Lecture #3

Electromagnetic Properties of Materials – Part 2
Nonlinear and Anisotropic Materials

Lecture Outline

- Nonlinear materials
- Anisotropic materials
- Tensor rotation and “unrotation”
- Dispersion relation and index ellipsoids
- Appendix
  - Rotation matrix for rotating $\vec{a}$ onto $\vec{b}$
  - Rotation matrix for rotating $(\vec{a}, \vec{b}, \vec{c})$ onto $(\vec{a}', \vec{b}', \vec{c}')$
All materials are nonlinear; some just have stronger nonlinear behavior than others.

For radio frequencies, materials tend to breakdown before they exhibit nonlinear properties. Nonlinear properties are commonly exploited in optics.

In general, the polarization of a material is a nonlinear function of the electric field and can be expressed as...

\[ P(\omega) = \varepsilon_0 \chi^{(1)}(\omega) E(\omega) + \varepsilon_0 \chi^{(2)}(\omega) E^2(\omega) + \varepsilon_0 \chi^{(3)}(\omega) E^3(\omega) + \cdots \]
“Potential Well” Description

$V$ is the “push” required to displace the charge by a distance $r$.

Linear materials have a parabolic potential well. $V \propto r^2$. This leads to a resonator that oscillates as a perfect sinusoid.

“Potential Well” for Nonlinear Materials

This type of resonance does not oscillate as a sinusoid. It can be seen as a series of sinusoids.

As bound charges are pushed very hard, the restoring force is no longer linear.

This results in anharmonic oscillation.

The oscillator is effectively resonating at multiple frequencies at the same time.
**Nonsymmetric Potentials**

This is a non-symmetrical potential and therefore exhibits a preferred direction for polarization.

The result is a rectified signal along with potentially other frequency content.

**Applications of Nonlinear Materials**

- **χ(1) Materials**
  - Ordinary linear materials

- **χ(2) Materials**
  - Rectification – can create a DC potential from an optical wave
  - Frequency doubling (second harmonic generation) – can make lasers at otherwise impossible wavelengths.
  - Parametric mixing – can provide sum and difference frequencies
  - Pockel’s effect – can introduce birefringence from an applied electric field.

- **χ(3) Materials**
  - Kerr effect – field dependent dielectric constant
  - Third harmonic generation – can generate very short wavelength waves.
  - Raman scattering – the mechanical vibration of a molecule can shift the frequency of the wave
  - Brillouin scattering – dielectric response changes with applied pressure
  - Two photon absorption – two photons are absorbed simultaneously where as a single photon would not be absorbed.
In some materials, charges are more easily displaced along certain directions. For this reason, the material can become polarized in a direction slightly different than the applied field. In this case, the susceptibility is a tensor quantity.

Imagine pushing at an angle against a sliding glass door. The door has a preferred direction for displacement. Real materials are not this dramatic!

\[ \bar{P}(\omega) = \varepsilon_0 \left[ \chi_e (\omega) \right] \bar{E}(\omega) \]

Isotropic materials are good for simple transmission of electromagnetic waves.

Anisotropic materials are good for controlling and manipulating the waves.
Atomic Scale Picture

Charges will oscillate differently in these two directions. Therefore, the susceptibility changes as a function of direction in the lattice.

Large $\varepsilon$

Small $\varepsilon$

Tensor Relations for Anisotropic Materials

The material polarization is now expressed as:

\[
\begin{bmatrix}
P_x(\omega) \\
P_y(\omega) \\
P_z(\omega)
\end{bmatrix} = \varepsilon_0 \begin{bmatrix} 
\chi_{xx}(\omega) & \chi_{yx}(\omega) & \chi_{xz}(\omega) \\
\chi_{yx}(\omega) & \chi_{yy}(\omega) & \chi_{yz}(\omega) \\
\chi_{xz}(\omega) & \chi_{yz}(\omega) & \chi_{zz}(\omega)
\end{bmatrix} \begin{bmatrix}
E_x(\omega) \\
E_y(\omega) \\
E_z(\omega)
\end{bmatrix}
\]

This is most often treated through a dielectric tensor.

\[\tilde{\varepsilon}_i(\omega) = \mathbf{1} + \chi_e(\omega)\]

The constitutive relation between $E$ and $D$ is then

\[
\begin{bmatrix}
D_x(\omega) \\
D_y(\omega) \\
D_z(\omega)
\end{bmatrix} = \varepsilon_0 \begin{bmatrix} 
\tilde{\varepsilon}_{xx}(\omega) & \tilde{\varepsilon}_{yx}(\omega) & \tilde{\varepsilon}_{xz}(\omega) \\
\tilde{\varepsilon}_{yx}(\omega) & \tilde{\varepsilon}_{yy}(\omega) & \tilde{\varepsilon}_{yz}(\omega) \\
\tilde{\varepsilon}_{xz}(\omega) & \tilde{\varepsilon}_{yz}(\omega) & \tilde{\varepsilon}_{zz}(\omega)
\end{bmatrix} \begin{bmatrix}
E_x(\omega) \\
E_y(\omega) \\
E_z(\omega)
\end{bmatrix}
\]

The dielectric tensor has Hermitian symmetry for the general lossy case.

\[E_{ij} = E_{ji}^*\]

This means the field components are no longer independent. 😊

But...it presents many new possibilities!!
Principle Axes

It is always possible to choose a coordinate system such that the dielectric tensor becomes diagonal.

\[
\begin{align*}
\hat{x} & \quad \hat{a} \\
\hat{y} & \Rightarrow \hat{b} \\
\hat{z} & \quad \hat{c}
\end{align*}
\]

where \( \hat{a}, \hat{b}, \) and \( \hat{c} \) are called the “Principal Axes of the Crystal.” \( \hat{a}, \hat{b}, \) and \( \hat{c} \) are not necessarily at 90° to each other.

\[
\begin{bmatrix}
D_a(\omega) \\
D_b(\omega) \\
D_c(\omega)
\end{bmatrix}
= \varepsilon_0
\begin{bmatrix}
\tilde{\varepsilon}_a(\omega) & 0 & 0 \\
0 & \tilde{\varepsilon}_b(\omega) & 0 \\
0 & 0 & \tilde{\varepsilon}_c(\omega)
\end{bmatrix}
\begin{bmatrix}
E_a(\omega) \\
E_b(\omega) \\
E_c(\omega)
\end{bmatrix}
\]

Alternative Description: There are only three degrees of freedom for 3D tensors. Numbers can only occur in the off-diagonal elements when the tensor is rotated.

Maxwell’s Equations with Anisotropic Materials

Maxwell’s equations remain unchanged.

\[
\nabla \times \vec{E} = -j\omega \vec{B} \quad \nabla \cdot \vec{D} = 0
\]

\[
\nabla \times \vec{H} = j\omega \vec{D} \quad \nabla \cdot \vec{B} = 0
\]

The constitutive relations now include tensors

\[
\vec{D} = [\varepsilon] \vec{E}
\]

\[
\vec{B} = [\mu] \vec{H}
\]

where

\[
\begin{bmatrix}
D_x \\
D_y \\
D_z
\end{bmatrix}
= \begin{bmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz}
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix}
\]
Symmetry and Anisotropy

<table>
<thead>
<tr>
<th>Anisotropy</th>
<th>Crystal Symmetry</th>
<th>Dielectric Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>Cubic</td>
<td>( \begin{bmatrix} \bar{\varepsilon} &amp; 0 &amp; 0 \ 0 &amp; \bar{\varepsilon} &amp; 0 \ 0 &amp; 0 &amp; \bar{\varepsilon} \end{bmatrix} )</td>
</tr>
<tr>
<td>Uniaxial</td>
<td>Hexagonal Tetragonal</td>
<td>( \begin{bmatrix} \varepsilon_0 &amp; 0 &amp; 0 \ 0 &amp; \varepsilon_0 &amp; 0 \ 0 &amp; 0 &amp; \varepsilon_0 \end{bmatrix} ) positive birefringence ( \varepsilon_0 &gt; \bar{\varepsilon} ) negative birefringence ( \varepsilon_0 &lt; \bar{\varepsilon} )</td>
</tr>
<tr>
<td>Biaxial</td>
<td>Monoclinic Triclinic Orthorhombic</td>
<td>( \begin{bmatrix} \bar{\varepsilon}_x &amp; 0 &amp; 0 \ 0 &amp; \bar{\varepsilon}_y &amp; 0 \ 0 &amp; 0 &amp; \bar{\varepsilon}_z \end{bmatrix} ) ( \bar{\varepsilon}_x &lt; \bar{\varepsilon}_y &lt; \bar{\varepsilon}_z )</td>
</tr>
</tbody>
</table>

Tensor Rotation and “Unrotation”
### Definition of a Rotation Matrix

Rotation matrix \([R]\) is defined as

\[
\vec{b} = \begin{bmatrix} R(\phi) \end{bmatrix} \vec{a}
\]

The rotation matrix should not change the amplitude. This implies that \([R]\) is unitary.

\[
|\vec{b}| = |\vec{a}|
\]

\[
[R]^{\dagger} = [R]^{-1}
\]

\[
[R][R]^{\dagger} = [R]^{\dagger} [R] = \mathbf{I}
\]

### Derivation of a 2D Rotation Matrix

Start with vector \(\vec{a}\) at angle \(\theta\).

\[
\vec{a} = a_x \hat{x} + a_y \hat{y} = a \begin{bmatrix} \cos \theta \hat{x} + \sin \theta \hat{y} \end{bmatrix}
\]

Add angle \(\phi\) to rotate the vector

\[
\vec{b} = a \begin{bmatrix} \cos(\theta + \phi) \hat{x} + \sin(\theta + \phi) \hat{y} \end{bmatrix}
\]

Apply trig identities

\[
\vec{b} = a \begin{bmatrix} (\cos \theta \cos \phi - \sin \theta \sin \phi) \hat{x} + (\sin \theta \cos \phi + \cos \theta \sin \phi) \hat{y} \\
(\cos \phi \hat{x} - \sin \phi \hat{y}) + (\sin \phi \hat{x} + \cos \phi \hat{y}) \end{bmatrix}
\]

\[
\begin{bmatrix} b_x \\ b_y \end{bmatrix} = \begin{bmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} a_x \\ a_y \end{bmatrix} = \begin{bmatrix} a_x \cos \phi - a_y \sin \phi \\ a_x \cos \phi + a_y \sin \phi \end{bmatrix}
\]

\[
[\begin{bmatrix} b_x \\ b_y \end{bmatrix}] = \begin{bmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{bmatrix} [\begin{bmatrix} a_x \\ a_y \end{bmatrix}]
\]

\[
[\begin{bmatrix} a_x \cos \phi - a_y \sin \phi \\ a_x \cos \phi + a_y \sin \phi \end{bmatrix}]
\]
3D Rotation Matrices

Rotation matrices for 3D coordinates can be written directly from the previous result.

\[
\begin{bmatrix}
1 & 0 & 0 \\
0 & \cos \phi & -\sin \phi \\
0 & \sin \phi & \cos \phi
\end{bmatrix}
\]

\[
\begin{bmatrix}
\cos \phi & 0 & \sin \phi \\
0 & 1 & 0 \\
-\sin \phi & 0 & \cos \phi
\end{bmatrix}
\]

\[
\begin{bmatrix}
\cos \phi & -\sin \phi & 0 \\
\sin \phi & \cos \phi & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

Tensor Rotation

Tensors are rotated using the same rotation matrices, but in a slightly different manner than vectors.

\[
\mathcal{E}^{(R)} = R_z(\phi) \mathcal{E} R_z(\phi)^{-1}
\]
Combinations of Rotations

Suppose we wish to first rotate about the x-axis by some angle, second rotate about the y-axis by some angle, and third rotate about the z-axis by some angle.

For vectors...

\[
\vec{b} = [R_z][R_y][R_x]\vec{a}
\]

For tensors...

\[
\begin{bmatrix} \mathcal{E}^{(R)} \end{bmatrix} = [R_z][R_y][R_x][\mathcal{E}][R_x]^{-1}[R_y]^{-1}[R_z]^{-1}
\]

Composite Rotation Matrix

We can combine multiple rotation matrices into a single composite rotation matrix \([R]\).

\[
[R] = [R_y][R_z][R_x]
\]

This equation implies we will rotate first about the x-axis, second about the z-axis, and third about the y-axis.

Vector rotation using the composite rotation matrix is

\[
\vec{b} = [R]\vec{a}
\]

Tensor rotation using the composite rotation matrix is

\[
\begin{bmatrix} \mathcal{E}^{(R)} \end{bmatrix} = [R][\mathcal{E}][R]^{-1}
\]
Animation of Tensor Rotation

![Animation of Tensor Rotation Diagram](image)

Order of Rotations Matter

The order that we multiply the rotation matrices controls the order that the rotations are performed.

\[
\vec{b} = \left[ R_z \left( -45^\circ \right) \right] \left[ R_y \left( 220^\circ \right) \right] \left[ R_x \left( 10^\circ \right) \right] \hat{a}
\]

1. First rotates about the \( x \)-axis by \( 10^\circ \).
2. Second rotates about the \( y \)-axis by \( 220^\circ \).
3. Third rotates about the \( z \)-axis by \( -45^\circ \).

In general, we do not get the same result when the order of rotation is changed.

\[
\left[ R_y \right] \left[ R_x \right] \neq \left[ R_x \right] \left[ R_y \right]
\]
Numerical Examples (1 of 2)

Given: \( \epsilon = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \)

Rotate about \( x \)-axis by 20°

\[
R_x(20°) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0.9397 & -0.3420 \\ 0 & 0.3420 & 0.9397 \end{bmatrix} \]

\( \epsilon' = \begin{bmatrix} 2.1170 & -0.3214 \\ 0 & 2.8830 \end{bmatrix} \)

Rotate about \( y \)-axis by 45°

\[
R_y(45°) = \begin{bmatrix} 0.7071 & 0.7071 & 0 \\ 0 & 1 & 0 \\ -0.7071 & 0.7071 & 0 \end{bmatrix} \]

\( \epsilon' = \begin{bmatrix} 0 & 0 & 1 \\ 2 & 0 & 0 \end{bmatrix} \)

Rotate about \( z \)-axis by 60°

\[
R_z(60°) = \begin{bmatrix} 0.5000 & -0.8660 & 0 \\ 0.8660 & 0.5000 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]

\( \epsilon' = \begin{bmatrix} 1.7500 & -0.4330 & 0 \\ -0.4330 & 1.2500 & 0 \\ 0 & 0 & 3 \end{bmatrix} \)

---

Numerical Examples (2 of 2)

Given: \( \epsilon = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \)

Rotate first about \( x \)-axis by 20° and second about the \( y \)-axis by 45°

\[
R_x(45°)R_x(20°) = \begin{bmatrix} 0.7071 & 0.2418 & 0.6645 \\ 0 & 0.9397 & -0.3420 \\ -0.7071 & 0.2418 & 0.6645 \end{bmatrix} \]

\( \epsilon' = \begin{bmatrix} 1.9415 & -0.2273 & 0.9415 \\ -0.2273 & 2.1170 & -0.2273 \\ 0.9415 & -0.2273 & 1.9415 \end{bmatrix} \)

Rotate first about \( z \)-axis by 60° and second about the \( y \)-axis by 45°

\[
R_y(45°)R_z(60°) = \begin{bmatrix} 0.3536 & -0.6124 & 0.7071 \\ 0.8660 & 0.5000 & 0 \\ -0.3536 & 0.6124 & 0.7071 \end{bmatrix} \]

\( \epsilon' = \begin{bmatrix} 2.3750 & -0.3062 & 0.6250 \\ -0.3062 & 1.2500 & 0.3062 \\ 0.6250 & 0.3062 & 2.3750 \end{bmatrix} \)

Rotate first about \( y \)-axis by 20°, second about the \( y \)-axis by 45°, and third about the \( z \)-axis by 60°

\[
R_y(60°)R_y(45°)R_z(20°) = \begin{bmatrix} 0.3536 & -0.6929 & 0.6284 \\ 0.6124 & 0.6793 & 0.4044 \\ -0.7071 & 0.2418 & 0.6645 \end{bmatrix} \]

\( \epsilon' = \begin{bmatrix} 2.2699 & 0.0377 & 0.6676 \\ 0.0377 & 1.7886 & 0.7017 \\ 0.6676 & 0.7017 & 1.9415 \end{bmatrix} \)
Tensor Unrotation (1 of 2)

A tensor can always be diagonalized along its principle axes.

\[
\mathbf{c} = \begin{bmatrix}
\varepsilon_a & 0 & 0 \\
0 & \varepsilon_b & 0 \\
0 & 0 & \varepsilon_c \\
\end{bmatrix}
\]

Principle Axes:
- \(\varepsilon_a\) is along \(\hat{a}\)
- \(\varepsilon_b\) is along \(\hat{b}\)
- \(\varepsilon_c\) is along \(\hat{c}\)

Convention:
- \(\varepsilon_a \leq \varepsilon_b \leq \varepsilon_c\)

But suppose we are given a general nine-element tensor.

\[
\mathbf{c}_{\text{rot}} = \begin{bmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \\
\end{bmatrix}
\]

How do we determine \(\varepsilon_{a, b, c}\) and the principle axes \(a, b,\) and \(c\)?

Tensor Unrotation (2 of 2)

We can relate the original tensor \(\mathbf{c}\) and the rotated tensor \(\mathbf{c}_{\text{rot}}\) through the composite rotation matrix \([R]\).

\[
\mathbf{c}_{\text{rot}} = [R][\mathbf{c}][R]^{-1}
\]

We calculate the eigen-vectors and eigen-values of \(\mathbf{c}_{\text{rot}}\).

\[
\mathbf{c}_{\text{rot}} \rightarrow [R] \text{ is the eigen-vector matrix of } \mathbf{c}_{\text{rot}} \\
[\mathbf{c}] \text{ is the eigen-value matrix of } \mathbf{c}_{\text{rot}}
\]
Determining Principle Axes (1 of 2)

What are the principle axes of \([\varepsilon_{\text{rot}}]\)?

Let's put the original principal axes \(a, b,\) and \(c\) into a matrix.

\[
\mathbf{\tilde{P}} = \begin{bmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{bmatrix}
\]

We are not rotating a tensor here so we don’t use \([R][P][R]^{-1} \). Now let's rotate them according to \([R]\) so they correspond to that of \([\varepsilon_{\text{rot}}]\).

\[
\mathbf{\tilde{P}_{\text{rot}}} = [R][\mathbf{\tilde{P}}]
\]

For the special case of orthorhombic symmetry, the principle axes start off as

\[
\mathbf{\tilde{P}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

\[
\mathbf{\tilde{P}_{\text{rot}}} = [R][I][R]
\]

We now have a second interpretation of the eigenvector matrix \([R]\). These are the principle axes of the rotated tensor (for orthorhombic symmetry).
Directly Setting the Principle Axes

We may know the orientation that we would like to place our tensor directly in terms of the desired crystal axes \( a, b, \) and \( c. \)

We place these into a matrix and interpret it as the composite rotation matrix.

\[
[R] = \begin{bmatrix}
a_x & b_x & c_x \\
a_y & b_y & c_y \\
a_z & b_z & c_z
\end{bmatrix}
\]

The rotated tensor can be directly calculated from \([R].\)

\[
[\hat{\varepsilon}_{\text{rot}}] = [R][\hat{\varepsilon}][R]^{-1}
\]
The Wave Vector

The wave vector (wave momentum) is a vector quantity that conveys two pieces of information:

1. **Wavelength and Refractive Index** – The magnitude of the wave vector tells us the spatial period $\lambda$ (wavelength) of the wave inside the material. When the free space wavelength is known, $|\vec{k}|$ conveys the material’s refractive index $n$ (more to be said later).

$$ |\vec{k}| = \frac{2\pi}{\lambda} = \frac{2\pi n}{\lambda_0} \quad \lambda_0 \equiv \text{free space wavelength} $$

2. **Direction** – The direction of the wave is perpendicular to the wave fronts (more to be said later).

$$ \vec{k} = k_a \hat{a} + k_b \hat{b} + k_c \hat{c} $$

Dispersion Relations

The dispersion relation for a material relates the wave vector to frequency. Essentially, it tells us the refractive index as a function of direction through a material.

It is derived by substituting a plane wave solution into the wave equation.

For an ordinary linear homogeneous and isotropic (LHI) material, the dispersion relation is:

$$ k_a^2 + k_b^2 + k_c^2 = k_0^2 n^2 $$

This can also be written as:

$$ \frac{k_a^2 + k_b^2 + k_c^2}{n^2} - k_0^2 = 0 $$
Index Ellipsoids

From the previous slide, the dispersion relation for a LHI material was:

\[ k_a^2 + k_b^2 + k_c^2 = k_0^2 n^2 \]

This defines a sphere called an “index ellipsoid.”

The vector connecting the origin to a point on the surface of the sphere is the \( k \)-vector for that direction. Refractive index is calculated from this.

\[ |\vec{k}| = k_0 n \]

For LHI materials, the refractive index is the same in all directions.

Think of this as a map of the refractive index as a function of the wave’s direction through the medium.

How to Derive the Dispersion Relation (1 of 2)

The wave equation in a linear homogeneous anisotropic material is:

\[ \nabla \times \nabla \times \vec{E} - k_0^2 \mu_0 \epsilon_0 \vec{E} = 0 \quad \text{We are ignoring the magnetic response here.} \]

The solution to this equation is still a plane wave, but our allowed values for \( k \) (modes) are more complicated.

\[ \vec{E} = \vec{E}_0 e^{-jk \cdot \vec{r}} \quad \vec{E}_0 = E_a \hat{a} + E_b \hat{b} + E_c \hat{c} \]

Substituting this solution into the wave equation leads to the following relation:

\[ \vec{k} \left( \vec{k} \cdot \vec{E}_0 \right) - |\vec{k}| \vec{E}_0 + k_0^2 \epsilon_0 \vec{E}_0 = 0 \]

This equation has the form: \((\cdot\cdot\cdot)\hat{a} + (\cdot\cdot\cdot)\hat{b} + (\cdot\cdot\cdot)\hat{c} = 0\)

Each \((\cdot\cdot\cdot)\) term has the form: \((\cdot\cdot\cdot)E_a + (\cdot\cdot\cdot)E_b + (\cdot\cdot\cdot)E_c = 0\)

Each vector component must be set to zero independently.

\(\hat{a}\) component: \((\cdot\cdot\cdot)E_a + (\cdot\cdot\cdot)E_a + (\cdot\cdot\cdot)E_a = 0\)

\(\hat{b}\) component: \((\cdot\cdot\cdot)E_a + (\cdot\cdot\cdot)E_b + (\cdot\cdot\cdot)E_b = 0\)

\(\hat{c}\) component: \((\cdot\cdot\cdot)E_a + (\cdot\cdot\cdot)E_c + (\cdot\cdot\cdot)E_c = 0\)

Matrix form...

\[
\begin{bmatrix}
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z \\
\end{bmatrix} = 0
\]
How to Derive the Dispersion Relation (2 of 2)

Solutions for $k$ are the eigen-values of the big matrix and derived by setting the determinant to zero.

$$\det\begin{pmatrix} (\ldots) & (\ldots) & (\ldots) \\ (\ldots) & (\ldots) & (\ldots) \\ (\ldots) & (\ldots) & (\ldots) \end{pmatrix} = 0$$

This leads to the following general equation:

$$\frac{k_a^2}{|\vec{k}|^2-k_0^2n_a^2} + \frac{k_b^2}{|\vec{k}|^2-k_0^2n_b^2} + \frac{k_c^2}{|\vec{k}|^2-k_0^2n_c^2} = 1$$

It can also be shown that given the wave vector, the polarization of the electric field is:

$$\vec{E}_0 = \left(\frac{k_a}{|\vec{k}|^2-k_0^2n_a^2}\right)\hat{a} + \left(\frac{k_b}{|\vec{k}|^2-k_0^2n_b^2}\right)\hat{b} + \left(\frac{k_c}{|\vec{k}|^2-k_0^2n_c^2}\right)\hat{c}$$

Generalized Dispersion Relation

Given the dielectric tensor..., \[\varepsilon_r = \begin{bmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_c \end{bmatrix} = \begin{bmatrix} n_a^2 & 0 & 0 \\ 0 & n_b^2 & 0 \\ 0 & 0 & n_c^2 \end{bmatrix}\]

The general form of the dispersion relation is:

$$\frac{k_a^2}{|\vec{k}|^2-k_0^2n_a^2} + \frac{k_b^2}{|\vec{k}|^2-k_0^2n_b^2} + \frac{k_c^2}{|\vec{k}|^2-k_0^2n_c^2} = 1$$

This can be written in a more useful form as:

$$|\vec{k}|^2 \left(\frac{k_a^2}{n_a^2n_c^2} + \frac{k_b^2}{n_b^2n_c^2} + \frac{k_c^2}{n_a^2n_b^2}\right) - k_0^2 \left(\frac{k_b^2}{n_a^2n_b^2} + \frac{k_c^2}{n_a^2n_c^2} + \frac{k_a^2}{n_b^2n_c^2}\right) + k_0^4 = 1$$
Dispersion Relation for Uniaxial Crystals

Uniaxial crystals have

\[ n_a = n_b = n_O \quad n_O = \text{ordinary refractive index} \]

\[ n_c = n_E \quad n_E = \text{extraordinary refractive index} \]

The general dispersion relation reduces to:

\[
\left( \frac{k_a^2 + k_b^2 + k_c^2}{n_O^2} - k_0^2 \right) \left( \frac{k_a^2 + k_b^2 + k_c^2}{n_E^2} - k_0^2 \right) = 0
\]

This has two solutions corresponding to the two polarizations (TE and TM).

This has two solutions corresponding to the two polarizations (TE and TM).

This first solution is the same as for an isotropic material. It acts like it is propagating through a isotropic material with index \( n_O \) so it is called the "ordinary wave."

The second solution is an ellipsoid. Depending on its direction, the effective refractive index will be somewhere between \( n_O \) and \( n_E \).

Index Ellipsoids for Uniaxial Crystals (1 of 2)

Ordinary Wave

\[
\left( \frac{k_a^2 + k_b^2 + k_c^2}{n_O^2} - k_0^2 \right) = 0
\]

Extraordinary Wave

\[
\left( \frac{k_a^2 + k_b^2 + k_c^2}{n_E^2} - k_0^2 \right) = 0
\]
Observations
• Both solutions share a common axis.
• This “common” axis looks isotropic with refractive index \( n_0 \) regardless of polarization.
• Since both solutions share a single axis, these crystals are called “uniaxial.”
• The “common” axis is called:
  - Optic axis
  - Ordinary axis
  - C axis
  - Uniaxial axis
• Deviation from the optic axis will result in two separate possible modes.

Dispersion Relation for Biaxial Crystals (1 of 2)

Biaxial crystals have all unique refractive indices. Most texts adopt the convention where

\[ n_a < n_b < n_c \]

The general dispersion relation cannot be reduced.

Notes and Observations
• The convention \( n_a < n_b < n_c \) causes the optic axes to lie in the \( a-c \) plane.
• The two solutions can be envisioned as one balloon inside another, pinched together so they touch at only four points.
• Propagation along either of the optic axes looks isotropic, thus the name “biaxial.”
Dispersion Relation for Biaxial Crystals (2 of 2)

There are three special cases when it can be simplified. We can cause these conditions by launching electromagnetic waves at the proper orientation.

\[
\begin{align*}
    k_a &= 0: \quad \left( k_b^2 + k_c^2 - k_0^2 n_a^2 \right) \left( \frac{k_b^2}{n_c^2} + \frac{k_c^2}{n_b^2} - k_0^2 \right) = 0 \\
    k_b &= 0: \quad \left( k_a^2 + k_c^2 - k_0^2 n_b^2 \right) \left( \frac{k_a^2}{n_c^2} + \frac{k_c^2}{n_a^2} - k_0^2 \right) = 0 \\
    k_c &= 0: \quad \left( k_a^2 + k_b^2 - k_0^2 n_c^2 \right) \left( \frac{k_a^2}{n_b^2} + \frac{k_b^2}{n_c^2} - k_0^2 \right) = 0
\end{align*}
\]

We see that each case has two separate solutions corresponding to the two polarizations (TE and TM).

Dispersion Surfaces of Magnetoelectric Materials

Magnetoelectric materials can exhibit up to 16 singularities.

\[
\tilde{D} = [\varepsilon] \tilde{E} + [\zeta] \tilde{H} \quad \text{and} \quad \tilde{B} = [\xi] \tilde{H} + [\sigma] \tilde{E}
\]
Direction of Power Flow

Isotropic Materials

Phase propagates in the direction of $\mathbf{k}$. Therefore, the refractive index derived from $|\mathbf{k}|$ is best described as the phase refractive index. Velocity here is the phase velocity.

Energy propagates in the direction of $\mathbf{P}$ which is always normal to the surface of the index ellipsoid. From this, we can define a group velocity and a group refractive index.

Anisotropic Materials

Illustration of $\mathbf{k}$ versus $\mathbf{\phi}$

Raymond C. Rumpf

Negative refraction into a photonic crystal.
Double Refraction in Anisotropic Materials

Isotropic Materials

Anisotropic Materials

Anisotropic materials have two index ellipsoids – one for each polarization. Wave energy can split between the two produce an ordinary and an extraordinary wave.

Appendix
Rotation Matrix \([R]\) that Rotates \(\vec{a}\) Onto \(\vec{b}\)

Normalize Vectors

\[
\hat{a} = \frac{\vec{a}}{|\vec{a}|} \quad \hat{b} = \frac{\vec{b}}{|\vec{b}|}
\]

Algorithm

\[
\vec{v} = \hat{a} \times \hat{b} \\
\hat{s} = |\vec{v}| \quad \text{i.e. } \sin \theta_{ab} \\
c = \hat{a} \cdot \hat{b} \quad \text{i.e. } \cos \theta_{ab}
\]

\[
[\vec{v} \times] = \begin{bmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{bmatrix}
\]

\[
[R] = [I] - [\vec{v} \times] - \left( \frac{1-c}{s^2} \right) [\vec{v} \times]^2
\]

\([R]\) is such that

\[
[R] \hat{a} = \hat{b}
\]

Rotation Matrix \([R]\) that Rotates \((\vec{a}, \vec{b}, \vec{c})\) Onto \((\vec{a}', \vec{b}', \vec{c}')\)

\[
[S_1] = \begin{bmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{bmatrix}
\]

\[
[S_2] = \begin{bmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{bmatrix}
\]

\[
[R] = [S_2][S_1]^{-1}
\]