# 3.23 Electrical, Optical, and Magnetic Properties of Materials

Fall 2007

# 3.23 Fall 2007 – Lecture 17

# FERMAT'S FIRST THEOREM

Hero

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Please see: http://en.wikipedia.org/wiki/Image:Ibn_haithem_portrait.jpg

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

Pierre-Louis
Moreau de
Maupertuis

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# 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

# Boundary conditions (Gauss theorem)

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

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

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# 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)

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

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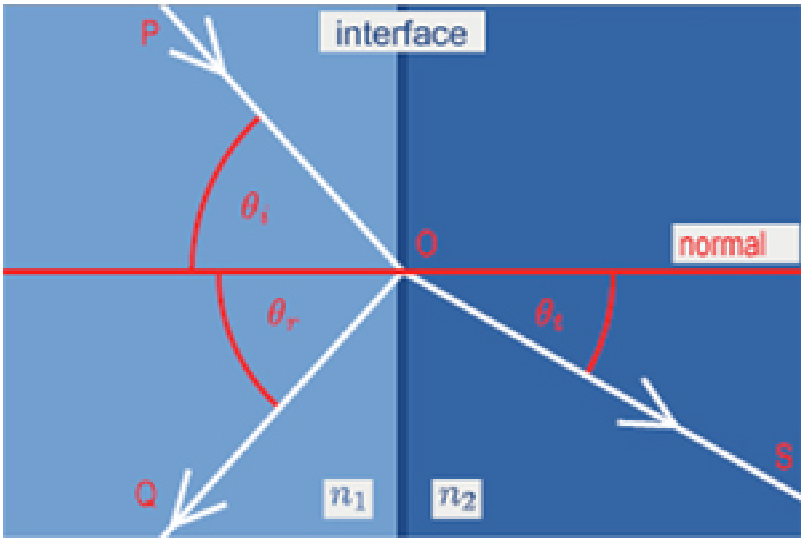
# Boundary conditions

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

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

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

# Snell's law



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

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

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

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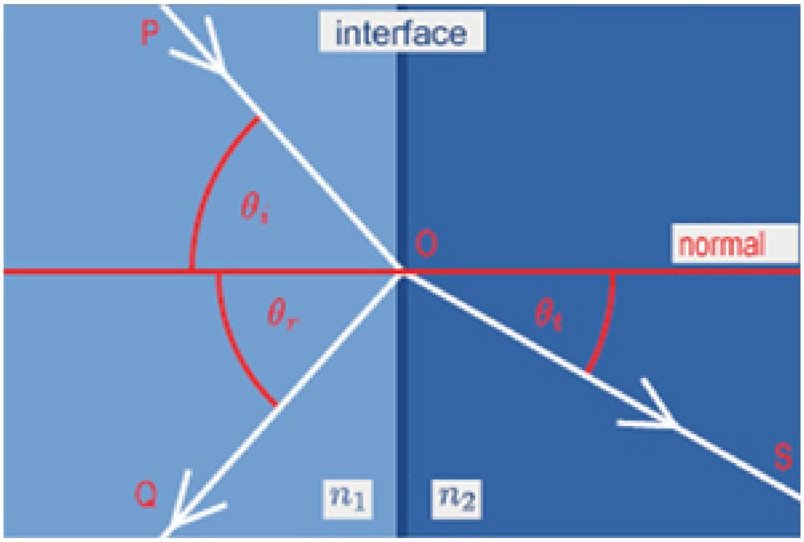
# Snell's law



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

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

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# Snell's law

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

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

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

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

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# Principle of least action

# Energy law

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

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

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

Apply Gauss's theorem

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

# 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

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

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

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# Optical processes

- Reflection and refraction
- Absorption
- Luminescence
- Scattering

# Optical coefficients

T: ratio of transmitted vs incident power

R+T=1 (no absorption, scattering)

Absorption:

Transmission:

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# Complex refractive index

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

# Complex refractive index

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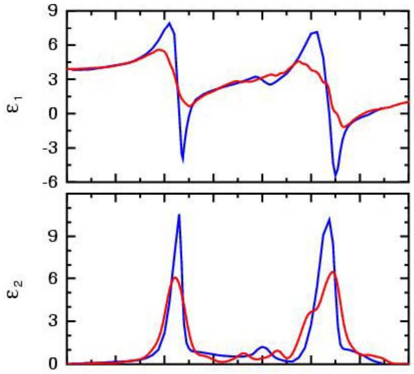
Please see any image of the structure of amorphous silica,
such as http://www.research.ibm.com/amorphous/figure1.gif.



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## Modeling Optical Constants with a Damped Harmonic Oscillator

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

## Modeling Optical Constants with a Damped Harmonic Oscillator

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

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

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

Atomic polarizability = α

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## 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

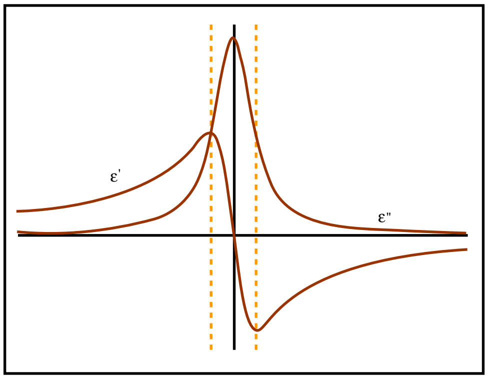
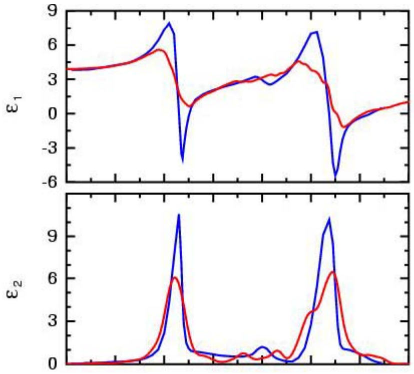


Figure by MIT OpenCourseWare.



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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. 1a and 2a in Giannozzi, Paolo, et al. "*Ab initio* Calculation of Phonon Dispersions in Semiconductors." *Physical Review B* 43 (March 15, 1991): 7231-7242.

# Optical materials

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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.

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# Transition rate for direct absorption

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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.