Lecture 3: Crystal Optics

Outline

- Homogeneous, Anisotropic Media
- Crystals
- Plane Waves in Anisotropic Media
- Wave Propagation in Uniaxial Media
- Reflection and Transmission at Interfaces

Homogeneous, Anisotropic Media

Introduction

- material equations for homogeneous anisotropic media
  \[
  \vec{D} = \varepsilon \vec{E}
  \]
  \[
  \vec{B} = \mu \vec{H}
  \]
- tensors of rank 2, written as 3 by 3 matrices
  - \(\varepsilon\): dielectric tensor
  - \(\mu\): magnetic permeability tensor
- examples:
  - crystals, liquid crystals
  - external electric, magnetic fields acting on isotropic materials (glass, fluids, gas)
  - anisotropic mechanical forces acting on isotropic materials

Properties of Dielectric Tensor

- Maxwell equations imply symmetric dielectric tensor
  \[
  \varepsilon = \varepsilon^T = \begin{pmatrix}
  \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
  \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\
  \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33}
\end{pmatrix}
  \]
- symmetric tensor of rank 2 \(\Rightarrow\) coordinate system exists where tensor is diagonal
- orthogonal axes of this coordinate system: principal axes
- elements of diagonal tensor: principal dielectric constants
- 3 principal indices of refraction in coordinate system spanned by principal axes
  \[
  \vec{D} = \begin{pmatrix}
  n_x^2 & 0 & 0 \\
  0 & n_y^2 & 0 \\
  0 & 0 & n_z^2
\end{pmatrix} \vec{E}
  \]
- \(x, y, z\) because principal axes form Cartesian coordinate system

Uniaxial Materials

- isotropic materials: \(n_x = n_y = n_z\) for any coordinate system
- anisotropic materials:
  - \(n_x \neq n_y \neq n_z\)
- uniaxial materials: \(n_x = n_y \neq n_z\)
- ordinary index of refraction:
  - \(n_0 = n_x = n_y\)
- extraordinary index of refraction:
  - \(n_e = n_z\)
- rotation of coordinate system around \(z\) does not change anything
- most materials used in polarimetry are (almost) uniaxial
**Crystals**

**Crystal Axes Terminology**
- **optic axis** is the axis that has a different index of refraction
- also called *c* or crystallographic axis
- **fast axis**: axis with smallest index of refraction
- ray of light going through uniaxial crystal is (generally) split into two rays
- **ordinary ray** (*o-ray*) passes the crystal without any deviation
- **extraordinary ray** (*e-ray*) is deviated at air-crystal interface
- two emerging rays have orthogonal polarization states
- common to use indices of refraction for ordinary ray \( (n_o) \) and extraordinary ray \( (n_e) \) instead of indices of refraction in crystal coordinate system
- \( n_e < n_o \): negative uniaxial crystal
- \( n_e > n_o \): positive uniaxial crystal

**Magnetic Field**
- constant, scalar \( \mu \), vanishing current density \( \Rightarrow \vec{H} \parallel \vec{B} \)
- \( \nabla \cdot \vec{H} = 0 \Rightarrow \vec{H} \perp \vec{k} \)
- \( \nabla \times \vec{H} = \frac{1}{c} \frac{\partial \vec{D}}{\partial t} \Rightarrow \vec{H} \perp \vec{D} \)
- \( \nabla \times \vec{E} = -\frac{\mu}{c} \frac{\partial \vec{H}}{\partial t} \Rightarrow \vec{H} \perp \vec{E} \)
- \( \vec{D}, \vec{E}, \) and \( \vec{k} \) all in one plane
- \( \vec{H}, \vec{B} \) perpendicular to that plane
- Poynting vector \( \vec{S} = \frac{c}{\mu} \vec{E} \times \vec{H} \)
- perpendicular to \( \vec{E} \) and \( \vec{H} \Rightarrow \vec{S} \) (in general) not parallel to \( \vec{k} \)
- energy (in general) not transported in direction of wave vector \( \vec{k} \)

**Plane Waves in Anisotropic Media**

**Displacement and Electric Field Vectors**
- plane-wave ansatz for \( \vec{D}, \vec{E}, \vec{H} \)
  \[
  \vec{E} = \vec{E}_0 e^{i(\vec{k} \cdot \vec{x} - \omega t)} \\
  \vec{D} = \vec{D}_0 e^{i(\vec{k} \cdot \vec{x} - \omega t)} \\
  \vec{H} = \vec{H}_0 e^{i(\vec{k} \cdot \vec{x} - \omega t)}
  \]
- no net charges in medium \( (\nabla \cdot \vec{D} = 0) \)
- \( \vec{D} \) perpendicular to \( \vec{k} \)
- \( \vec{D} \) and \( \vec{E} \) not parallel \( \Rightarrow \vec{E} \) not perpendicular to \( \vec{k} \)
- wave normal, energy flow not in same direction, same speed

**Relation between \( \vec{D} \) and \( \vec{E} \)**
- combine Maxwell, material equations in principal coordinate system
  \[
  \mu D_i = \mu \varepsilon_i E_i = n^2 \left( \vec{E}_i - s_i \left( \vec{E} \cdot \vec{s} \right) \right) \quad i = 1 \ldots 3
  \]
- \( \vec{s} = \vec{k} / |\vec{k}| \): unit vector in direction of wave vector \( \vec{k} \)
- \( n \): refractive index associated with direction \( \vec{s} \), i.e. \( n = n(\vec{s}) \)
- 3 equations for 3 unknowns \( \vec{E}_i \)
- eliminate \( \vec{E} \) assuming \( \vec{E} \neq 0 \Rightarrow \text{Fresnel equation} \)
  \[
  \frac{s_x^2}{r^2 - \mu \varepsilon_x} + \frac{s_y^2}{r^2 - \mu \varepsilon_y} + \frac{s_z^2}{r^2 - \mu \varepsilon_z} = 1
  \]
- with \( r^2 = \mu \varepsilon_i \)
  \[
  s_x^2 (s_x^2 - s_y^2) (s_x^2 - s_z^2) + s_y^2 (s_y^2 - s_x^2) (s_y^2 - s_z^2) + s_z^2 (s_z^2 - s_x^2) (s_z^2 - s_y^2) = 0
  \]
Electric Field in Anisotropic Material

- with arbitrary constant $a$, electric field vector given by
  \[ \vec{E} = a \left( \begin{array}{c} \frac{s_x}{n^2 - n_0^2} \\ \frac{s_y}{n^2 - n_0^2} \\ \frac{s_z}{n^2 - n_0^2} \end{array} \right) \]

- quadratic equation in $n \Rightarrow$ generally two solutions for given direction $\vec{s}$
- electric field can also be written as
  \[ \vec{E}_k = \frac{n^2 s_k (\vec{E} \cdot \vec{s})}{n^2 - \mu \epsilon_k} \]

- system of 3 equations can be solved for $E_k$
- denominator vanishes if $\vec{k}$ parallel to a principal axis $\Rightarrow$ treat separately

Non-Absorbing, Non-Active, Anisotropic Materials

- $\vec{k}$ not parallel to a principal axis $\Rightarrow$ ratio of 2 electric field components $k$ and $l$
  \[ \frac{E_k}{E_l} = \frac{s_k (n^2 - \mu \epsilon_l)}{s_l (n^2 - \mu \epsilon_k)} \]

- ratio is independent of electric field components
- $n^2$ and $\epsilon_i$ real $\Rightarrow$ ratios are real $\Rightarrow$ electric field is linearly polarized
- in non-absorbing, non-active, anisotropic material, 2 waves propagate that have different linear polarization states and different directions of energy flows
- direction of vibration of $\vec{D}$ corresponding to 2 solutions are orthogonal to each other (without proof)
  \[ \vec{D}_1 \cdot \vec{D}_2 = 0 \]

Wave Propagation in Uniaxial Media

Introduction

- uniaxial media $\Rightarrow$ dielectric constants:
  \[ \epsilon_x = \epsilon_y = n_0^2 \]
  \[ \epsilon_z = n_e^2 \]

- second form of Fresnel equation reduces to
  \[ (n^2 - n_0^2) \left[ n_0^2 \left( s_x^2 + s_y^2 \right) (n^2 - n_0^2) + s_z^2 n_e^2 (n^2 - n_0^2) \right] = 0 \]

- two solutions $n_1$, $n_2$ given by
  \[ n_1^2 = n_0^2 \]
  \[ \frac{1}{n_2^2} = \frac{s_x^2 + s_y^2}{n_0^2} + \frac{s_z^2}{n_e^2} \]

Propagation in General Direction

- (unit) wave vector direction in spherical coordinates
  \[ \vec{s} = \left( \begin{array}{c} s_x \\ s_y \\ s_z \end{array} \right) = \left( \begin{array}{c} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{array} \right) \]

  - $\theta$: angle between wave vector and optic axis
  - $\phi$: azimuth angle in plane perpendicular to optic axis

  \[ \frac{1}{n_2^2} = \frac{\cos^2 \theta}{n_0^2} + \frac{\sin^2 \theta}{n_e^2} \]
  \[ n_2 (\theta) = \frac{n_0 n_e}{\sqrt{n_0^2 \sin^2 \theta + n_e^2 \cos^2 \theta}} \]

- take positive root, negative value corresponds to waves propagating in opposite direction
Ordinary and Extraordinary Rays

- from before

\[
\frac{1}{n_2^2} = \frac{\cos^2 \theta}{n_0^2} + \frac{\sin^2 \theta}{n_e^2} \\
n_2(\theta) = \sqrt{\frac{n_0^2 \sin^2 \theta + n_e^2 \cos^2 \theta}{n_0 n_e}}
\]

- \(n_2\) varies between \(n_0\) for \(\theta = 0\) and \(n_e\) for \(\theta = 90^\circ\)
- first solution propagates according to ordinary index of refraction, independent of direction \(\Rightarrow\) ordinary beam or ray
- second solution corresponds to extraordinary beam or ray
- index of refraction of extraordinary beam is (in general) not the extraordinary index of refraction

Ordinary Beam

- ordinary beam speed independent of wave vector direction
  
  \[
  \mu D_i = \mu_e \vec{E}_i = n_i^2 \left( \vec{E}_i - s_i \left( \vec{E}_i \cdot \vec{s}_i \right) \right), \ i = 1 \cdots 3 \text{ to hold for any direction } \vec{s}_i, \vec{E}_o \cdot \vec{s}_i = 0 \text{ and } E_{o,z} = 0
  \]
- electric field vector of ordinary beam
  (with real constant \(a_o \neq 0\))
  
  \[
  \vec{E}_o = a_o \begin{pmatrix} \sin \phi \\ - \cos \phi \\ 0 \end{pmatrix}
  \]
- ordinary beam is linearly polarized
- \(\vec{D}_o\) perpendicular to plane formed by wave vector \(\vec{k}\) and \(c\)-axis
- displacement vector \(\vec{D}_o = n_0 \vec{E}_o \parallel \vec{E}_o\)
- Poynting vector \(\vec{S}_o \parallel \vec{k}\)

Extraordinary Ray

- since \(\vec{D}_e \cdot \vec{k} = 0\) and \(\vec{D}_e \cdot \vec{B}_o = 0 \Rightarrow\) unique solution (up to real constant \(a_e\))
  
  \[
  \vec{D}_e = a_e \begin{pmatrix} \cos \theta \cos \phi \\ \cos \theta \sin \phi \\ - \sin \theta \end{pmatrix}
  \]
- since \(E_e \cdot D_o = 0, D_e = \epsilon \vec{E}_e\)
  
  \[
  \vec{E}_e = a \begin{pmatrix} n_0^2 \cos \theta \cos \phi \\ n_0^2 \cos \theta \sin \phi \\ - n_0^2 \sin \theta \end{pmatrix}
  \]
- uniaxial medium \(\Rightarrow\) \(\vec{E}_o \cdot \vec{E}_o = 0\)
- however, \(\vec{E}_e \cdot \vec{k} \neq 0\)

Dispersion Angle

- angle between \(\vec{k}\) and Poynting vector \(\vec{S} = \) angle between \(\vec{E}\) and \(\vec{D}\)
  
  \[
  \tan \alpha = \frac{\left| \vec{E}_e \times \vec{D}_e \right|}{\vec{E}_e \cdot \vec{D}_e} = \frac{(n_e^2 - n_0^2) \tan \theta}{n_e^2 + n_0^2 \tan^2 \theta} = \frac{2}{\sin 2\theta} \frac{(n_e^2 - n_0^2)}{n_0^2 \sin^2 \theta + n_e^2 \cos^2 \theta}
  \]
- equivalent expression
  
  \[
  \alpha = \theta - \arctan \left( \frac{n_0^2}{n_e^2} \tan \theta \right)
  \]
- for given \(\vec{k}\) in principal axis system, \(\alpha\) fully determines direction of energy propagation in uniaxial medium
- for \(\theta\) approaching \(\pi/2\), \(\alpha = 0\)
- for \(\theta = 0\), \(\alpha = 0\)
Propagation Direction of Extraordinary Beam

- angle $\theta'$ between Poynting vector $\vec{S}$ and optic axis
  \[ \tan \theta' = \frac{n_o^2}{n_e^2} \tan \theta \]
- ordinary and extraordinary wave do (in general) not travel at the same speed
- phase difference in radians between the two waves given by
  \[ \frac{\omega}{c} (n_2(\theta) d_e - n_o d_o) \]
- $d_o, d_e$: geometrical distances traveled by ordinary and extraordinary rays

Propagation Perpendicular to c Axis

- plane wave propagating perpendicular to c-axis $\Rightarrow \theta = \pi/2$
  \[ \vec{E}_o = \begin{pmatrix} \sin \phi \\ -\cos \phi \\ 0 \end{pmatrix} \]
- $\vec{E}_o$ perpendicular to plane formed by $\vec{k}$ and c-axis
- electric field vector of extraordinary wave
  \[ \vec{E}_e = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \]
- $\vec{E}_e$ parallel to c-axis
- direction of energy propagation of extraordinary wave parallel to $\vec{k}$ since $\vec{E}_e \parallel \vec{D}_e$

Phase Delay between Ordinary and Extraordinary Rays

- ordinary and extraordinary wave propagate in same direction
- ordinary ray propagates with speed $\frac{c}{n_o}$
- extraordinary beam propagates at different speed $\frac{c}{n_e}$
- $\vec{E}_o, \vec{E}_e$ perpendicular to each other $\Rightarrow$ plane wave with arbitrary polarization can be (coherently) decomposed into components parallel to $\vec{E}_o$ and $\vec{E}_e$
- 2 components will travel at different speeds
- (coherently) superposing 2 components after distance $d$ $\Rightarrow$ phase difference between 2 components $\frac{\omega}{c} (n_e - n_o) d$ radians
- phase difference $\Rightarrow$ change in polarization state
- basis for constructing linear retarders
special cases reduce complexity of equations

\[ n_2(\theta) = \frac{n_0 n_e}{\sqrt{n_0^2 \sin^2 \theta + n_e^2 \cos^2 \theta}} \]

- \( n_2 \): direction-dependent index of refraction of the extraordinary ray
- \( n_0 \): ordinary index of refraction
- \( n_e \): extraordinary index of refraction
- \( \theta \): angle between extraordinary wave vector and optic axis

extraordinary ray is not parallel to its wave vector

give angle between the two is \textit{dispersion angle}.

\[ \tan \alpha = \frac{(n_0^2 - n_e^2) \tan \theta}{n_0^2 + n_e^2 \tan^2 \theta} \]

Extraordinary Ray Refraction for General Case

\[ \begin{align*}
\cos \phi_2 &= \frac{c_x c_y (n_0^2 - n_e^2) \pm n_0 \sqrt{c_x^2 + c_y^2 (c_x^2 - n_0^2) - (n_0^2 - n_e^2)(c_x^2 + c_y^2)}}{n_0^2 + c_x^2 (n_0^2 - n_e^2)} \\
\end{align*} \]

propagation vector of extraordinary ray

\[ \begin{align*}
S_x &= \cos \alpha \cos \phi_2 - \frac{\sin \alpha \sin \phi_2 (c_x \sin \phi_2 - c_y \cos \phi_2)}{\sqrt{c_x^2 + (c_y \sin \phi_2 - c_x \cos \phi_2)^2}} \\
S_y &= \cos \alpha \sin \phi_2 - \frac{\sin \alpha \cos \phi_2 (c_y \sin \phi_2 - c_x \cos \phi_2)}{\sqrt{c_x^2 + (c_y \sin \phi_2 - c_x \cos \phi_2)^2}} \\
S_z &= \sin \alpha \frac{c_y}{\sqrt{c_x^2 + (c_y \sin \phi_2 - c_x \cos \phi_2)^2}} \\
\end{align*} \]

\( \vec{c} \) optic axis vector \( \vec{c} = (c_x, c_y, c_z)^T \)
\( \vec{S} \) propagation direction of extraordinary ray \( \vec{S} = (S_x, S_y, S_z)^T \)
\( \theta_1 \): angle between \( \vec{k}_1 \) and interface normal
\( \theta_2 \): angle between \( \vec{k}_0 \) and interface normal
\( \alpha \): dispersion angle
Normal Incidence

- normal incidence $\Rightarrow \theta_1 = 0, \theta_1 = \theta_2 = 0$
- choose plane formed by surface normal and crystal axis
- both wave vectors and ordinary ray not refracted
- extraordinary ray refracted by dispersion angle $\alpha$

\[ \alpha = \theta - \arctan \left( \frac{n_0^2}{n_e^2} \tan \theta \right) \]

Optic Axis in Plane of Incidence and Plane of Interface

- $\theta + \theta_2 = \pi/2 \Rightarrow \cot \theta_2 = \frac{n_0}{n_e} \cot \theta_1$
- $\theta_1$: angle between surface normal and ordinary ray or wave vector
  \[ \sin \theta_1 = n_0 \sin \theta_1 \]
- extraordinary wave sees equivalent refractive index
  \[ n_2 = \sqrt{n_e^2 + \sin^2 \theta_1 \left( 1 - \frac{n_0^2}{n_e^2} \right)} \]
- direction of Poynting vector
  \[ S_x = \cos(\theta_2 + \alpha) \]
  \[ S_y = \sin(\theta_2 + \alpha) \]
  \[ S_z = 0 \]
- determine dispersion angle $\alpha$ and add to $\theta_2$ to obtain direction of extraordinary ray

Optic Axis Perpendicular to Plane of Incidence

- $c$-axis perpendicular to plane of incidence $\Rightarrow \theta = \frac{\pi}{2}, n_2 \left( \frac{\pi}{2} \right) = n_e$
- extraordinary wave vector obeys Snell’s law with index $n_e$
- $\theta = \frac{\pi}{2} \Rightarrow$ dispersion angle $\alpha = 0$
- Poynting vector $\parallel$ wave vector, extraordinary beam itself obeys Snell’s law with $n_e$
- double refraction only for non-normal incidence

Interface from Uniaxial Medium to Isotropic Medium

- ordinary ray follows Snell’s law
- transmitted extraordinary wave vector and ray coincide
- exit of extraordinary wave on interface defined by extraordinary ray
- extraordinary wave vector follows Snell’s law with index $n_2(\theta)$
  \[ n_1 \sin \theta_E = n_2 \sin \theta_U \]
- $n_1$ index of isotropic medium
- $\theta_E$ angle of wave/ray vector with surface normal in isotropic medium
- $n_2, \theta_U$ corresponding values for extraordinary wave vector in uniaxial medium
- $n_2$ is function of $\theta$ normally already known from beam propagation in uniaxial medium
- $\theta_U$ is function of geometry of interface,
- plane-parallel slab of uniaxial medium, $\theta_E = \theta_1$, (in general) extraordinary beam displaced on exit
Total Internal Reflection (TIR)

- TIR also in anisotropic media
- \( n_0 \neq n_e \Rightarrow \) one beam may be totally reflected while other is transmitted
- principal of most crystal polarizers
- example: calcite prism, normal incidence, optic axis parallel to first interface, exit face inclined by 40°
- \( \Rightarrow \) extraordinary ray not refracted, two rays propagate according to indices \( n_o, n_e \)
- at second interface rays (and wave vectors) at 40° to surface
- 632.8 nm: \( n_o = 1.6558, n_e = 1.4852 \)
- requirement for total reflection \( \frac{n_i}{n_U} \sin \theta > 1 \)
- with \( n_i = 1 \Rightarrow \) extraordinary ray transmitted, ordinary ray undergoes TIR