Linear crystal optics for monochromatic plane waves

The physics of three-wave mixing in anisotropic crystals can be conveniently separated into three topics: how a light wave is changed when it enters or exits the crystal, how a light wave propagates in the crystal, and how three-wave mixing occurs in the crystal. Each of these topics can be considered at different levels of complexity, but each begins with a treatment of monochromatic plane waves. This chapter is devoted to the first two topics, linear propagation of monochromatic plane waves in a crystal, and their behavior on entering or exiting the crystal. Chapters 3 & 4 will explain nonlinear mixing of the monochromatic plane waves. Once the behavior of monochromatic plane waves is thoroughly explored, we will show in subsequent chapters how linear combinations of monochromatic plane waves are used to construct realistic beams and pulses, and how the equations that describe those realistic cases are derived and applied.

As a starting point we rewrite Maxwell’s equations specifically for monochromatic plane waves. Following the customary procedure, we write the vectors for the polarization, the electric field, and the displacement in complex notation,

\[ P = \frac{1}{2} \left[ P e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} + P^* e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} \right], \quad (2.1) \]
\[ E = \frac{1}{2} \left[ E e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} + E^* e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} \right], \quad (2.2) \]
\[
\mathbf{D} = \frac{1}{2} \left[ \mathbf{D} e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} + \mathbf{D}^* e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} \right].
\] (2.3)

The actual fields are represented by the real quantities \(\mathbf{P}, \mathbf{E},\) and \(\mathbf{D}\), but for many calculations it is more convenient to use the complex envelope functions \(\mathbf{D}, \mathbf{E},\) and \(\mathbf{P}\). These complex vectors are in general functions of \((x, y, z, t)\). However, for monochromatic plane waves, they are independent of space and time so we omit these arguments in this chapter, and treat the envelope functions as simple complex vectors.

We substitute the expansions of Eqs. (2.1)-(2.3) in the wave equation, Eq. (1.13)
\[
\nabla \times \nabla \times \mathbf{E} = -\mu_0 \frac{\partial^2}{\partial t^2} \mathbf{D} = -\mu_0 \frac{\partial^2}{\partial t^2} \left[ \epsilon_0 \mathbf{E} + \mathbf{P} \right].
\] (2.4)

The operator \(\nabla\) becomes \((\pm i\mathbf{k})\) when it operates on the exponent \((\pm i\mathbf{k} \cdot \mathbf{r})\). Similarly the operator \((\partial/\partial t)\) becomes \((\pm i\omega)\) when it operates on the exponent \((\pm i\omega t)\). Making these substitutions in Eq. (2.4) and equating the positive (or negative) frequency components on each side of the equation yields
\[
\mathbf{k} \times \mathbf{k} \times \mathbf{E} = -\mu_0 \omega^2 \mathbf{D}.
\] (2.5)

In deriving this equation we assumed that \(\mathbf{E}\) and \(\mathbf{D}\) do not change on propagation, so this is a wave equation for eigenpolarized light. This expression implies that \(\mathbf{D}\) must be normal to \(\mathbf{k}\), but \(\mathbf{D}\) is not necessarily parallel to \(\mathbf{E}\). However, \(\mathbf{k}, \mathbf{D},\) and \(\mathbf{E}\) must lie in a single plane.

We use a similar procedure to rewrite the Poynting vector equation to find the energy flow for monochromatic plane waves. We start with Eq. (1.16), the general Poynting vector equation,
\[
\mathbf{S} = \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B} = \mathbf{E} \times \mathbf{H}.
\] (2.6)

For monochromatic plane waves the third Maxwell equation, Eq. (1.3), relates \(\mathbf{H}\) to \(\mathbf{E}\) for eigenpolarized light in a nonmagnetic material by
\[
\mathbf{H} = \frac{\mathbf{k} \times \mathbf{E}}{\mu_0 \omega}.
\] (2.7)

Substituting the expansions for \(\mathbf{E}\) and \(\mathbf{H}\) in Eq. (2.6), equating equal frequency components, and using Eq. (2.7) plus
\[
\epsilon_0 \mu_0 c^2 = 1,
\] (2.8)

we arrive at
\[
\langle \mathbf{S} \rangle = \frac{n \epsilon_0 c}{2} |\mathbf{E}|^2 \hat{\mathbf{e}} \times \hat{\mathbf{k}} \times \hat{\mathbf{e}},
\] (2.9)
where the angle brackets around $S$ indicate a time average over the optical cycle. We only care about the time averaged values, so we will leave the brackets off in the remainder of the book, and $S$ will be understood to be the time averaged Poynting vector. The unit vector $\hat{e}$ is parallel to the electric field, and the unit vector $\hat{k}$ is parallel to the propagation vector (normal to the wave fronts). From Eq. (2.9) we see that the flow of optical energy, represented by $S$, is perpendicular to $E$, but not necessarily parallel to $k$. However, $S$, $E$, and $\hat{k}$ must lie in a single plane.

It is a good idea to memorize the two pairings of orthogonal vectors we have just derived, $(E \perp S)$ and $(D \perp k)$.

The remainder of this chapter consists of finding solutions to Eq. (2.5) in anisotropic crystals. The solutions will allow us to explore linear propagation in biaxial crystals, and to show how uniaxial and isotropic crystals are special cases of biaxial crystals. I choose this approach because it is not difficult to understand propagation in biaxial crystals, and also because the popular nonlinear crystals of the KTP family (KTP, RTP, KTA, RTA, CTA), plus several borate crystals (LBO, CBO, BiBO, YCOB, GdCOB), and KNbO$_3$ are all biaxial.

Our discussion of light propagation in biaxial crystals will progress from a word-and-diagram geometrical sketch to a more mathematical description based on that geometrical picture, and finally to more abstract mathematical derivations based directly on Maxwell’s equations and crystal dielectric tensors.

### 2.1 A geometrical description

The word picture presented in this section is adapted from Born and Wolf’s classic text *Principles of Optics* [1]. We consider only crystals that are nonmagnetic ($M=0$) and nonconductive ($J=0$).

The solution to the wave equation for eigenpolarized light,

$$k \times k \times E = -\mu \omega^2 D,$$  \hspace{1cm} (2.10)

can be broken into two steps. The first step is to relate $D$ to $E$ in a general way. The second step is to find the particular paired values of $D$ and $E$ that solve the wave equation.

#### 2.1.1 Relating $D$ to $E$

Any two vector quantities in a nonisotropic crystal are generally related by a $(3 \times 3)$ tensor. In our case of $D$ and $E$, the relation is

$$D = \epsilon \cdot E,$$  \hspace{1cm} (2.11)
where $\epsilon$ is the symmetric $(3 \times 3)$ dielectric tensor. It will be more convenient to use this equation in the form

$$E = \epsilon^{-1} \cdot D.$$  \hfill (2.12)

As we discuss in Chapter 13, Eq. (2.12) can be associated with a three dimensional ellipsoid with principal axes $n_x$, $n_y$, and $n_z$ defined by

$$n_x = \sqrt{\epsilon_{xx}/\epsilon_o},$$  \hfill (2.13)

$$n_y = \sqrt{\epsilon_{yy}/\epsilon_o},$$  \hfill (2.14)

$$n_z = \sqrt{\epsilon_{zz}/\epsilon_o}.$$  \hfill (2.15)

This ellipsoid has various names in the literature. We will call it the $D$-ellipsoid because, as we will see, it relates a given $D$ to its paired $E$. The $D$-ellipsoid is diagrammed in Fig. 2.1 where, for the purpose of illustration, the ellipticity is greatly exaggerated. In practice the lengths of the principal axes usually differ by 5% or less.

For biaxial crystals the three principal axes have different lengths, and we adopt the standard labeling with $(n_x < n_y < n_z)$. For uniaxial crystals two of the axes have equal length, while for isotropic crystals all three axes have equal length. These are limiting cases of the biaxial crystal, so an understanding of biaxial crystals will be easy to apply to them. We will
relate the orientation of the $D$-ellipsoid to the underlying crystal structure in Chapter 15. For now it is sufficient to know the $D$-ellipsoid exists for any crystal.

The $D$-ellipsoid represents the dielectric response for all orientations of $D$. If $D$-extended is drawn as a vector from the origin through the ellipsoid surface, the electric field $E$ associated with $D$ is parallel to the surface normal of the ellipsoid at the point where $D$ intersects the surface. In general $E$ is not quite parallel to $D$. The two are exactly parallel only when they are aligned with one of the principal axes of the $D$-ellipsoid.

### 2.1.2 Finding the eigenpolarizations

As we showed earlier, the relation ($D \perp k$) must hold in order to satisfy the wave equation. If we consider a wave propagating along direction $\hat{k}$, as shown in Fig. 2.2, $D$ must lie in the plane normal to $\hat{k}$. This plane passes through the center of the $D$-ellipsoid and intersects the ellipsoid in an ellipse that we can call the $n$-ellipse. The $E$ field associated with $D$ must be aligned normal the $D$-ellipsoid and thus normal to the $n$-ellipse. However, $E$ does not generally lie in the plane of the $n$-ellipse.

![FIGURE 2.2. $D$-ellipsoid and propagation vector, $k$. The plane normal to $k$ that passes through the origin intersects the $D$-ellipsoid in the $n$-ellipse indicated by the heavy line. The eigenpolarization planes coincide with the major and minor axes of this $n$-ellipse, and the associated refractive indices are equal to the semi major and semi minor axes of the ellipse.](image)

In order to satisfy the wave equation, $E$ must lie in the same plane as $k$ and $D$. Otherwise the vector quantities on the two sides of Eq. (2.10)
would not be parallel. This condition can be met only if $D$ lies along one of the principal axes of the $n$-ellipse. There are two possible solutions to the wave equation corresponding to $D$ lying along either of the principal axes of the $n$-ellipse. The $D$ vectors of the two solutions are thus orthogonal to one another, and in combination with $k$ define two eigenpolarization planes that contain $k$ and the paired solutions for $D$ and $E$. Only waves with $D$ aligned along the major or minor axis of the $n$-ellipse propagate without changes to the direction of $D$ or $E$, that is as eigenpolarizations. The corresponding two refractive index values correspond to the lengths of the two principal axes of the $n$-ellipse. We use $hi$ or $lo$ to label the eigenpolarization associated with the higher or lower refractive index.

To summarize, the problem of finding the eigenpolarizations and their refractive indices is reduced to the problem of constructing the $D$-ellipsoid based on the crystal’s dielectric tensor, followed by defining a propagation vector $k$. The $n$-ellipse is then defined in the plane normal to $k$, and the two eigenpolarization planes are those defined by $k$ and the major and minor axes of the $n$-ellipse. The two corresponding refractive indices are given by the lengths of the semi major and semi minor axes of the $n$-ellipse.

### 2.1.3 Optical axes of biaxial crystals

Suppose we start with the propagation vector parallel to the $z$ axis of the $D$-ellipsoid and continuously rotate it in the $xz$ plane until it is parallel to $x$. Initially, when the propagation is along $z$, the $n$-ellipse lies in the $xy$ plane, and $n_{hi}$, the higher index, must be equal to $n_y$, and $n_{lo}$ must be equal to $n_x$. As the propagation direction rotates away from $z$ toward the $x$, the $n$-ellipse pivots about the $y$-axis. Thus the $y$ direction remains an eigenpolarization with the refractive index $n_y$, but the second refractive index increases as the angle increases, going from $n_x$ for propagation along $z$ to $n_z$ for propagation along $x$. The second index starts out smaller than $n_y$ and finishes larger than $n_y$, so at some intermediate angle it must be equal to $n_y$. At that angle the $n$-ellipse must be a circle with both refractive indices equal to $n_y$. This propagation direction is known as the optic axis, and its angle relative to $z$ is traditionally labeled $\Omega$. By symmetry there must be a second equivalent optic axis on the opposite side of the $z$-axis at ($-\Omega$). As the propagation angle sweeps through $\Omega$ the major and minor axes of the $n$-ellipse swap places. For angles smaller than $\Omega$ the major axis is parallel to $y$, while for angles larger than $\Omega$ the minor axis is parallel to $y$. 
2.1.4 Propagation outside the principal planes

When the $k$-vector lies outside the three principal planes, $xy$, $xz$, or $yz$, the $n$-ellipse and its eigenpolarization directions are generally rotated so the eigenpolarizations do not align with the axes of the $D$-ellipsoid. Figure 2.3 illustrates the two eigenpolarization directions for various propagation direction lying in one octant for the biaxial crystal KNbO$_3$. The eigenpolarizations twist as the propagation direction changes, but they are always orthogonal to one another. The other octants are images of this one reflected in the three principal planes, $xy$, $yz$, and $xz$. The angle of the optical axis, $\Omega$, uniquely determines the entire eigenpolarization map for a crystal. All crystals with identical optical axis directions share the same eigenpolarization map.

![Figure 2.3](image)

**FIGURE 2.3.** Eigenpolarization pairs plotted against the propagation direction in one octant of the biaxial crystal KNbO$_3$. The polarization directions for the $lo$ refractive index follow lines originating on the $yz$ arc, while the polarization directions for the $hi$ refractive index follow lines originating on the $xy$ arc. The optic axis is labeled $oa$. The other octants are reflections of this one in the three principal planes, $xy$, $yz$, or $xz$. 
2.1.5 Poynting vector walk off

As described earlier, the electric field $\mathbf{E}$ paired with $\mathbf{D}$ is normal to the surface of the $D$-ellipsoid at the point where $\mathbf{D}$ intersects it, so $\mathbf{E}$ is not in general parallel to $\mathbf{D}$. For an eigenpolarization the point of intersection coincides with either the major or the minor axis of the $n$-ellipse, so the tilt of $\mathbf{E}$ must lie in the plane containing both $\mathbf{D}$ and $\mathbf{k}$. The small angle between $\mathbf{D}$ and $\mathbf{E}$ is conventionally labeled $\rho$. $\mathbf{E}$ is tilted relative to $\mathbf{D}$ in the direction of diminishing refractive index.

Recall that $\mathbf{E}$ and $\mathbf{S}$ are orthogonal. This implies that the angle between $\mathbf{k}$ and $\mathbf{S}$ is also $\rho$. Each of the eigenpolarizations has an associated Poynting vector walk off angle that we label $\rho_{hi}$ or $\rho_{lo}$. These tilts are illustrated in Fig. 2.4.

![Figure 2.4](image)

**FIGURE 2.4.** Vectors $\mathbf{D}_{hi}$, $\mathbf{E}_{hi}$, $\mathbf{S}_{hi}$, and $\mathbf{k}$ lie in a single plane while vectors $\mathbf{D}_{lo}$, $\mathbf{E}_{lo}$, $\mathbf{S}_{lo}$, and $\mathbf{k}$ lie in an orthogonal plane. Walk off angle $\rho_{hi}$ is the angle between $\mathbf{D}_{hi}$ and $\mathbf{E}_{hi}$ and also the angle between $\mathbf{k}$ and $\mathbf{S}_{hi}$. Walk off angle $\rho_{lo}$ is the angle between $\mathbf{D}_{lo}$ and $\mathbf{E}_{lo}$ and also the angle between $\mathbf{k}$ and $\mathbf{S}_{lo}$.

Because walk off occurs in the eigenpolarization planes, the lines in Fig. 2.3 that show the eigenpolarization directions also indicate the directions of the two Poynting vector walk off angles. For the $hi$ eigenpolarization (curves originating on the $xy$ arc), the energy flow is tilted along the $hi$ eigenpolarization direction in the direction away from the $xy$ plane, while for the $lo$-index polarization (curves originating on the $yz$ plane) the
energy flow is tilted along the lo eigenpolarization direction toward the yz plane.

Walk off always tilts S toward the direction of lower refractive index, so if \( \mathbf{k} \) is pivoted slightly in the plane of the lo eigenpolarization in the direction of walk off, \( n_{lo} \) decreases but \( n_{hi} \) is unaltered. This means that the lines in Fig. 2.3 that indicate the directions of the lo eigenpolarization (curves originating on the yz plane) are also curves of constant \( n_{hi} \). Similarly, the hi eigenpolarization directions (curves originating on the xy plane) are curves of constant \( n_{lo} \). For example, for propagation directions lying in the yz plane, the hi eigenpolarization lies in the yz plane and \( n_{hi} \) varies with angle, but the lo eigenpolarization is normal to the yz plane and \( n_{lo} = n_x \), independent of angle. Similarly, along each of the lines originating on the xy arc, \( n_{lo} \) is constant, with a different value for each line, varying from \( n_x \) for the line lying in the yz plane to \( n_y \) for the line lying in the xz plane and terminating at the optic axis.

For propagation in a principal plane one of the walk off angles becomes zero. For example, propagation in the yz plane makes \( (\rho_{lo} = 0) \), while propagation in the xy plane makes \( (\rho_{hi} = 0) \). Propagation in the xz plane makes \( (\rho_{lo} = 0) \) for directions between \( oa \) and \( x \), and \( (\rho_{hi} = 0) \) for directions between \( oa \) and \( z \).

### 2.1.6 Hi and lo index surfaces

We have explained that there are two refractive indices associated with each propagation direction. They can be represented by double surfaces as shown in Fig. 2.5. The distance from the origin to the outer surface along any propagation direction is \( n_{hi} \). The distance to the inner surface is \( n_{lo} \). The two surfaces touch only at their point of intersection with the optic axes. The Poynting vector for a beam with lo polarization is normal to the inner surface, the Poynting vector for the beam with hi polarization is normal to the outer surface. The corresponding \( \mathbf{E} \) fields are tangent to the surfaces.

### 2.1.7 Uniaxial crystals

The symmetry of the crystal structure for certain classes of crystals requires that two of the principal refractive indices be exactly equal (see Chapter 15). In the transition from biaxial to uniaxial there are two possibilities: the intermediate index \( n_y \) can approach the high index \( (n_y \to n_z) \) or the low index \( (n_y \to n_x) \). If \( (n_y \to n_z) \), the two optic axes tilt toward the \( x \) axis, while if \( (n_y \to n_x) \), the optic axes tilt toward the \( z \) axis. The left diagram in Fig. 2.6 shows the eigenpolarization directions for the crystal DLAP which has principal indices at 1064 nm of \( (n_x = 1.496), (n_y = 1.558) \),
FIGURE 2.5. The two $n$ surfaces. The distance from the origin to the outer surface at each value of $(\theta, \phi)$ is $n_{hi}(\theta, \phi)$, while the distance to the inner surface is $n_{lo}(\theta, \phi)$. The $\mathbf{E}$ field for an eigenpolarization is tangent to the corresponding surface, and its Poynting vector $\mathbf{S}$ is normal to the corresponding surface. The optic axis $oa$ is the only point where the two surfaces touch.

and ($n_z = 1.565$). Its optic axis lies near the $x$ axis. The right diagram in Fig. 2.6 shows the eigenpolarization directions for the crystal KTA which has principal indices at 1064 nm of ($n_x = 1.782$), ($n_y = 1.787$), and ($n_z = 1.868$). Its optic axis lies near the $z$ axis.

If $n_y$ becomes exactly equal to $n_x$ the two optic axes merge into a single optic axis oriented along $z$. The eigenpolarization directions then lie along the latitude and longitude lines as shown in Fig. 2.7. The $hi$-index wave, polarized along a line of constant longitude, is called the extraordinary, or $e$-wave, while the $lo$-index wave, polarized along a line of constant latitude, is called the ordinary, or $o$-wave. The $n_o$ surface is spherical with radius $n_x (= n_y)$, while the $n_e$ surface is an oblate ellipsoid of revolution with polar radius of $n_x (= n_y)$ and equatorial radius $n_z$. The left hand diagram
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FIGURE 2.6. Eigenpolarization and walk off directions for DLAP (left) and KTA (right). The line labeled \( oa \) is the optic axis. The other octants are reflections of this one in the three principal planes.

of Fig. 2.8 shows a slice through the double \( n \)-surface for such a positive uniaxial crystal. The \( o \)-wave has no Poynting vector walk off, while the walk off of the \( e \)-wave is toward the \( z \) axis.

On the other hand, if \( n_y \) becomes exactly equal to \( n_z \), the crystal is negative uniaxial and the two optic axes converge to a single axis lying along \( x \). The eigenpolarization contours converge on the \( x \) axis rather than the \( z \) axis. However, for such crystals it is customary to abandon the convention \( (n_x < n_y < n_z) \) and relabel the unique axis from \( x \) to \( z \). The eigenpolarization directions then are identical to those shown in Fig. 2.7. The ordinary or \( n_o \) surface is again spherical while the extraordinary or \( n_e \) surface is a prolate ellipsoid of revolution. A cross section through the double index surfaces for a negative uniaxial crystal shown on the right in Fig. 2.8. Poynting vector walk off of the \( e \)-wave is away from the \( z \) axis for a negative uniaxial crystal.

2.1.8 Isotropic crystals

If \( (n_x = n_y = n_z) \), all three refractive indices are equal so the \( D \)-ellipsoid is a sphere. The crystal is isotropic, meaning all propagation directions and polarizations are equivalent. There are no unique eigenpolarization directions determined by the crystal’s dielectric response, so all polarizations are eigenpolarizations.

Exercise 1 illustrates computation of the \( hi \) and \( lo \) refractive indices plus the walk off angles, for any propagation direction in a biaxial or uniaxial crystal using the SNLO function RefInd.