Chapter 8. Optical Properties

Index of Refraction

Optical properties of materials: Refraction, reflection, absorption, light emission
(Relation between them)

- Index of refraction without absorption:

$$r = c/v = \sqrt{\varepsilon_r \mu_r}$$

ε_r: dielectric constant
μ_r: permeability

- Index of refraction with absorption:

$$r^* = r + i\Gamma$$

Γ: absorption index

- Absorption constant (α):

$$\alpha = \frac{2\omega\Gamma}{c} = \frac{4\pi\Gamma}{\lambda}$$

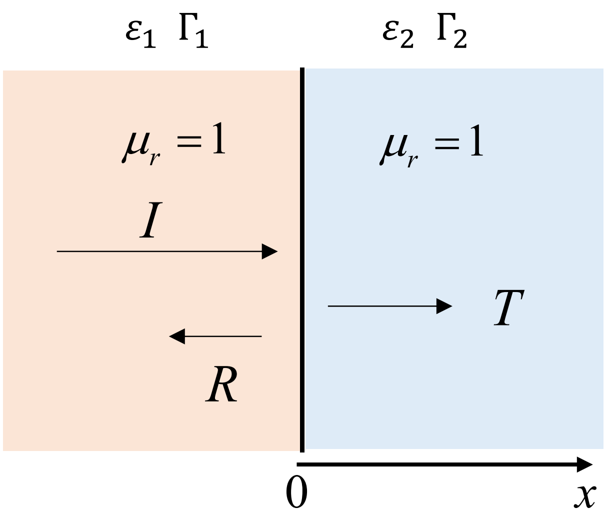
- Relationship between r and α

$$r^2 - \Gamma^2 = \varepsilon_r \mu_r$$

$$r^2 = \varepsilon_r \mu_r + \frac{c^2 \alpha^2}{4\omega^2}$$

: The refractive index can be determined by first calculating $\alpha(\omega)$ from a specific absorption mechanism.

Reflection



Electric (E_y) and magnetic (H_z)components are continuous and conserved across $x = 0$

I : Incident electric and magnetic waves
R : Reflected electric and magnetic waves
T : Transmitted electric and magnetic waves
$\boxed{I = R + T}$ [energy conservation]

ε: dielectric constant
Γ: absorption index
r: index of refraction

For an interface between a vacuum and a material without absorption on either side,

$$R = \frac{(r-1)^2}{(r+1)^2}$$

For an interface between a vacuum and a material with index of refraction (r) and absorption index (Γ),

$$R = \frac{(r-1)^2 + \Gamma^2}{(r+1)^2 + \Gamma^2}$$

$$\boxed{R = \frac{(r_2 - r_1)^2 + (\Gamma_2 - \Gamma_1)^2}{(r_2 + r_1)^2 + (\Gamma_2 + \Gamma_1)^2}}$$ [general form]

Reflection

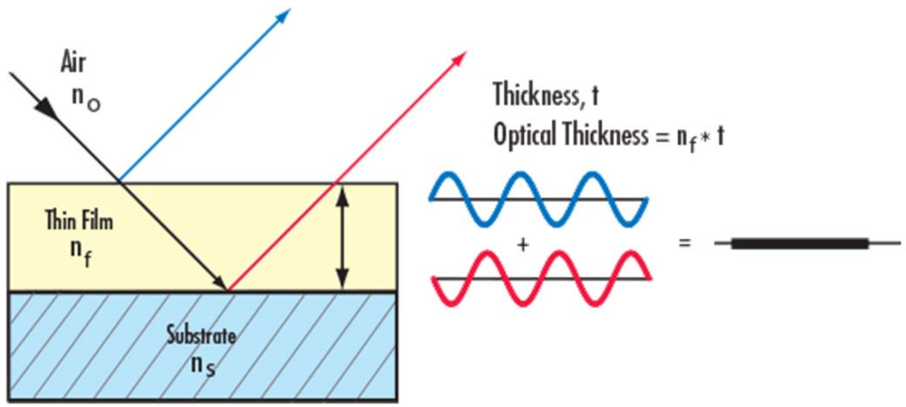
$$R = \frac{(r-1)^2 + \Gamma^2}{(r+1)^2 + \Gamma^2}$$

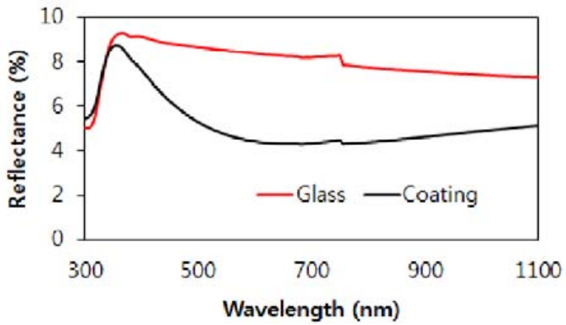
: For a strongly absorbing material with high Γ, R should be unity ($R \rightarrow 1$)

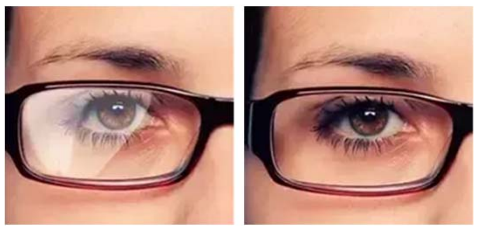
Q: A material with higher absorption index can reflect more light. True or false?

A: The absorbed light cannot penetrate the material ($T = 0$). Due to energy conservation, the light should be reflected. ($R = I - T \approx 1$)

ex) Antireflection coating (MgF_2)

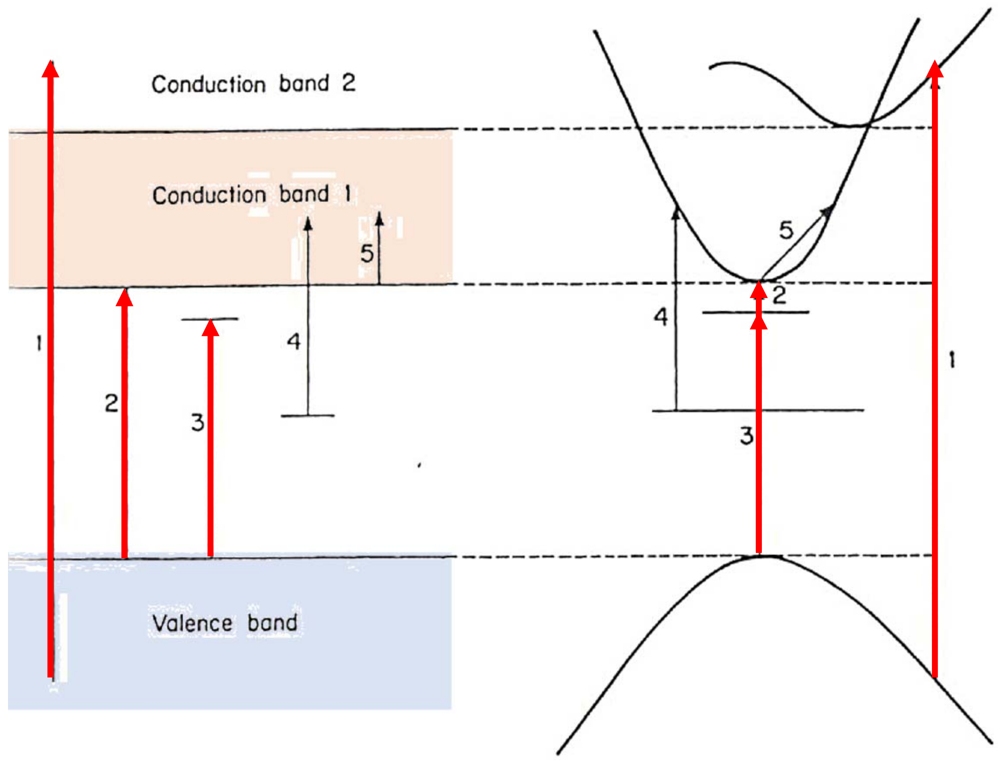






Summary of absorption processes

1) Electron transition from the valence band to higher-lying conduction bands. Continuous high absorption processes. Absorp. Coef. (α) = $10^5 \sim 10^6$ cm^{-1}
2) Electron transition from the valence band to the lowest-lying conduction band with a minimum required energy of the forbidden band gap. Direct or indirect transition.
3) Optical transition producing bound electron-hole pair (excitons), requiring less energy than to produce a free electron-hole pair by the system. For free carriers, excitons should be thermally dissociated. The excitons can recombine with the emission of light or phonons.

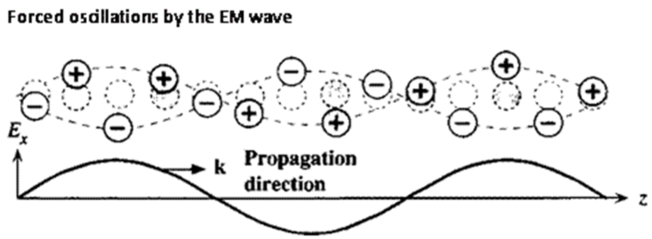


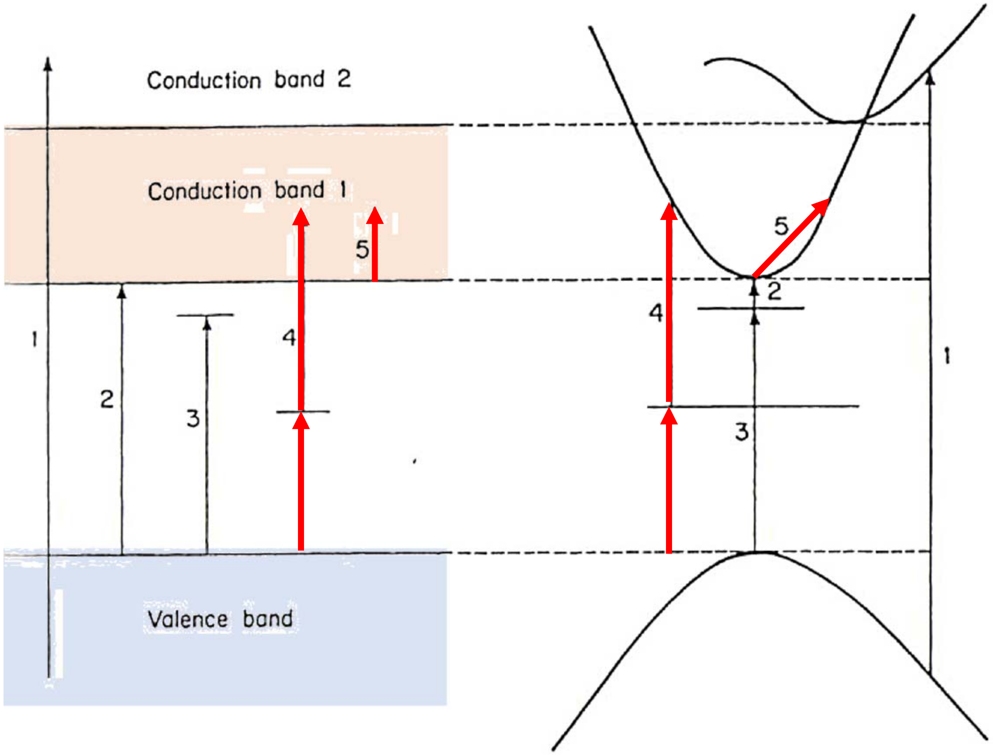
Summary of absorption processes

4) Midgap states by imperfections, such as defects and impurities. Discrete levels within a band gap. Absorp. Coef. (α) < 10^3 cm^{-1}

5) Absorption by free carriers. Transition to higher energy states within the same band or to higher bands. It involves the absorption of both photons and phonons because both *E* an *k* must be change in the transition.

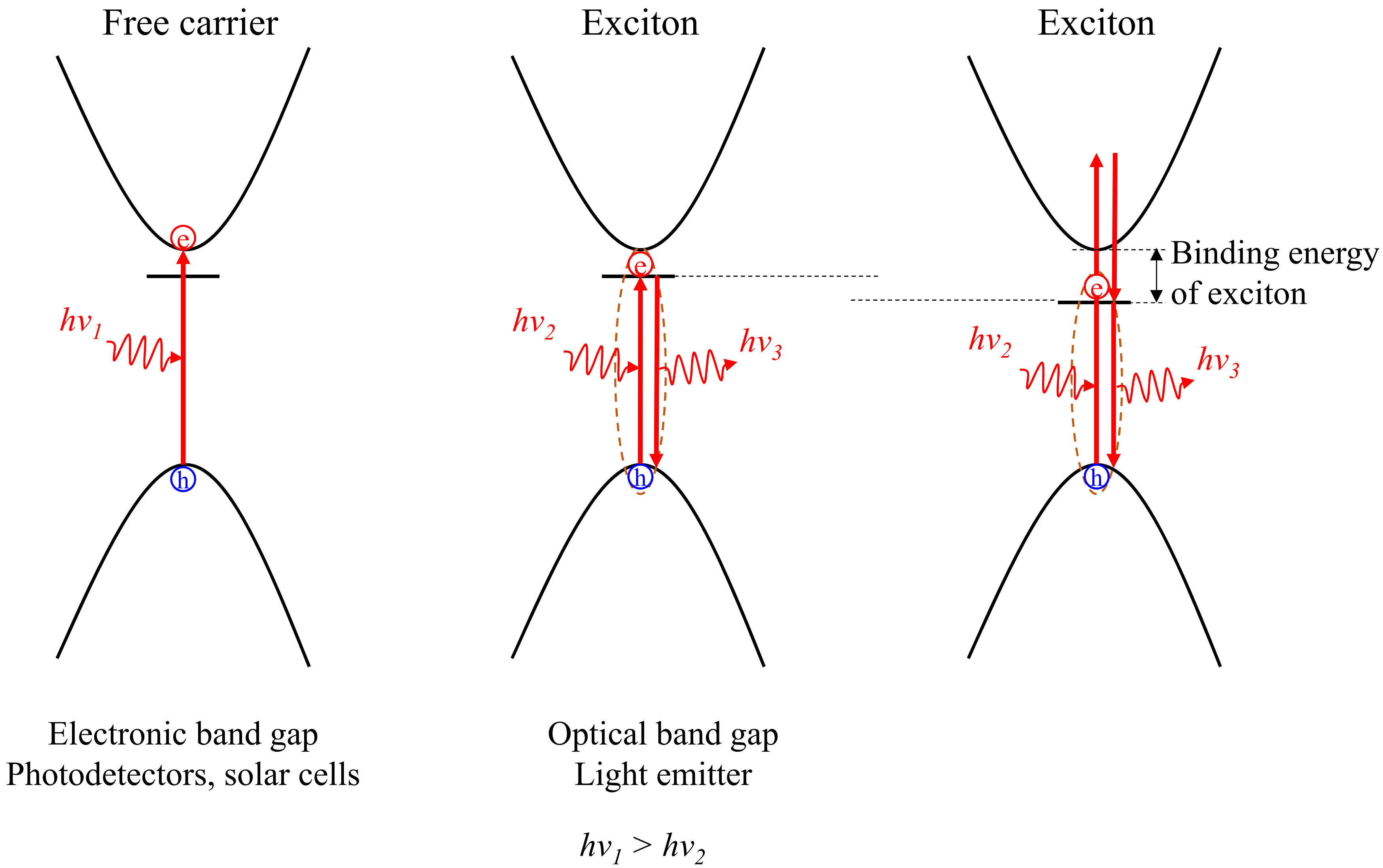
6) Reststrahlen absorption (ch. 3) – interaction between light wave and lattice wave. (Does not involve electronic transition.)





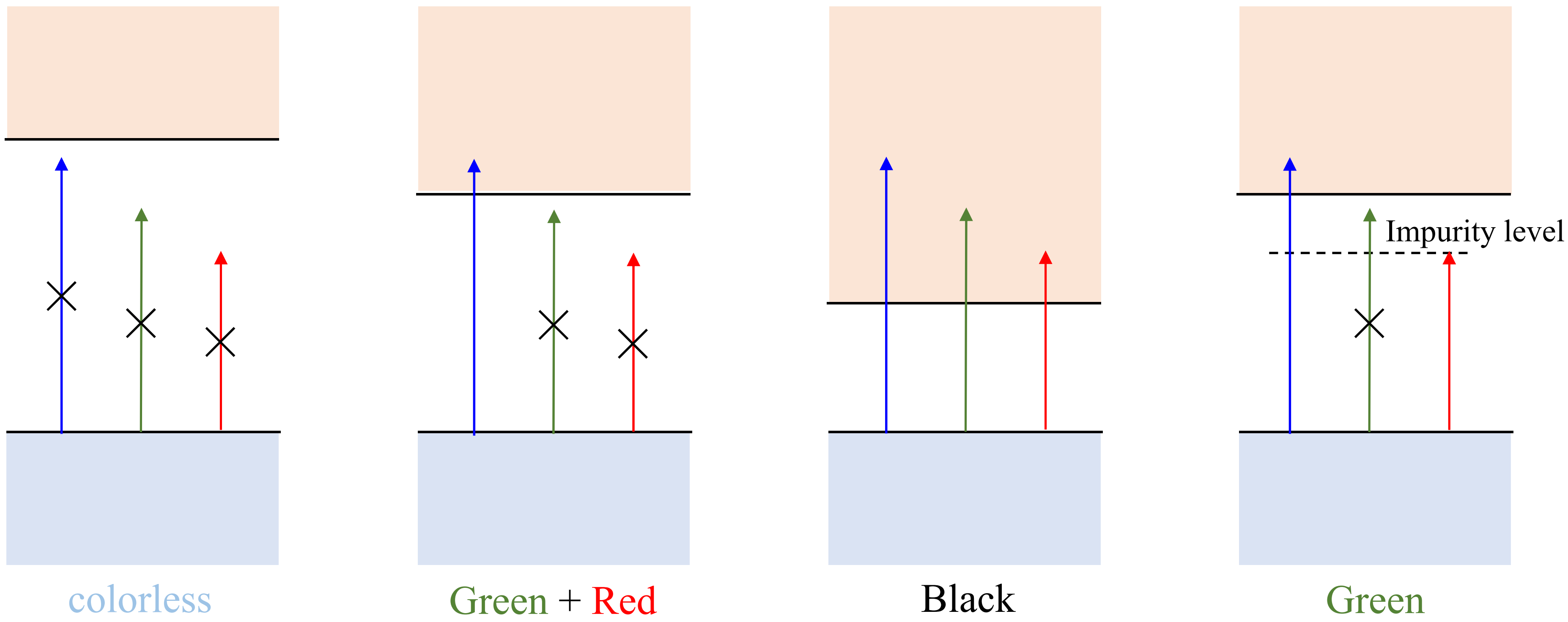
Higher photon energy is required for transition in order of 1 to 6.
ex) E_{ph} in process 1 > E_{ph} in process 2 > E_{ph} in process 3 > E_{ph} in process 4 …

Summary of absorption processes

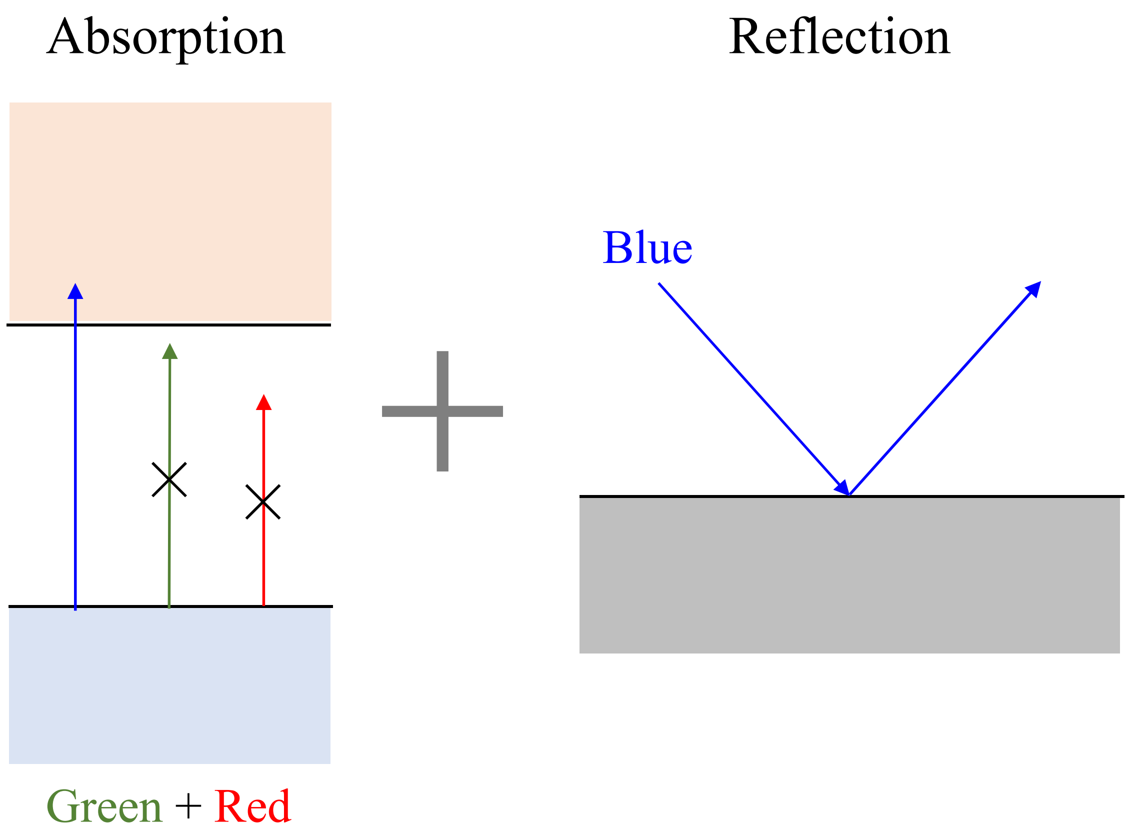


Transition across the band gap

- The band-to-band transition are the cause of the fundamental absorption edge of the material, and hence of the apparent *color* by *transmission* of many semiconductors.



Transition across the band gap



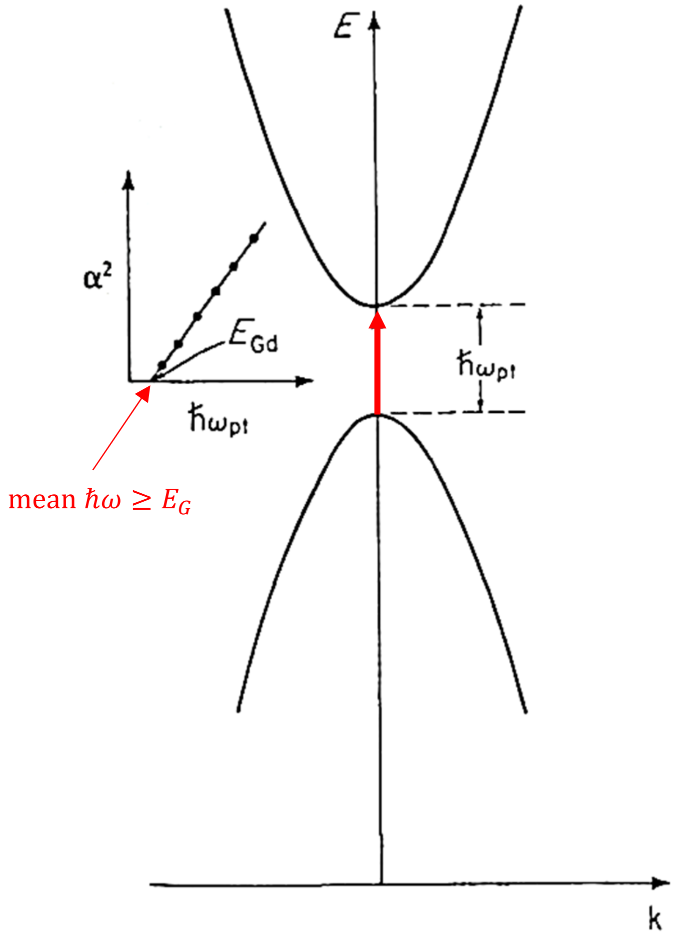
= Green + Red + Blue

However, reflection is not dominant rather than transmission. So, Blue is weak.

Band-to-band transition

[Direct band gap]

Transition between the conduction band and valence band extrema at the same value of k



- Energy conservation

$$\hbar\omega_{pt} = E_{Gd} + \frac{\hbar^2 {k_0}^2}{2m_r^*}$$

E_{Gd}: direct band gap
k_0: k value for optical transition
m_r^*: reduced mass

$$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

- Momentum conservation

$$\Delta k \sim K_{photon} \sim 0$$

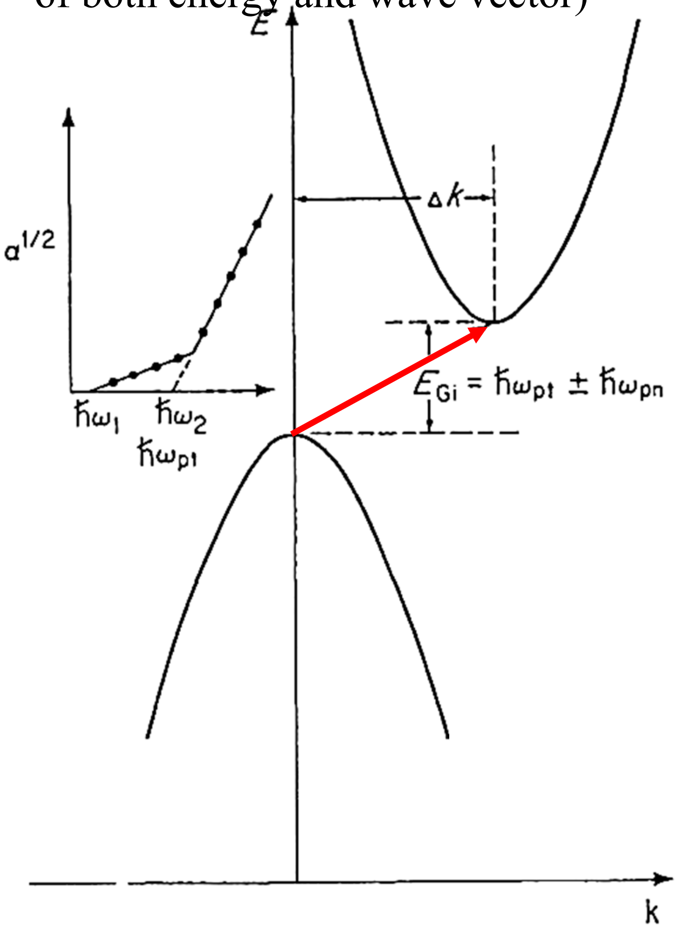
- Transmission probability (absorption coef.)

$$\alpha \propto \left(\hbar\omega_{pt} - E_{Gd}\right)^{1/2}$$

: The values of α increases rapidly with photon energy larger than EG to values in the range of 10^5~10^6 cm^{-1}. This relation holds only for a small range of photon energies greater than E_G. In the plot of α^2 vs. $\hbar\omega_{pt}$, the intercept is E_{Gd}.

Band-to-band transition

[Indirect band gap]
Transition between the extrema of conduction and valence bands at different points in *k* space. (Change of both energy and wave vector)



- Energy conservation

$$\Delta E = \hbar\omega_{pt} \pm \hbar\omega_{pn}$$

Phonon energy absorbed or emitted.

+ : absorption
− : emission

- Momentum conservation

$$\Delta k = K_{pt} \pm K_{pn} = K_{pn}$$

Wave vector

- Transmission probability (absorption coef.)

$$\alpha \propto \left[\underbrace{\frac{\left(\hbar\omega_{pt} + \hbar\omega_{pn} - E_{Gi}\right)^2}{e^{\hbar\omega_{pn}/kT} - 1}}_{\text{Phonon absorption}} + \underbrace{\frac{\left(\hbar\omega_{pt} - \hbar\omega_{pn} - E_{Gi}\right)^2 e^{\hbar\omega_{pn}/kT}}{e^{\hbar\omega_{pn}/kT} - 1}}_{\text{Phonon emission}} \right]$$

In the plot of $\alpha^{1/2}$ vs. $\hbar\omega_{pt}$, two straight lines with intercepts of $\hbar\omega_1$ and $\hbar\omega_2$.

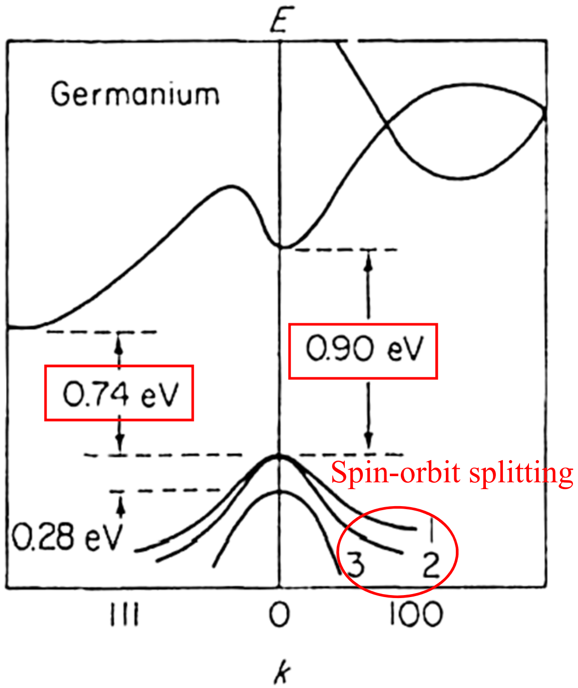
$$E_{Gi} = \frac{\hbar\omega_1 + \hbar\omega_2}{2}$$

$$\hbar\omega_{pn} = \frac{\hbar\omega_2 - \hbar\omega_1}{2}$$

Indirect band gap materials

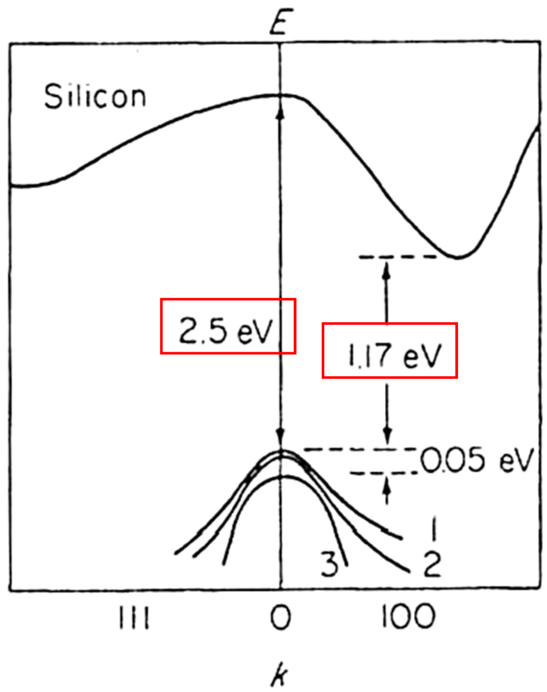
Ge

- E_{Gi}=0.74 eV corresponding to a conduction band minimum at the 111 zone face
- A direct band gap of 0.90 eV at k=0

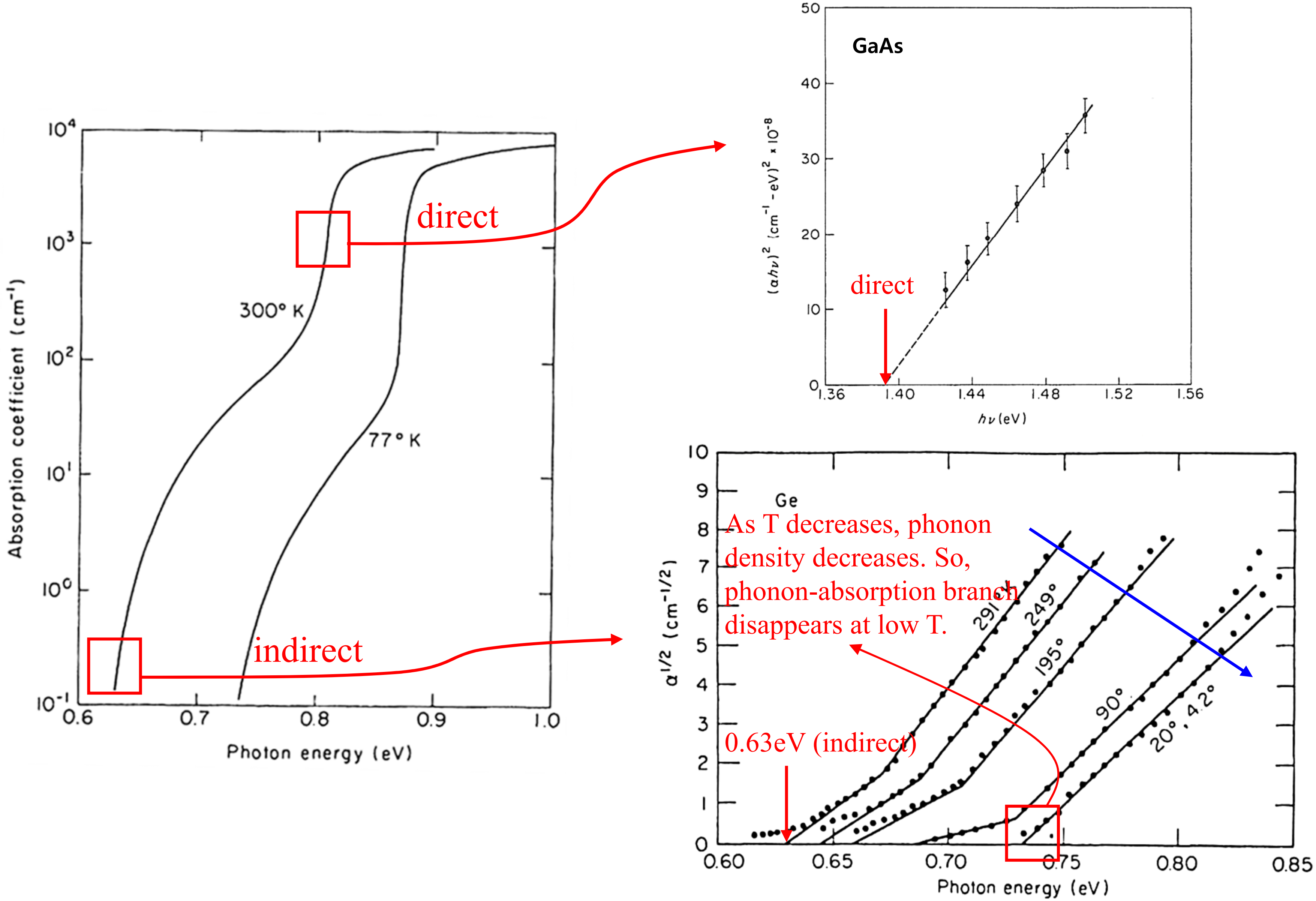


Si

- E_{Gi}=1.17 eV in the 100 direction about 85% of the way to the zone face
- A direct band gap of 2.5 eV at k=0

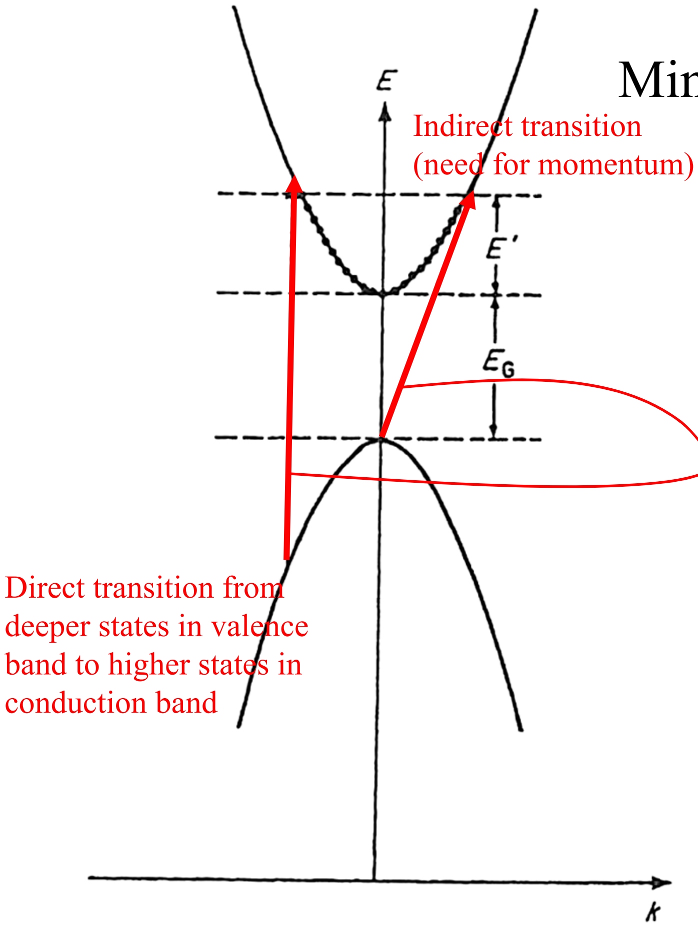


Indirect band gap materials



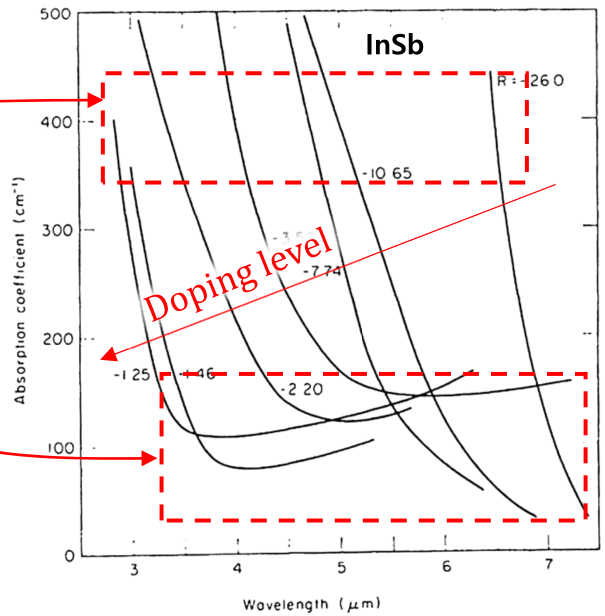
Degenerate semiconductors

- "Degenerate" means that E_F lies in a conduction band.
  (different from "degenerate" in chapter 3)
- Optical absorption edge ~ a function of carrier density if free electrons fill up the lowest states in the conduction band by a large density of impurities.



Minimum photon energy for transition: $\hbar\omega_{pt} \geq E_G + E'$

where $E' = (E_F - E_c)$, the height of the Fermi level above the bottom of the conduction band

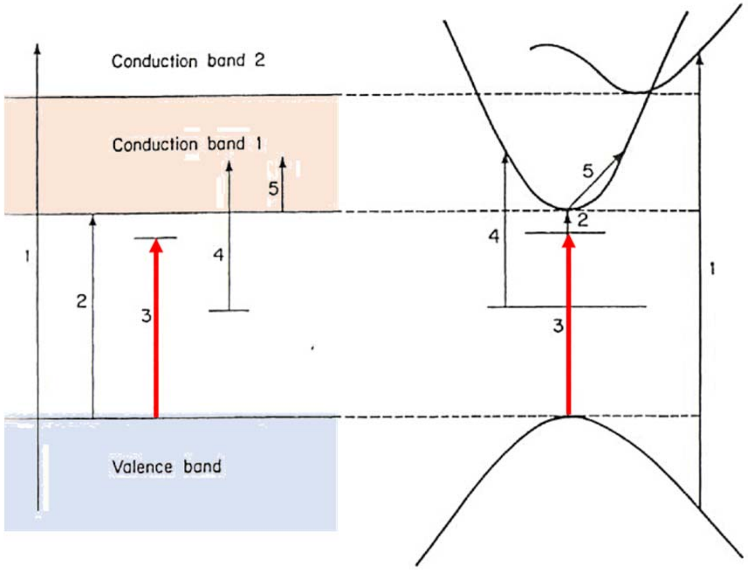


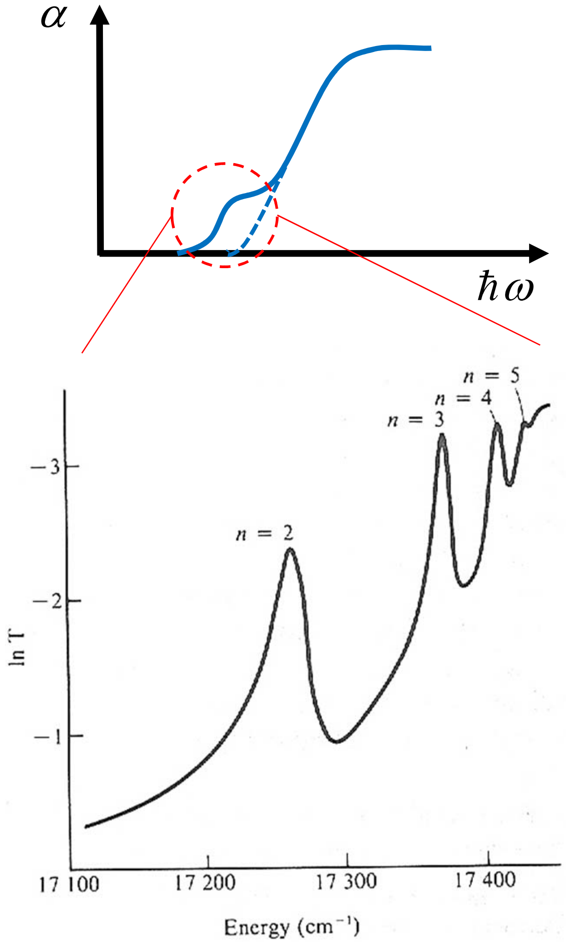
R_H: Hall constant
$n = 6.25 \times 10^{17}/R_H$

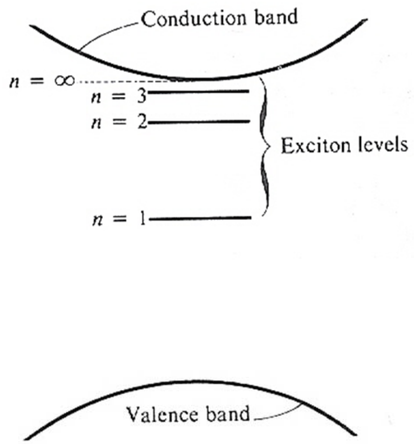
1r

Excitons

: Bound electron-hole pairs, Neutral in charge







Allowed energy states for exciton (from hydrogen model)

Excitons

- Binding energy or dissociation energy of exciton

$$E_{ex,\,\mathrm{n}} = \frac{M_r/m}{{\varepsilon_r}^2 n^2} E_H$$

where E_H is the ground state energy of the isolated hydrogen atom (-13.5 eV) and M_r is a reduce mass

$$\frac{1}{M_r} = \frac{1}{{m_e}^*} + \frac{1}{{m_h}^*}$$

- Exciton binding energy is a strong function of dielectric constant ε_r

$$E_H = -13.5\ eV \qquad {m_e}^* = {m_h}^* = m \qquad \varepsilon_r = 10 \Rightarrow E_{ex,\,\mathrm{n}} = -\frac{0.067}{n^2} eV$$

:Dissociation rate of exciton is high at high T due to thermal energy.

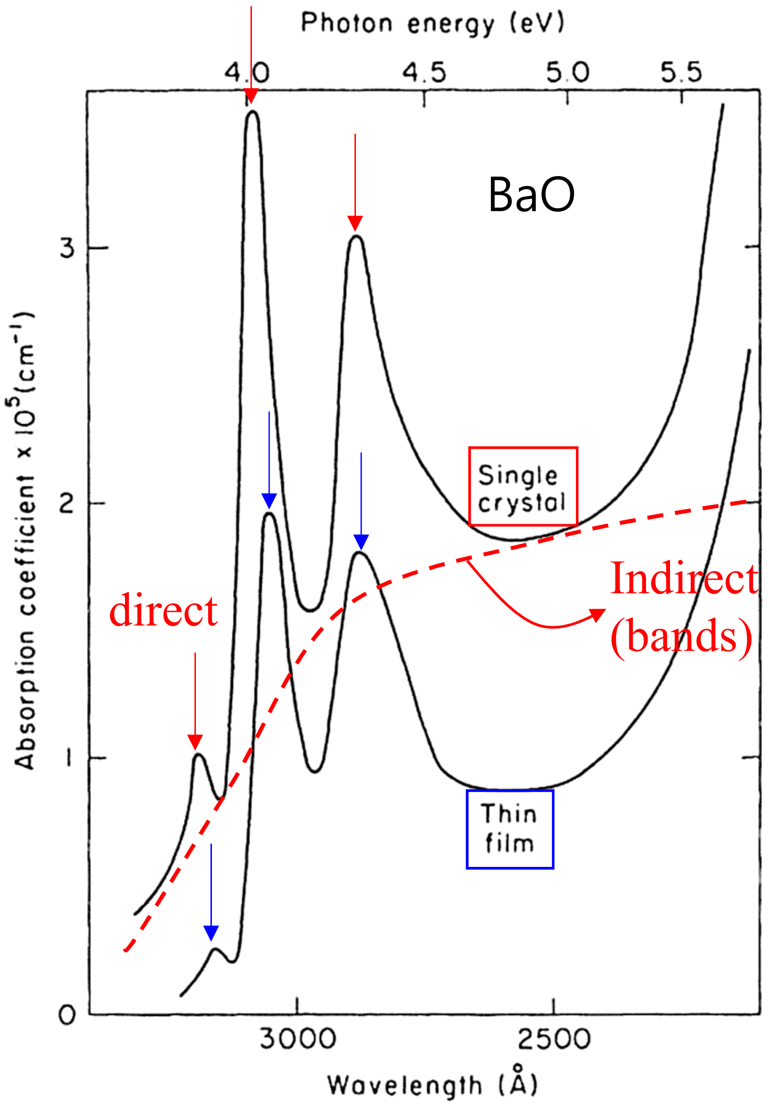
- An exciton can diffuse in a crystal and transport energy (binding energy of exciton). The total energy of an exciton is

$$E = \underbrace{\frac{\hbar K_{ex}^2}{2(m_e^* + m_h^*)}}_{} + E_{ex,n}$$

Kinetic energy of exciton for direct and indirect optical absorption

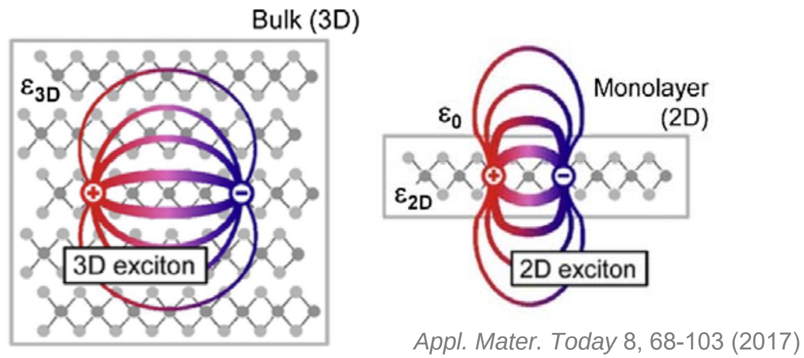
$$\begin{cases} K_{ex} \approx 0 \text{ for direct transition} \\ K_{ex} \approx K_{pn} \text{ for indirect transition} \end{cases}$$

Excitons

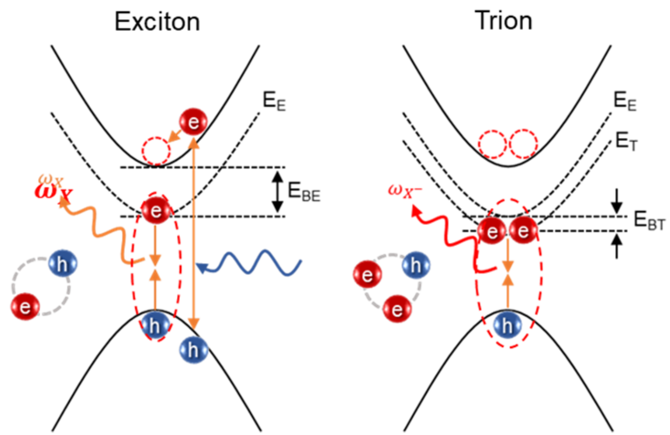


Shift of direct transition peaks shows that binding energy of exciton increases as the thickness of a material decreases due to dielectric screening and spatial confinement.

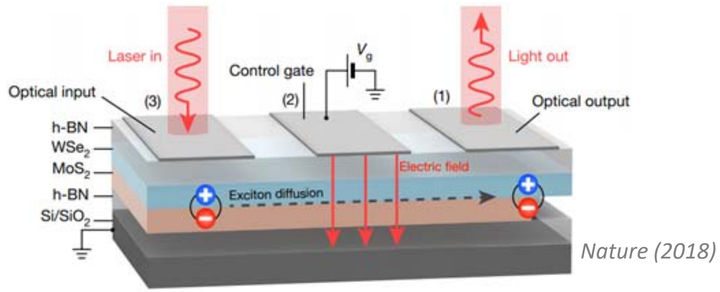
Excitons in 2D



Large binding E of excitons in 2D ~ 300-400 meV



Observation of exciton complexes, such as trions (e-e-h pairs) and bi-excitons (e-h-e-h pairs)



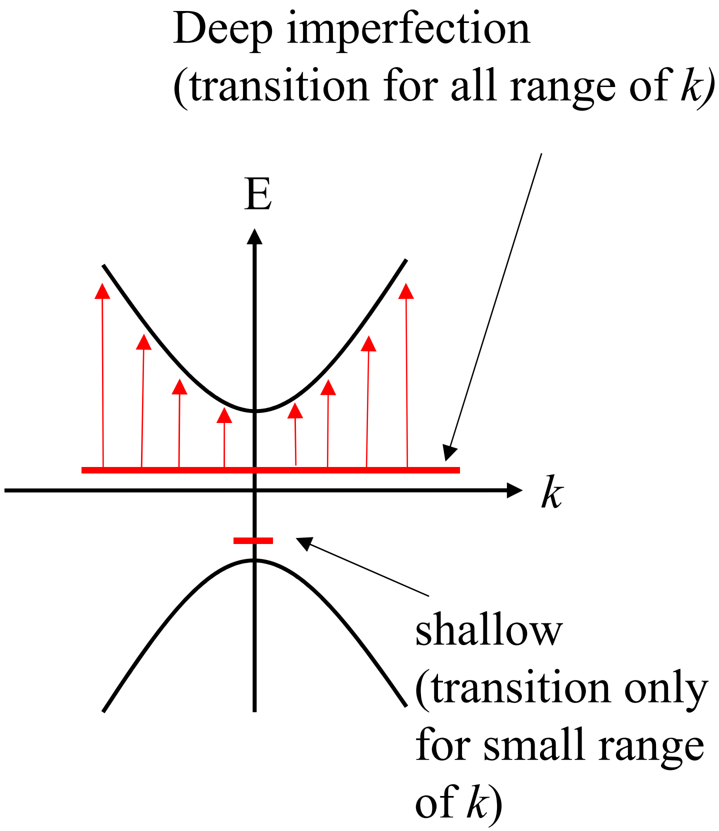
Transport of excitons in stacked 2D heterostructure

Imperfections

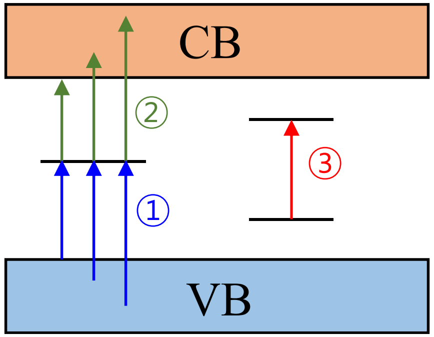
: localized energy levels by imperfections that exist only in relatively small regions of space around imperfections. They are indicated by a short line in a flat band diagram.

- Deep imperfections
  : highly localized
  Uncertainty Δx is small, but Δk is large.

- Shallow imperfections
  : small energy difference between the imperfection energy levels and conduction (valence) band edge
  Uncertainty Δx is large, but Δk is small.



Imperfections



- Transition ① and ②: absorption consists of a threshold followed by a region of higher absorption.
- Transition ③: a narrow peak at the energy separation between the two levels.

- Types of imperfections
  - Point imperfections: vacancy or misplaced atoms
  - Impurities
  - Larger structural defects: dislocations, grain boundaries, surfaces

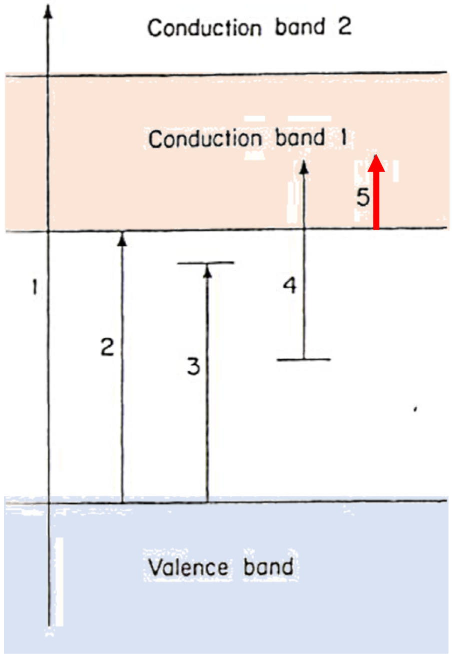
Absorption constant for the transitions of ① and ②

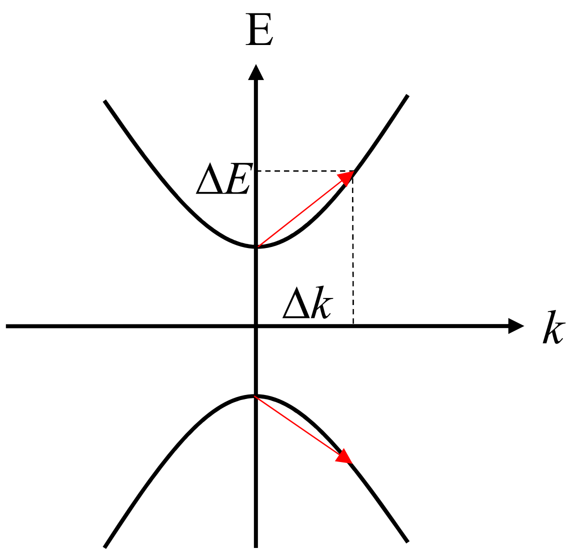
$$\alpha = S_{\mathrm{opt}} N_{\mathrm{I}}$$

where S_{opt} is the optical cross section (10^{-15} to 10^{-17} cm^2)and N_{I} the density of imperfections (10^{14} to 10^{18} cm^{-3})

Free carriers

: Indirect process involving both a photon and a phonon





need both ΔE and Δk

Indirect absorption involving both a photon and a phonon

$\alpha \propto \lambda^{n}$ (n=2~3)

Relation between absorption and conductivity

$\alpha_{\sigma} \propto \sigma / rc\varepsilon_0$

Plasma Resonance Absorption

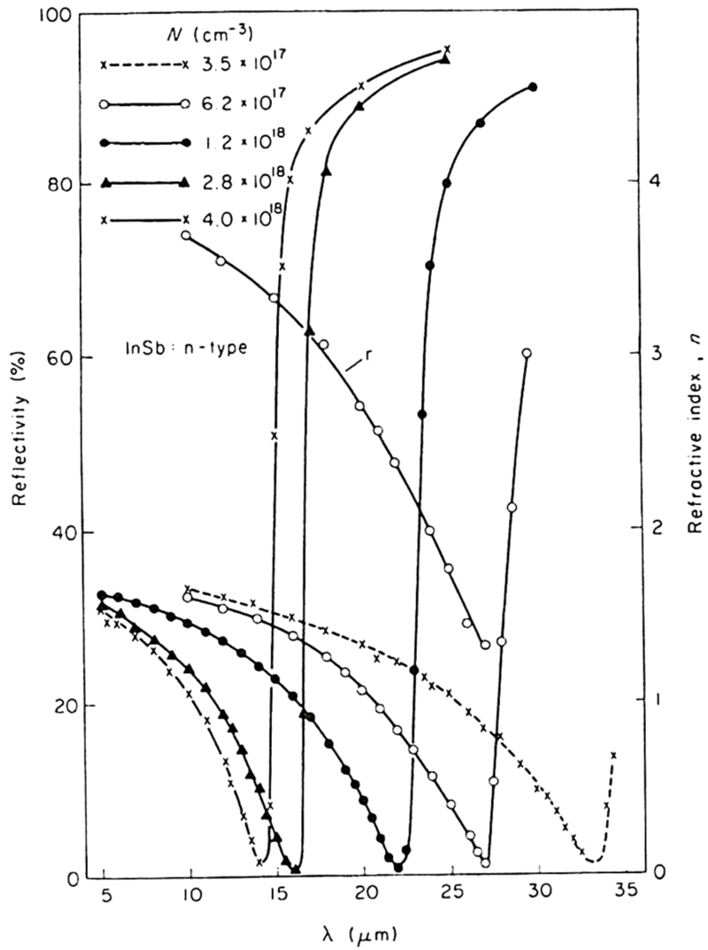
- Optical transition due to collective action of the carriers
- Collection of free electrons to be displayed a distance ξ by an electric field E

$$E = \frac{nq\xi}{\varepsilon_0}$$

$$nm_e^* \frac{d^2\xi}{dt^2} = -nqE = -4\pi n^2 q^2 \xi$$

$$\frac{d^2\xi}{dt^2} + \omega_p^2 \xi = 0$$

$$\omega_p = \left(\frac{nq^2}{\varepsilon_0 m_e^*}\right)^{\frac{1}{2}}$$



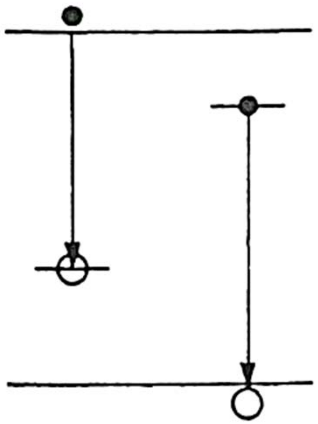
- When the frequency of the incident radiation is equal to the plasma resonance frequency, strong absorption occurs.

Photoelectronic effects

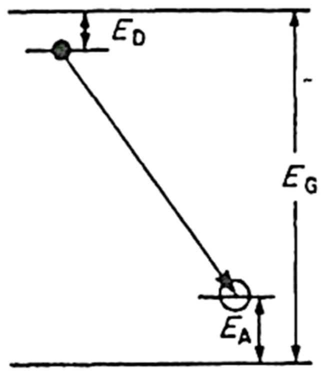
: related to light emission or light detection. (=optoelectronics)

- Results of absorption
  - If electrons are excited to conduction band, the free carrier density increases to enhance the conductivity (Photoconductivity)
  - When the excited electrons give up their energy and return to their initial states, the energy can be emitted as photons (Luminescence)

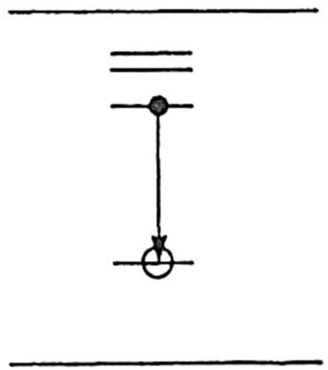
    ex) photoluminescence, cathodoluminescence, electron-beam induced current (EBIC)



Recombination between free carrier and trapped carrier

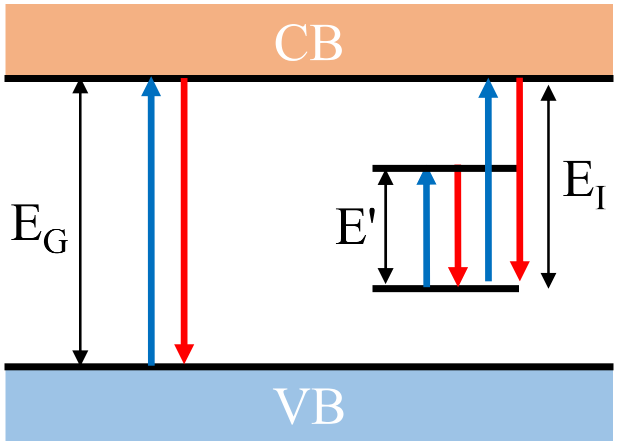


Pair-recombination between trapped carriers



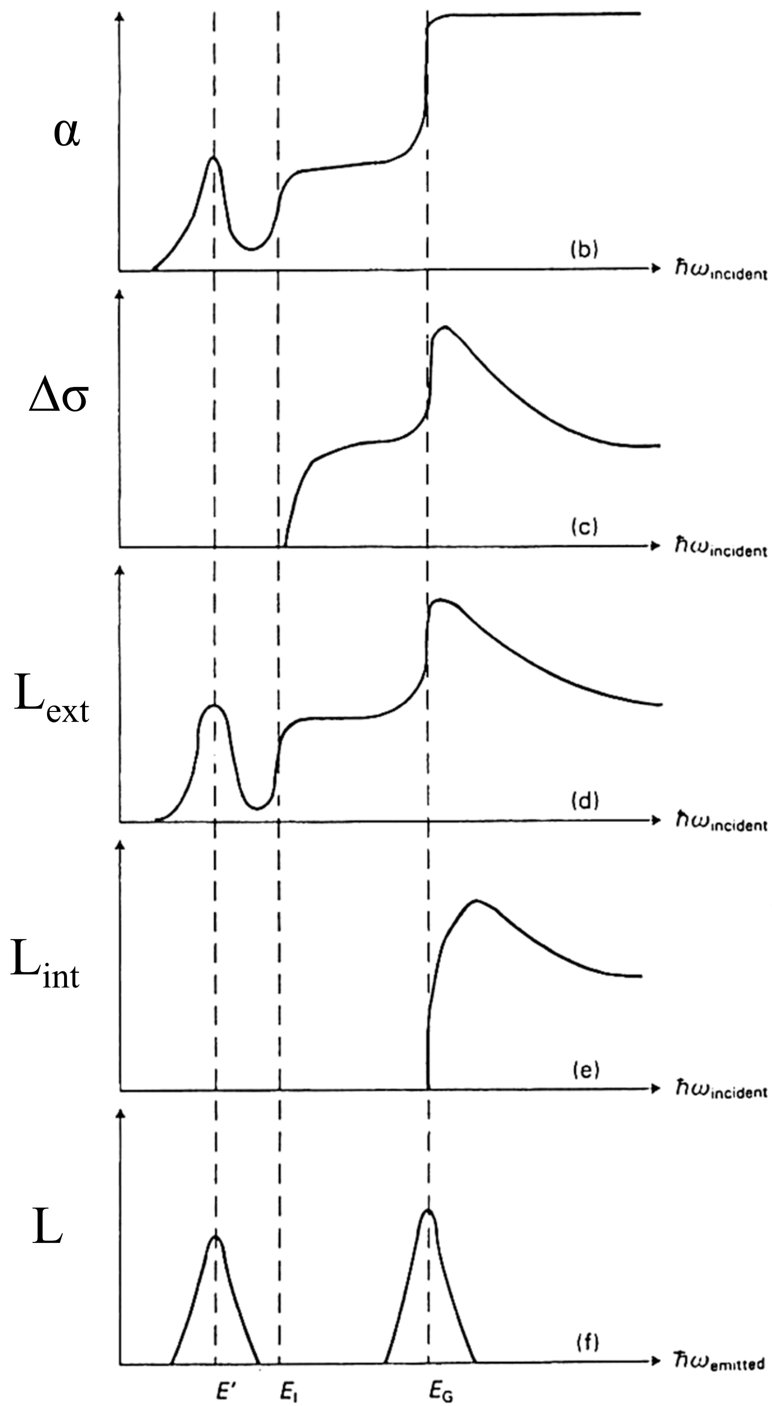
Recombination within atomic levels of impurity ionriers

Optical spectra



Intrinsic luminescence

extrinsic luminescence



Optical spectra