3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

3.23 Fall 2007 – Lecture 17

FERMAT'S FIRST THEOREM

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Pierre-Louis Moreau de Maupertuis

Abū ʿAlī al-Ḥasan ibn al-Ḥasan ibn al-Haytham

Hero

Last time

1. Electric field, polarization, displacement, susceptibility
2. Maxwell's equations
3. Potentials and gauges
4. Electromagnetic waves (no free charges, currents)
5. Refractive index, phase and group velocity

Study

- (mostly read) Fox, Optical Properties of Solids: 1.1 to 1.4, 2.1 to 2.2.3, 3.1 to 3.3

Polarization, transversality of EM fields

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

$k_x x + k_y y + k_z z$

$$\boxed{\vec{\nabla}\cdot\vec{E}} \qquad \vec{\nabla}\cdot\vec{H} = 0$$

$$\frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} = 0$$

$$\Downarrow$$

$$E_{0x}(-ik_x)e^{i(\omega t - \vec{k}\cdot\vec{r})}$$

$$E_{0x}k_x + E_{0y}k_y + E_{0z}k_z = 0 \Longleftrightarrow \vec{E}_0\cdot\vec{k} = 0$$

Boundary conditions (Gauss theorem)

$$\int_{volume} \vec{\nabla} \cdot \vec{B} dv = \int_{surface} \vec{B} \cdot \hat{n} dS = 0$$

$$\int_{volume} \vec{\nabla} \cdot \vec{D} dv = \int_{surface} \vec{D} \cdot \hat{n} dS = 4\pi \int_{volume} \rho dv$$

Boundary conditions

$$\hat{n} \cdot \left(\vec{B}_2 - \vec{B}_1 \right) = 0$$

$$\hat{n} \cdot \left(\vec{D}_2 - \vec{D}_1 \right) = \sigma \ \left(\sigma = \text{surface charge density} \right)$$

Boundary conditions (Stokes theorem)

$$\int_{surface} \vec{\nabla} \times \vec{E} \cdot \hat{n} dS = \int_{line} \vec{E} \cdot d\vec{r}$$

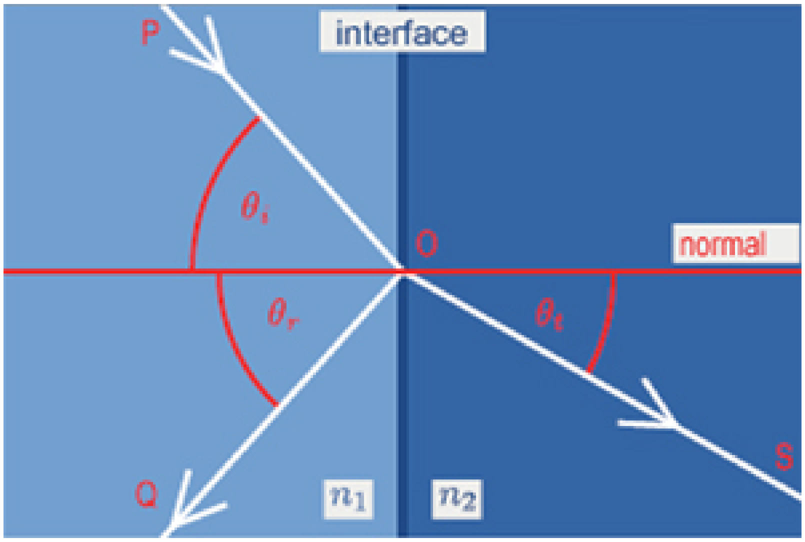
Boundary conditions

$$\hat{n} \times \left(\vec{E}_2 - \vec{E}_1 \right) = 0$$

$$\hat{n} \times \left(\vec{H}_2 - \vec{H}_1 \right) = \vec{K}$$

$$\left(\vec{K} = \text{surface current density} \right)$$

Snell's law



$\vec{E}_i e^{i\omega t - i\vec{k}_i\cdot\vec{r}}$ incident wave

$\vec{E}_r e^{i\omega t - i\vec{k}_r\cdot\vec{r}}$ reflected wave

$\vec{E}_t e^{i\omega t - i\vec{k}_t\cdot\vec{r}}$ transmitted wave

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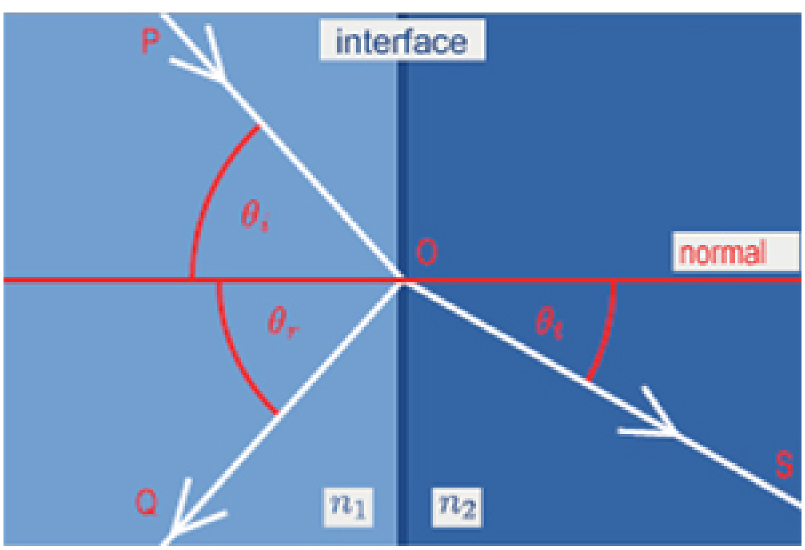
Snell's law



$$\left|\vec{k}_i\right| = \left|\vec{k}_r\right| = \frac{\omega n_1}{c}$$

$$\left|\vec{k}_t\right| = \frac{\omega n_2}{c}$$

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Snell's law

$$\boxed{\left(\vec{k}_1 \cdot \vec{r}\right)_{x=0} = \left(\vec{k}_1' \cdot \vec{r}\right)_{x=0} = \left(\vec{k}_2 \cdot \vec{r}\right)_{x=0}}$$

$$\left(k_{1y} y + k_{1z} z\right) = \left(k_{1y}' y + k_{1z}' z\right) = \left(k_{2y} y + k_{2z} z\right) \rightarrow k_{1y} = k_{1y}' = k_{2y}$$

and $k_{1z} = k_{1z}' = k_{2z}$

$$\left(\vec{k}_{1t} \cdot \vec{r}_t\right) = \left(\vec{k}_{1t}' \cdot \vec{r}_t\right) = \left(\vec{k}_{2t} \cdot \vec{r}_t\right)$$

Snell's law

$$\left|\vec{k}_1\right| = \left|\vec{k}_1'\right| = n_1 \frac{\omega}{c}$$

$$\left|\vec{k}_2\right| = n_2 \frac{\omega}{c}$$

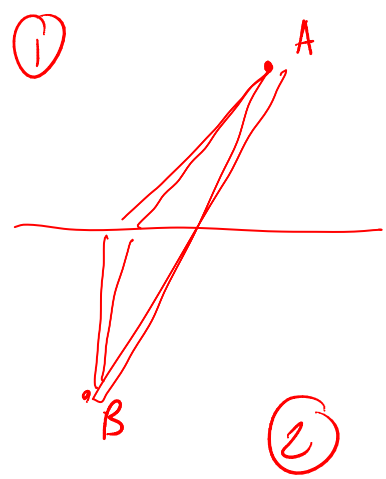
$$k_{iz} = k_{tz} \rightarrow \left|k_i\right| \sin\theta_1 = \left|k_t\right| \sin\theta_2$$

$$\frac{\omega n_1}{c} \sin\theta_1 = \frac{\omega n_2}{c} \sin\theta_2$$

Snell's law

$$\left.\begin{aligned} k_{1z} &= \left|\vec{k}_1\right| \sin\theta_1 = n_1 \frac{\omega}{c} \sin\theta_1 \\ k_{2z} &= \left|\vec{k}_2\right| \sin\theta_2 = n_2 \frac{\omega}{c} \sin\theta_2 \end{aligned}\right\} n_1 \sin\theta_1 = n_2 \sin\theta_2$$

Principle of least action



Energy law

$$\boxed{\vec{E}\cdot\vec{\nabla}\times\vec{H}-\vec{H}\cdot\vec{\nabla}\times\vec{E}}=\frac{4\pi}{c}\vec{J}\cdot\vec{E}+\frac{1}{c}\vec{E}\cdot\frac{\partial\vec{D}}{\partial t}+\frac{1}{c}\vec{H}\cdot\frac{\partial\vec{B}}{\partial t}$$

$$\vec{E}\cdot\vec{\nabla}\times\vec{H}-\vec{H}\cdot\vec{\nabla}\times\vec{E}=-\vec{\nabla}\cdot\left(\vec{E}\times\vec{H}\right)$$

$$\rightarrow\frac{4\pi}{c}\vec{J}\cdot\vec{E}+\frac{1}{c}\vec{E}\cdot\frac{\partial\vec{D}}{\partial t}+\frac{1}{c}\vec{H}\cdot\frac{\partial\vec{B}}{\partial t}+\vec{\nabla}\cdot\left(\vec{E}\times\vec{H}\right)=0$$

Apply Gauss's theorem

$$\int_V\frac{4\pi}{c}\vec{J}\cdot\vec{E}dv+\int_V\left(\frac{1}{c}\vec{E}\cdot\frac{\partial\vec{D}}{\partial t}+\frac{1}{c}\vec{H}\cdot\frac{\partial\vec{B}}{\partial t}\right)dv+\int_S\left(\vec{E}\times\vec{H}\right)\cdot\hat{n}dS=0$$

Energy law

$$\frac{1}{4\pi}\vec{E}\cdot\frac{\partial\vec{D}}{\partial t}=\frac{1}{4\pi}\vec{E}\cdot\frac{\partial\varepsilon\vec{E}}{\partial t}=\frac{1}{8\pi}\frac{\partial\varepsilon\vec{E}^2}{\partial t}=\frac{1}{8\pi}\frac{\partial\left(\vec{E}\cdot\vec{D}\right)}{\partial t}$$

$$\frac{1}{4\pi}\vec{H}\cdot\frac{\partial\vec{B}}{\partial t}=\frac{1}{8\pi}\frac{\partial\left(\vec{H}\cdot\vec{B}\right)}{\partial t}$$

Energy conservation

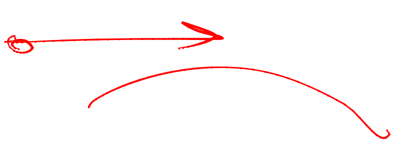
$$\int \cancel{\vec{J}\cdot\vec{E}\,dv} + \frac{\partial}{\partial t}\int \underbrace{\left(\vec{E}\cdot\vec{D}+\vec{H}\cdot\vec{B}\right)}_{\substack{\text{total energy stored in electrical}\\ \text{and magnetic field}\\ \text{per volume}}} dv + \int \underbrace{\left(\vec{E}\times\vec{H}\right)}_{\substack{\text{energy surface}\\ \text{flux per unit area}}} \cdot\hat{n}\,dS = 0$$

POYNTING

$$\vec{S} = \frac{c}{4\pi}\vec{E}\times\vec{H}$$

Optical processes

- Reflection and refraction
- Absorption
- Luminescence
- Scattering



3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

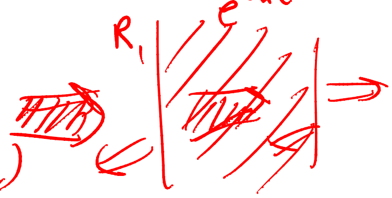
Optical coefficients

T: ratio of transmitted vs incident power

R+T=1 (no absorption, scattering)

Absorption: $dI = -\alpha \, dz \, I \Rightarrow I(z) = I_0 e^{-\alpha z}$

Transmission: $T = (1-R_1)\, e^{-\alpha \ell}\, (1-R_2)$



Complex refractive index

$$\boxed{\tilde{n} = n + ik}$$

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

$$k = \frac{\omega n}{c} \Rightarrow \frac{\omega}{c}(n + ik)$$

$$\vec{E}_0 \, e^{-k\omega z/c} \, e^{i(\omega n z/c - \omega t)}$$

$$\varepsilon = n^2 \Rightarrow \tilde{\varepsilon} = \tilde{n}^2 = \varepsilon_1 + i\varepsilon_2$$

Complex refractive index

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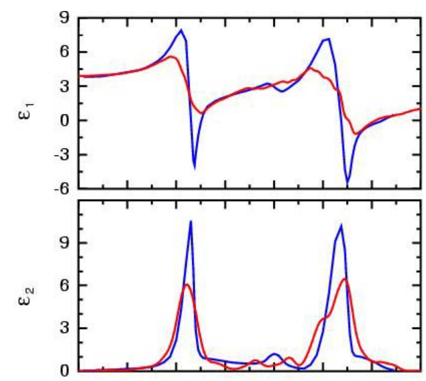
Please see any image of the structure of amorphous silica,
such as http://www.research.ibm.com/amorphous/figure1.gif.



Modeling Optical Constants with a Damped Harmonic Oscillator

$$\underbrace{m_0 \frac{d^2X}{dt^2}}_{acceleration} + \underbrace{m_0\gamma\frac{dX}{dt}}_{dissipation} + \underbrace{m_0\omega_0^2 X}_{harmonic\ restoring\ force} = \underbrace{-eE(t)}_{time\ dependent\ electric\ field}$$

$$E(t) = E\, e^{-i\omega t - \phi}$$

$$X(t) = X_0\, e^{-\omega t - \phi'}$$

$$-m_0\omega^2 X_0 \cancel{e^{-i\omega t}} - i m_0\gamma\omega X_0 \cancel{e^{-i\omega t}} + m_0\omega_0^2 X_0 \cancel{e^{-i\omega t}} = -\mathcal{E}_0 \cancel{e^{-i\omega t}}$$

Modeling Optical Constants with a Damped Harmonic Oscillator

$$X_0 = \frac{-eE_0}{m_0\left(\omega_0^2 - \omega^2 - i\gamma\omega\right)}$$

$X = X_0 e^{-i\omega t}$

$$P_{resonant} = Np = -NeX = \underbrace{\frac{Ne^2}{m_0\left(\omega_0^2 - \omega^2 - i\gamma\omega\right)}}_{\alpha} E$$

$$D = E + 4\pi P + 4\pi P_{resonant} = E + 4\pi\chi E + 4\pi \underbrace{\frac{Ne^2}{m_0\left(\omega_0^2 - \omega^2 - i\gamma\omega\right)}}_{\alpha} E = \varepsilon E$$

Atomic polarizability = α

Modeling Optical Constants with a Damped Harmonic Oscillator

$$\varepsilon = \underbrace{1 + 4\pi\chi + 4\pi \frac{Ne^2\left(\omega_0^2 - \omega^2\right)}{m_0\left(\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2\right)}}_{\varepsilon_1} - i\,\underbrace{4\pi \frac{Ne^2\gamma\omega}{m_0\left(\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2\right)}}_{\varepsilon_2}$$

$$\varepsilon = \left(n + ik\right)^2 = \underbrace{n^2 - k^2}_{\varepsilon_1} + i\,\underbrace{2nk}_{\varepsilon_2}$$

Amorphous silica

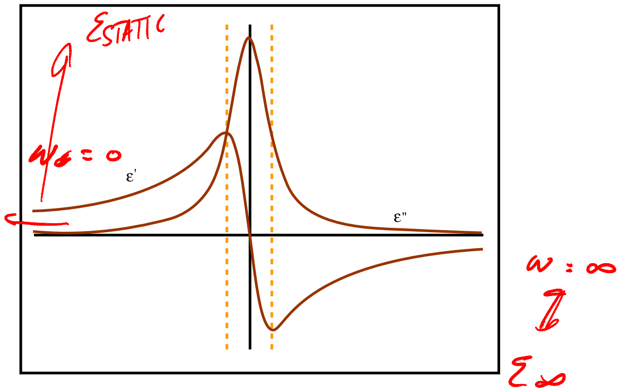
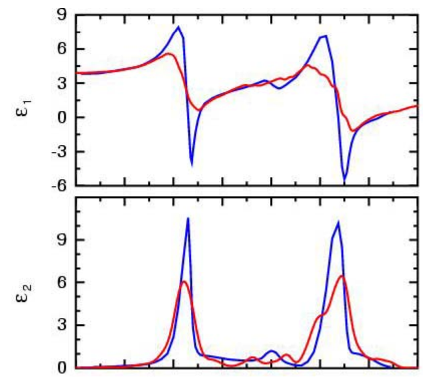


Figure by MIT OpenCourseWare.



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Optical materials

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Please see: Fig. 1.4 in Fox, Mark. *Optical Properties of Solids*. Oxford, England: Oxford University Press, 2001.

Infrared active modes

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Please see: Fig. 1.7 in Fox, Mark. *Optical Properties of Solids*. Oxford, England: Oxford University Press, 2001.

Optical materials

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Please see: Fig. 1.5 in Fox, Mark. *Optical Properties of Solids.* Oxford, England: Oxford University Press, 2001.

Transition rate for direct absorption

$W_{i \to f} =$

$= \frac{2\pi}{\hbar} |\langle f | H' | i \rangle|^2 g(\hbar\omega)$

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Please see any diagram of GaAs energy bands,
such as http://ecee.colorado.edu/~bart/book/book/chapter2/gif/fig2_3_6.gif.