Fundamentals of Solid State Physics

Origin of Optical Properties

Xing Sheng 盛兴

Department of Electronic Engineering
Tsinghua University
xingsheng@tsinghua.edu.cn

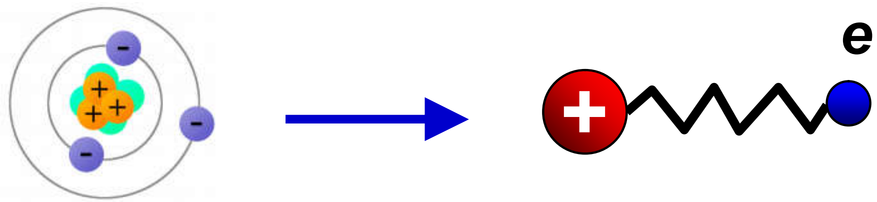
Outline

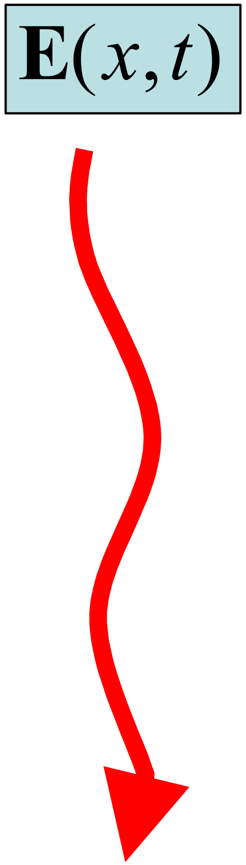
$$\tilde{n} = n + i\kappa$$

- **Refractive index**
  - **dipole polarization - oscillator model**
- **Absorption**
  - **damped oscillator**
  - **free carriers, band transitions, optical phonons, defects, ...**

Origin of ε_r and $\tilde{n}$

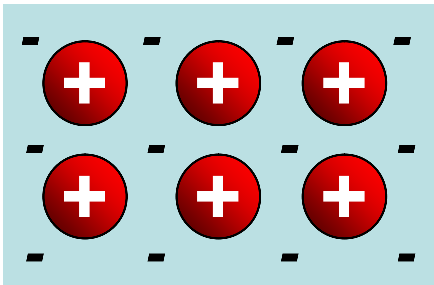
- **Interaction between EM wave and charges (electrons, ions, etc.) in the solids**
  - **Oscillation between electrons and nuclei**



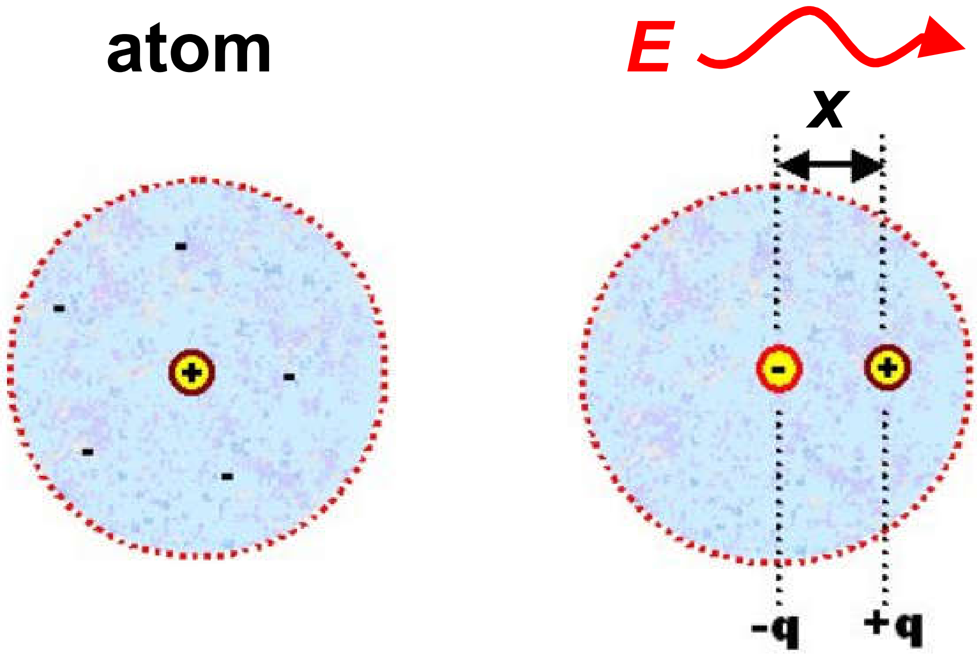


  - **Oscillation between ions (phonon)**

  - **Oscillation of free electron gas**



The Dipole Polarization



Polarization (极化)

$$\mathbf{P} = nq\mathbf{x}$$

n - density of dipoles
q - unit charge
x - displacement

$$\begin{aligned}\mathbf{D} &= \varepsilon_0\mathbf{E} + \mathbf{P} \\ &= \varepsilon_0\mathbf{E} + \sum \mathbf{P}_{\text{dipole}} \\ &= \varepsilon_0\mathbf{E} + \sum nq\mathbf{x}\end{aligned}$$

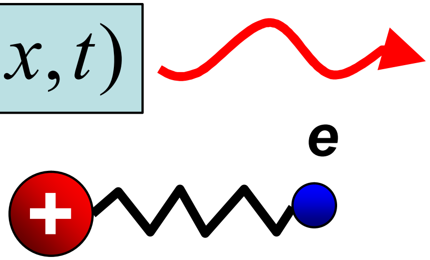
$$\mathbf{D} = \varepsilon_0\varepsilon_r\mathbf{E}$$

$$\rightarrow \quad \varepsilon_r = 1 + \sum \frac{nq\mathbf{x}}{\varepsilon_0\mathbf{E}}$$

dielectric constant = vacuum + all the dipoles

The Dipole Oscillator Model

$\mathbf{E}(x,t)$



oscillation frequency

$$\omega_0 = \sqrt{\frac{K}{m}}$$

$$m\frac{dv}{dt} + m\frac{v}{\tau} + Kx = eE(t)$$

Lorentz Model

$$m\frac{d^2x}{dt^2} + \frac{m}{\tau}\frac{dx}{dt} + m\omega_0{}^2 x = eE(t)$$

acceleration **damping relaxation** **Spring force** **Electric force**

The Dipole Oscillator Model

Lorentz Model

$$m\frac{d^2x}{dt^2} + \frac{m}{\tau}\frac{dx}{dt} + m\omega_0^{\ 2}x = eE(t)$$

$$x = x_0 e^{-i\omega t}$$

$\rightarrow$

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

$\rightarrow$

$$\varepsilon_r = 1 + \frac{nq\mathbf{x}}{\varepsilon_0 \mathbf{E}} = 1 + \frac{ne^2}{\varepsilon_0 m}\cdot\frac{1}{\omega_0^{\ 2} - \omega^2 - i\omega/\tau}$$

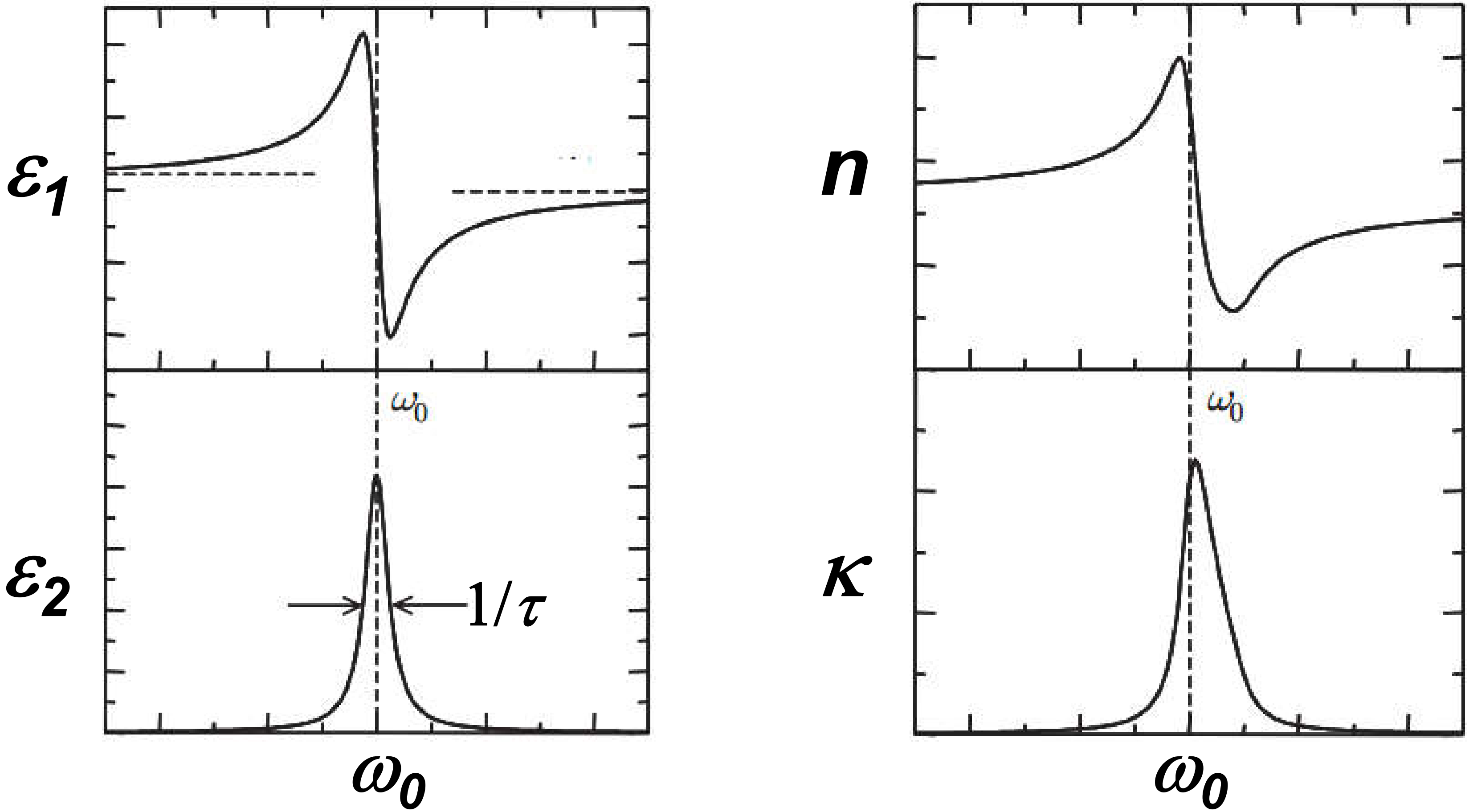
contribution of one resonance

The Dipole Oscillator Model

$$\tilde{\varepsilon}_r = \varepsilon_1 + i\varepsilon_2$$

$$\tilde{n} = \sqrt{\tilde{\varepsilon}_r} = n + i\kappa$$

resonance at ω_0

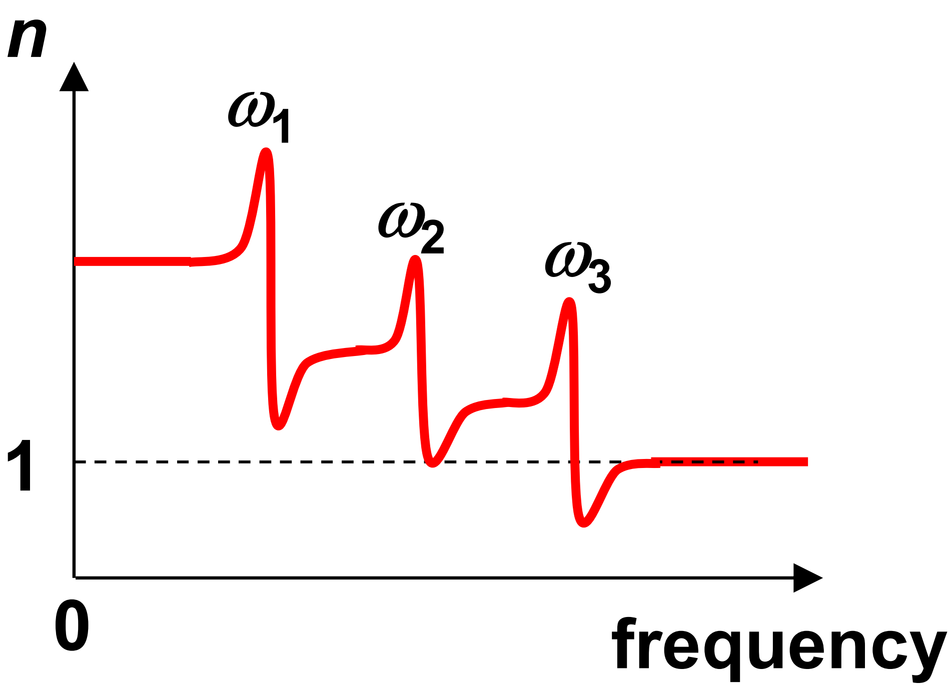


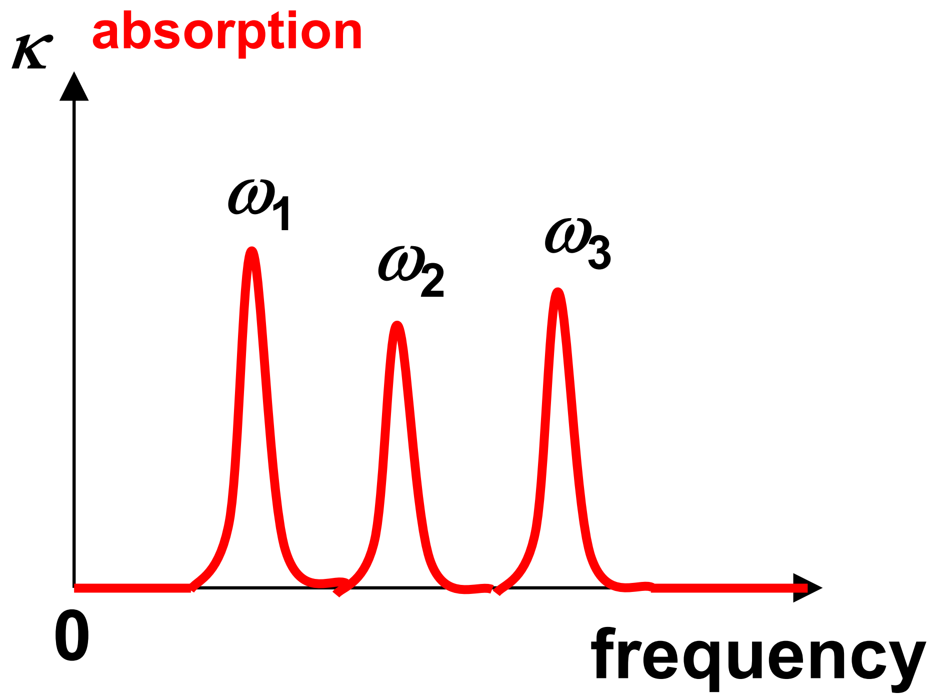
The Dipole Oscillator Model

Multiple resonances

$$\varepsilon_r = 1 + \sum \frac{nq\mathbf{x}}{\varepsilon_0 \mathbf{E}}$$

$$= 1 + \frac{ne^2}{\varepsilon_0 m} \cdot \sum_j \frac{1}{\omega_j^{\,2} - \omega^2 - i\omega/\tau_j}$$



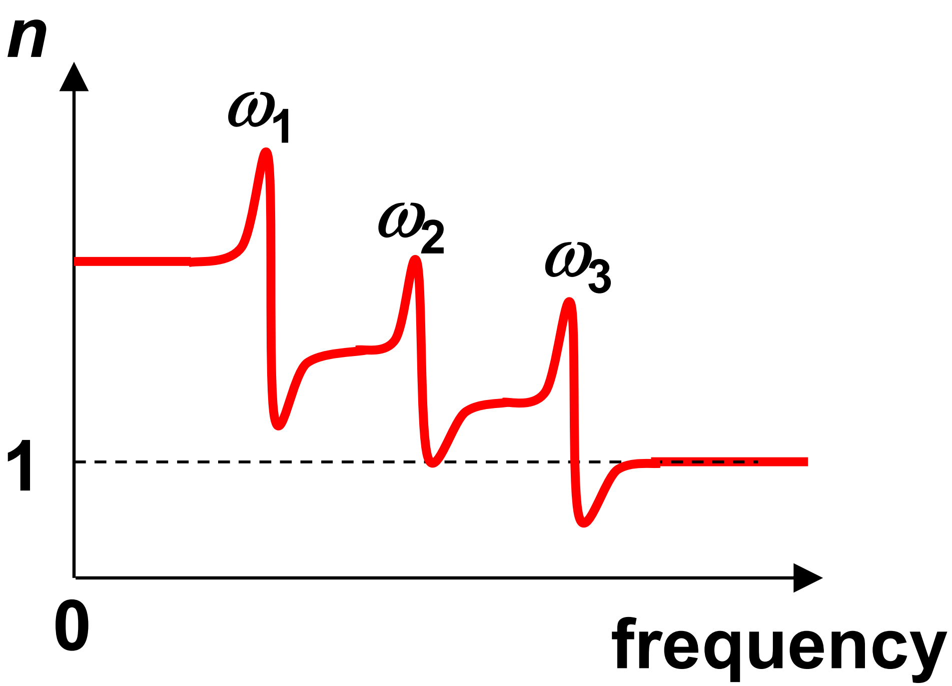


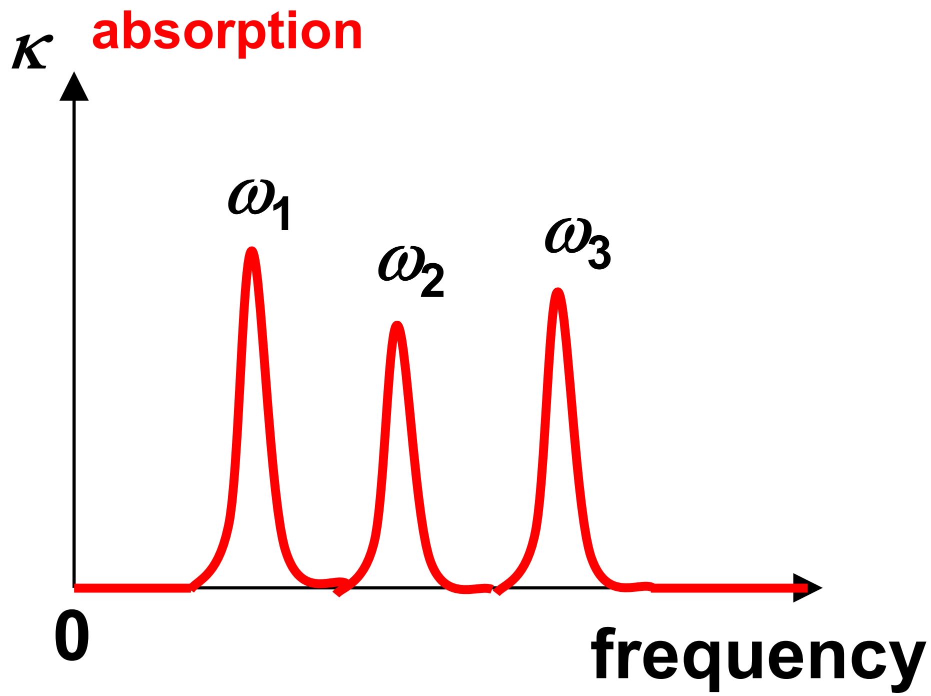
The Dipole Oscillator Model

When $\omega \sim 0$, n and ε_r is constant (dielectric) in DC field

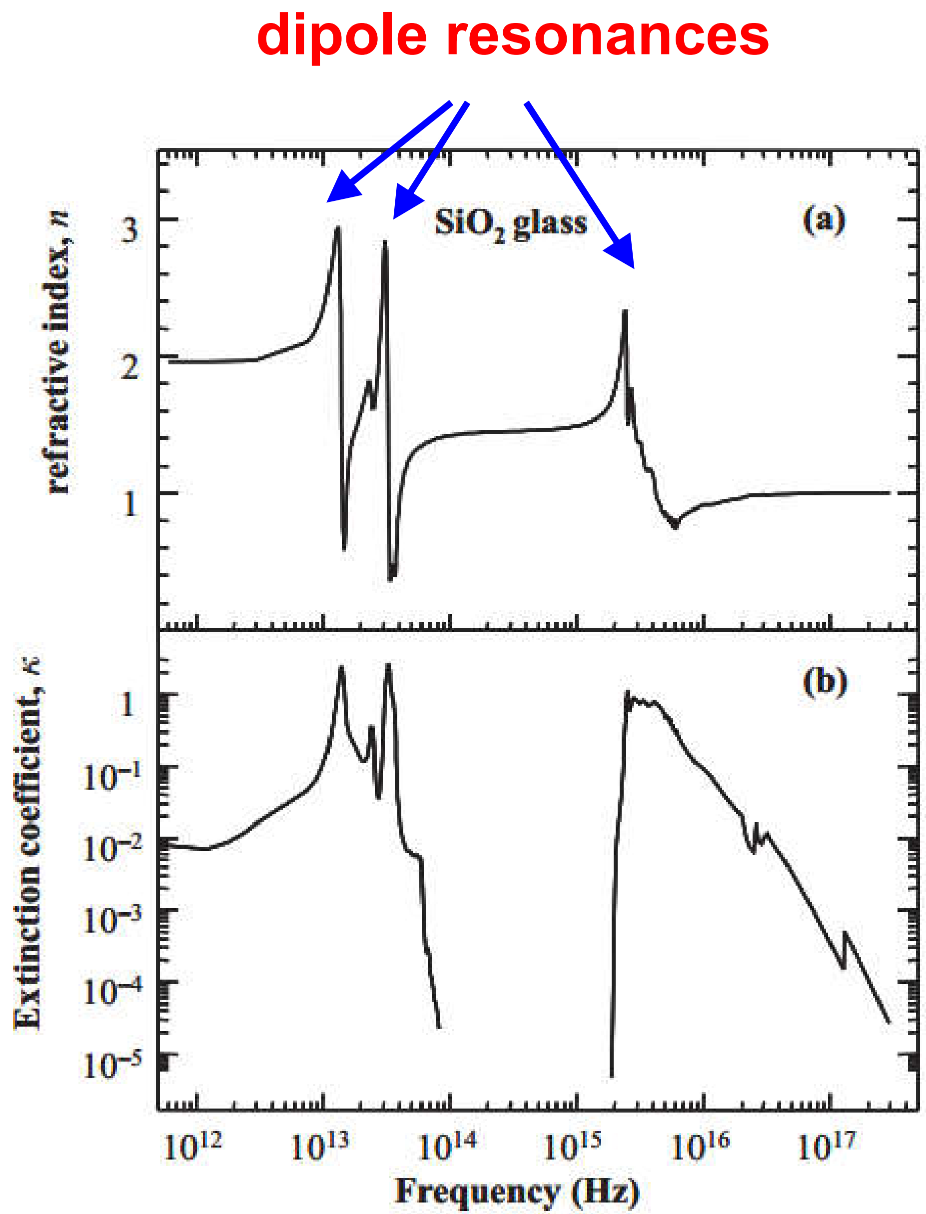
When ω is at resonance, strong absorption

When $\omega = +\infty$, $n = 1$, $\kappa = 0$. Transparent like vacuum (High frequency x-rays and γ-rays can penetrate most materials)

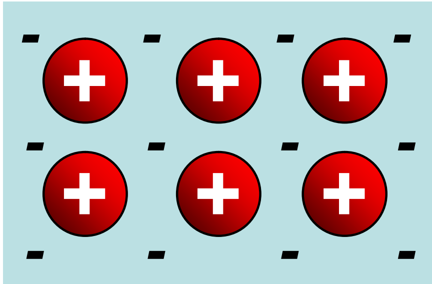




Example: SiO_2 glass



Free Electrons in Metals



The Drude Model: Free electron 'gas'

- **Independent**
  - electrons do not interact with each other
- **Free**
  - electrons do not interact with ions, except collision
- **Collision**
  - electrons are scattered by the ions instantaneously
- **Relaxation time τ**
  - average time between two collisions
  - electron mean free path $l = v^*\tau$
- **Maxwell-Boltzmann distribution**
  - average kinetic energy

$$\frac{1}{2}mv^2 = \frac{3}{2}kT$$

P. Drude
1863–1906

Free Electrons in Metals

Drude-Lorentz Model

$$F = m\frac{dv}{dt} + m\frac{v}{\tau} = eE(t)$$

τ - relaxation time (s)

when *E* is constant, *v* is constant

$$v = eE\frac{\tau}{m}$$

$$\mu = \frac{v}{E} = e\frac{\tau}{m}$$

mobility

$$\sigma = ne\mu = ne^2\frac{\tau}{m}$$

conductivity

$$j = nev = \sigma E$$

Ohm's law

Free Electrons in Metals

Drude-Lorentz Model

$$F = m\frac{dv}{dt} + m\frac{v}{\tau} = eE(t)$$

when interacting with AC field (Optical wave)

$$m\frac{d^2x}{dt^2} + \frac{m}{\tau}\frac{dx}{dt} = eE(t) = eE_0 e^{-i\omega t}$$

$$x = x_0 e^{-i\omega t}$$

$$\rightarrow \quad x = -\frac{e}{m(\omega^2 + i\omega/\tau)}E$$

$$\rightarrow \quad \varepsilon_r = 1 + \frac{nq\mathbf{x}}{\varepsilon_0 \mathbf{E}} = 1 - \frac{ne^2}{\varepsilon_0 m}\cdot\frac{1}{\omega^2 + i\omega/\tau}$$

Free Electrons in Metals

$$\varepsilon_r = 1 + \frac{nq\mathbf{x}}{\varepsilon_0 \mathbf{E}} = 1 - \frac{ne^2}{\varepsilon_0 m} \cdot \frac{1}{\omega^2 + i\omega/\tau}$$

For a weakly damp system, 1/$\tau \approx$0

$$\rightarrow \varepsilon_r = 1 - \frac{ne^2}{\varepsilon_0 m} \cdot \frac{1}{\omega^2} = 1 - \frac{\omega_p^{\ 2}}{\omega^2}$$

$$\omega_p = \sqrt{\frac{ne^2}{\varepsilon_0 m}}$$

plasma frequency (Hz)

Plasma frequency (ω_p) represents the oscillation of the whole electron gas in the solid.

Free Electrons in Metals

$$\tilde{n} = \sqrt{\varepsilon_r} = \sqrt{1 - \frac{\omega_p^{\ 2}}{\omega^2}}$$

$$R = \left| \frac{\tilde{n} - 1}{\tilde{n} + 1} \right|^2$$

When $\omega < \omega_p$, $\tilde{n}$ is purely imaginary. R = 100%.

Metals are like a mirror at low frequency.

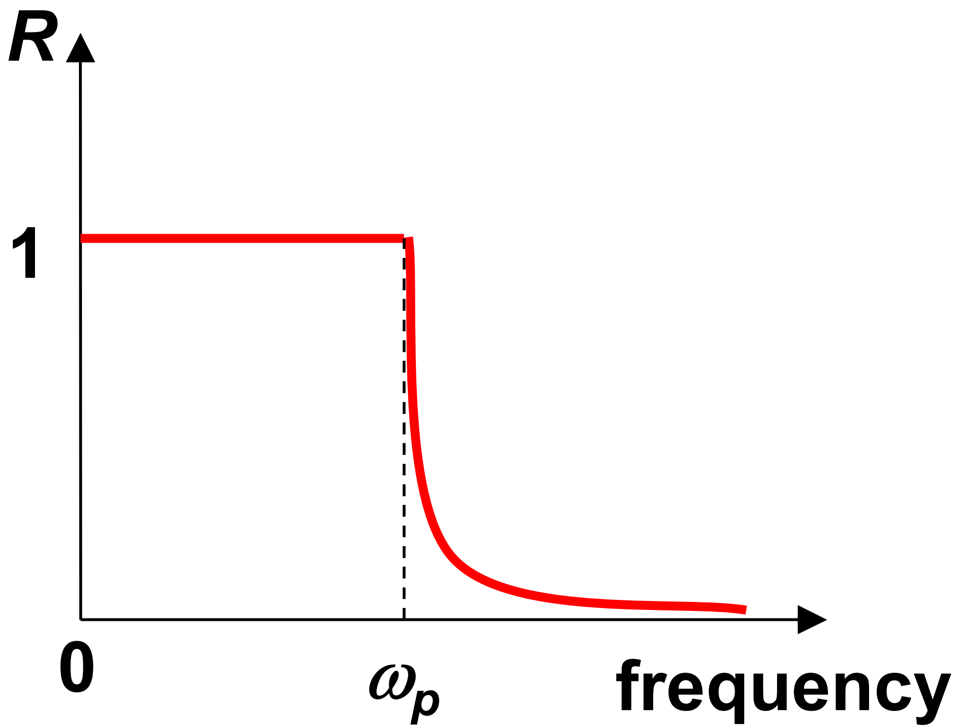
When $\omega > \omega_p$, $\tilde{n}$ is real. R decreases when ω increases
When $\omega = +\infty$, $\tilde{n}$ = 1, R = 0. Transparent like vacuum

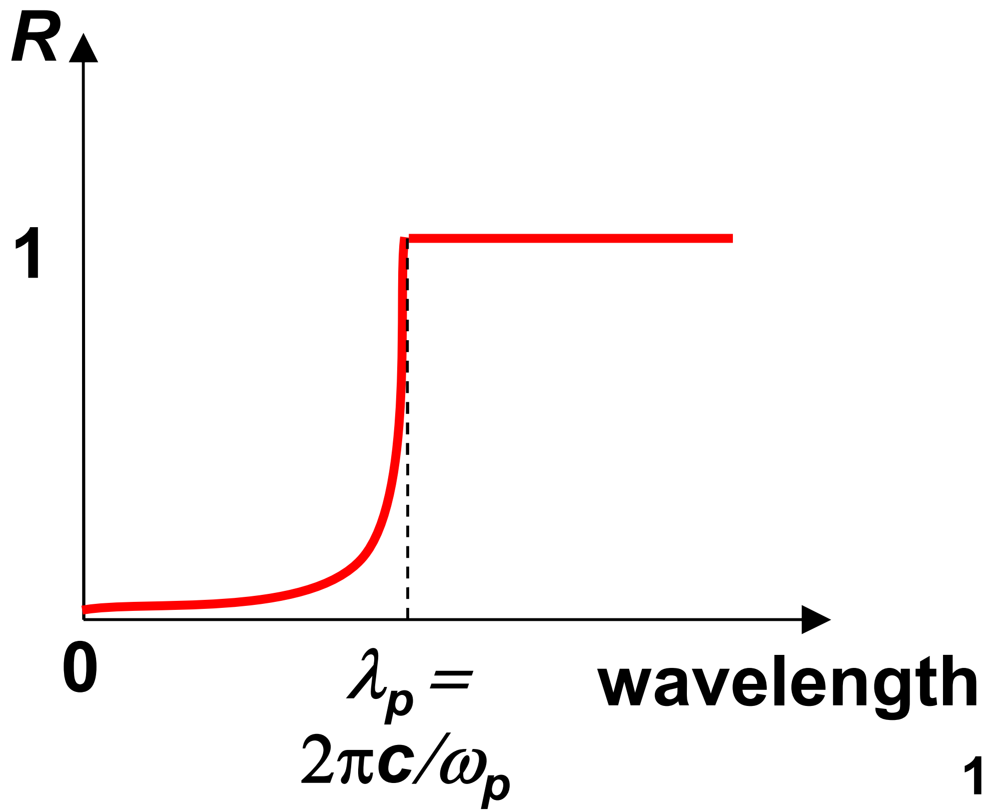
(High frequency x-rays and γ-rays can penetrate most materials)

Reflectivities of Metals

$$\tilde{n} = \sqrt{\varepsilon_r} = \sqrt{1 - \frac{{\omega_p}^2}{\omega^2}}$$

$$R = \left|\frac{\tilde{n} - 1}{\tilde{n} + 1}\right|^2$$

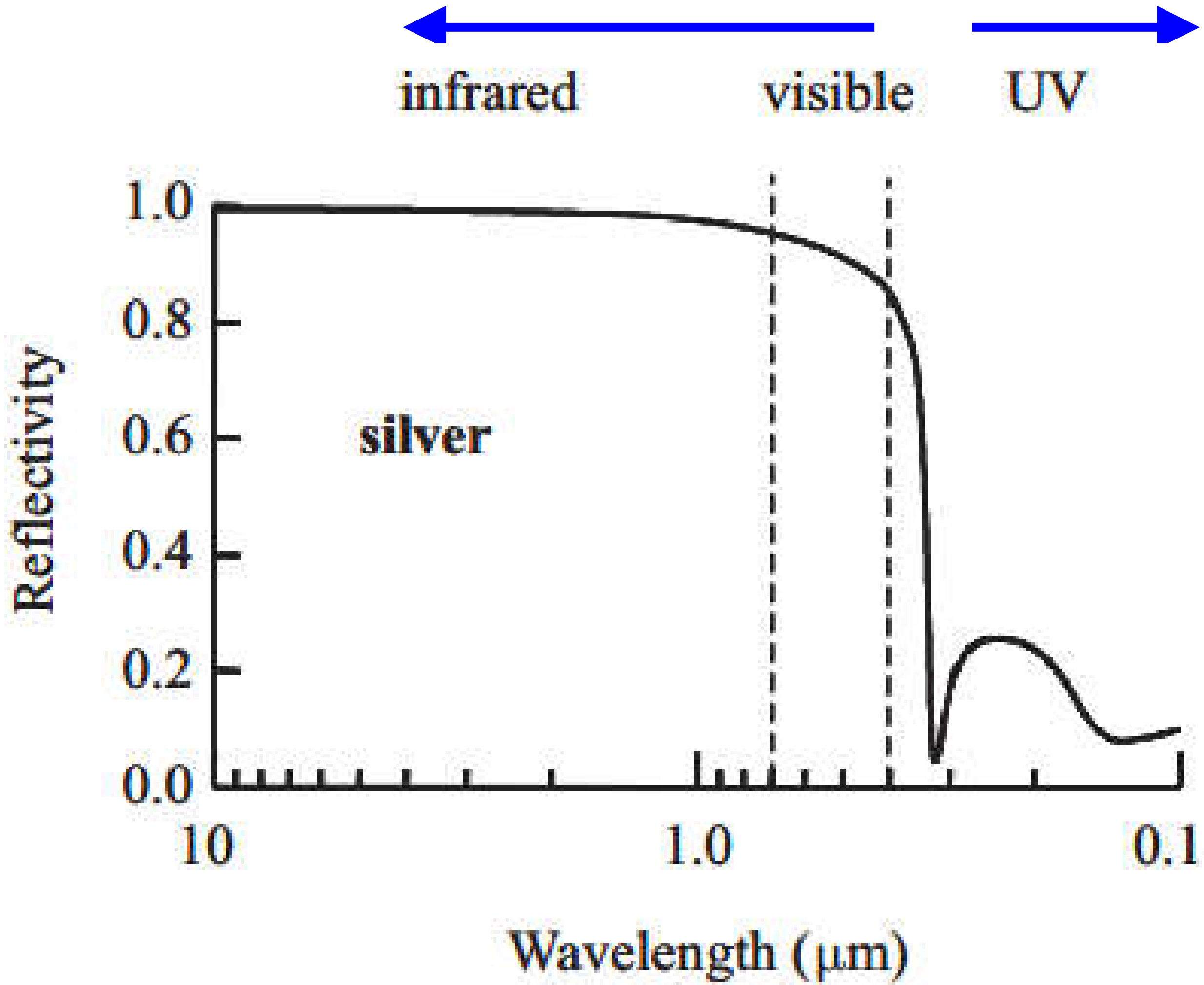




Example: Silver

reflection at long wavelength (infrared and visible)

Transmission at short wavelength (ultraviolet)



Silver mirror

Example: Metals

transmission at high frequency **reflection at low frequency**

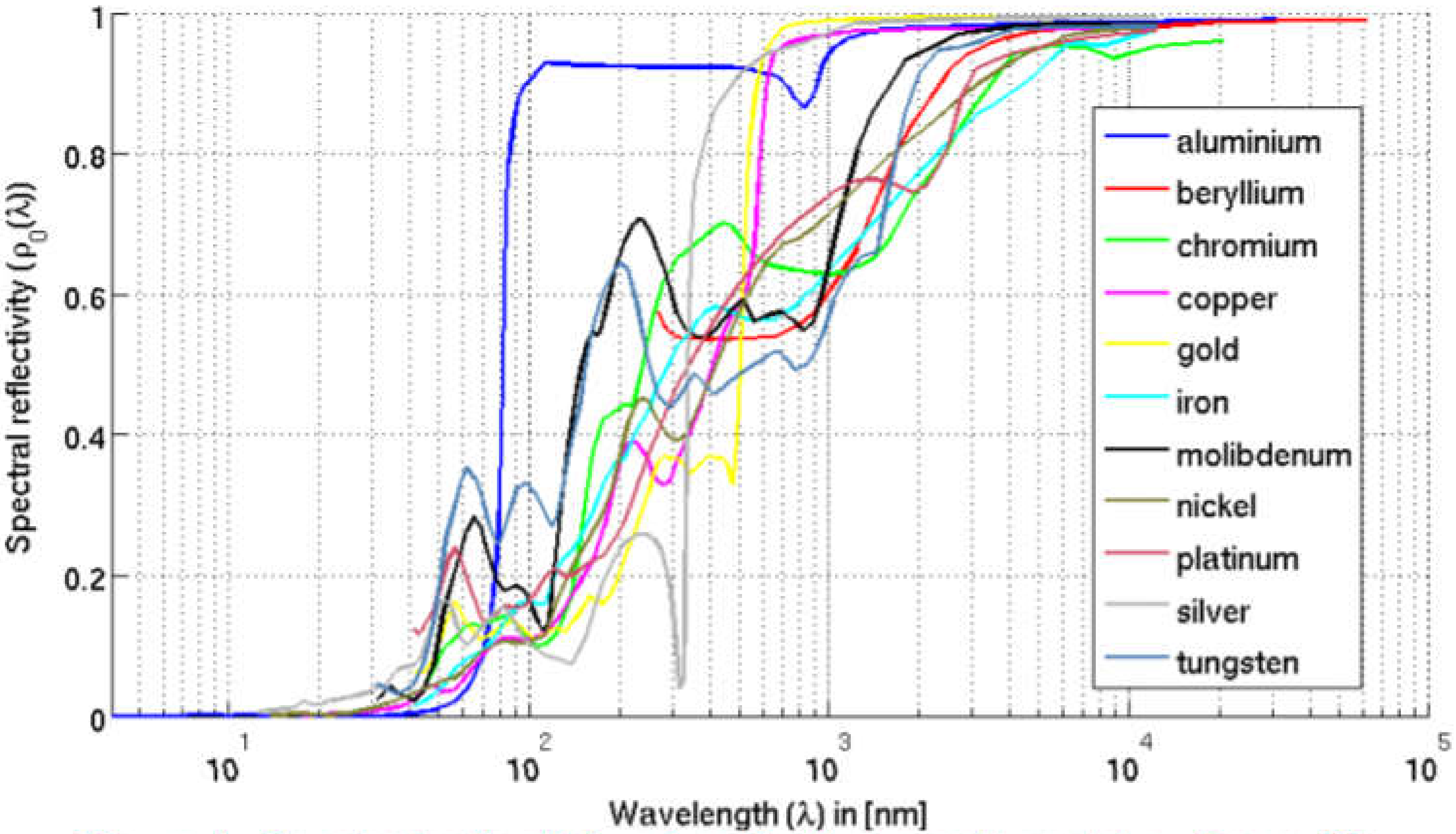


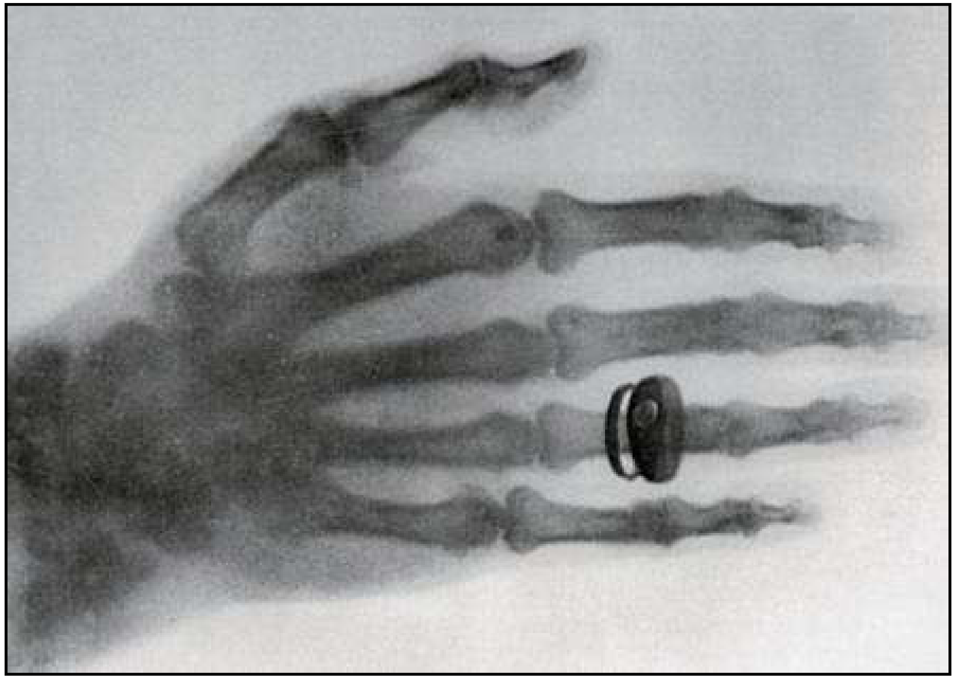
Figure 1: Spectral reflectivity of perfectly smooth metal surfaces [3]

dx.doi.org/10.3929/ethz-a-006206911

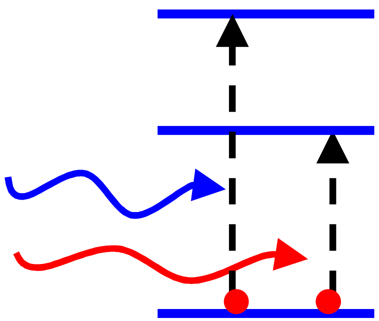
Q: Why does Aluminum have the shortest cutoff wavelength?

Example - X-ray Transmission

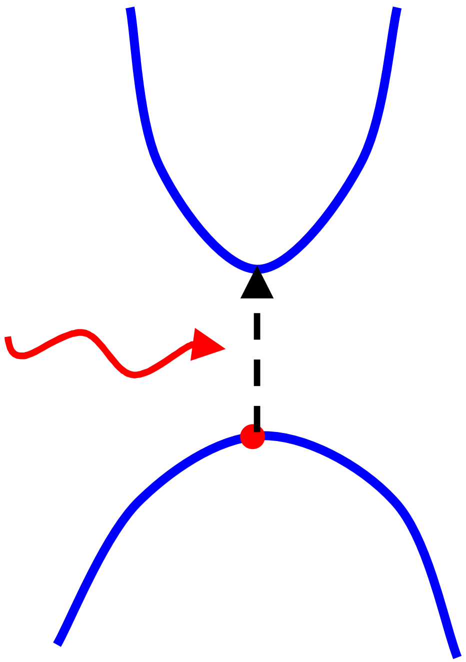
- X-ray has higher transmission for light atoms (water, skin, fat, etc.)
- X-ray has higher absorption and reflection for heavy atoms (bones, metals, etc.)



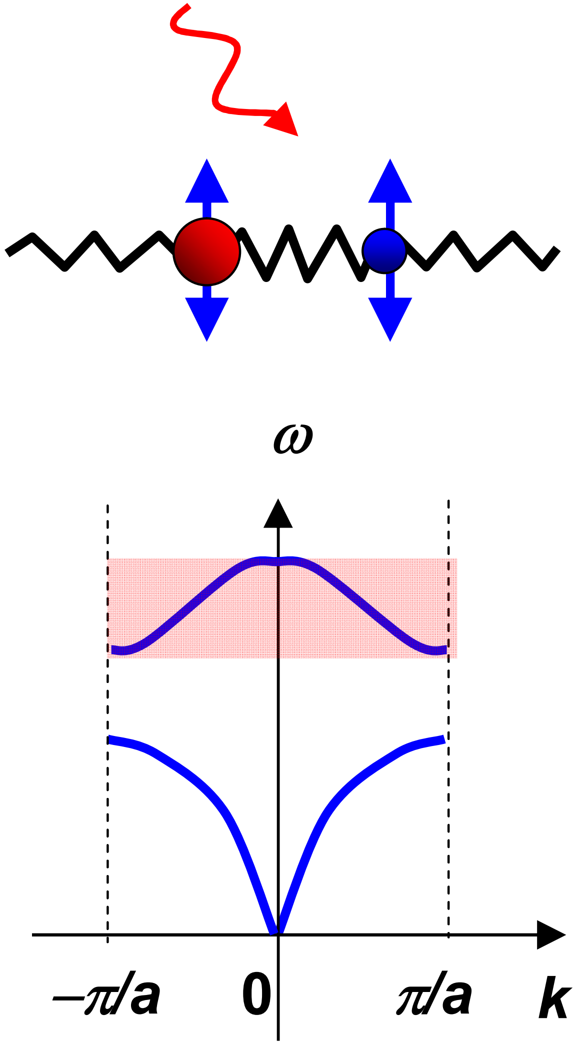
Origin of Optical Absorption κ



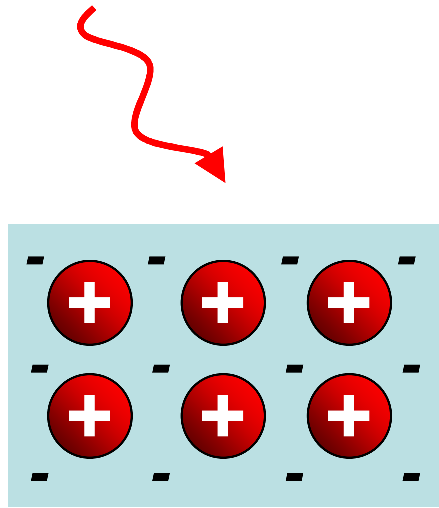
energy levels
(atoms,
defects, ...)



above band gap
(electronic
band theory)

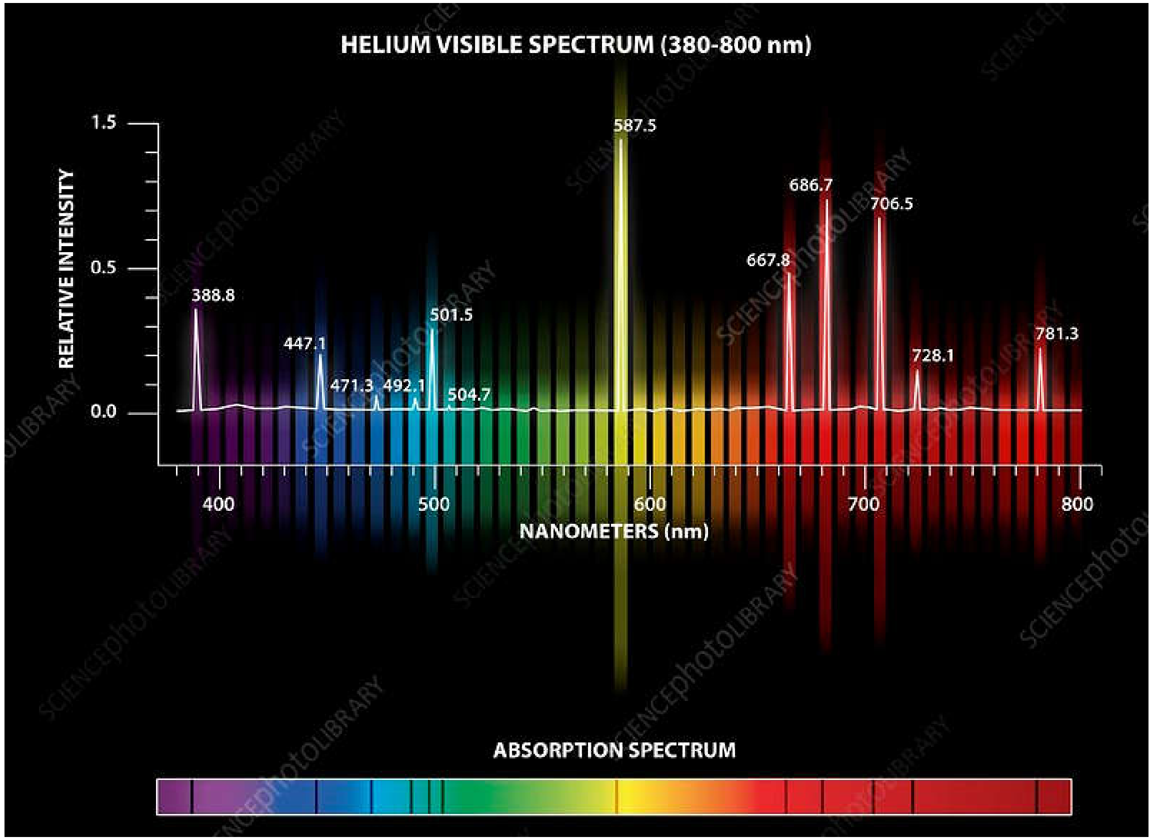


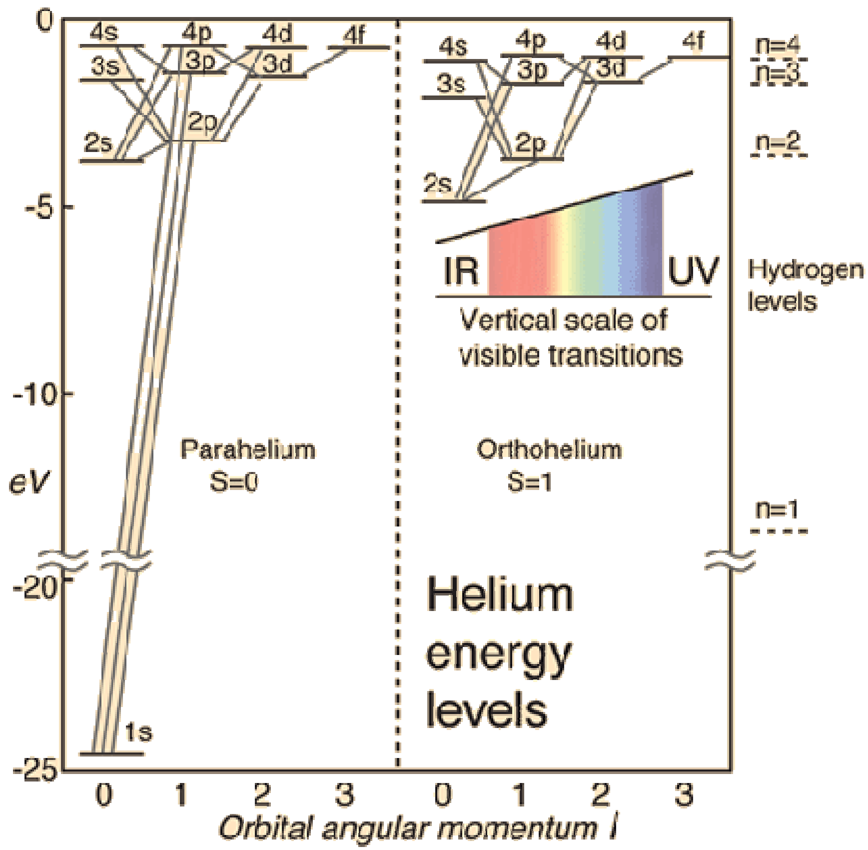
optical phonons
(Lorentz Model)



free carriers
(Drude Model)

Example: Helium





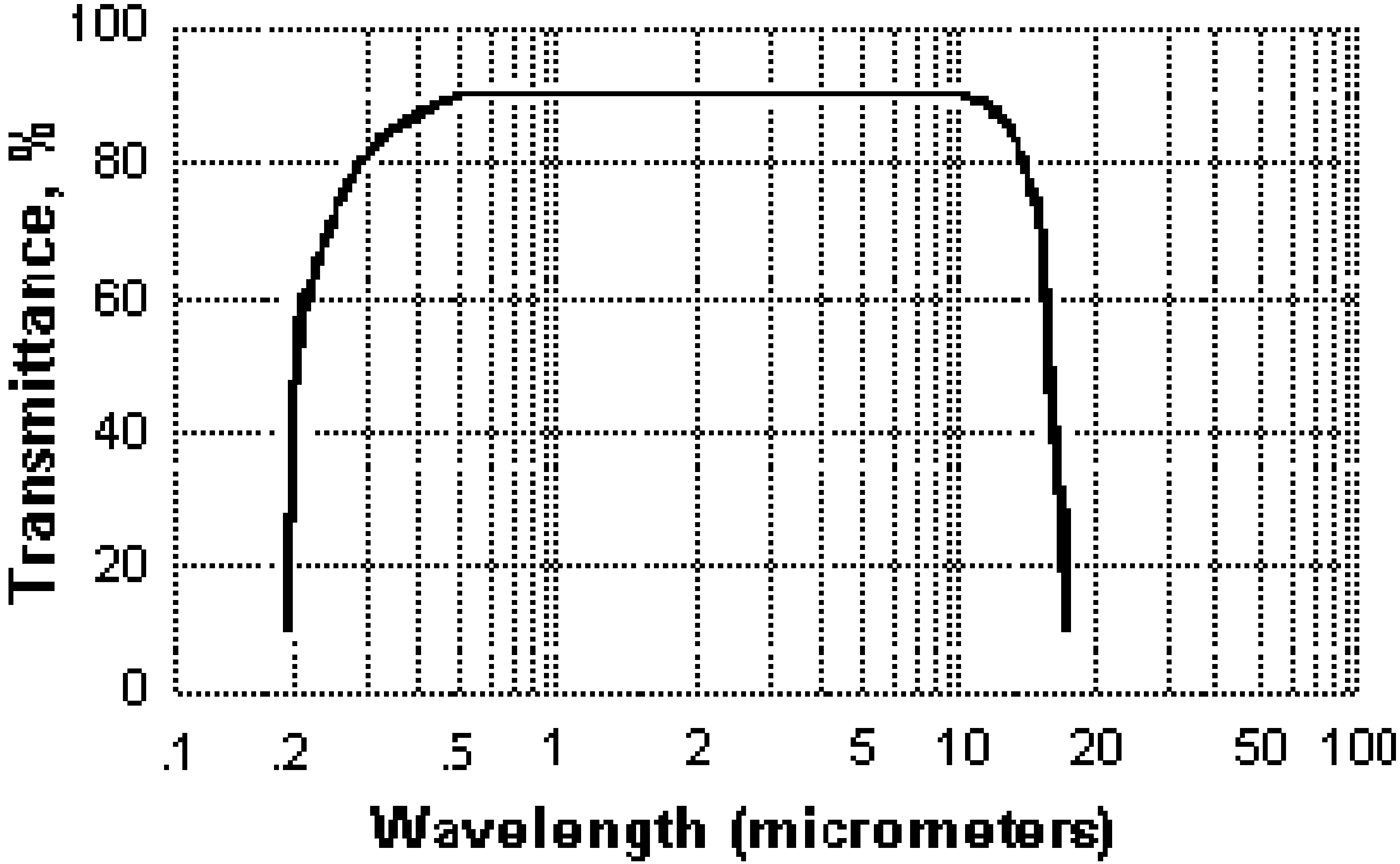
https://www.sciencephoto.com/media/673903/view/helium-emission-and-absorption-spectra
http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/helium.html

Example: NaCl

absorption above band gap (E_g ~ 8.5 eV)

transparent

absorption by crystal vibration ($2\pi\omega_{max}/c$ ~ 10 um)

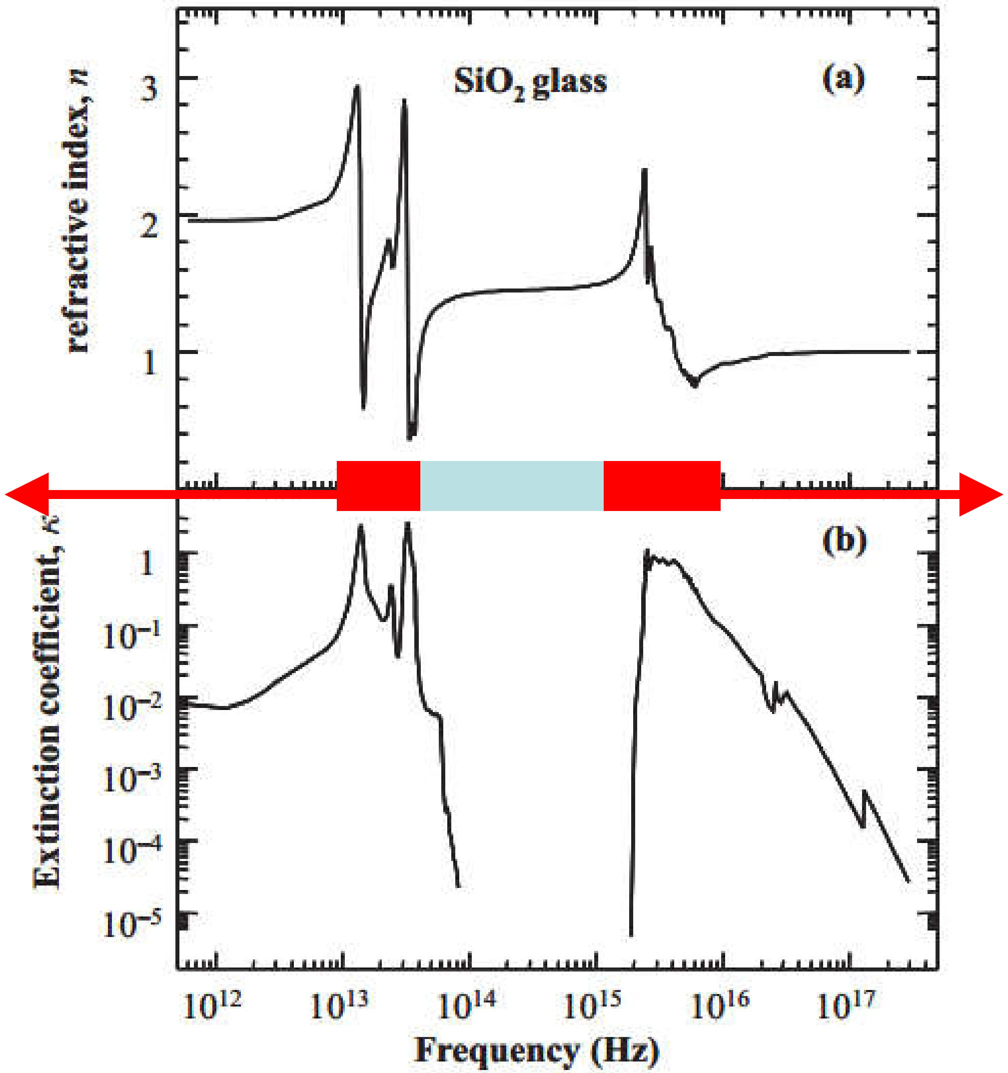


http://www.crystaltechno.com/NaCl_en.htm

Example: SiO_2 glass

transparent in the visible
(n = 1.4)

infrared absorption of optical phonons (crystal vibration)



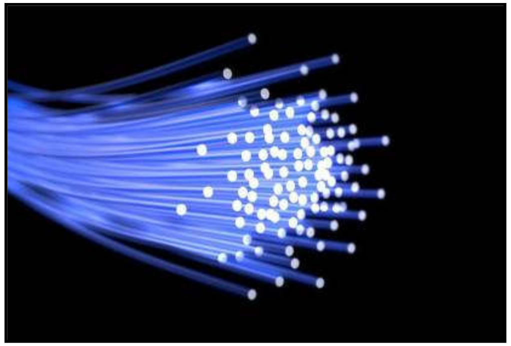
ultraviolet absorption above band gap ($E_g \approx$9 eV)

Impurities in SiO_2

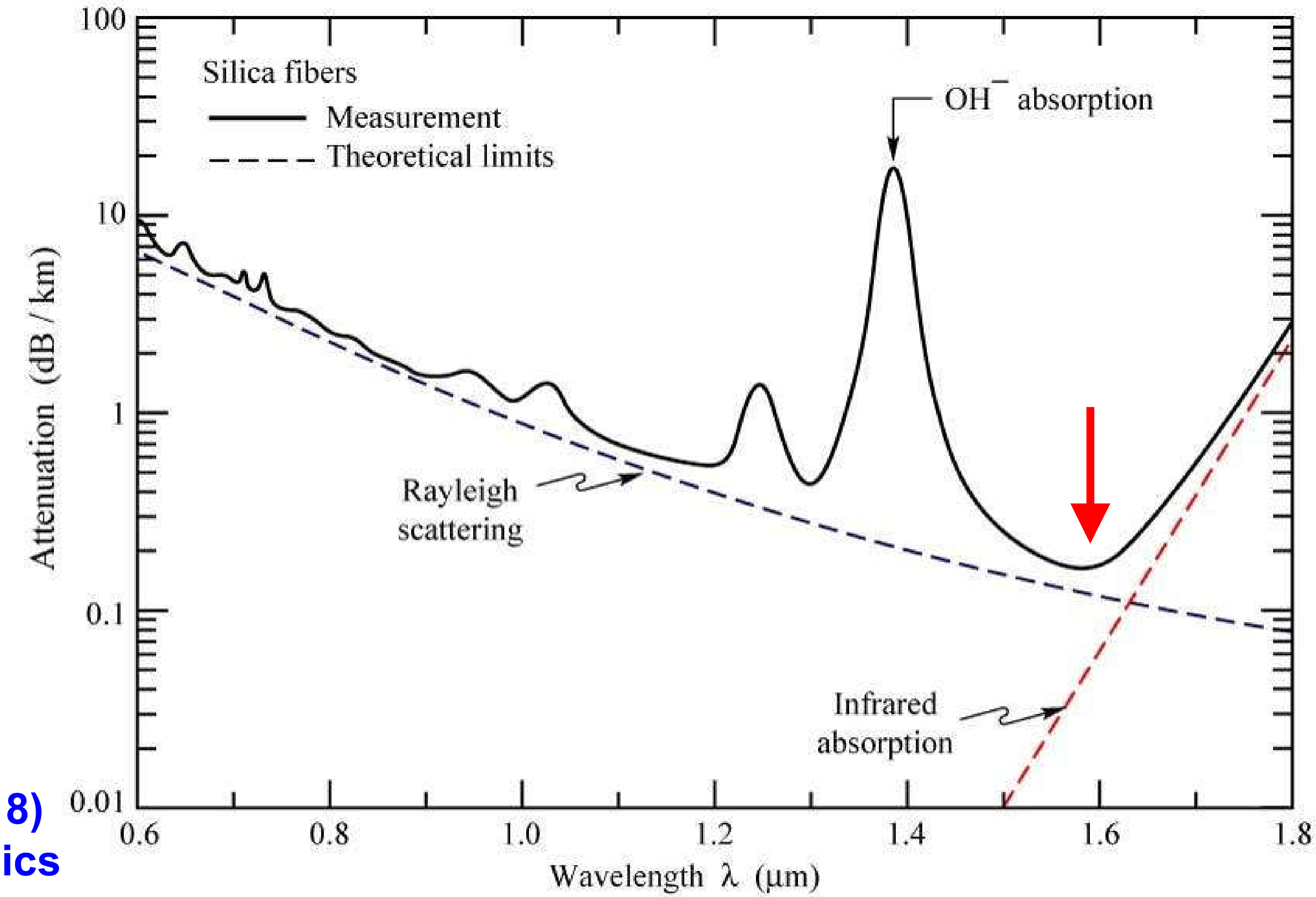
- **Why is desert yellow?**
  - because of Fe_2O_3

- **Why is beer bottle green?**
  - because of FeO

Pure SiO_2 - Optical Fibers



K. Kao (高锟) (1933–2018)
2009 Nobel Prize in Physics



minimum loss at 1550 nm, 0.2 dB/km
~ 2% loss every kilometer

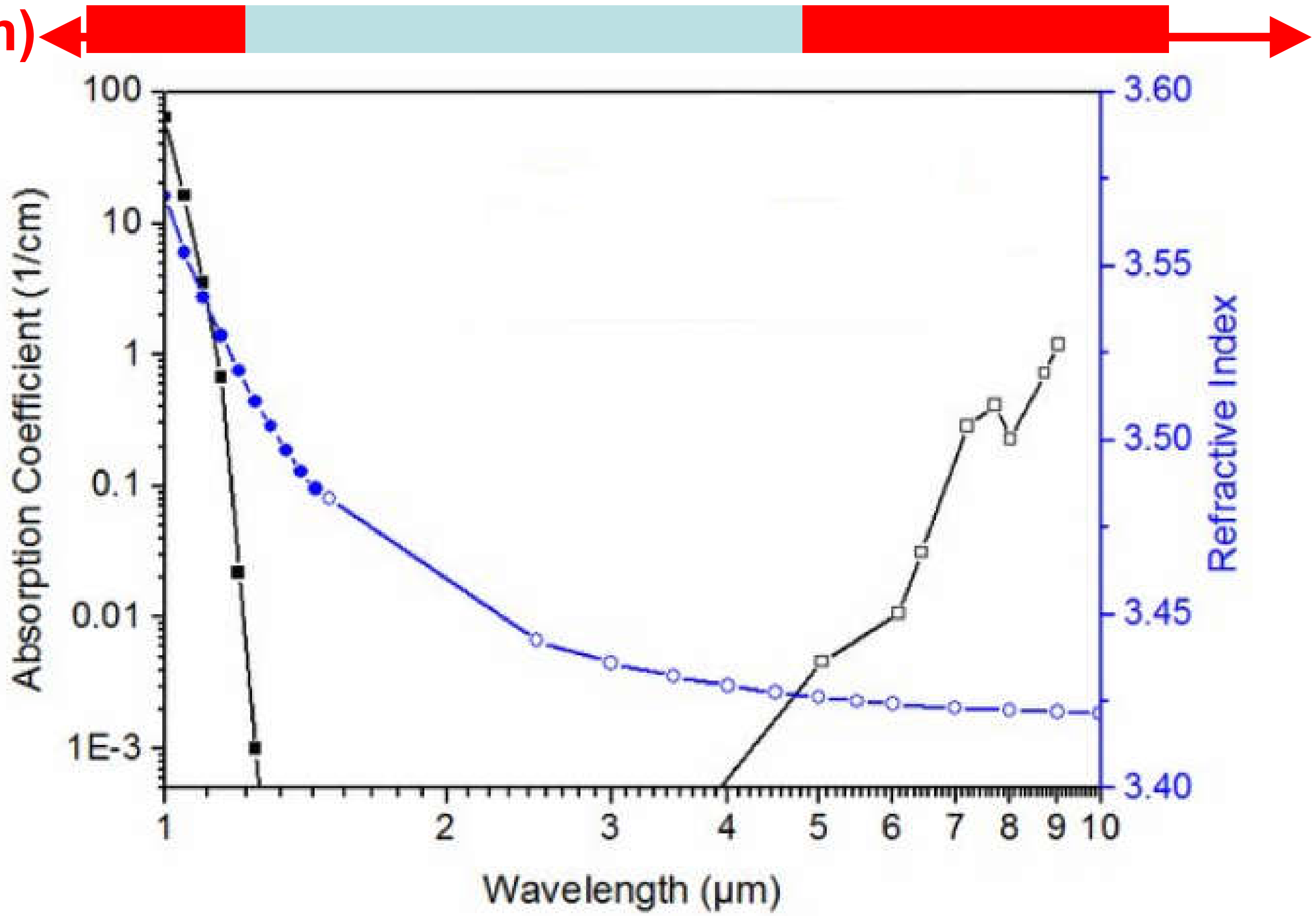
K. C. Kao, G. A. Hockham, *Proc. IEE* **113,** 1151 (1966)

Example - Silicon

absorption above band gap (E_g = 1.1 eV) (λ < 1.2 um)

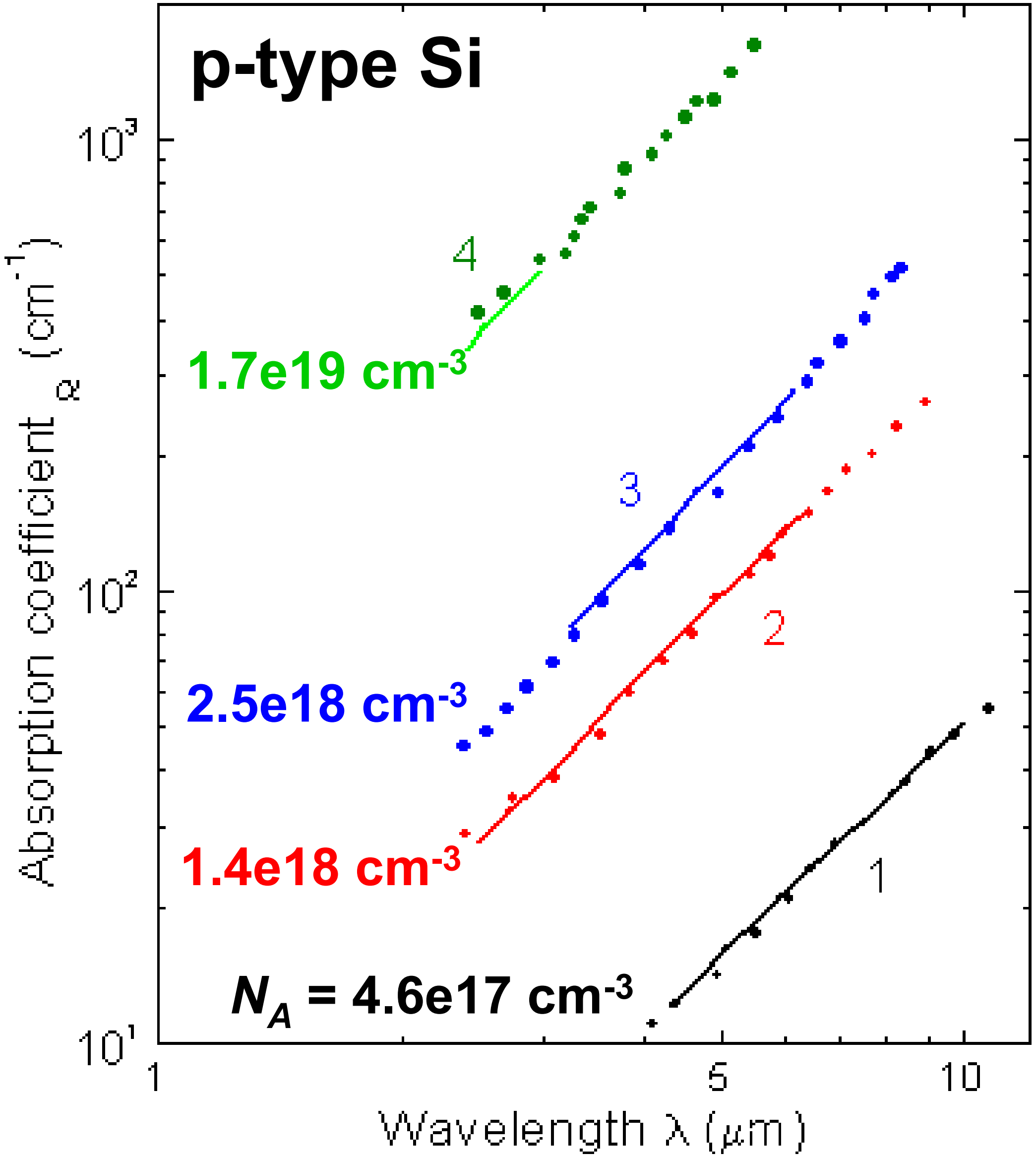
transparent in the near-infrared (n ~ 3.5)

absorption of optical phonons and free carriers



https://www.researchgate.net/publication/299465370_Silicon-germanium_for_photonic_applications

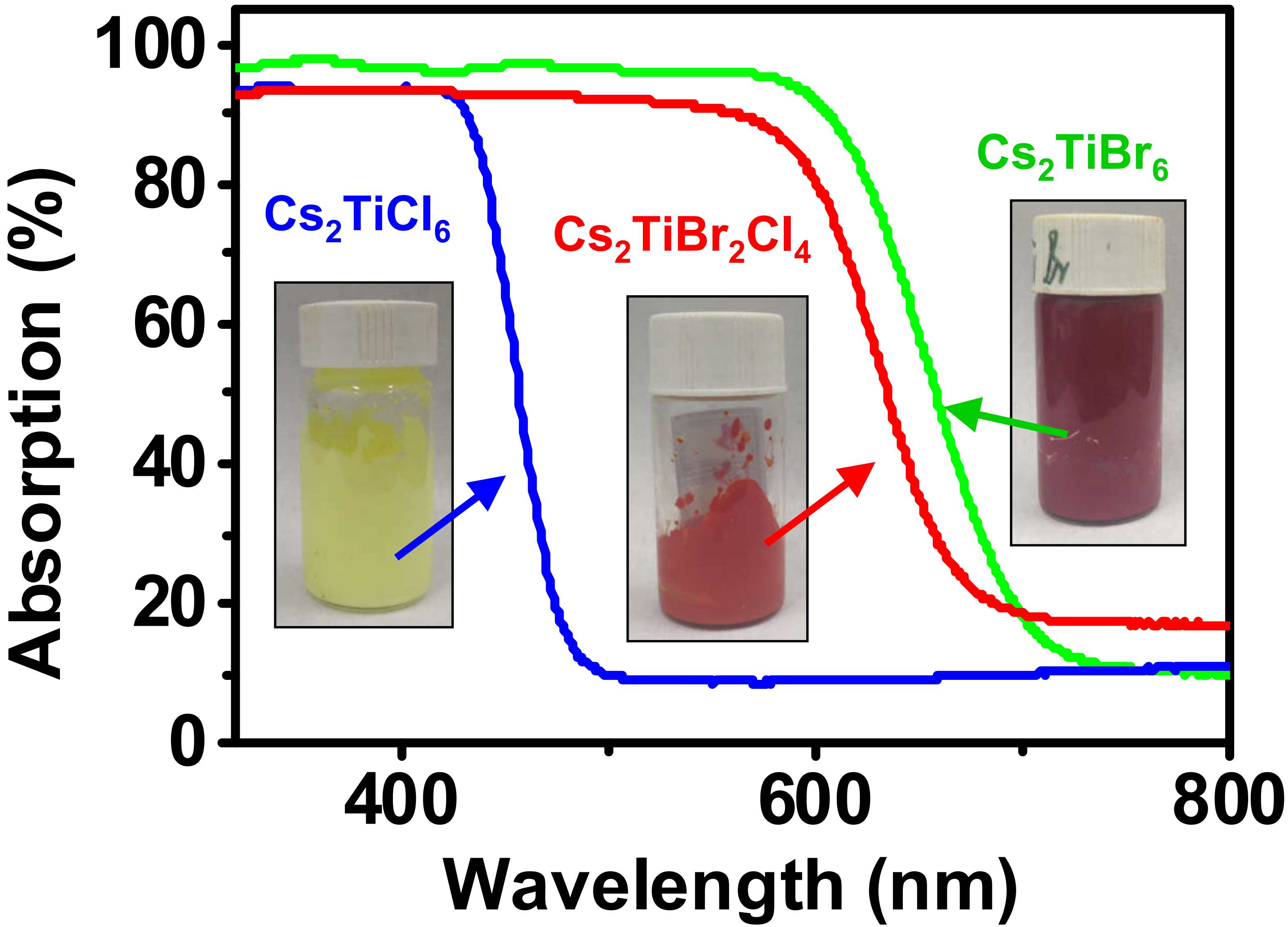
Example - Silicon (with dopants)



increased absorption caused by free carriers

H. Hara, Y. Nishi, *J. Phys. Soc. Jpn.* **21,** 1222 (1966)

Absorption and Colors

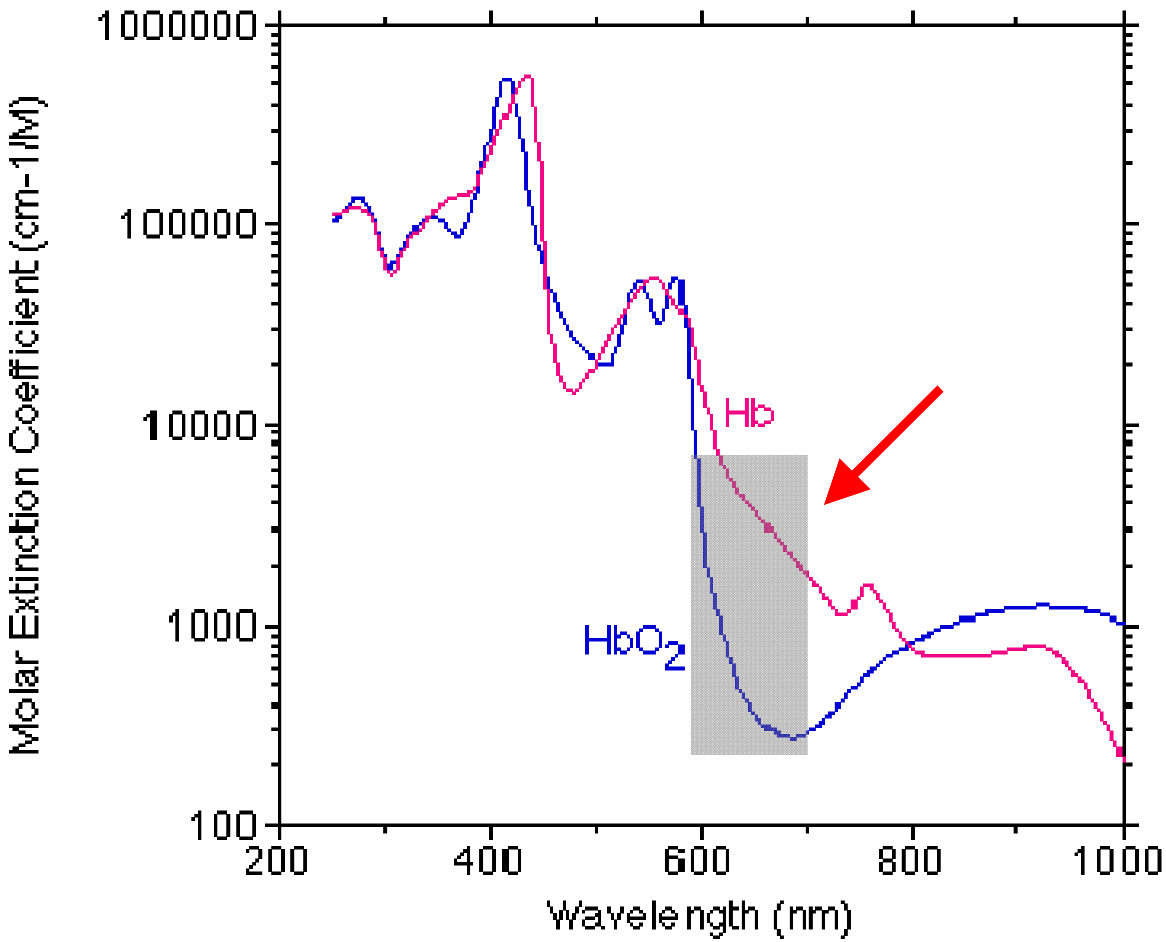


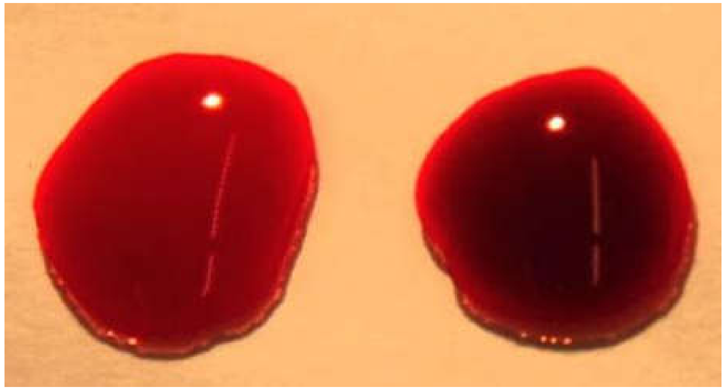
D. Kong, *et al*, *J. Mater. Chem. C* **8,** 1591 (2020)

Example: Hemoglobin (Hb, 血红蛋白)

Hb 脱氧血红蛋白　　**HbO_2 氧合血红蛋白**

Hb has higher red absorption than HbO_2





Arterial blood
动脉血

Venous blood
静脉血

oximeter

https://omlc.org/spectra/hemoglobin/index.html

Thank you for your attention