be found in existing literature.

To find an expression for the path of a light ray, we will use Eq. (29). 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. Recall that, since we are primarily interested in the energy transfer of a light ray, we have defined a ray to be an integral curve of the Poynting vector, given by Eq. (24). According to Eq. (23), the direction of the Poynting vector \(\mathbf{S}\) is the same as the direction of \(\nabla_{\mathcal{H}} \mathcal{H}.\) Hence, we can write a set of equations for the ray path given by

$$\frac{d\mathbf{r}}{d\tau} = \alpha \mathbf{E}, \hspace{1cm} i = x,y,z,$$  \hspace{1cm} (30)

where the factor \(\alpha\) is an arbitrary function of \(\tau\) and only depends on the choice for the parameter \(\tau.\) 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. [36], p. 110) reading

$$\frac{dp_i}{d\tau} = -\alpha \frac{\partial \mathcal{H}}{\partial p_i}, \hspace{1cm} i = x,y,z,$$  \hspace{1cm} (31)

for the same \(\alpha\) as in Eq. (30). The next step is crucial, since we apply a classical-mechanical interpretation to the light rays: a mathematical light ray is considered the trajectory of a particle with coordinates \(\mathbf{r}=(x,y,z)\) and generalized momentum \(\mathbf{p}=(p_x,p_y,p_z)\) (cf. [36], p. 115), which satisfy Eqs. (30) and (31), 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. (29) represents a Hamiltonian system with canonical equations given by

$$\frac{d(x,y,z)}{d\tau} = \alpha \nabla_{\mathcal{H}} \mathcal{H},$$  \hspace{1cm} (32)

$$\frac{dp_x}{d\tau} = -\alpha \nabla_{\mathcal{H}} \mathcal{H},$$  \hspace{1cm} (33)

where the ray position \(\mathbf{r}(\tau)\) and momentum \(\mathbf{p}(\tau)\) are functions of the parameter \(\tau.\) Equations (32) and (33) are also called the Hamilton equations. Equation (32) 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. (33).

The Hamilton equations form a set of six coupled first-order differential equations with six unknowns: the vector components of \(\mathbf{r}(\tau)\) and \(\mathbf{p}(\tau).\) These can be solved either analytically or numerically. However, before we can apply these equations we must calculate the right-hand sides. Below, we will introduce expressions for the vector components of \(\nabla_{\mathcal{H}} \mathcal{H}\) and \(\nabla_{\mathcal{H}} \mathcal{H},\) by using Eq. (29).

Recall that we have allowed for inhomogeneous principal dielectric constants, i.e., their values are position dependent. Then, the partial derivatives of \(\mathcal{H}\) with respect to position read

$$\frac{\partial \mathcal{H}}{\partial x} = 2|\mathbf{p}|^2 \left[ e_u(p \cdot \hat{u}) \frac{\partial \hat{u}}{\partial x} + e_v(p \cdot \hat{v}) \frac{\partial \hat{v}}{\partial x} + e_w(p \cdot \hat{w}) \frac{\partial \hat{w}}{\partial x} \right] + 2 e_v e_w \hat{v} \cdot (p \times \hat{v}) + \hat{u}$$

$$\cdot \left( \frac{\partial p_x}{\partial \tau} \right) \hat{u} \cdot (p \times \hat{v}) + 2 e_v e_w \left[ \frac{\partial \hat{u}}{\partial \tau} \cdot (p \times \hat{v}) + \hat{u} \cdot (p \times \hat{v}) \right]$$

$$\cdot \left( \frac{\partial p_y}{\partial \tau} \right) \hat{u} \cdot (p \times \hat{w}) + 2 e_u e_w \left[ \frac{\partial \hat{u}}{\partial \tau} \cdot (p \times \hat{w}) + \hat{v} \cdot (p \times \hat{w}) \right]$$

$$\cdot \left( \frac{\partial p_z}{\partial \tau} \right) \hat{v} \cdot (p \times \hat{w}) + \h \frac{\partial e_u}{\partial \tau} \cdot \frac{\partial e_v}{\partial \tau} \cdot \frac{\partial e_w}{\partial \tau},$$

$$i = x,y,z,$$  \hspace{1cm} (34)

where \(\h\) is a function of the partial derivatives of the dielectric constants with respect to position, given by
\[ h = |p|^2 \left[ \frac{\partial v}{\partial t} (p \cdot \hat{u})^2 + \frac{\partial v}{\partial x} (p \cdot \hat{v})^2 + \frac{\partial w}{\partial x} (p \cdot \hat{w})^2 \right] \]

\[ + \left[ \hat{u} \cdot (p \times \hat{v}) \right]^2 \frac{\partial}{\partial t} (e_w e_v) + \left[ \hat{u} \cdot (p \times \hat{w}) \right]^2 \frac{\partial}{\partial t} (e_w e_w) \]

\[ + \left[ \hat{v} \cdot (p \times \hat{w}) \right]^2 \frac{\partial}{\partial t} (e_w e_v) + \frac{\partial}{\partial t} (e_w e_w), \quad i = x, y, z. \] (35)

The partial derivatives of \( H \) with respect to the wave normal components yield

\[ \frac{\partial H}{\partial p_i} = 2|p|^2 [e_u (p \cdot \hat{u}) \hat{u}_i + e_v (p \cdot \hat{v}) \hat{v}_i + e_w (p \cdot \hat{w}) \hat{w}_i] \]

\[ + 2p_i [e_u (p \cdot \hat{u})^2 + e_v (p \cdot \hat{v})^2 + e_w (p \cdot \hat{w})^2 - e_v e_v - e_w e_w] \]

\[ - e_u e_u - 2e_u e_v (\hat{u} \cdot \hat{v}) \hat{u} \cdot (p \times \hat{v}) \]

\[ - 2e_u e_w (\hat{u} \times \hat{w}) \hat{u} \cdot (p \times \hat{w}) \]

\[ - 2e_v e_w (\hat{v} \times \hat{w}) \hat{v} \cdot (p \times \hat{w}), \quad i = x, y, z. \] (36)

Equation (34) contains \( \hat{u}(r) \), \( \hat{v}(r) \) and \( \hat{w}(r) \) and their partial derivatives with respect to position. This can be expressed in terms of the directors \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \) using Eq. (26).

Hence, we conclude that if \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \) and their partial derivatives with respect to position are known, the curved light paths of light rays in anisotropic media can be calculated with Eqs. (32)–(36).

In practice, the Hamilton equations can be solved as follows. If we redefine \( \tau \) such that \( \alpha = 1 \), the corresponding Hamilton equations are

\[ \frac{dr^i(\tau)}{d\tau} = \nabla_p \mathcal{H}(\mathbf{d}), \]

\[ \frac{dp^i(\tau)}{d\tau} = -\nabla_p \mathcal{H}(\mathbf{d}), \] (37)

with \( \nabla_p \mathcal{H} \) and \( \nabla_p \mathcal{H} \) as defined in Eqs. (34)–(36). This set of six coupled first-order 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

\[ \mathbf{r}(\tau_0) = (x_0, y_0, z_0), \]

\[ \mathbf{p}(\tau_0) = \mathbf{p}_0. \] (38)

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 \( \mathbf{p}(\tau_0 + N \Delta \tau) \) and the corresponding wave normal \( \mathbf{p}(\tau_0 + N \Delta \tau) \) and the corresponding wave normal \( \mathbf{p}(\tau_0 + N \Delta \tau) \). For an arbitrary interval \([\tau_N, \tau_N + \Delta \tau] \), with \( N \in \mathbb{N} \). For an arbitrary interval \([\tau_N, \tau_N + \Delta \tau] \), the \( x \), \( y \), and \( z \) components of the position and wave normal are given by

\[ i(\tau_N + \Delta \tau) = i(\tau_N) + \Delta \tau \frac{\partial H}{\partial p_i}(\tau_N), \] (39)

with the partial derivatives of \( H \) given by Eqs. (34)–(36). In this way, we can obtain the ray paths of the transmitted waves in the bulk material.

### 6. Biaxially Anisotropic Interfaces

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. To calculate the optical properties at an anisotropic interface, it is necessary to calculate the wave field at an interface, according to Eq. (1). In earlier work, we have discussed a procedure for uniaxial anisotropic interfaces in detail (cf. [12]). For biaxially anisotropic interfaces, the procedure is largely the same. Only the formulas for the polarization vectors and the wave normals at an interface change for biaxial anisotropy. In Section 4, we have already derived the vector equations for the electric and magnetic polarization vectors (in the principal coordinate system). In this section, we present a procedure for the calculation of the reflected and refracted wave normals at a biaxially anisotropic interface with arbitrary orientation and/or anisotropic properties. In addition, we briefly discuss the procedure for the calculation of the Fresnel coefficients. As an example, we work out the procedure for an isotropic–biaxial interface.

#### A. Procedure for the Calculation of the Optical Properties of Biaxial Interfaces

In practice, one usually begins the process of ray tracing in an isotropic medium. Hence, we will discuss the optical properties of an isotropic–biaxial interface in this subsection. By using the same procedure, the optical properties of other types of interfaces, such as uniaxial–biaxial or biaxial–biaxial interfaces, can be calculated as well.

First, we consider a normalized incident Poynting vector \( \langle \hat{S} \rangle \) of a wave incident to a plane boundary that forms the interface between two different transparent media. This vector defines the direction of the energy transfer of a wave. In isotropic media, the incident wave normal is then given by

\[ p_i = n \langle \hat{S} \rangle, \] (41)

where \( n \) is the index of refraction of the isotropic medium. In anisotropic media, the incident wave normal at an interface is known from the calculations in the bulk material (see Section 5).

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

\[ p_i \times \hat{n} = p \times \hat{n}, \] (42)

where \( \hat{n} \) is the local normal vector to the boundary and \( p \) is the corresponding transmitted or reflected wave normal. Snell’s law demands that the tangential component of the wave normal \( (p_{\text{tan}}) \) is continuous across the bound-
ary. Given the incident wave normal \( p_i \), the tangential wave normal \( p_n \) can be calculated by subtracting the normal component from the incident wave normal, yielding

\[
p_n = p_i - (p_i \cdot \hat{n}) \hat{n}.
\]  

(43)

According to Snell’s law, the waves can be either reflected or refracted. In what follows, we will derive a general procedure for the calculation of the reflected and refracted wave normals in biaxially anisotropic media.

The refracted wave normals are determined by substitution of the vector

\[
p = p_n + \xi \hat{n}, \quad \xi \geq 0,
\]  

(44)

in the equation \( H = 0 \) and solve for \( \xi \). Since the biaxial optical indicatrix consists of two shells, there are two solutions for \( \xi \) and therefore two solutions for \( p \). However, in general, the optical indicatrix can have any arbitrary orientation at an interface. Furthermore, Eq. (9) only applies in the principal coordinate system \( \{\hat{x}, \hat{y}, \hat{z}\} \), and the principal wave normal \( p_n \) should be transformed to a coordinate system in which Eq. (9) does apply. Consider a matrix \( M \), which represents a linear orthogonal transformation that transforms a vector on the Cartesian basis \( \{\hat{x}, \hat{y}, \hat{z}\} \) to the basis \( \{\hat{u}, \hat{v}, \hat{w}\} \), the principal coordinate system. Then, the “new input” vectors are given by \( \hat{n}^p = M \hat{n} \) and \( p_n^p = M p_n \), where the index \( p \) denotes the principal coordinate system.

With the vectors in the principal coordinate system, we can determine the refracted wave normals with Eqs. (9) and (44). If we substitute Eq. (44) into Eq. (9), we obtain an equation for \( \xi \) of the fourth degree. Obviously, \( n_u = \xi \leq n_w \) and we can find numerical solutions by any of the standard methods described in Press et al. (cf. [37], Chapter 9, p. 355). Alternatively, an analytical procedure for solving a polynomial of the fourth degree is described in Griffiths (cf. [38], p. 32). When the solutions for \( \xi \) and \( p^p \) are obtained, they can be applied to Eq. (17) to calculate the corresponding polarization vectors in the principal coordinate system. Finally, the vectors \( \hat{n}^p, p_n^p, p^p \), and the resulting polarization vectors are transformed back to the coordinate system \( \{\hat{x}, \hat{y}, \hat{z}\} \). To this end, we apply the inverse of the matrix \( M \), denoted by \( M^{-1} \).

For reflected waves at a biaxially anisotropic interface, Eq. (44) changes into \( p = p_n^p - \xi \hat{n} \), with \( \xi \geq 0 \). Of course now the indicatrix in the reflected medium should be used. For any arbitrary type of Hamiltonian (isotropic, uniaxial, or biaxial), the reflected wave normals and the corresponding polarization vectors can be calculated according to the same procedure.

Since we now know the refracted and reflected wave normals and the corresponding polarization vectors, we are left with the calculation of the complex amplitude \( \tilde{E} \) of the wave field at an interface. The complex amplitudes of the reflected and refracted waves are the Fresnel coefficients. The Fresnel coefficients can be calculated from the boundary conditions for an electromagnetic field at an interface between two (an)isotropic media. The boundary conditions demand that across the boundary, the tangential components of the field vectors \( \tilde{E} \) and \( \tilde{H} \) should be continuous (cf. [39], p. 18). Application of the boundary conditions yields four linear equations with four unknowns: the Fresnel coefficients. With the Fresnel coefficients, the wave field at an anisotropic interface is known. From the wave field we can calculate the time-averaged Poynting vectors and the corresponding phases and intensity transmittance factors. The method for the calculation of the Fresnel coefficients at an uniaxially anisotropic interface is discussed in detail in [4, 12]. For biaxially anisotropic interfaces, the same method applies. Also in biaxially anisotropic media, there are two kinds of waves (eigenmodes), but we can no longer speak of ordinary and extraordinary waves. In this paper, we will not work out this procedure again.

We conclude that we have a procedure for the calculation of the optical wave field at a biaxial interface. This procedure is largely the same as the procedure for a uniaxially anisotropic interface and applies to isotropic–biaxial, uniaxial–biaxial, and biaxial–biaxial interfaces. Knowing the optical wave field at the interface, we can proceed to calculate optical properties of the bulk material with the help of the theory described in Section 5.

### B. Conical Refraction

Consider a linearly polarized beam of light that is refracted at a homogeneous biaxially anisotropic interface in the direction of one of the optical axes. Then the Poynting vector of a refracted light ray, which is perpendicular to the optical indicatrix, is determined by the corresponding polarization vector of the light ray (see Fig. 2). At the position where the two sheets of the biaxial optical indicatrix touch each other, there exists an infinite number of possible polarization vectors. Each of the possible polarization vectors at the common point of intersection has a corresponding Poynting vector. Although the Poynting vectors of these eigenmodes are all different in direction, there is a common wave normal, which in the principal coordinate system is given by

\[
p = \pm \frac{e_u (e_i - e_u)}{e_w - e_u} \hat{u} + 0 \hat{v} \pm \frac{e_u (e_i - e_v)}{e_w - e_u} \hat{w}.
\]  

(45)

Now let us consider an unpolarized beam of light that is refracted along the optical axis [with a wave normal given by Eq. (45)] at the interface of a homogeneous biaxially anisotropic medium. Due to the optical properties described above, the incident beam of light is transformed to a hollow cone of light; see Fig. 4(a). This is a phenomenon known as internal conical refraction (cf. [25], p. 688). Similarly, there is also a set of wave normals that have a common Poynting vector. In this case, an unpolarized incident beam of light is also transformed to a hollow cone by a biaxially anisotropic medium; see Fig. 4(b). This phenomenon is known as external conical refraction.

In the geometrical-optics approach, we can calculate the light distribution due to conical refraction with the method presented in Subsection 6.A. In what follows, we will simulate an example of internal conical refraction. Figure 5(a) shows an unpolarized incident beam of light with a solid angle dΩ, propagating in the direction of the vertical z axis. The light is refracted at the interface of a homogeneous biaxial medium. One of the optical axes of the biaxial medium is aligned with the z axis. Due to the
biaxial anisotropic properties, the incident light beam is transformed to a cone of light with semiangle \( \theta \), as depicted in Fig. 5(b).

The incident light beam is defined by all light rays confined in the solid angle \( d\Omega \). We define the initial position of the incident light beam at \( (x,y,z) = (0,0,0) \). There, the incident light rays, which are randomly polarized, are refracted and split into two eigenmodes. We calculate the ray paths of these eigenmodes inside the homogeneous biaxial medium and the corresponding transmittance factors. At \( z = 100 \), we define a matrix in \( x \) and \( y \) that is used to bin the \( x \) and \( y \) coordinates of ray paths. The number of rays collected by each matrix element is a measure for the intensity. In this way, the intensity distribution at \( z = 100 \) is calculated. Figure 6 shows the results for different solid angles. The number of rays that is traced for each image is 30,000. In Fig. 6(a) the incident beam of light has a solid angle of \( 1 \times 10^{-3} \text{ sr} \) whereas in Figs. 6(b) and 6(c) the solid angles are \( 4 \times 10^{-3} \) and \( 9 \times 10^{-3} \text{ sr} \), respectively. The disklike appearance of the light distributions changes with the solid angle: the disk edge increases with increasing \( d\Omega \). In addition, the intensity decreases with increasing \( d\Omega \) since the incident light is spread over a bigger area. The semiangle \( \theta \) of the light cone can be expressed in terms of the principal indices of refraction of the biaxial medium, yielding [cf. \( [32] \), p. 291, Eq. (2.5)]

\[
\theta = \frac{\sqrt{(n_{oo} - n_{ee})(n_{ee} - n_{oo})}}{n_{ee}},
\]

with the angle \( \nu \) in radians. For the principal indices defined above, Eq. (46) yields \( \nu = 7.63^\circ \). In Fig. 5(a), the semiangle \( \nu \) is approximately 7.62°, which is in good agreement with Eq. (46).

Conical refraction only occurs when the incident light beam is accurately aligned with the optical axis of the biaxial medium. If the light beam is not aligned with the optical axis, we simply obtain two independent refracted eigenmodes for each individual light ray. Effectively, the incident light beam is split up into two beams, a phenomenon that is called double refraction. Figure 7 shows three simulations of the light distribution at \( z = 100 \) for different angles of the optical axis in the \( xz \) plane. The solid angle of the incident beam is \( d\Omega = 1 \times 10^{-3} \text{ sr} \). In Fig. 7(a) the optical axis is at 2.7° with the vertical \( z \) axis. In this case we observe double refraction and the two resulting light beams are centered in the \( xz \) plane. Figure 7(b) shows the result for the optical axis at 1.0° with the \( z \) axis. Here, part of the light fulfills the conditions for conical refraction and we can already observe the formation of a hollow

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**Fig. 4.** When an unpolarized beam of light is refracted along the optical axis of a biaxially anisotropic medium, the light beam is transformed to a hollow cone of light; see (a). This phenomenon is known as internal conical refraction. The refracted light rays of the beam inside the biaxial medium have a common wave normal. In the case when the refracted light rays of the beam have a common Poynting vector, we observe external conical refraction; see (b).

**Fig. 5.** Unpolarized beam of light incident to a biaxial medium with one of the optical axes aligned with the vertical \( z \) axis; see (a). Internal conical refraction occurs and the incident beam is transformed to a cone of light with semiangle \( \nu \). At \( z = 100 \) the light distribution is calculated; see (b).

**Fig. 6.** (Color online) Light intensity distribution at \( z = 100 \) for different values of the solid angle \( d\Omega \). For (a)–(c) the solid angles are \( 1 \times 10^{-3} \text{ sr}, 4 \times 10^{-3} \text{ sr}, \) and \( 9 \times 10^{-3} \text{ sr} \), respectively. The unpolarized beam of light enters the biaxial medium at the origin. Apparently, the disk edge increases with increasing solid angle. In addition, the intensity decreases with increasing solid angle.
cone of light. Finally, in Fig. 7(c), the optical axis is aligned with the z axis and this image is equivalent to the situation in Fig. 6(a).

In general, conical refraction contains both ray and wave-optics effects [32–35]. Therefore, conical refraction is often termed conical diffraction. A full discussion would be two refracted rays for each incident ray. Then we will calculate the directions of propagation and the intensity paths of the refracted rays in the bulk material. The initial 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 (transparent) conducting plate at \( z=0 \), where \( \mathbf{w}=(0,0,1) \). The incident rays are linearly polarized in the yz-plane and have an angle of incidence of 10° with the z axis in the same plane. With a uniaxially anisotropic director profile, the refracted rays in the upper half-space \( z>0 \) would be extraordinary [12]. But now, the field is so high, that the principal w axis follows the electric field direction. Hence, the unit vector \( \mathbf{w} \) due to the electric field of the point charge \( q \) is:

\[
\mathbf{w}(x,y,z) = \frac{\mathbf{E}(x,y,z)}{|\mathbf{E}(x,y,z)|}, \quad z \geq 0.
\]

Figure 9 shows \( \mathbf{w}(x,y,z) \) in the xz plane for \( a=50 \), \( x \in [-50,50] \) and \( z \in [0,100] \). We assume that the principal \( u \) axes is in the direction of the vector \( \mathbf{w} \times \mathbf{z} \). The principal \( v \) axis is then in the direction of \( \mathbf{w} \times \mathbf{u} \), as indicated in Fig. 9.

The biaxial medium in the upper half-space \( z>0 \) is taken with principal indices of refraction \( n_u=1.3, n_v=1.5 \), and \( n_w=1.7 \). The lower half-space \( z<0 \) is assumed to be glass with an index of refraction \( n_{glass}=1.5 \).

We will use the theory discussed in Subsection 6.A to calculate the directions of propagation and the intensity transmittance factors of the rays propagating from the glass into the anisotropic medium. In general, there will be two refracted rays for each incident ray. Then we will use the Hamilton equations (32)–(36) to calculate the ray paths of the refracted rays in the bulk material. The initial 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 (transparent) conducting plate at \( z=0 \), where \( \mathbf{w}=(0,0,1) \). The incident rays are linearly polarized in the yz-plane and have an angle of incidence of 10° with the z axis in the same plane. With a uniaxially anisotropic director profile, the refracted rays in the upper half-space \( z>0 \) would be extraordinary [12]. But now,
the director profile is biaxially anisotropic and the terms ordinary and extraordinary no longer apply. In the bulk material, we will assume that only the optical indicatrix changes with position and that the magnitude of the dielectric constants is homogeneous, i.e., \( h = 0 \) [see Eq. (35)]. 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 10 shows the ray paths of two refracted rays corresponding to a ray incident at the position \((x_0, y_0, z_0)\) =\((5, -9, 0)\). Figures 10(a) and 10(b) show the image projections in the \(xz\) and \(yz\) planes, respectively. Figure 10(c) shows the top view of the two ray paths. Finally, Fig. 10(d) shows an oblique projection of the two ray paths. Apparently, both ray paths are curved and they seem to be repelled by the region above the point charge. The left and right ray paths in Fig. 10(a) correspond to an intensity transmittance factor \( T_1 = 0.2210 \) and \( T_2 = 0.7777 \), respectively. The reflected ray in the glass \( z = 100 \) has an intensity reflectance factor \( R = 0.0013 \). As expected, the sum of \( T_1 \), \( T_2 \), and \( R \) exactly add up to 1.0000.

At \( z = 100 \), a matrix in \( x \) and \( y \) is defined that is used to collect 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 $I$ at $z=100$ should give us an idea of the optical behavior. In Fig. 11, we show the intensity distribution at $z=100$ for the uniaxial director profile with $n_o=1.5$ and $n_e=1.7$ [see Figs. 11(a)–11(c)] and the biaxial director profile [see Figs. 11(d)–11(f)]. The number of rays that is traced for each individual image is 25,000. The white square (at $z=0$) indicates the boundary in which the initial positions of the incident rays lie. In Figs. 11(a) and 11(d), the center of the white square is exactly below the point charge. Figure 11(a) shows how the square light source at $z=0$ is transformed to a ring-shaped light distribution (similar to the results presented in [12], but now with an angle of incidence of $10^\circ$). Clearly, we observe a different intensity distribution in Fig. 11(d). In contrast with Fig. 11(a), this figure shows the light distribution due to the presence of two independent eigenmodes. The biaxial anisotropic properties of the director profile generate a twofold light distribution. Moreover, the total light distribution shows three compact regions of high intensity, located above two corners of the white square and the (positive) $y$ axis.

In Figs. 11(b), 11(c), 11(e), and 11(f) the white square is moved from its initial position along the line $x=y$. It is clear that the intensity distribution changes with the position of the square. In the limit where the square is far away from the point charge, the image of the square light source at $z=100$ is again a square.

8. CONCLUSIONS

In view of the recent introduction of biaxially anisotropic nematic liquid crystals, we have introduced a new polarized ray-tracing method for biaxially anisotropic media. With this ray-tracing method, we are now able to calculate the ray paths of light rays in the bulk material of inhomogeneous biaxially anisotropic media. In addition, the theory enables us to calculate the optical properties of curved interfaces with arbitrary orientation and/or anisotropic properties, including the effect of conical refraction. For a general approach, the ray-tracing formulas are presented in a concise vector notation. In the limit where material properties change from biaxial to uniaxial, the biaxial theory evolves to the uniaxial theory presented in [12]. Altogether, this paper explains a method for assessing the optical properties of inhomogeneous biaxially anisotropic media in three dimensions.

In our way of presenting the theory, the formulas produced by our analysis are ready for use and easy to implement in a ray-tracing simulation program. To prove this, we have implemented the vector equations in a ray-tracing program. This ray-tracing program is applied to an artificial biaxially anisotropic gradient-index profile in three dimensions. In the presented simulations the difference between the optical behavior of a uniaxial and a biaxial director profile has been demonstrated. It has been shown that, given an arbitrary director profile, either uniaxial or biaxial, our method can be applied to assess the optical properties of an anisotropic optical system.

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