Lecture 21

Reminder/Introduction to Wave Optics

Program:

- 1. Maxwell's Equations.
- 2. Magnetic induction and electric displacement.
- 3. Origins of the electric permittivity and magnetic permeability.
- 4. Wave equations and optical constants.
- 5. The origins and frequency dependency of the dielectric constant.

Questions you should be able to answer by the end of today's lecture:

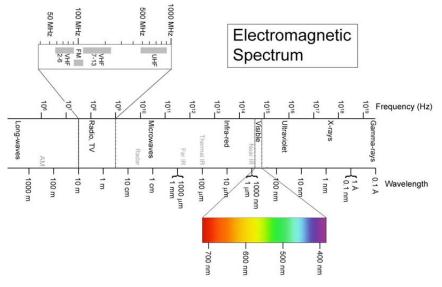
- 1. What are the equations determining propagation of the waves in the media?
- 2. What are the relationships between the electric field and electric displacement and magnetic field and magnetic induction?
- 3. What is the nature of the polarization? How can we gain intuition about the dielectric constant for a material?
- 4. How do Maxwell's equations lead to the wave nature of light?
- 5. What is refractive index and how it relates to the dielectric constant? How does it relate to the speed of light inside the material?
- 6. What is the difference between the phase and group velocity?

Response of materials to electromagnetic waves - propagation of light in solids.

We classified materials with respect to their conductivity and related the observed differences to the existence of band gaps in the electron energy eigenvalues. The optical properties are determined to a large extent by the electrons and their ability to interact with the electromagnetic field, thus the conductivity classification of materials, which was a result of the band structure and band filling, is also useful for classifying the optical response. The most widely used metric for quantifying the optical behavior of materials is the index of refraction, which captures the extent to which the electromagnetic wave interacts with the material.

Figure removed due to copyright restrictions. Graph showing index of refraction vs. wavelength in microns: Unknown source.

When we talk about optical properties of material, we generally refer to light with wavelengths between the ultraviolet and infrared regions of optical spectrum ($\sim 100 \text{ nm} - 10 \mu \text{m}$).



Electromagnetic spectrum. (This image is in the public domain.)

These wavelengths are significantly larger than the lattice constant of the crystalline materials or the diameters of the atoms, so we can consider EM radiation as waves rather than particles.

The wave nature of EM radiation is described precisely by Maxwell's equations:

Maxwell's Equations:

$$\vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = \mathbf{0}$$
$$\vec{\nabla} \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = \vec{J}$$
$$\vec{\nabla} \cdot \vec{B} = \mathbf{0}$$
$$\vec{\nabla} \cdot \vec{D} = \rho$$

The two quantities used to describe the electromagnetic field are:

 $\vec{E} = (E_x, E_y, E_z)$ - Electric field

$$\vec{H} = (H_x, H_y, H_z)$$
 - Magnetic Field

The two quantities used to describe the effect of the electromagnetic field on the matter:

$$\vec{D} = (D_x, D_y, D_z)$$
 - Electric displacement

 $\vec{B} = (B_x, B_y, B_z)$ - Magnetic induction

Taking into account the vector nature of the fields, Maxwell's equations can be written as 8 scalar equations with 12 variables $(E_x, E_y, E_z, H_x, H_y, H_z, D_x, D_y, D_z, B_x, B_y, B_z)$, so in order to

obtain a unique solution we need additional relations. These equations are called constitutive relations or the material equations:

$$\vec{D} = \varepsilon \vec{E} = \varepsilon_0 \vec{E} + \vec{P}$$
$$\vec{B} = \mu \vec{H} = \mu_0 \vec{H} + \vec{M}$$

Where μ , and ε are the second order tensors called the magnetic permeability and electric permittivity respectively. \vec{P} is electric polarization and \vec{M} magnetization.

The origins of polarization. Oscillator model.

Here will take a simple classical approach to gain some intuition about polarization. Similar discussion may be applied to derivation of magnetization, where instead of electric dipoles we can talk about magnetic dipoles.



The ion-electron dipoles are constantly oscillating (electrons have thermal velocity that allows them to move away from the ions but then they are pulled back by the Coulombic force). Then we can describe the distance between the electron and an ion using an oscillatory equation:

$$\frac{d^2x}{dt^2} + \omega_0^2 x = 0$$

Where ω_0 , the natural frequency, is determined by the temperature and material properties (size of atoms etc.)

But what happens when we add the external EM field?

In a simplest case when the EM wave propagates through the material it's wavelength is significantly larger than the lattice constant or the size of the atoms, so locally we can approximate electric field alternating in space with a field that is locally constant in space: $\vec{E} = \vec{E}_0 e^{ikx} e^{-i\omega t} \Rightarrow \vec{E} = \vec{E}_0 e^{-i\omega t}$

Then electrons bound to ions would be pushed in the direction opposite to the applied field orienting the ion-electron dipoles in the direction of the field \vec{E}_0 . The electric field will act as a driving force applied to our oscillating dipoles. Then the equation above becomes:

$$\frac{d^2\vec{x}}{dt^2} + \omega_0^2\vec{x} = \frac{\vec{F}}{m}, \text{ where } \vec{F} = q\vec{E} = q\vec{E}_0e^{-i\omega t}$$

Since the dipole moment is: $\vec{p} = q\vec{x}$, then the polarization of the entire material is the sum of all the *N* dipoles inside it: $\vec{P} = N\vec{p} = Nq\vec{x}$

Then we can rewrite the equation for the forced oscillator to get the equation for polarization:

$$Nq \frac{d^2 \vec{x}}{dt^2} + Nq \omega_0^2 \vec{x} = Nq \frac{q\vec{E}}{m} \Longrightarrow \frac{d^2 \vec{P}}{dt^2} + \omega_0^2 \vec{P} = \frac{Nq^2}{m\varepsilon_0 \omega_0^2} \varepsilon_0 \omega_0^2 \vec{E}$$
$$\frac{d^2 \vec{P}}{dt^2} + \omega_0^2 \vec{P} = \omega_0^2 \varepsilon_0 \chi_0 \vec{E}, \quad \chi_0 = \frac{Nq^2}{m\varepsilon_0 \omega_0^2}$$

It is reasonable that under applied electric field the dipoles will oscillate with the same frequency as the applied field:

$$\vec{E} = \vec{E}_0 e^{-i\omega t} \Longrightarrow \vec{P} = \vec{P}_0 e^{-i\omega t}$$

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Then substituting this solution into the equation above, we find:

$$\frac{d^2 P}{dt^2} + \omega_0^2 \vec{P} = \omega_0^2 \varepsilon_0 \chi_0 \vec{E} \Longrightarrow -\omega^2 \vec{P} + \omega_0^2 \vec{P} = \omega_0^2 \varepsilon_0 \chi_0 \vec{E}$$
, where $\chi(\omega)$ is the electric susceptibility.
$$\vec{P} = \frac{\omega_0^2 \varepsilon_0 \chi_0}{\omega_0^2 - \omega^2} \vec{E} = \varepsilon_0 \chi(\omega) \vec{E}, \quad \chi(\omega) = \chi_0 \frac{\omega_0^2}{\omega_0^2 - \omega^2}$$
, where $\chi(\omega)$ is the electric susceptibility.

Then the electric displacement:

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon_0 \vec{E} + \varepsilon_0 \chi \vec{E} = \varepsilon_0 (1 + \chi) \vec{E} = \varepsilon \vec{E}$$
$$\vec{D} = \varepsilon \vec{E}, \quad \varepsilon = \varepsilon_0 (1 + \chi)$$

Absorptive materials – damped oscillator model.

Many materials have relatively low refractive indices and yet transmission through them is also very low. It turns out that the model above does not include an important characteristic of the medium – absorption.

Take a closer look at the expression for electric susceptibility. When the frequency of the applied EM field, ω , approaches the natural frequency of the material, ω_0 , the electric susceptibility $\chi(\omega)$ should go to infinity, which is unrealistic:

$$\chi(\omega) = \chi_0 \frac{\omega_0^2}{\omega_0^2 - \omega^2} \xrightarrow{\omega \to \omega_0} \infty$$

It reasonable to think that every driven oscillator should resist the applied force, i.e. there is damping. Damping is akin to friction and hence is proportional to the velocity $\frac{d\vec{x}}{dt}$, which in our

case translates into the first derivative of the polarization: $Nq \frac{d\vec{x}}{dt} = \frac{d\vec{P}}{dt}$

$$\frac{d^{2}\vec{P}}{dt^{2}} + \sigma \frac{d\vec{P}}{dt} + \omega_{0}^{2}\vec{P} = \omega_{0}^{2}\varepsilon_{0}\chi_{0}\vec{E} \Longrightarrow -\omega^{2}\vec{P} - i\sigma\omega\vec{P} + \omega_{0}^{2}\vec{P} = \omega_{0}^{2}\varepsilon_{0}\chi_{0}\vec{E}$$
$$\vec{P} = \frac{\omega_{0}^{2}\varepsilon_{0}\chi_{0}}{\omega_{0}^{2} - \omega^{2} - i\sigma\omega}\vec{E} = \varepsilon_{0}\chi(\omega)\vec{E}$$

$$\chi(\omega) = \chi_0 \frac{\omega_0^2 (\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + (\sigma \omega)^2} + \chi_0 \frac{i\omega_0^2 \sigma \omega}{(\omega_0^2 - \omega^2)^2 + (\sigma \omega)^2} = \chi'(\omega) + i\chi''(\omega)$$

In Figure:

) LIXUH UHP RYHG GXH WR FRS\LLIK WUHVWULFWURQV 6HH) LI 6DOHK %DKDD (\$ and 0 DOYLQ & DUO7HLFK.) *XQGDP HQWDOY RI 3KRWRQLFV* QG HG : LOPH

$$v = \frac{\omega}{2\pi}, \ \Delta v = \frac{\sigma}{2\pi}$$
$$Q = \frac{\omega_0}{\sigma}$$

Using complex variable analysis it is also possible to show that and depend on each other through the Kramers-Kronig relationships:

$$\chi'(\omega) = \frac{2}{\pi} \int_{0}^{\infty} \frac{s\chi''(s)}{s^2 - \omega^2} ds$$
$$\chi''(\omega) = \frac{2}{\pi} \int_{0}^{\infty} \frac{\omega\chi'(s)}{s^2 - \omega^2} ds$$

The dielectric constant can then also be written as:

$$\varepsilon = \varepsilon_0 (1 + \chi) = \varepsilon_0 (1 + \chi') + i\varepsilon_0 \chi'' = \varepsilon' + i\varepsilon''$$

Later we will also show that in the absence of magnetization index of refraction can be found as:

$$n' = \sqrt{\frac{\varepsilon}{\varepsilon_0}} = \sqrt{1 + \chi' + i\chi''} = n + i\alpha$$

Where *n* is the index of refraction the way you've learned it in optics and α is an absorption coefficient.

Effect of material structure on optical constants

While our simple analysis above provides us with intuition about the origins of the dielectric constant, in general in crystals the response to the EM field will be dependent on the direction of the field with respect to the orientation of crystal lattice and dielectric and magnetic permittivities are tensors. However, one can always define coordinate axes (principal axes) such that the dielectric (and magnetic) tensor is diagonal:

$$\varepsilon = \begin{bmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{bmatrix} \text{ and } \mu = \begin{bmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{bmatrix}$$

Cubic or amorphous materials are isotropic, i.e. $\varepsilon_1 = \varepsilon_2 = \varepsilon_3$. Example: Yttrium Aluminum Garnet Y₃Al₅O₁₂ (cubic).

Trigonal, tetragonal, and hexagonal are uniaxial, i.e. $\varepsilon_1 \neq \varepsilon_2 = \varepsilon_3$ Example: Lithium Niobate LiNbO₃ (trigonal).

Triclinic, monoclinic, orthorhombic are biaxial, i.e. $\varepsilon_1 \neq \varepsilon_2 \neq \varepsilon_3$.

Comments:

- 1. When μ and ε are field dependent the material is called non-linear. This generally occurs in the presence of strong electromagnetic fields.
- 2. For simplicity we will assume that the materials are optically isotropic meaning, i.e. $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = \varepsilon$, and consequently $\vec{E} \parallel \vec{D}, \vec{H} \parallel \vec{B}$.
- 3. The first equation defines the dielectric function ε (or permittivity) in terms of the electric field and polarization.

Wave Equations and Monochromatic Plane Waves

Assuming an isotropic, weakly absorbing ($\varepsilon'' \approx 0$) media and no surface charge or current:

$$\vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0 \xrightarrow{\frac{1}{\mu}} \frac{1}{\mu} \vec{\nabla} \times \vec{E} + \frac{\partial \vec{H}}{\partial t} = 0 \xrightarrow{\overline{\nabla} \times} \vec{\nabla} \times \left(\frac{1}{\mu} \vec{\nabla} \times \vec{E}\right) + \frac{\partial}{\partial t} \vec{\nabla} \times \vec{H} = 0$$

$$\vec{\nabla} \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = 0 \xrightarrow{\frac{\partial}{\partial t}} \frac{\partial}{\partial t} \vec{\nabla} \times \vec{H} = \varepsilon \frac{\partial^2 \vec{E}}{\partial t^2}$$

$$\vec{\nabla} \times \left(\frac{1}{\mu} \vec{\nabla} \times \vec{E}\right) + \varepsilon \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \Longrightarrow -\vec{\nabla}^2 \vec{E} + \mu \varepsilon \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

$$\vec{\nabla}^2 \vec{E} - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0, \ c = \frac{c_0}{n} = \frac{1}{\sqrt{\mu \varepsilon}}, \ c_0 = \frac{1}{\sqrt{\mu \varepsilon_0}} \ and \ n = \frac{c_0}{c} = \sqrt{\frac{\mu \varepsilon}{\mu_0 \varepsilon_0}} = \sqrt{\mu_r \varepsilon_r}$$

Here c_0 is the speed of light in vacuum and c is the speed of light inside the material. ε_r , μ_r are dimensionless constants for a given isotropic material. n is the index of refraction of the material.

The analogous equation can be derived for the magnetic field. Together these equations are called wave equations:

$$\vec{\nabla}^2 \vec{E} - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$
$$\vec{\nabla}^2 \vec{H} - \frac{1}{c^2} \frac{\partial^2 \vec{H}}{\partial t^2} = 0$$

Solutions to the wave equations can take different forms: plane waves, cylindrical waves or spherical waves. For simplicity, we will focus on the most commonly used solution – the harmonic plane wave.

As we remember plane waves have the following structure:

$$\vec{E}(x, y, z) = \vec{E}_0 e^{i\vec{k}\vec{r} - i\omega t}$$
$$\vec{H}(x, y, z) = \vec{H}_0 e^{i\vec{k}\vec{r} - i\omega t}$$

Substituting these solutions into the wave equation, we find the dispersion relation between the frequency and the wavevector for the EM waves.

$$\omega = c \left| \vec{k} \right|$$
$$\left| \vec{k} \right| = \frac{2\pi}{\lambda} = \frac{n}{c_0} \omega$$

Note, that the frequency ω does not change depending on the material, but the wavevector \vec{k} the wavelength λ change.

In the following sections we will examine the meaning and significance of each one of the quantities defining the plane wave. In particular: the complex amplitude \vec{E}_0 related to the wave polarization, the frequency ω defining the photon energy, and the wavevector \vec{k} related to the direction of propagation and wavelength of EM radiation inside the media.

Phase velocity:

The plane wave $\vec{E}(x, y, z) = \vec{E}_0 e^{i\vec{k}\cdot\vec{r} - i\omega t}$ is a complex function with a phase: $\phi = \vec{k}\cdot\vec{r} - \omega t$

If we consider the fronts, i.e. the surfaces of constant phase: $\omega t - \vec{k} \cdot \vec{r} = const$

We can find that these constant fronts are moving with a velocity:

$$\vec{v}_{phase} = \frac{\omega}{|k|} \hat{k} = \frac{c_0}{n} \hat{k} = c\hat{k}, \ \hat{k}$$
 is the direction vector defined by the direction of the wavevector.

The phase velocity is different (and in most cases lower) inside materials as compared to its value in vacuum.

Wave packets and group velocity:

A monochromatic wave (single ω) is an idealization, which in practice does not exist. Instead, we typically consider a superposition of monochromatic waves, a wavepacket:

$$E(r,t) = \int_{0}^{\infty} a_{\omega}(\vec{r}) e^{i\vec{k}\cdot\vec{r}-i\omega t} d\omega$$

Where $a_{\alpha}(\vec{r})$ are the amplitudes of the Fourier components constituting the wavepacket.

A very narrow packet or a nearly monochromatic wave consists of a few non-zero Fourier components with frequencies within narrow $\Delta \omega$ region around ω .

While each plane wave front moves with its corresponding phase velocity, the center of the wavepacket moves with the group velocity:

$$\vec{v}_{group} = \frac{\partial \omega}{\partial k}$$

Using dispersion relation we can find: $v_{group} = \frac{\partial \omega}{\partial k} = \frac{1}{\frac{\partial k}{\partial \omega}} = \frac{1}{\frac{\partial}{\partial \omega} \left(\frac{n}{c_0}\omega\right)}$

If the refractive index does not depend on frequency: $n \neq f(\omega) \Rightarrow v_{group} = v_{phase} = \frac{c_0}{n}$

If the refractive index depends on frequency then: $v_{group} \neq v_{phase}$. And the material is called dispersive.

Transverse nature of EM fields:

The solutions of the wave equation are in general vector quantities:

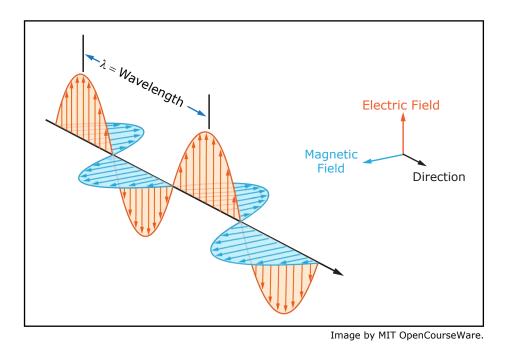
$$\vec{E}(x, y, z) = E_x \hat{x} + E_y \hat{y} + E_z \hat{z}$$

In a medium that is homogeneous and charge free:

$$\vec{\nabla} \cdot \vec{E} = 0 \Longrightarrow ik_x E_x + ik_y E_y + ik_z E_z = 0 \Longrightarrow \vec{E} \cdot \vec{k} = 0 \Longrightarrow \vec{E} \perp \vec{k}$$
$$\vec{\nabla} \cdot \vec{H} = 0 \Longrightarrow ik_x H_x + ik_y H_y + ik_z H_z = 0 \Longrightarrow \vec{H} \cdot \vec{k} = 0 \Longrightarrow \vec{H} \perp \vec{k}$$

The equations above state that EM fields are transverse, i.e. the fields oscillate in the pla ne that is perpendicular to the direction of the wave front propagation.

From the equation:
$$\vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0 \Rightarrow \vec{\nabla} \times \vec{E} + \mu \frac{\partial \vec{H}}{\partial t} = 0$$
 we can also conclude that: $\vec{E} \perp \vec{H}$



Energy Law of Electromagnetic fields

Electromagnetic theory interprets the light intensity as the energy flux of the field. We can find this energy flux using Maxwell's equations.

In the absence of currents and stored charges:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \\ \vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t} \\ \Rightarrow \qquad \vec{E} \cdot \vec{\nabla} \times \vec{H} = \vec{E} \cdot \frac{\partial \vec{D}}{\partial t} \\ \vec{E} \cdot \vec{\nabla} \times \vec{H} = \vec{E} \cdot \frac{\partial \vec{D}}{\partial t} \\ \Rightarrow \qquad \vec{E} \cdot \vec{\nabla} \times \vec{H} = \vec{E} \cdot \frac{\partial \vec{D}}{\partial t} \\ \Rightarrow \vec{E} \cdot \vec{\nabla} \times \vec{H} = \vec{E} \cdot \frac{\partial \vec{D}}{\partial t}$$

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By using a vector multiplication property: $\vec{E} \cdot \vec{\nabla} \times \vec{H} - \vec{H} \cdot \vec{\nabla} \times \vec{E} = -\vec{\nabla} \cdot (\vec{E} \times \vec{H})$

We can derive:
$$\vec{E} \cdot \frac{\partial \vec{D}}{\partial t} + \vec{H} \cdot \frac{\partial \vec{B}}{\partial t} + \vec{\nabla} \cdot (\vec{E} \times \vec{H}) = 0$$

By integrating over volume and employing Gauss theorem: $\int \vec{\nabla} (\vec{E} \times \vec{H}) dV = \int (\vec{E} \times \vec{H}) \cdot \hat{n} dS$

We find:
$$\int \left(\vec{E} \cdot \frac{\partial \vec{D}}{\partial t} + \vec{H} \cdot \frac{\partial \vec{B}}{\partial t} \right) dV + \int \left(\vec{E} \times \vec{H} \right) \cdot \hat{n} \, dS = 0$$

By using the relationships between \vec{E} and \vec{D} , and \vec{H} and \vec{B} :

$$\vec{E} \cdot \frac{\partial \vec{D}}{\partial t} = \vec{E} \cdot \frac{\partial \vec{E} \vec{E}}{\partial t} = \frac{1}{2} \frac{\partial \vec{E} \vec{E}^2}{\partial t} = \frac{1}{2} \frac{\partial \left(\vec{E} \cdot \vec{D}\right)}{\partial t}$$
$$\vec{H} \cdot \frac{\partial \vec{B}}{\partial t} = \frac{1}{2} \frac{\partial \left(\vec{H} \cdot \vec{B}\right)}{\partial t}$$

Which leads us to an energy conservation equation:

$$\frac{\partial}{\partial t} \int \underbrace{\frac{1}{2} \left(\vec{E} \cdot \vec{D} + \vec{H} \cdot \vec{B} \right)}_{\text{energy stored in electrical}} dV + \int \underbrace{\left(\vec{E} \times \vec{H} \right)}_{\text{energy surface}} \cdot \hat{n} \, dS = 0$$

The second integral term represents the energy flow and is known as the Poynting vector:

$$\vec{S} = \vec{E} \times \vec{H}$$

Note that $\vec{S} \parallel \vec{k}$, which means that the energy is carried in the direction of the wave front propagation.

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