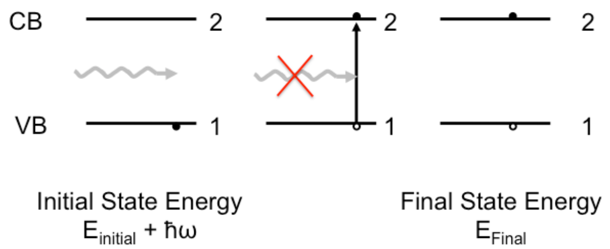
EEE6212
"Semiconductor Materials" -Optical Transitions

Professor Richard Hogg,
Centre for Nanoscience & Technology, North Campus
Tel 0114 2225168,
Email - r.hogg@shef.ac.uk

Outline

- Absorption
- Spontaneous emission
- Stimulated emission
- Density of states
- Occupancy
- Summary

Absorption



Photon is annihilated and gives energy up to an electron and promotes it to a higher energy level. "Stimulated" – in response to a passing photon

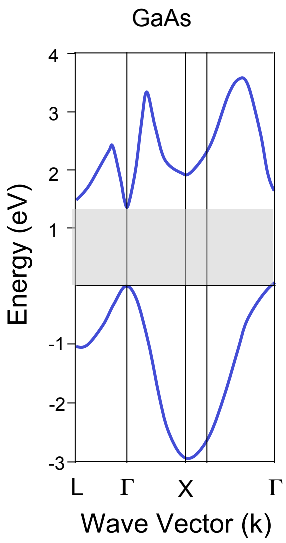
Fundamental absorption – exciting electrons from valence band to conduction band

Conserve Momentum

Momentum of electron at Brillouin Zone edge
$p = k\hbar = \pi h/2\pi a$
a=interatomic spacing ~ 3×10^{-10} m

Momentum of photon = h/λ
λ~840 nm = 8.4×10^{-7} m

Photon Momentum ~1000th that of electron so is essentially vertical when plotted on electron E-k graph



Absorption Rate

Will look later at how quantum mechanics can be used to calculate transition rates. Initially we will use the original Einstein coefficients for these transition rates

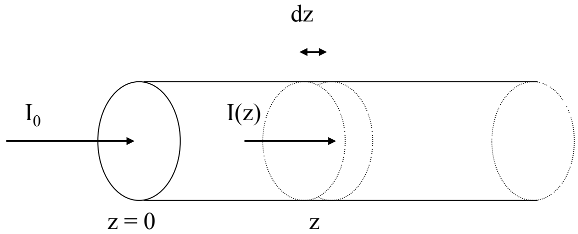
Absorption probability

= B_{12}x photon density x density of e in VB x density of h in CB

B_{12} is a rate coefficient for absorption (s^{-1})

Recombination probability proportional to photon density – "stimulated" absorption

Absorption Coefficient



I_0 photons incident/unit area/unit time at z = 0.

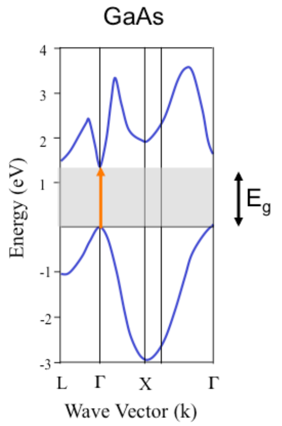
Absorption reduces I_0 to I(z) at z.

In a further distance dz number of photons absorbed is $\alpha I(z)dz = -dI$.

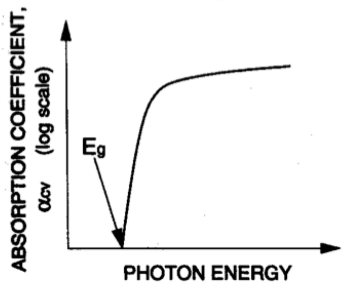
Hence, $dI/dz = -\alpha I(z)$, so $I(z) = \text{const.}x\exp(-\alpha z) = I_0\exp(-\alpha z)$.

α = absorption coefficient = inverse absorption length - dimensions 1/L.
Typically $\alpha = 10^6\ m^{-1}$ for GaAs at energy just above the band gap.

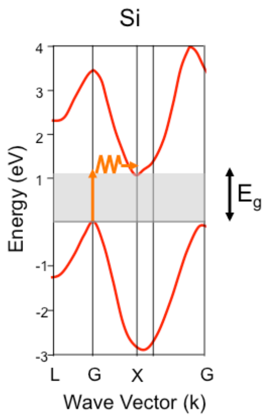
Direct Band-Gap



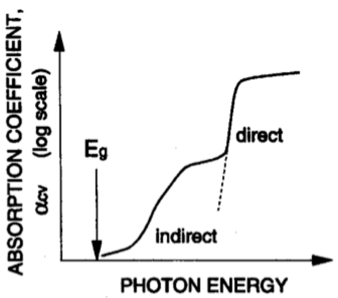
Direct Band-gap



Indirect Band-gap

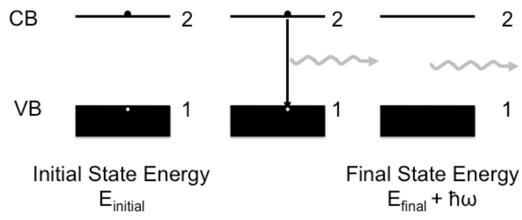


Indirect Band-gap



Indirect Absorption process only possible by phonon emission

Spontaneous Emission

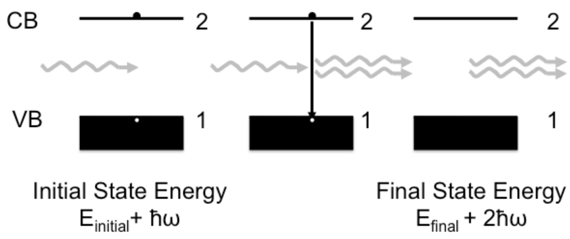


Recombination without any apparent provocation

Rate = A_{21} x density of e in CB x density of h in VB

Photons are created with random direction and phase

Stimulated Emission



Recombination rate proportional to photon density

Photons created are identical in energy, phase, direction to stimulating photon

Rate = B_{21} x density of e in CB x density of h in VB x photon density

Einstein Coefficients

A_{21} – Spontaneous emission rate from 2 to 1

B_{12} – (Stimulated) Absorption rate from 1 to 2

B_{21} – (Stimulated) Emission rate from 2 to 1

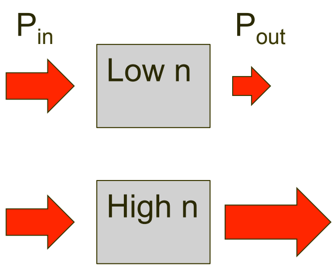
Formulated before quantum mechanics, A & B coefficients are proportional to "Oscillator Strength"

In quantum picture rate is governed by Fermi's Golden Rule

Absorption/Stimulated Emission

SE Rate = B_{21} x density of e in CB x density of h in VB x photon density

Abs Rate = B_{12}x density of e in VB x density of h in CB x photon density



Fermi's Golden Rule

$$W_{i \to f} = \frac{2\pi}{\hbar}|M|^2 g(\hbar\omega)$$

W – transition rate
i – initial
f - final
ħ – reduced Planck constant
M – matrix element
g(ħω) – joint density of states

In all cases, we can see that the density of states, and their occupancy is important. Park this for now…

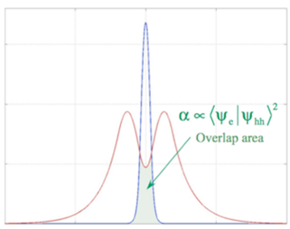
Matrix Element

Matrix element describes effect of external perturbation of light on electrons

(See Fox pages…..)

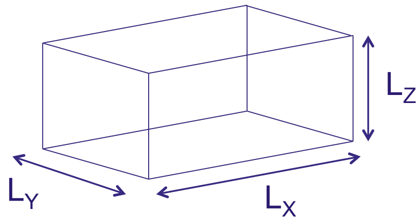
Important factors are the overlap of the initial and final wavefunctions

$$M = \langle f|H'|i\rangle = \int \psi_f^*(\mathbf{r})\, H'(\mathbf{r})\, \psi_i(\mathbf{r})\, d^3\mathbf{r},$$



Density of States

Want to evaluate g(E)dE
Density of states over a given interval at energy E



$$\psi(x,y,z) = \sin(k_x x)\sin(k_y y)\sin(k_z z)$$

$$k_x L_x = \pi n_x, k_y L_y = \pi n_y, k_z L_z = \pi n_z, \text{ for } n_x, n_y, n_z \text{ integers}$$

K-Space

Each state in k-space occupies k-space volume V_k

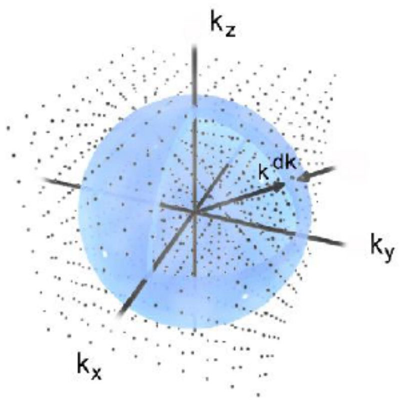
$V_k = k_X \cdot k_Y \cdot k_Z$

$V_k = (\pi/L_X) \cdot (\pi/L_Y) \cdot (\pi/L_Z)$

Number of states per volume in k-space is reciprocal of this
$=L_X L_Y L_Z/\pi^3$
$=V/\pi^3$

-V is the volume of the semiconductor in real space

Number of States for Given IkI



Construct a spherical shell of radius IkI and thickness dk

Volume of this spherical shell in k-space is $4\pi k^2 dk$

Number of k-states within the shell – k-space volume x k-space state density

$$g(k)dk = 4\pi k^2 \left[\frac{V}{\pi^3}\right] dk$$

Contd. (1)

Each state can hold 2 spins so x2

$$g(k)dk = 8\pi k^2 \left[\frac{V}{\pi^3}\right] dk$$

Each octant is indistinguishable so x 1/8

$$g(k)dk = \pi k^2 \left[\frac{V}{\pi^3}\right] dk = \left[\frac{Vk^2}{\pi^2}\right] dk$$

Need to convert to E not k

$$p = \hbar k \,, E = p^2 / 2m^* \quad E = \frac{\hbar^2 k^2}{2m^*}$$

Rewriting and noting E is w.r.t. E_C

$$k^2 = \frac{(E - E_c)2m^*}{\hbar^2}$$

Contd. (2)

Differentiation $$2kdk = \frac{2m^* dE}{\hbar^2}$$

Combine two previous Eqns
$$dk = \frac{2m^* dE}{2k\hbar^2} = \frac{m^* dE}{k\hbar^2} = \frac{m^* dE}{\hbar^2 \sqrt{2m^*(E-E_c)/\hbar^2}}$$
$$= \frac{m^* dE}{\hbar\sqrt{2m^*(E-E_c)}}$$

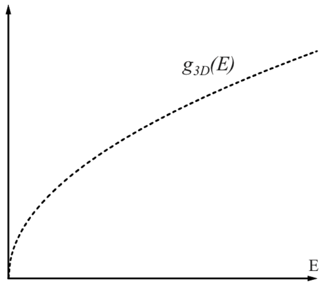
Next put this into $$g(k)dk = \pi k^2 \left[\frac{V}{\pi^3}\right] dk = \left[\frac{Vk^2}{\pi^2}\right] dk$$

Contd. (3)

Gives
$$g(k)dk = \frac{Vk^2}{\pi^2} \frac{m^* dE}{\hbar\sqrt{2m^*(E-E_c)}}$$
$$= \frac{V\left[2m^*(E-E_c)/\hbar^2\right](m^* dE)}{\pi^2\hbar\left[2m^*(E-E_c)\right]^{1/2}}$$
$$= \frac{Vm^*\left[2m^*(E-E_c)\right]^{1/2}}{\pi^2\hbar^3} dE$$

Divide by V $$g(E)dE = \frac{m^*\left[2m^*(E-E_c)\right]^{1/2}}{\pi^2\hbar^3} dE$$

Density of States



$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}$$

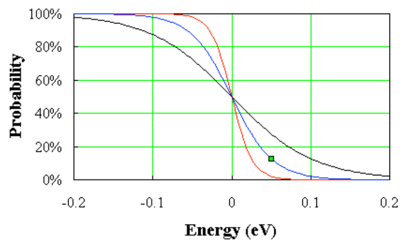
Importance of m*

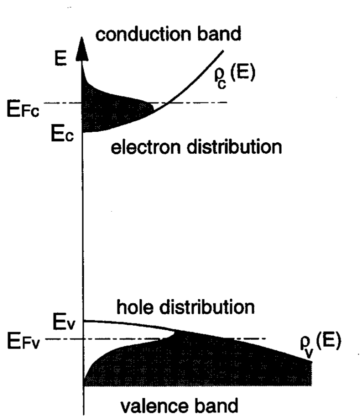
High effective mass – high density of states

Carrier Distribution

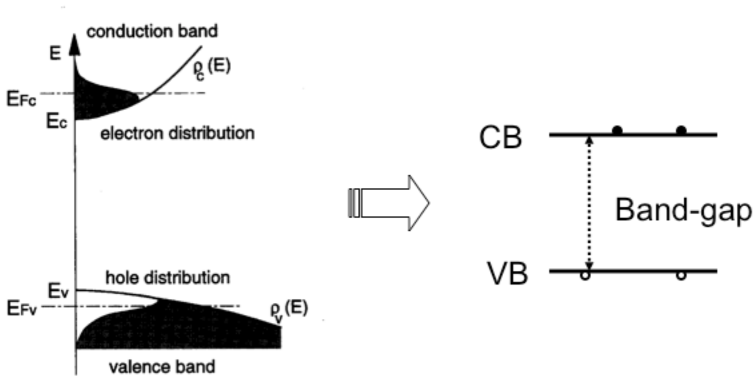
Electrons and holes have thermal energy

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}}$$





Behind the scenes….



Summary

- Discussed the optical transitions and their probabilities/ rates
- Touched upon matrix element
- Looked at density of states for a bulk material
- Introduced Fermi-function to describe carrier distribution

