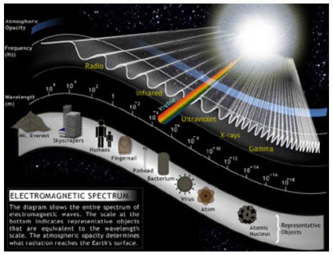
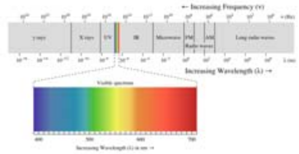
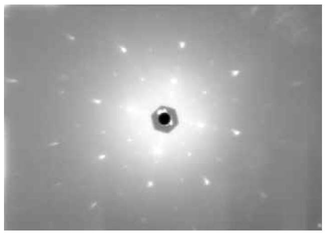




Phys 774:
Principles of Spectroscopy



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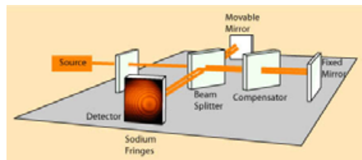
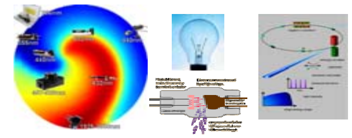
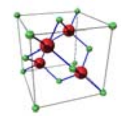


Linear Spectroscopy



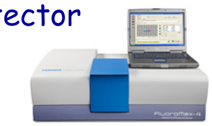
Source of Radiation
or Excitation

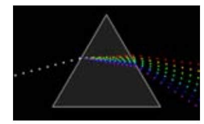
Sample

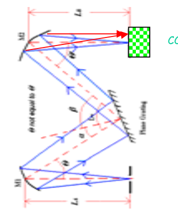


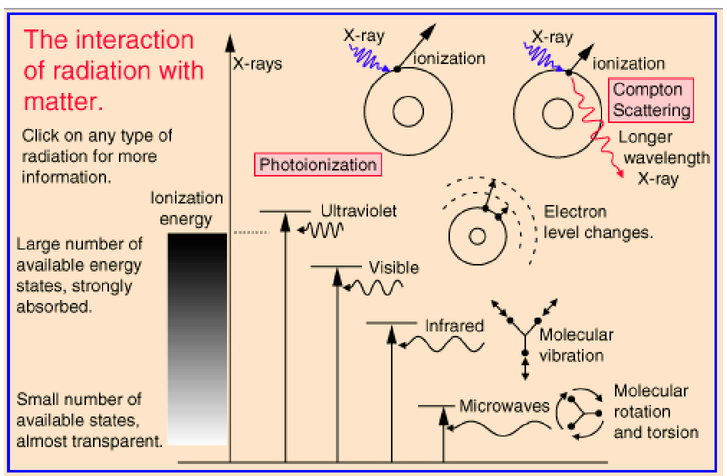
Processes in the SAMPLES
- Transmission / Reflection /Absorption
- Linear Spectroscopy
- Dielectric function approach

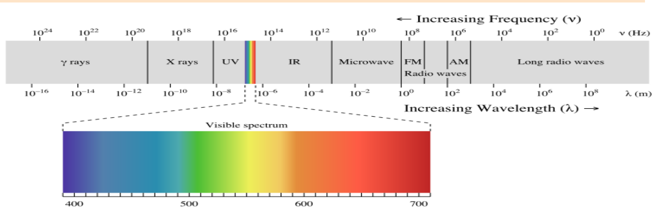
Spectrometer +
Detector



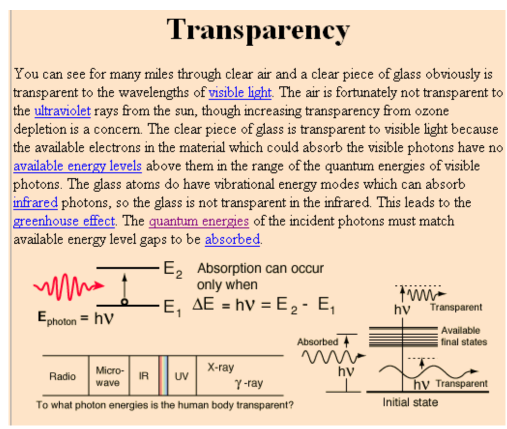






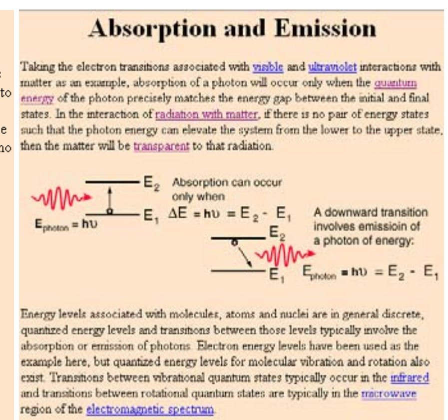


The interaction of radiation with matter



Transparency

You can see for many miles through clear air and a clear piece of glass obviously is transparent to the wavelengths of visible light. The air is fortunately not transparent to the ultraviolet rays from the sun, though increasing transparency from ozone depletion is a concern. The clear piece of glass is transparent to visible light because the available electrons in the material which could absorb the visible photons have no available energy levels above them in the range of the quantum energies of visible photons. The glass atoms do have vibrational energy modes which can absorb infrared photons, so the glass is not transparent in the infrared. This leads to the greenhouse effect. The quantum energies of the incident photons must match available energy level gaps to be absorbed.

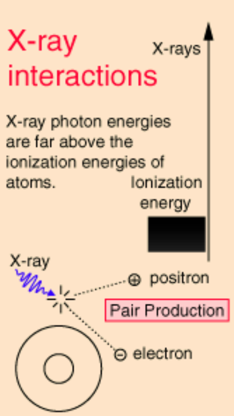


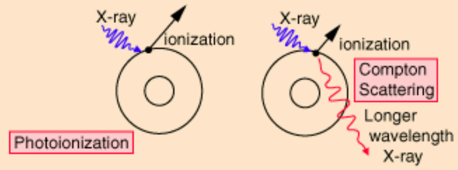
Absorption and Emission

Taking the electron transitions associated with visible and ultraviolet interactions with matter as an example, absorption of a photon will occur only when the quantum energy of the photon precisely matches the energy gap between the initial and final states. In the interaction of radiation with matter, if there is no pair of energy states such that the photon energy can elevate the system from the lower to the upper state, then the matter will be transparent to that radiation.

Energy levels associated with molecules, atoms and nuclei are in general discrete, quantized energy levels and transitions between those levels typically involve the absorption or emission of photons. Electron energy levels have been used as the example here, but quantized energy levels for molecular vibration and rotation also exist. Transitions between vibrational quantum states typically occur in the infrared and transitions between rotational quantum states are typically in the microwave region of the electromagnetic spectrum.

The interaction of radiation with matter



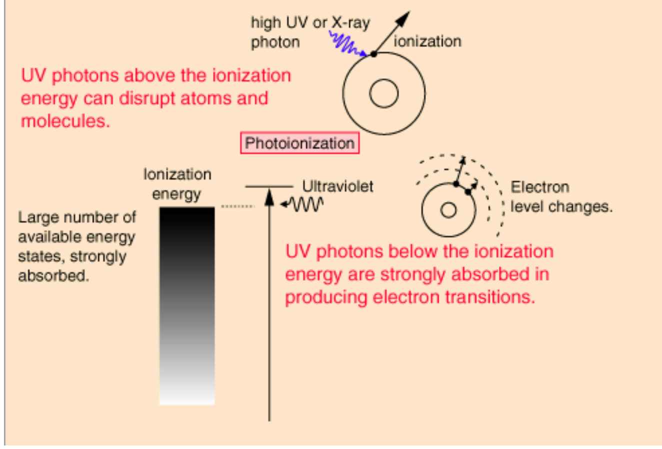


Since the quantum energies of x-ray photons are much too high to be absorbed in electron transitions between states for most atoms, they can interact with an electron only by knocking it completely out of the atom. That is, all x-rays are classified as ionizing radiation. This can occur by giving all of the energy to an electron (photoionization) or by giving part of the energy to the electron and the remainder to a lower energy photon (Compton scattering). At sufficiently high energies, the x-ray photon can create an electron positron pair.

http://www4.nau.edu/microanalysis/Microprobe/Course%20Overview.html

The interaction of radiation with matter

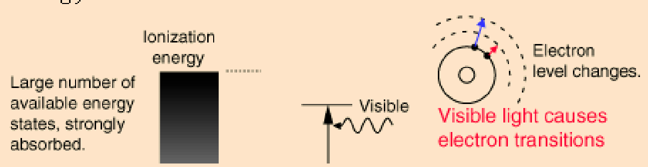
Ultraviolet Interactions



The interaction of radiation with matter

Visible Light Interactions

The primary mechanism for the absorption of visible light photons is the elevation of electrons to higher energy levels. There are many available states, so visible light is absorbed strongly. With a strong light source, red light can be transmitted through the hand or a fold of skin, showing that the red end of the spectrum is not absorbed as strongly as the violet end.

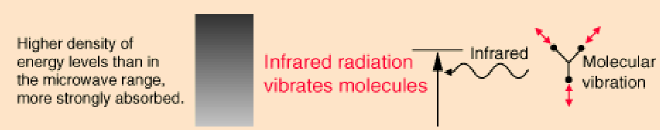


While exposure to visible light causes heating, it does not cause ionization with its risks. You may be heated by the sun through a car windshield, but you will not be sunburned - that is an effect of the higher frequency uv part of sunlight which is blocked by the glass of the windshield.

The interaction of radiation with matter

Infrared Interactions

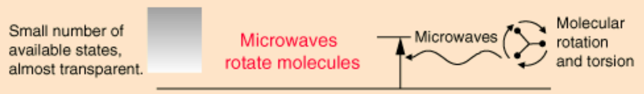
The quantum energy of infrared photons is in the range 0.001 to 1.7 eV which is in the range of energies separating the quantum states of molecular vibrations. Infrared is absorbed more strongly than microwaves, but less strongly than visible light. The result of infrared absorption is heating of the tissue since it increases molecular vibrational activity. Infrared radiation does penetrate the skin further than visible light and can thus be used for photographic imaging of subcutaneous blood vessels.



The interaction of radiation with matter

Microwave Interactions

The quantum energy of microwave photons is in the range 0.00001 to 0.001 eV which is in the range of energies separating the quantum states of molecular rotation and torsion. The interaction of microwaves with matter other than metallic conductors will be to rotate molecules and produce heat as result of that molecular motion. Conductors will strongly absorb microwaves and any lower frequencies because they will cause electric currents which will heat the material. Most matter, including the human body, is largely transparent to microwaves. High intensity microwaves, as in a microwave oven where they pass back and forth through the food millions of times, will heat the material by producing molecular rotations and torsions. Since the quantum energies are a million times lower than those of x-rays, they cannot produce ionization and the characteristic types of radiation damage associated with ionizing radiation.



The interaction of radiation with matter

Maxwell's equations (c.g.s. units)

$$\nabla \times \vec{H} - \frac{1}{c}\frac{\partial \vec{D}}{\partial t} = \frac{4\pi}{c}\vec{j}$$

$$\nabla \times \vec{E} + \frac{1}{c}\frac{\partial \vec{B}}{\partial t} = 0$$

$$\nabla \cdot \vec{D} = 0$$

$$\nabla \cdot \vec{B} = 0$$

Materials equations

$$\vec{D} = \varepsilon \vec{E}$$

$$\vec{B} = \mu \vec{H}$$

$$\vec{j} = \sigma \vec{E}$$

Solution

$$\nabla^2 \vec{E} = \frac{\varepsilon\mu}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} + \frac{4\pi\sigma\mu}{c^2}\frac{\partial \vec{E}}{\partial t}$$

$$\nabla^2 \vec{H} = \frac{\varepsilon\mu}{c^2}\frac{\partial^2 \vec{H}}{\partial t^2} + \frac{4\pi\sigma\mu}{c^2}\frac{\partial \vec{H}}{\partial t}.$$

EM wave

$$\vec{E} = \vec{E}_0 e^{i(\vec{K}\cdot\vec{r} - \omega t)}$$

$$-K^2 = -\frac{\varepsilon\mu\omega^2}{c^2} - \frac{4\pi i\sigma\mu\omega}{c^2}.$$

Loss part of K-vector

The interaction of radiation with matter

Complex Dielectric Function

$$\vec{D} = \varepsilon \vec{E}$$

$$\vec{B} = \mu \vec{H}$$

$$\vec{j} = \sigma \vec{E}$$

$$\varepsilon_{\text{complex}} = \varepsilon + \frac{4\pi i\sigma}{\omega} = \varepsilon_1 + i\varepsilon_2.$$

$$\tilde{N}(\omega) = \sqrt{\mu\varepsilon_{\text{complex}}} = \sqrt{\varepsilon\mu\left(1 + \frac{4\pi i\sigma}{\varepsilon\omega}\right)} = \tilde{n}(\omega) + i\tilde{k}(\omega).$$

we will relate these quantities in two ways:

1. to observables such as the reflectivity which we measure in the laboratory,
2. to properties of the solid such as the carrier density, relaxation time, effective masses, energy band gaps, etc.

$$\vec{E}(z,t) = \vec{E}_0 e^{-i\omega t}\exp\left(i\frac{\omega z}{c}\sqrt{\varepsilon\mu}\sqrt{1 + \frac{4\pi i\sigma}{\varepsilon\omega}}\right)$$

$$\varepsilon_1 = \tilde{n}^2 - \tilde{k}^2$$

$$\varepsilon_2 = 2\tilde{n}\tilde{k}$$

$\lambda >> a_0 \rightarrow q \approx 0$

The interaction of radiation with matter

EM wave:

In vacuum: $\varepsilon = 1, \mu = 1, \sigma = 0$

$$\vec{D} = \varepsilon \vec{E}$$

$$\vec{B} = \mu \vec{H}$$

$$\vec{j} = \sigma \vec{E}$$

$$\vec{E} = \vec{E}_0 e^{i(\vec{K}\cdot\vec{r} - \omega t)}$$

$$\vec{E}(z,t) = \vec{E}_0 e^{-i\omega t}\exp\left(i\frac{\omega z}{c}\sqrt{\varepsilon\mu}\sqrt{1 + \frac{4\pi i\sigma}{\varepsilon\omega}}\right)$$

Can measure usually only E^2 $\quad I(z) = I_0 e^{-\alpha_{\text{abs}}(\omega) z}$

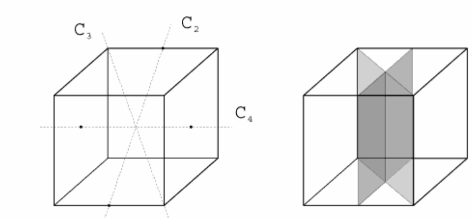
Typical absorption length: $\quad \frac{1}{\alpha_{\text{abs}}} = \frac{c}{2\omega\tilde{k}(\omega)}$

Dielectric function is a tensor

Important for crystals !

$$\vec{D} = \hat{\varepsilon}(\omega)\vec{E}$$

$$\vec{j} = \hat{\sigma}(\omega)\vec{E}$$

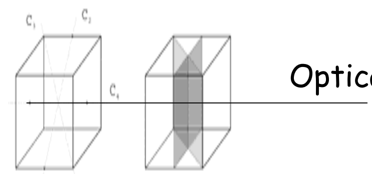


$$\boldsymbol{j} = \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{E}.$$

$$\boldsymbol{j} = \begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix}, \quad \boldsymbol{E} = \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}, \quad \hat{\boldsymbol{\sigma}} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

$$j_x = \sigma_{xx}E_x + \sigma_{xy}E_y + \sigma_{xz}E_z$$
$$j_y = \sigma_{yx}E_x + \sigma_{yy}E_y + \sigma_{yz}E_z$$
$$j_z = \sigma_{zx}E_x + \sigma_{zy}E_y + \sigma_{zz}E_z$$

Optical birefringence spectroscopy



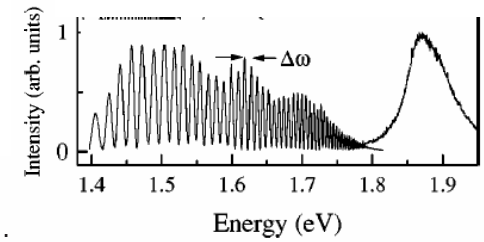
$$\vec{D} = \hat{\varepsilon}(\omega)\vec{E}$$

$$\varepsilon_{zz}(\omega) \neq \varepsilon_{xx}(\omega) = \varepsilon_{yy}(\omega)$$

$$\Delta n = (n_\perp - n_\parallel).$$

$$\Delta n(\lambda) d = M\lambda,$$

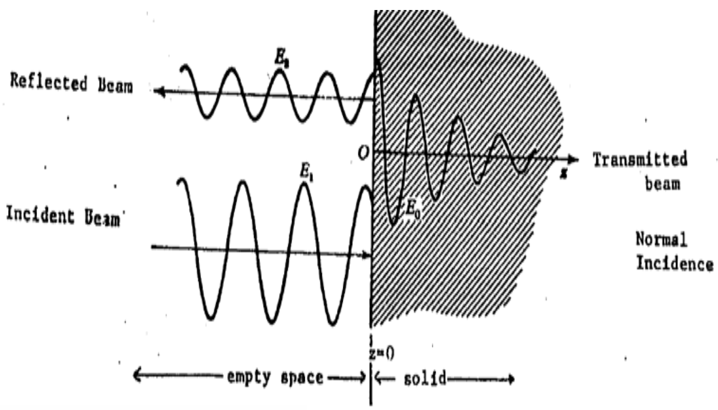
$$I(\omega) \sim \sin^2\left[\frac{d}{2c}\Delta n(\omega)\omega\right].$$



Linear spectroscopy

Schematic diagram for normal incidence reflectivity

$$\mathcal{R} = \left|\frac{E_2}{E_1}\right|^2$$



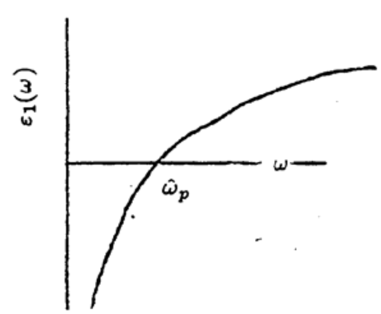
$$\mathcal{R} = \left|\frac{1 - \tilde{N}_{\text{complex}}}{1 + \tilde{N}_{\text{complex}}}\right|^2 = \frac{(1-\tilde{n})^2 + \tilde{k}^2}{(1+\tilde{n})^2 + \tilde{k}^2}$$

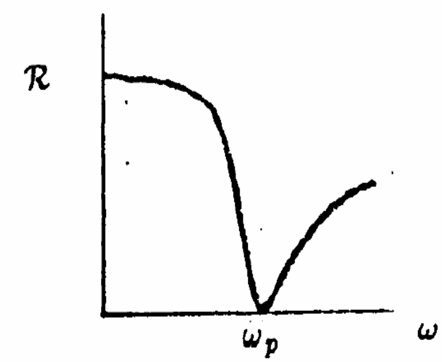
$$1 = \mathcal{R} + \mathcal{A} + \mathcal{T}$$

Contributions to Dielectric Function

The Free Carrier Contribution

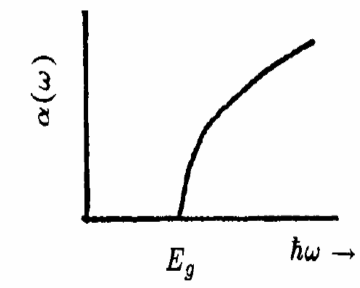
The Plasma Frequency



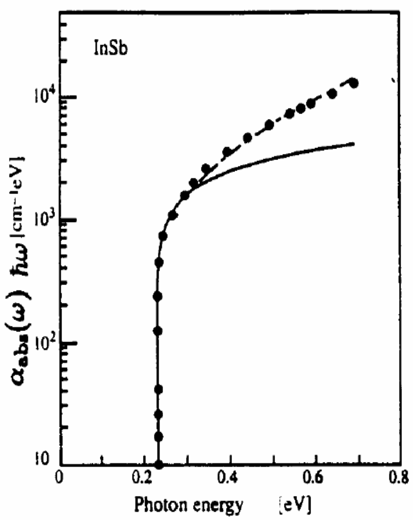


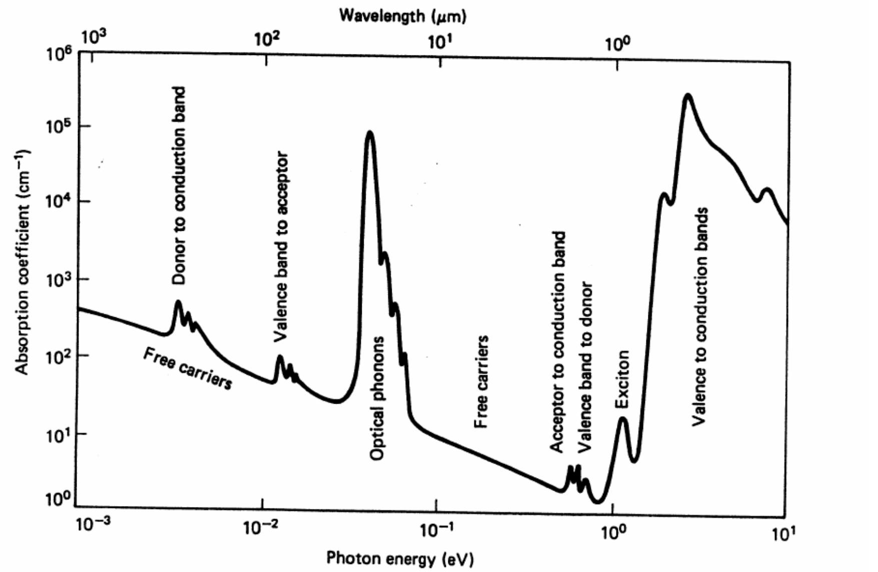
$$\omega_p^2 = \frac{4\pi n e^2}{m\varepsilon_{\text{core}}}$$

Linear spectroscopy of semiconductors and dielectrics



Frequency dependence of the absorption coefficient near a threshold for interband transitions.





Hypothetical absorption spectrum for a typical III-V semiconductor as a function of phonon energy.

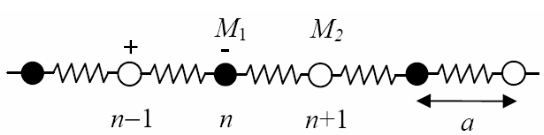
Ionic polarizability / Phonon contribution

Evaluate the dielectric constant of an ionic crystal.

Ionic polarizability is related to the motion of ions.

Recall the linear chain model we used to describe lattice vibrations:

Equations of motion in the presence of external field:



$$M_1 \frac{d^2 u_n}{dt^2} = -C(2u_n - u_{n+1} - u_{n-1}) - e^* E$$

$$M_2 \frac{d^2 u_{n+1}}{dt^2} = -C(2u_{n+1} - u_{n+2} - u_n) + e^* E$$

e^* - effective charge,

E – external field;

assume $E = E_0 e^{i(qx-\omega t)}$

also assume long wavelength, $\lambda >> a_0 \rightarrow q \approx 0 \Rightarrow$

$$u_n = u_{0-} e^{-i\omega t} \qquad u_{n+1} = u_{0+} e^{-i\omega t}$$

Substitute this solution into equations of motion, solve for u_{0+}, u_{0-}

Get $$u_{0-} = -\frac{e^*}{M_1(\omega_t^2 - \omega^2)} E_0 \qquad u_{0+} = \frac{e^*}{M_2(\omega_t^2 - \omega^2)} E_0$$

where $\omega_t = \sqrt{2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right)}$ - transverse optical phonon frequency at $q = 0$

The ionic polarization P_i is then $P_i = n_m e^*(u_{0+} - u_{0-})$

(n_m – number of dipoles per unit volume); $P = \varepsilon_0 \chi E$

relative permittivity: $\varepsilon_r = \varepsilon/\varepsilon_0 = 1 + \chi$; $\chi = \chi_{el} + \chi_i$

Get $$\varepsilon_r(\omega) = 1 + \chi_{el} + \frac{n_m e^*}{M_R \varepsilon_0 (\omega_t^2 - \omega^2)}$$

where $M_R = \left(\frac{1}{M_1} + \frac{1}{M_2}\right)^{-1} = \frac{M_1 M_2}{M_1 + M_2}$ - reduced mass

At high frequencies, $\omega >> \omega_t$, the ionic term vanishes: $\varepsilon_{r\infty} = 1 + \chi_{el}$

at $\omega = 0$,

$$\varepsilon_{r0} = 1 + \chi_{el} + \frac{n_m e^*}{M_R \varepsilon_0 \omega_t^2}$$

can rewrite

$$\varepsilon_r(\omega) = 1 + \chi_{el} + \frac{n_m e^*}{M_R \varepsilon_0 \omega_t^2 (1 - \omega^2/\omega_t^2)} = \varepsilon_{r\infty} + \frac{\varepsilon_{r0} - \varepsilon_{r\infty}}{1 - \omega^2/\omega_t^2}$$

Note that $\varepsilon_r(\omega_t) \to \infty$. Also, $\varepsilon_r(\omega) = 0$ at $\omega_l = \left(\frac{\varepsilon_{r0}}{\varepsilon_{r\infty}}\right)^{1/2} \omega_t$

Between ω_t and ω_l $\varepsilon_r(\omega) < 0 \Rightarrow$ index of refraction is imaginary:

$$N(\omega) = \sqrt{\varepsilon_r} = i \cdot k(\omega)$$ wave is reflected

Physical meaning of ω_l - the frequency of longitudinal optical phonon

$$\nabla \cdot \mathbf{D} = \varepsilon(\nabla \cdot \mathbf{E}) = 0$$

$$\nabla \times \vec{H} - \frac{1}{c}\frac{\partial \vec{D}}{\partial t} = \frac{4\pi}{c}\vec{j}$$
$$\nabla \times \vec{E} + \frac{1}{c}\frac{\partial \vec{B}}{\partial t} = 0$$
$$\nabla \cdot \vec{D} = 0$$
$$\nabla \cdot \vec{B} = 0$$

TO phonons:

no field in z direction; from the symmetry of the problem:

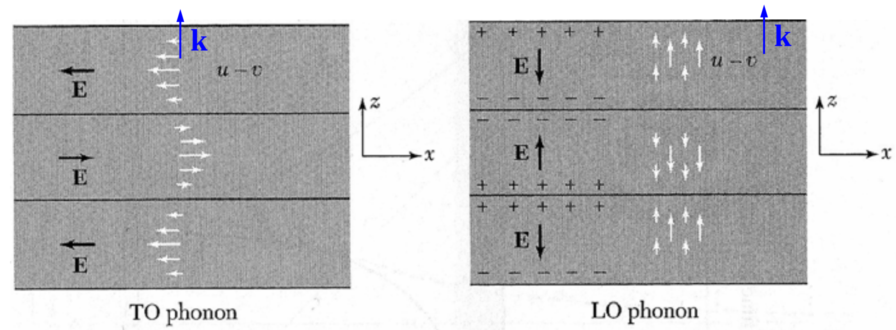
$$\frac{\partial E_x}{\partial x} = 0 \Rightarrow \nabla \cdot \mathbf{E} = 0$$

LO phonons:

macroscopic field along z

$$\frac{\partial E_z}{\partial z} \neq 0 \Rightarrow \nabla \cdot \mathbf{D} = 0$$

only if $\varepsilon(\omega) = 0$



TO phonon LO phonon

Lyddane-Sachs-Teller relation

We had $\varepsilon_r(\omega) = \varepsilon_{r\infty} + \frac{\varepsilon_{r0} - \varepsilon_{r\infty}}{1 - \omega^2/\omega_t^2}$ and $\omega_l^2 = \frac{\varepsilon_{r0}}{\varepsilon_{r\infty}} \omega_t^2$

combine, get

$$\varepsilon_r(\omega) = \varepsilon_{r\infty} \frac{\omega_l^2 - \omega^2}{\omega_t^2 - \omega^2} \quad \text{or} \quad \frac{\varepsilon_{r0}}{\varepsilon_{r\infty}} = \frac{\omega_l^2}{\omega_t^2}$$

If many phonon branches:

$$\boxed{\varepsilon(\omega) = \varepsilon_\infty \prod_j \frac{\omega_{LO_j}^2 - \omega^2}{\omega_{TOj}^2 - \omega^2}}$$

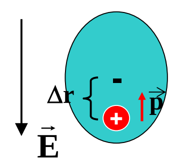
Electronic polarizability

For an accurate quantitative description, quantum mechanics is needed

But we can get some general ideas with classical approach

Recall our model of atom:

Displaced electronic cloud feels a restoring force, which is linear (for small displacements)



Total force $\mathbf{F} = e\mathbf{E} - \kappa\Delta\mathbf{r} = m\frac{d^2}{dt^2}\Delta\mathbf{r}$

κ = spring constant

m = mass

For simplicity consider one-dimensional case ($\Delta\mathbf{r}$ parallel to x)

Without an external field: $$-kx = m\frac{d^2x}{dt^2}$$

Equation for harmonic oscillator. Solution: harmonic vibration

$x(t) = x_0 e^{-i\omega_0 t}$ with frequency $\omega_0 = \sqrt{k/m}$

Now, have electromagnetic wave with field $E(t)=E_0 e^{-i\omega t}$

Force $F(t)=eE_0 e^{-i\omega t}$

Equation of motion becomes (forced oscillator) $$eE_o e^{-i\omega t} - m\omega_0^2 x = m\frac{d^2x}{dt^2}$$

Look for a solution $x(t)=x_0 e^{-i\omega t}$

get $$x(t) = \frac{e/m}{\omega_0^2 - \omega^2} E_o e^{-i\omega t} = \frac{e/m}{\omega_0^2 - \omega^2} E(t)$$

$$x(t) = \frac{e/m}{\omega_0^2 - \omega^2} E(t)$$

Expect strong response (large x), $\Rightarrow$ large susceptibility $\chi \Rightarrow$ large refractive index n at $\omega \approx \omega_0$

Dipole moment $p = qx$, so polarization $P = eNZx$
(N atoms per unit volume, Z electrons per atom) $\Rightarrow$

$$P = \frac{e^2 ZN/m}{\omega_0^2 - \omega^2} E$$

Recall $P = \varepsilon_0 \chi E$ and $\varepsilon = \varepsilon_0(1+\chi)$

get $$\chi = \frac{NZe^2}{\varepsilon_0 m}\frac{1}{(\omega_0^2 - \omega^2)}$$ or $$\varepsilon = \varepsilon_0\left(1 + \frac{NZe^2}{\varepsilon_0 m}\frac{1}{(\omega_0^2 - \omega^2)}\right)$$

and $$n^2(\omega) = \frac{\varepsilon}{\varepsilon_0} = 1 + \frac{NZe^2}{\varepsilon_0 m}\left(\frac{1}{\omega_0^2 - \omega^2}\right)$$

Now, consider damping force proportional to speed :

$$F_{damp} = -m\gamma\frac{dx}{dt}$$

Equation of motion becomes (damped oscillator):

$$eE_o e^{-i\omega t} - m\omega_0^2 x - m\gamma\frac{dx}{dt} = m\frac{d^2x}{dt^2}$$

Again, look for a solution $x(t)=x_0 e^{-i\omega t}$

get $$x(t) = \frac{e}{m}E(t)\frac{1}{\omega_0^2 - \omega^2 + i\omega\gamma}$$

Same form as before, just includes damping

Therefore $$n^2(\omega) = \frac{\varepsilon}{\varepsilon_0} = 1 + \frac{NZe^2}{\varepsilon_0 m}\left(\frac{1}{\omega_0^2 - \omega^2 + i\omega\gamma}\right)$$

n is complex for nonzero damping: $\tilde{n} = n_R + in_I$

and $\mathbf{k} = \tilde{n}\mathbf{k}_0$, $k = \tilde{n}k_0$ - complex wavenumber

What does it mean?

$$E = E_0 e^{i(kx-\omega t)} = E_0 e^{i[n_R + in_I]k_0 x - i\omega t} = E_0 e^{-n_I k_0 x} e^{i(n_R k_0 x - \omega t)}$$

or $E = \tilde{E}_0 e^{i(n_R k_0 x - \omega t)}$ where $\tilde{E}_0 = E_0 e^{-n_I k_0 x}$

Amplitude decays as wave propagates – absorption; results from damping

Usually write $\tilde{n} \to n + i\frac{\alpha}{2k_0}$ instead of $n_R + in_I$

Then $\tilde{E}_0 = E_0 e^{-\alpha x/2}$

and intensity $I \propto \tilde{E}_0^2 = I_0 e^{-\alpha x}$

α - ***absorption coefficient*** (m^{-1})

Reflectivity at normal incidence (in air)

Field amplitude: $r = \frac{n-1}{n+1}$ power (intensity): $R = |r|^2 = \frac{(n-1)^2}{(n+1)^2}$

If $\tilde{n} = n_R + in_I$ then $R = |r|^2 = rr^* = \frac{(n_R-1)^2 + n_I^2}{(n_R+1)^2 + n_I^2}$

As we've seen, the dielectric function and refractive index are generally complex: $\varepsilon_r = \varepsilon_r' + i\varepsilon_r''$ $\tilde{n} = n_R + in_I$

$\varepsilon_r' = n_R^2 - n_I^2$; $\varepsilon_r'' = 2n_R n_I$

n_I is called *extinction coefficient*

We obtained

$$n^2(\omega) = \frac{\varepsilon}{\varepsilon_0} = 1 + \underbrace{\frac{NZe^2}{\varepsilon_0 m}\left(\frac{1}{\omega_0^2 - \omega^2 + i\omega\gamma}\right)}_{\chi_e(\omega)}$$

Quantum mechanics gives similar result: $\alpha_e(\omega) = \frac{e^2}{m}\sum_j \frac{f_j}{\omega_j^2 - \omega^2 + i\omega\gamma_j}$

Many resonant frequencies ω_j correspond to energy transitions

Weighting factors f_j called oscillator strengths

(related to transition matrix elements)

Optical properties of conductive solids (metals)

conductivity of a medium σ: $\mathbf{J} = \sigma\mathbf{E}$

Including conductivity in Maxwell's equations in the medium:

$$\nabla \times \mathbf{B} = \mu\mathbf{J} + \mu\varepsilon\frac{\partial \mathbf{E}}{\partial t}$$

leads to wave equation: $\nabla^2\vec{\mathbf{E}} = \mu\sigma\frac{\partial \mathbf{E}}{\partial t} + \mu\varepsilon\frac{\partial^2 \mathbf{E}}{\partial t^2}$

Differs from a "standard" wave equation by the first term in the right part

Still, look for plane wave solution: $\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}$

$$\nabla^2\vec{\mathbf{E}} = \mu\sigma\frac{\partial \mathbf{E}}{\partial t} + \mu\varepsilon\frac{\partial^2 \mathbf{E}}{\partial t^2} \qquad \vec{\mathbf{E}}(\vec{\mathbf{r}},t) = \vec{\mathbf{E}}_0 e^{i(\vec{\mathbf{k}}\cdot\vec{\mathbf{r}} - \omega t)}$$

applying ∇^2 to plane wave gives $\nabla^2\vec{\mathbf{E}} = -k^2\vec{\mathbf{E}}$

$\partial/\partial t \to -i\omega$; $\partial^2/\partial t \to -\omega^2$ get $-k^2\vec{\mathbf{E}} = -i\omega\mu\sigma\vec{\mathbf{E}} - \mu\varepsilon\omega^2\vec{\mathbf{E}}$

so

$$k^2 = \mu\varepsilon\omega^2 + i\omega\mu\sigma = \mu_0\varepsilon_0\omega^2\left(\frac{\mu\varepsilon}{\mu_0\varepsilon_0} + i\frac{\mu\sigma}{\mu_0\varepsilon_0\omega}\right) \qquad k_0 = \mu_0\varepsilon_0\omega^2 = \frac{\omega^2}{c^2}$$

assume nonmagnetic: $\mu = \mu_0$ get $k = k_0\sqrt{\frac{\varepsilon}{\varepsilon_0} + i\frac{\sigma}{\varepsilon_0\omega}} = \tilde{n}k_0$

complex refractive index: $\tilde{n} = \left(\frac{\varepsilon}{\varepsilon_0} + i\frac{\sigma}{\varepsilon_0\omega}\right)^{1/2} = n_R + in_I = n_R + i\frac{\alpha}{2k_0}$

α - absorption coefficient (m^{-1}); $\tilde{E}_0 = E_0 e^{-\alpha x/2}$ and $I = I_0 e^{-\alpha x}$

Reflection from metals

Have complex refractive index n_t: $\tilde{n} = \left(\frac{\varepsilon}{\varepsilon_0} + i \frac{\sigma}{\varepsilon_0 \omega} \right)^{1/2} = n_I + i \frac{\alpha}{2k_0}$

n_R, $n_I = \alpha/2k_0$ are real

Reflectivity at normal incidence (in air) $R = |r|^2 = rr^* = \frac{(n_R - 1)^2 + n_I^2}{(n_R + 1)^2 + n_I^2}$

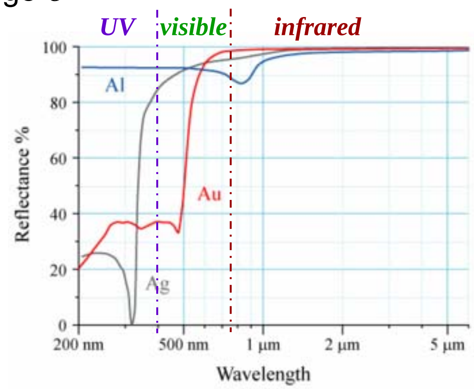
Consider a very good metal: large σ (e.g. silver: $\sigma \approx 6 \cdot 10^7\ \Omega^{-1}\text{m}^{-1}$)

For $\lambda = 500$ nm and $\epsilon \approx \epsilon_0$

$$\frac{\sigma}{\epsilon_0 \omega} \approx 2000$$

then $\frac{\alpha}{2k_0} = n_I >> n_R - 1$

$$\Rightarrow R \to 1$$



Dispersion equation in metals

The dispersion we got in a model of oscillating electrons:

$$n^2(\omega) = 1 + \frac{Ne^2}{\varepsilon_0 m} \left(\frac{1}{\omega_0^2 - \omega^2 + i\omega\gamma} \right)$$

$\omega_0 = \sqrt{k/m_e}$

k – "spring constant"
m_e – electron mass

in metal, there are free electrons – no restoring force $\Rightarrow \omega_0 = 0$

Still, there may be bound electrons, too.

So

$$n^2(\omega) = 1 + \frac{Ne^2}{\varepsilon_0 m} \left(\underbrace{\frac{1}{-\omega^2 + i\omega\gamma_e}}_{\text{free electrons}} + \underbrace{\sum_j \frac{f_j}{\omega_{0j}^2 - \omega^2 + i\omega\gamma_j}}_{\text{bound electrons (like in dielectric)}} \right)$$

If we neglect the contribution of bound electrons and also neglect free electron damping γ_e

Then $n^2(\omega) = 1 - \frac{Ne^2}{\varepsilon_0 m \omega^2}$

Introduce $\omega_p = \sqrt{\frac{Ne^2}{\varepsilon_0 m_e}}$ ***- plasma frequency***

Then $n^2(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$

Below ω_p refractive index is complex – absorption;

above ω_p n is real, free electron absorption is small

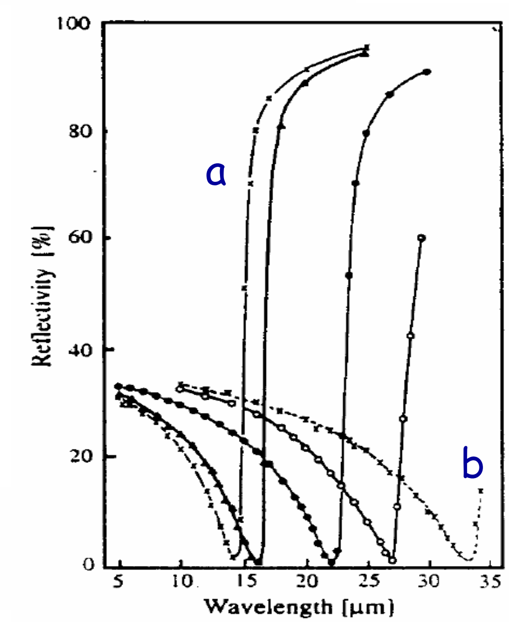
For most metals ω_p lies in the UV range

The Free Carrier Contribution

Where carrier concentration is higher? Choose between *a* and *b*. Show work

Plasma edges observed in the room temperature reflectivity spectra of n-type InSb with carrier concentration n varying between 3.5×10^{17} cm^{-3} and 4.0×10^{18} cm^{-3}.

$$\omega_p^2 = \frac{4\pi n e^2}{m \varepsilon_{\text{core}}}$$



Summary

- Ionic contribution to dielectric function is related to lattice vibrations and exhibits dispersion in infrared region, given by the Lyddane-Sachs-Teller relation:

$$\varepsilon(\omega) = \varepsilon_\infty \prod_{\mathrm{j}} \frac{\omega^2_{LO_j} - \omega^2}{\omega^2_{TOj} - \omega^2}$$

- Electronic polarizability is given by

$$\alpha(\omega) = \frac{e^2}{m}\left(\underbrace{\frac{1}{-\omega^2 + i\omega\gamma_e}}_{\text{free electrons}} + \underbrace{\sum_j \frac{f_j}{\omega_{0j}^2 - \omega^2 + i\omega\gamma_j}}_{\text{bound electrons}}\right)$$

- Dielectric function and refractive index are generally complex:

$\varepsilon_r = \varepsilon_r' + i\varepsilon_r''$; $\tilde{n} = n_R + in_I$; $\varepsilon_r' = n_R^2 - n_I^2$; $\varepsilon_r'' = 2n_R n_I$

absorption coefficient $\alpha = 2k_0 n_I$ n_I - extinction coefficient