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

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Fermi’s Golden Rule

Study

- Fox, Optical Properties of Solids: 3.1 to 3.6 (skip 3.3.5 and 3.3.6), 4.1, 4.2, and Appendix B.2
Boundary conditions

\[ \hat{n} \cdot (\vec{B}_2 - \vec{B}_1) = 0 \]

\[ \hat{n} \cdot (\vec{D}_2 - \vec{D}_1) = \sigma \ (\sigma = \text{surface charge density}) \]

\[ \hat{n} \times (\vec{E}_2 - \vec{E}_1) = 0 \]

\[ \hat{n} \times (\vec{H}_2 - \vec{H}_1) = \vec{K} \]

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

Snell’s law

\[
\left( \vec{k}_1 \cdot \vec{r}_i \right) = \left( \vec{k}'_1 \cdot \vec{r}_i \right) = \left( \vec{k}_2 \cdot \vec{r}_i \right)
\]

\[
k_{1z} = \left| \vec{k}_1 \right| \sin \theta_1 = n_1 \frac{\omega}{c} \sin \theta_1 \quad n_1 \sin \theta_1 = n_2 \sin \theta_2
\]

\[
k_{2z} = \left| \vec{k}_2 \right| \sin \theta_2 = n_2 \frac{\omega}{c} \sin \theta_2
\]

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Energy conservation

\[ \int \mathbf{J} \cdot \mathbf{E} \, dv + \frac{\partial}{\partial t} \int \left( \mathbf{E} \cdot \mathbf{D} + \mathbf{H} \cdot \mathbf{B} \right) \, dv + \int \mathbf{E} \times \mathbf{H} \cdot \mathbf{n} \, dS = 0 \]

- total energy stored in electrical and magnetic field per volume
- energy surface flux per unit area

\[ \mathbf{S} = \frac{c}{4\pi} \mathbf{E} \times \mathbf{H} \]

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:

Modeling Optical Constants with a Damped Harmonic Oscillator

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

$$\varepsilon = 1 + 4\pi \chi + 4\pi \frac{Ne^2 \left( \omega_0^2 - \omega^2 \right)}{m_0 \left( \omega_0^2 - \omega^2 \right)^2 + \gamma^2 \omega^2} \frac{-i4\pi}{\varepsilon_1} \frac{Ne^2 \gamma \omega}{m_0 \left( \omega_0^2 - \omega^2 \right)^2 + \gamma^2 \omega^2}$$
Amorphous silica

Figure by MIT OpenCourseWare.

Kramers-Kronig relations

\[
n(\omega) = 1 + \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\kappa(\omega')}{\omega' - \omega} d\omega'
\]

\[
\kappa(\omega) = -\frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{n(\omega') - 1}{\omega' - \omega} d\omega'
\]
Optical materials

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Infrared active modes

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Please see Fig. 1a and 2a in Giannozzi, Paolo, et al. 
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Interband absorption

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Direct and indirect transitions

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Please see: Fig. 3.2 in Fox, Mark. *Optical Properties of Solids*. Oxford, England: Oxford University Press, 2001.
Transition rate for direct absorption

Transition rates: perturbing Hamiltonian
Transition rates: perturbing Hamiltonian

Transition rate for direct absorption