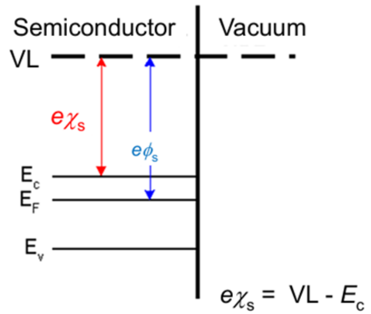
Lecture 12 – 04/12/2024

- Absorption
    - Optical transitions and Fermi’s Golden Rule
    - Optical susceptibility
    - Absorption and gain in semiconductors
    - Bernard-Duraffourg condition

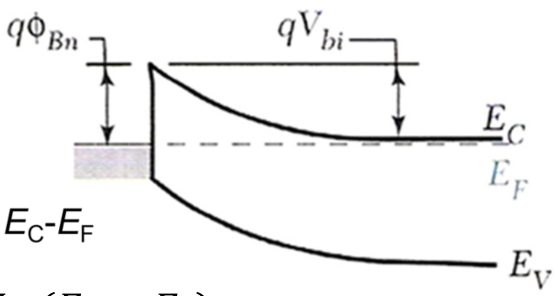
Summary Lecture 11

Work function and electron affinity



Metal-semiconductor junction

- Creation of a depletion region
- Schottky barrier: $e\phi_B = E_c(0)\text{-}E_F$
- Vacuum level continuous and // to the band edges:



$e\phi_{Bn} = e(\phi_m\text{-}\chi)$

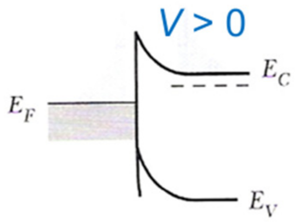
$eV_{bi} = e\phi_{Bn}$ - eV_n with $eV_n = E_C\text{-}E_F$

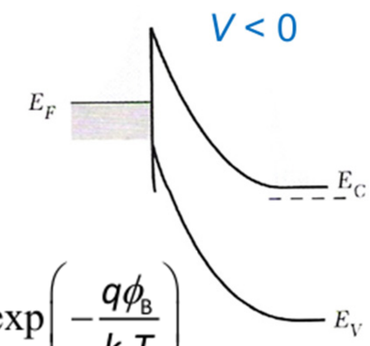
- Surface states: $\sigma = -eN_{SS}(E_F - E_0)$

$$\downarrow$$

$$V_{bi} = -\frac{\sigma W}{2\varepsilon}$$

Schottky diode





$$J(V) = J_S\left[\exp\left(\frac{qV}{k_BT}\right) - 1\right] \text{ with } J_S = A^*T^2\exp\left(-\frac{q\phi_B}{k_BT}\right)$$

Ohmic contact

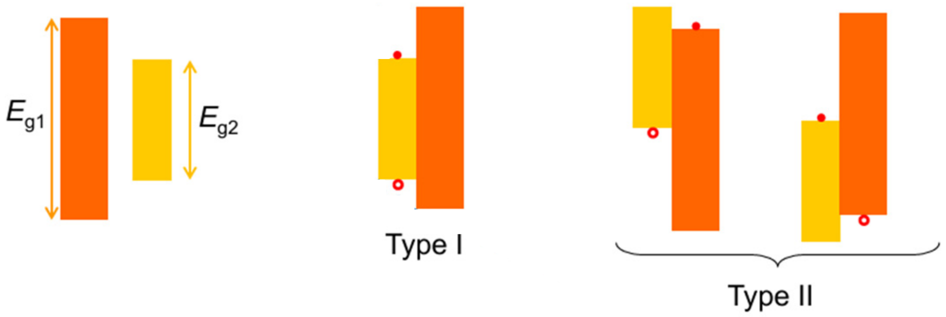
↳ Negligible contact resistance vs series resistance of the semiconductor

$$R_C = \left(\frac{\partial J}{\partial V}\right)^{-1}_{V=0} = \frac{k_B}{eA^*T}\exp\left(\frac{q\phi_B}{k_BT}\right)$$

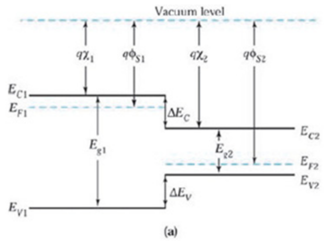
- Low barrier height required
- Heavy doping ⟶ tunneling current dominates

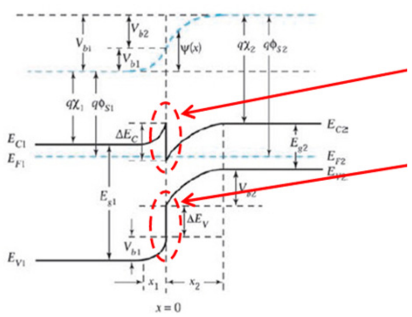
Summary Lecture 11

Heterostructures



- E_F is constant
- Bandgap is conserved inside a structure
- Vacuum level continuous and // to the band edges
- Singularity for one of the bands and an abrupt jump for the other





SiO2

Dielectric commonly used in industry for surface passivation that offers a tunable capacitance

Si(solid) + O_2(dry oxygen) → SiO_2(solid) — Dry oxidation

or Si(solid) + $2H_2O$(steam) → SiO_2(solid) + $2H_2$ — Wet oxidation

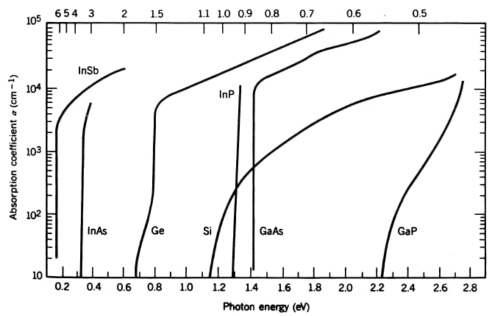
- The oxidation rate in steam is about 5 to 10 times higher than for dry oxygen
- Short reaction times: $d \propto t$
- Prolonged oxidation: $d \propto \sqrt{t}$
- Si (100) orientation: reasonably fast oxidation rate under steam growth (at 1250°C, 400 nm after 10' and ~1 µm after 1h)

Absorption

$h\nu > E_g$: $I_{transmitted} = I_{initial} \exp(-\alpha L)$

α increases with E_g

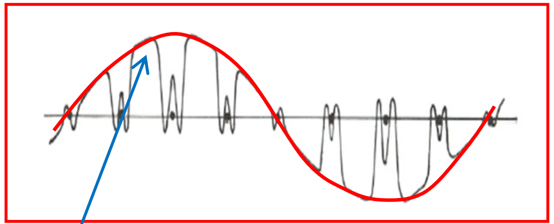
The optical properties of many materials are explained by E_g value and doping/impurity bands



Direct bandgap: absorption increases abruptly at E_g
Indirect bandgap: gradual increase

Bloch waves: wavefunction of a particle in a periodic potential

$$\mathrm{H}_e \psi_{n,\mathbf{k}}(\mathbf{r}) = \left(\frac{p^2}{2m} + V(\mathbf{r}) \right) \psi_{n,\mathbf{k}}(\mathbf{r}) = E_{n,\mathbf{k}} \psi_{n,\mathbf{k}}(\mathbf{r})$$



with $V(\mathbf{r})$ which is periodic: $V(\mathbf{r}+\mathbf{T}) = V(\mathbf{r})$

The eigenfunctions can be written as follows:

Reminder + to be admitted

$$\psi_{n,\mathrm{k}}(\mathrm{r}) = \boxed{\frac{u_{n,\mathrm{k}}(\mathrm{r})}{\sqrt{V_s}}} \boxed{e^{-i\mathrm{kr}}}$$

Volume of the solid

Plane wave ≈ envelope function, slow spatial variations

Bloch functions:

- $u_{n,\mathbf{k}}$ functions vary rapidly at the lattice scale
- same symmetry as $V(\mathbf{r})$, i.e., $u_{\mathbf{k}}(\mathbf{r}+\mathbf{T}) = u_{\mathbf{k}}(\mathbf{r})$

Absorption in direct bandgap semiconductors

Let us consider the wavefunction of an electron of wavevector **k** within a band *n*:

$$\Psi_{n,\mathbf{k}}(\mathbf{r}) = \frac{u_{n,\mathbf{k}}(\mathbf{r})}{\sqrt{V_s}} e^{-i\mathbf{k}.\mathbf{r}}$$

If a semiconductor experiences a perturbation due to an electromagnetic (EM) wave of wavevector $\mathbf{k}_{\mathrm{op}}$ and electric field **E**, the perturbation Hamiltonian can be described by:

$$\hat{\mathrm{W}}(\mathbf{r},t) = \hat{\mathrm{W}}\cos(\mathbf{k}_{\mathrm{op}}.\mathbf{r} - \omega t) = -q\mathbf{E}.\hat{\mathbf{r}}\cos(\mathbf{k}_{\mathrm{op}}.\mathbf{r} - \omega t)$$

position operator

Dipolar approximation

This perturbation couples the states $|\Psi_{n,\mathbf{k}}\rangle$ and $|\Psi_{n',\mathbf{k}'}\rangle$ and the transition rate (expressed in s^{-1}) from the first state to the second one is given by **Fermi's Golden Rule**:

$$\boxed{P_{n,\mathbf{k},n',\mathbf{k}'} = \frac{\pi}{2\hbar}\left|\left\langle \Psi_{n',\mathbf{k}'}\middle|\hat{\mathrm{W}}\middle|\Psi_{n,\mathbf{k}}\right\rangle\right|^2 \delta\left(E_{n',\mathbf{k}'} - E_{n,\mathbf{k}} - \hbar\omega\right)}$$

$E_{n',\mathbf{k}'} - E_{n,\mathbf{k}} = \hbar\omega \quad \Rightarrow$ *energy conservation*

Nota bene: The shape of $P_{n,\mathbf{k},n',\mathbf{k}'}$ is that obtained for transitions induced between a discrete level and a continuum state by single frequency excitation (cf., e.g., *Optoelectronics* by E. Rosencher and B. Vinter or C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics*, (Wiley-VCH, Weinheim, 2020))

Absorption in semiconductors

Interband dipole matrix element VB $\rightarrow$ CB

$$\langle \Psi_{\mathrm{c},\mathbf{k}'} | \hat{\mathrm{W}} | \Psi_{\mathrm{v},\mathbf{k}} \rangle = -\frac{qE}{V_{\mathrm{s}}}\int_{\text{lattice}} u^{*}_{\mathrm{c},\mathbf{k}'}(\mathbf{r}) e^{i\mathbf{k}'\mathbf{r}}\, \mathbf{r}\, e^{-i\mathbf{k}_{\mathbf{op}}\mathbf{r}}\, u_{\mathrm{v},\mathbf{k}}(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}} d^3 r$$

$$= -\frac{qE}{V_{\mathrm{s}}}\sum_j e^{i(\mathbf{k}'-\mathbf{k}_{\mathbf{op}}-\mathbf{k})\mathbf{r}_j} V_j \times \frac{1}{V_j}\int_{V_j} u^{*}_{\mathrm{c},\mathbf{k}'}(\mathbf{r})\,\mathbf{r}\,u_{\mathrm{v},\mathbf{k}}(\mathbf{r}) d^3 r$$

$V_j << V_s$

Unit cell volume

$$= -\frac{qE}{V_{\mathrm{s}}}\int_{\text{lattice}} e^{i(\mathbf{k}'-\mathbf{k}_{\mathbf{op}}-\mathbf{k})\mathbf{r}} d^3 r \times r_{\mathrm{vc}} = -qE\,\delta(\mathbf{k}'-\mathbf{k}_{\mathbf{op}}-\mathbf{k}) \times r_{\mathrm{vc}}$$

During the electron-photon interaction, momentum conservation is also ensured:

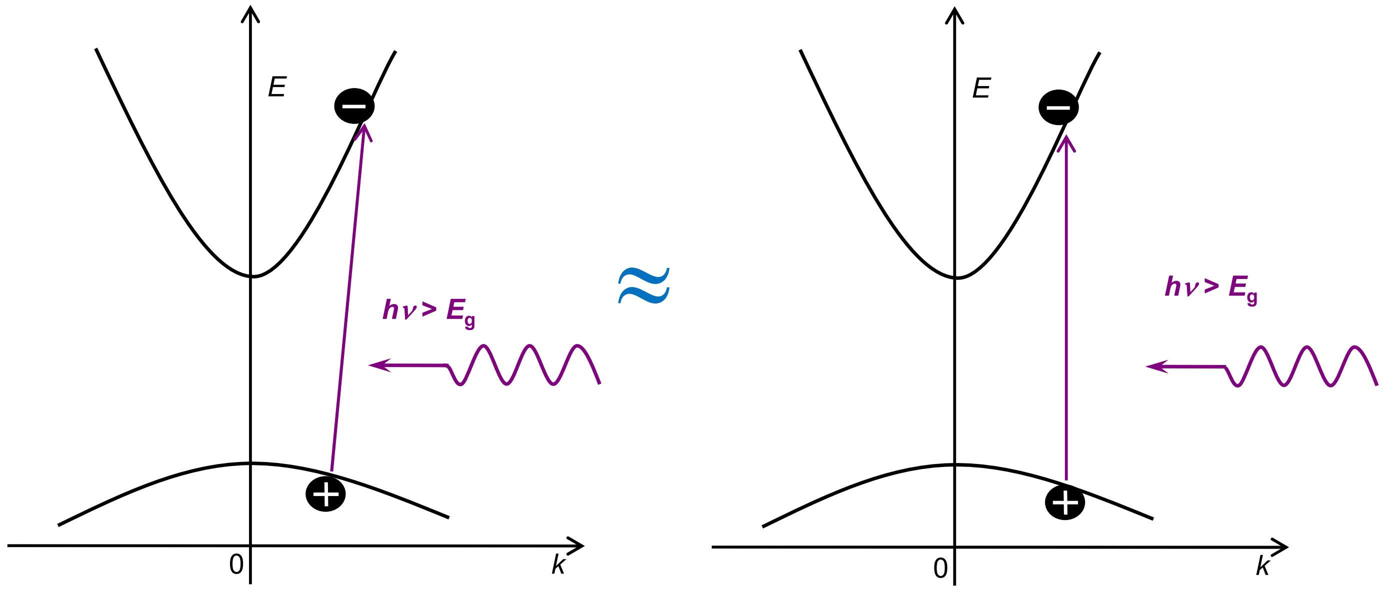
$$\boxed{\mathbf{k}' = \mathbf{k} + \mathbf{k}_{\mathbf{op}}}$$

Absorption in semiconductors

$k_{op} = 2\pi/\lambda \approx 10^4\text{-}10^6\ \mathrm{cm}^{-1}$ and $k = 2\pi/a \approx 10^8\ \mathrm{cm}^{-1}$

$$\mathbf{k}' \approx \mathbf{k} \qquad \mathbf{k}' = \mathbf{k} + \mathbf{k}_{op}$$

Optical transitions are nearly vertical in reciprocal space



Absorption in semiconductors

$\mathbf{r}_{\mathbf{vc}}$ is the interband dipolar optical matrix element between VB → CB

$$\left\langle \Psi_{\mathrm{c},\mathbf{k}'} \middle| \hat{\mathrm{W}} \middle| \Psi_{\mathrm{v},\mathbf{k}} \right\rangle = -qE\delta(\mathbf{k}' - \mathbf{k}_{\mathbf{op}} - \mathbf{k}) \times r_{\mathrm{vc}}$$

One can show that: $$\boxed{r_{\mathrm{vc}} = \frac{\hbar}{E_{\mathrm{g}}}\sqrt{\frac{E_{\mathrm{p}}}{2m_0}}}$$

E_{p} Kane energy (20-22 eV) = P^2

6 Å for GaAs (1.42 eV)

22 Å for InAs (0.35 eV)

Cf. Lecture 3, slides 7-8

In usual direct band gap SCs (i.e., zinc blende III-V SCs), we set $x_{\mathrm{vc}}^2 = 2/3 r_{\mathrm{vc}}^2$ (contribution of HH and LH subbands only for near band edge optical transitions due to the large spin-orbit interaction):

$$\boxed{x_{\mathrm{vc}}^2 = \frac{1}{3}\frac{\hbar^2}{E_{\mathrm{g}}^2}\frac{E_{\mathrm{p}}}{m_0}}$$

x_{vc} is used in the calculation of the absorption coefficient

Absorption and susceptibility in semiconductors

Linear optical susceptibility and absorption

Some basic elements:

Polarization of a medium:

polarizability of the medium

$$P(t) = \Re(\varepsilon_0 \chi(\omega) E e^{i\omega t})$$

$$\text{with} \quad \chi(\omega) = \chi_{\Re}(\omega) + i\chi_{\Im}(\omega)$$

$\chi_{\Re}$ Real part of the susceptibility in phase with the EM wave: instantaneous response of the system

$\Rightarrow$ **refractive index**

$\chi_{\Im}$ Imaginary part of the susceptibility in quadrature with the EM wave: dissipation within the system

$\Rightarrow$ **absorption**

Absorption and susceptibility in semiconductors

Maxwell's equations

In a polarizable non-magnetic medium without charge:

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$$

$$\nabla \times \mathbf{B}(\mathbf{r},t) = \frac{1}{\varepsilon_0 c^2}\frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t)$$

$$\text{with } \mathbf{D}(\mathbf{r},t) = \boxed{\varepsilon_0\mathbf{E} + \mathbf{P}} + \mathbf{P}_{\mathrm{res}} = \boxed{\varepsilon\mathbf{E}} + \mathbf{P}_{\mathrm{res}}$$

D is the displacement vector, **P** is the polarization vector of the host medium far from the resonance, and $\mathbf{P}_{\mathbf{res}}$ is the polarization vector close to the resonance (i.e., that of our two-level system)

as $\mathbf{P}_{\mathbf{res}} = \varepsilon_0\chi(\omega)\mathbf{E}$ then $\mathbf{D} = \varepsilon(1+\varepsilon_0\chi(\omega)/\varepsilon)\mathbf{E}$

Absorption and susceptibility in semiconductors

Maxwell's equation solutions

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 \Re[e^{-i(\mathbf{kr}-\omega t)}]$$ with $\mathbf{D} = \varepsilon(1+\varepsilon_0\chi(\omega)/\varepsilon)\mathbf{E}$

EM waves propagating in a non-magnetic and isotropic medium

$$\mu_0 \partial^2 \mathbf{D} / \partial t^2 = \nabla^2 \mathbf{E} \quad \Rightarrow \quad \mu_0 \omega^2 \varepsilon(1+\varepsilon_0\chi(\omega)/\varepsilon) = k^2$$

Complex number!

n_{op} is the refractive index which is defined such as $n_{op} = \sqrt{\dfrac{\varepsilon}{\varepsilon_0}}$ and $\mu_0\varepsilon_0 c^2 = 1$

Then the dispersion relation between ω and k is $\boxed{k = |\mathbf{k}| = \dfrac{n_{op}\omega}{c}\left|1+\dfrac{\varepsilon_0}{\varepsilon}\chi(\omega)\right|^{1/2}}$

Absolute value ≠ modulus

Cf. section 3.4, *Optoelectronics*, Rosencher-Vinter

Absorption and susceptibility in semiconductors

$$|\mathbf{k}| = \frac{n_{\text{op}}\omega}{c}\left|1 + \frac{\varepsilon_0}{\varepsilon}\chi(\omega)\right|^{1/2}$$

with $\chi(\omega) = \chi_{\Re}(\omega) + i\chi_{\Im}(\omega)$

k then writes (with χ <<1)

$$k = \frac{n_{\text{op}}\omega}{c}\left(1 + \frac{\varepsilon_0}{2\varepsilon}\chi_{\Re}\right) + i\frac{\omega}{2n_{\text{op}}c}\chi_{\Im}$$

$$= k_{\Re} + ik_{\Im}$$

Absorption and susceptibility in semiconductors

The expression of **k** is introduced in $\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0\Re[e^{-i(\mathbf{kr}-\omega t)}]$

$$\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0 e^{k_{\Im}r}\,\Re[e^{-i(k_{\Re}r-\omega t)}]$$

$$k=\frac{n_{op}\omega}{c}\left(1+\frac{\varepsilon_0}{2\varepsilon}\chi_{\Re}\right)+i\frac{\omega}{2n_{op}c}\chi_{\Im}=k_{\Re}+i\,k_{\Im}$$

$$=\mathbf{E}_0 e^{-\frac{\alpha}{2}r}\,\Re[e^{-i(k_{\Re}r-\omega t)}]$$

with $$\boxed{\alpha(\omega)=-2k_{\Im}=-\frac{\omega}{cn_{op}}\chi_{\Im}\quad(\chi_{\Im}<0)}$$

Absorption coefficient

The intensity of an EM wave propagating within an absorbing medium is given by:

$$\boxed{I(z)=I_0 e^{-\alpha z}}$$

Beer-Lambert law

Total susceptibility in semiconductors (2-band approximation)

$$\chi(\omega) = 2\sum_{\mathbf{k}} \frac{q^2 x_{vc}(\mathbf{k})^2 T_2}{2\varepsilon_0 \hbar} \frac{(\omega-\omega_{vc}(\mathbf{k}))T_2 - i}{(\omega-\omega_{vc}(\mathbf{k}))^2 T_2^2 + 1}\left(N_v(\mathbf{k}) - N_c(\mathbf{k})\right)$$

Optical susceptibility for transitions between quasi-discrete levels

spin

carrier relaxation time ≈ 100 fs

particle densities

See Chapters 3 & 7 Rosencher-Vinter

To account for a single type of valence band
(factor overlooked by Rosencher & Vinter)

$$2\sum_{\mathbf{k}_n \in 1^{st} BZ} \leftrightarrow \int_{\mathbf{k}} \rho(\mathbf{k}) d^3\mathbf{k} \leftrightarrow \int_E \rho(E) dE$$

$$\rho_c(k) = \rho_v(k) = \frac{V}{4\pi^3}$$

$$N_v(\mathbf{k}) - N_c(\mathbf{k}) = \rho_c d^3\mathbf{k}\left[f_v(E_v(\mathbf{k})) - f_c(E_c(\mathbf{k}))\right]$$

Infinitesimal density for the d^3**k** element

$$\boxed{\chi(\omega) = \frac{q^2 x_{vc}^2 T_2}{2\varepsilon_0 \hbar}\int_{E_g/\hbar}^{\infty} \rho_j(\omega_{vc}) d\omega_{vc}\left[f_v(E_v) - f_c(E_c)\right]\frac{(\omega-\omega_{vc})T_2 - i}{(\omega-\omega_{vc})^2 T_2^2 + 1}}$$

Optical susceptibility associated with an interband transition in a bulk direct bandgap semiconductor (within the 2-band approximation)

$$\frac{1/\pi T_2}{(\omega-\omega_{vc})^2 + (1/T_2)^2} \Leftrightarrow \delta(\omega-\omega_{vc})$$

Important mathematical step!

Absorption and susceptibility in semiconductors

Absorption coefficient calculation

$$\boxed{\alpha(\omega) = -\frac{\omega}{c n_{\mathrm{op}}} \chi_{\Im}}$$

In a semiconductor the imaginary part of the optical susceptibility $\chi_{\Im}$ writes as:

$$\boxed{\chi_{\Im}(\omega) = -\frac{q^2 x_{\mathrm{vc}}^2 \pi}{2\varepsilon_0 \hbar} \rho_j(\omega)\left[f_{\mathrm{v}}\left(E_{\mathrm{v}}(\mathbf{k})\right) - f_{\mathrm{c}}\left(E_{\mathrm{c}}(\mathbf{k})\right)\right]}$$

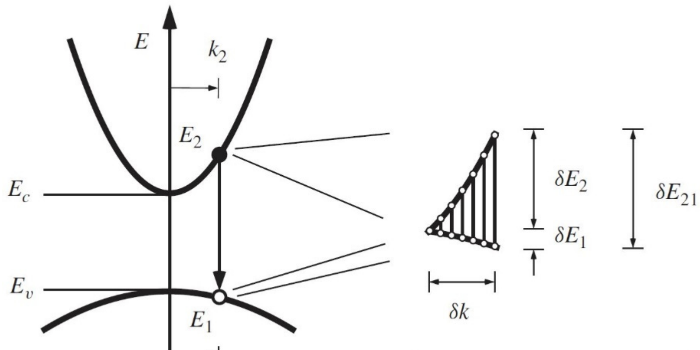
f_{v}, f_{c} Fermi-Dirac distributions (using quasi-Fermi levels since the system is driven out of equilibrium)

x_{vc} Dipole matrix element

$\rho_j(\omega)$ **Joint density of states** (3D case) $\Rightarrow$ the number of transition pairs within δk is equal to the number of states in either the conduction or valence band

$$\boxed{\rho_j(\omega) = \frac{1}{2\pi^2}\left(\frac{2m_{\mathrm{r}}}{\hbar}\right)^{3/2} (\omega - E_{\mathrm{g}}/\hbar)^{1/2}}$$

with $\frac{1}{m_{\mathrm{r}}} = \frac{1}{m_{\mathrm{e}}} + \frac{1}{m_{\mathrm{h}}}$ *and m_{r} is the reduced mass*



#states/volume = $\rho(E)\delta E$

Absorption in semiconductors

$$\hbar\omega = E_c(\mathbf{k}) - E_v(\mathbf{k}) = E_g + \frac{\hbar^2\mathbf{k}^2}{2m_r}$$

with

$$E_c(\mathbf{k}) = E_g + \frac{\hbar^2\mathbf{k}^2}{2m_e} = E_g + \frac{m_r}{m_e}(\hbar\omega - E_g)$$

$$E_v(\mathbf{k}) = -\frac{\hbar^2\mathbf{k}^2}{2m_h} = -\frac{m_r}{m_h}(\hbar\omega - E_g)$$

Finally

semiconductor medium gain

$$\alpha(\omega) = -\gamma(\omega) = \alpha_0(\omega)\left[f_v(\hbar\omega) - f_c(\hbar\omega)\right]$$ ***Absorption in a semiconductor***

with $$\boxed{\alpha_0(\omega) = \frac{q^2 x_{vc}^2\omega}{4\pi\varepsilon_0\hbar n_{op}c}\left(\frac{2m_r}{\hbar}\right)^{3/2}\sqrt{\omega - E_g/\hbar}}$$

Absorption without carriers in the bands

Gradual increase of $\alpha_0(\omega)$ with increasing SC bandgap

Bernard-Duraffourg condition

$$\boxed{\alpha(\omega) = \alpha_0(\omega)\left[f_v(\hbar\omega) - f_c(\hbar\omega)\right]}$$

Expression also valid out of thermal equilibrium

with $\alpha_0(\omega) = \dfrac{q^2 x_{vc}^2 \omega}{4\pi\varepsilon_0 \hbar n_{op} c}\left(\dfrac{2m_r}{\hbar}\right)^{3/2}\sqrt{\omega - E_g/\hbar}$

Absorption without carriers in the bands

quasi-Fermi levels

$$f_c(\hbar\omega) > f_v(\hbar\omega) \quad \Rightarrow \quad \boxed{E_{Fc} - E_{Fv} > \hbar\omega > E_g}$$

Bernard-Duraffourg condition

Light gets amplified only once the Bernard-Duraffourg condition is fulfilled, i.e., when the semiconducting medium exhibits optical gain!

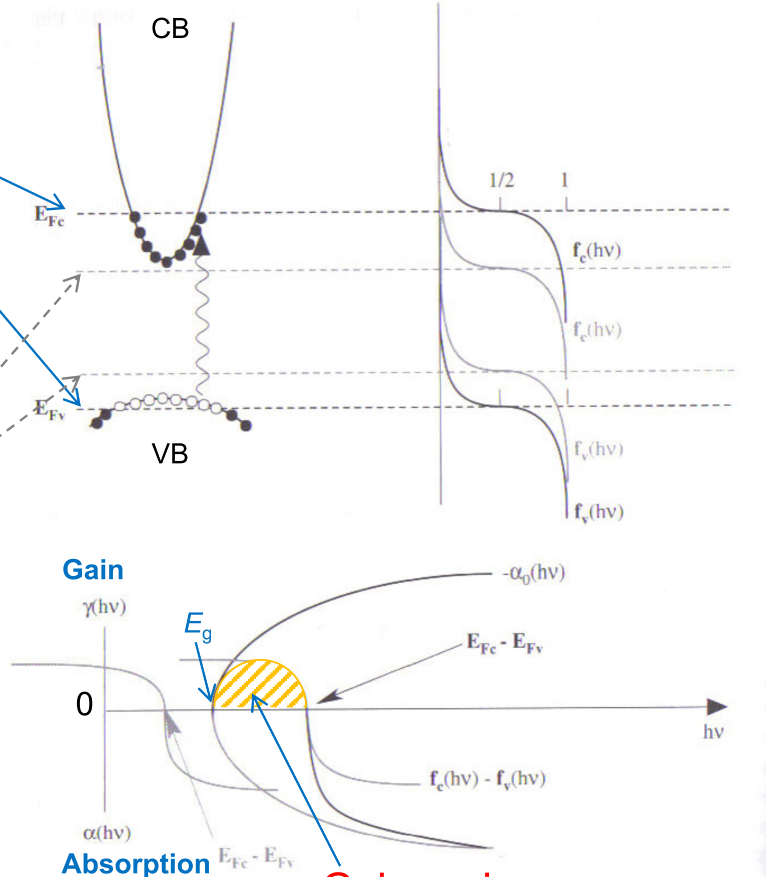
$\Rightarrow$ **Necessary condition for the achievement of lasing in a semiconducting medium**

Absorption in semiconductors

$$\boxed{E_{Fc} - E_{Fv} > \hbar\omega > E_g}$$

- Strong excitation
  - ✓ At least one of the bands is degenerate
  - ✓ All the states satisfying the *B-D* inequality are "fully occupied", i.e., the SC is transparent for those λ!
- Weak or moderate excitation
  - ✓ None of the bands are degenerate, i.e., $n < N_C$ and $p < N_V \Rightarrow$ use of Boltzmann approximation
  - ✓ $\Rightarrow$ photon absorption is still at play since there are available states in the CB where e⁻ from the VB can be promoted

System driven out of equilibrium



Gain region
$\Rightarrow$ Light amplification

Absorption and gain in semiconductors

Example: quasi-Fermi levels in bulk GaAs

Non-degenerate case

$$E_{F_n} = E_C - k_B T \ln\left(\frac{N_C}{n}\right)$$

$$E_{F_p} = E_V + k_B T \ln\left(\frac{N_V}{p}\right)$$

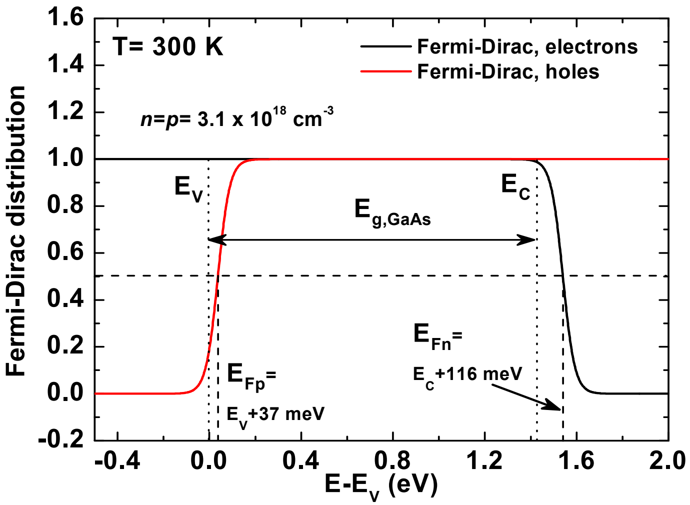
effective DOS

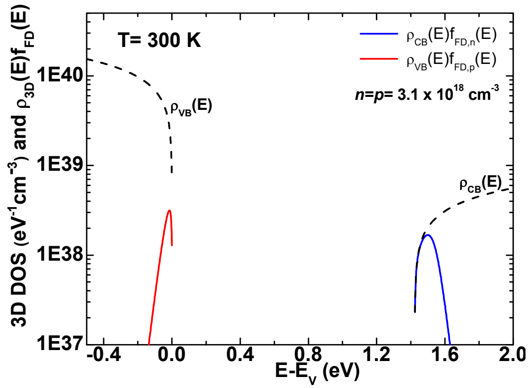
Degenerate case

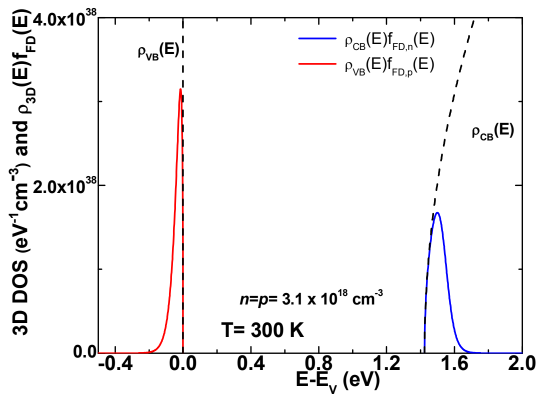
$$E_{F_n} = E_C + \frac{\hbar^2}{2m_C}\left(3\pi^2 n\right)^{2/3}$$

$$E_{F_p} = E_V - \frac{\hbar^2}{2m_V}\left(3\pi^2 p\right)^{2/3}$$

$$\boxed{N_{C,V} = \frac{1}{4}\left(\frac{2m^*_{C,V} k_B T}{\pi\hbar^2}\right)^{3/2}}$$







E_{Fn}-E_{Fp} > E_g, i.e., Bernard-Duraffourg condition is fulfilled!

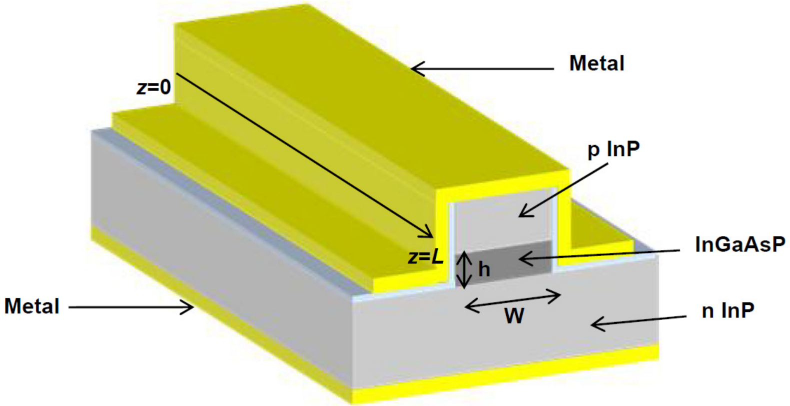
General comments on absorption in semiconductors

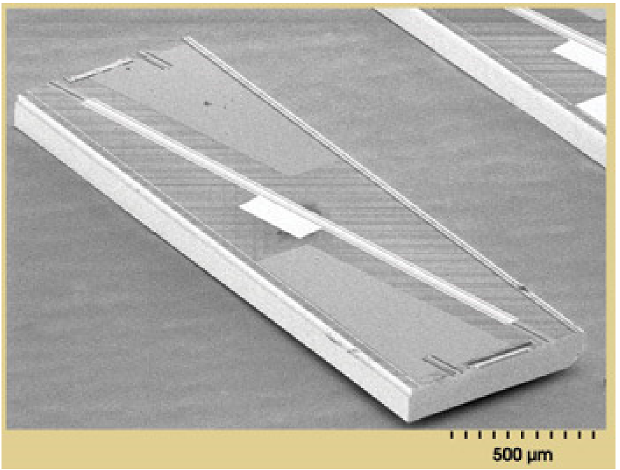
- In bulk semiconductors, there is a *continuum of absorbing states for photons fulfilling the condition $\hbar\omega \geq E_g$* (inherited from the joint-DOS) $\Rightarrow$ to be clearly separated from the case of dilute media (e.g., gases) where absorption occurs between quasi-discrete states (hence the use of a Lorentzian lineshape)

- Light emission will mostly occur in the vicinity of the bandgap because intraband relaxation processes via phonon emission are more efficient than the spontaneous emission process (to be discussed and validated in Lecture 14)

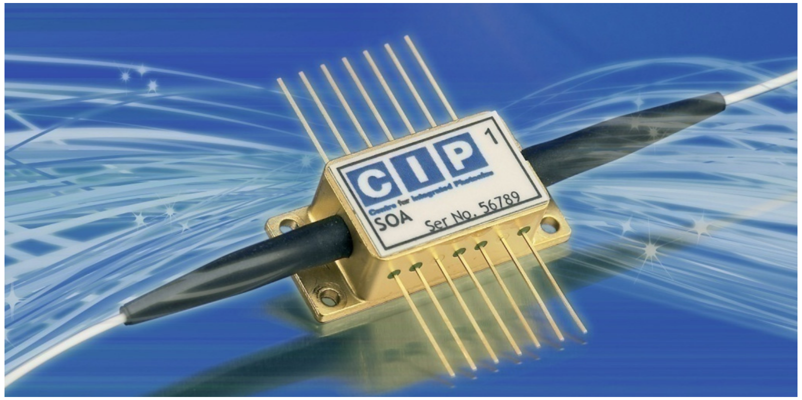
- Do not mix up between the extent of the gain region and the emission linewidth of a laser! At this stage we can only say that lasing will occur in the gain region…

Semiconductor optical amplifier (SOA)





Light amplification via stimulated emission occurs while it propagates inside the waveguide

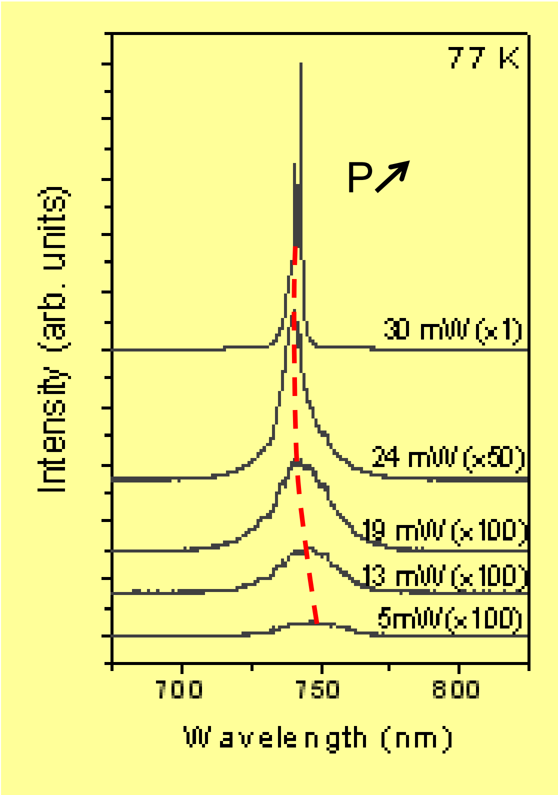


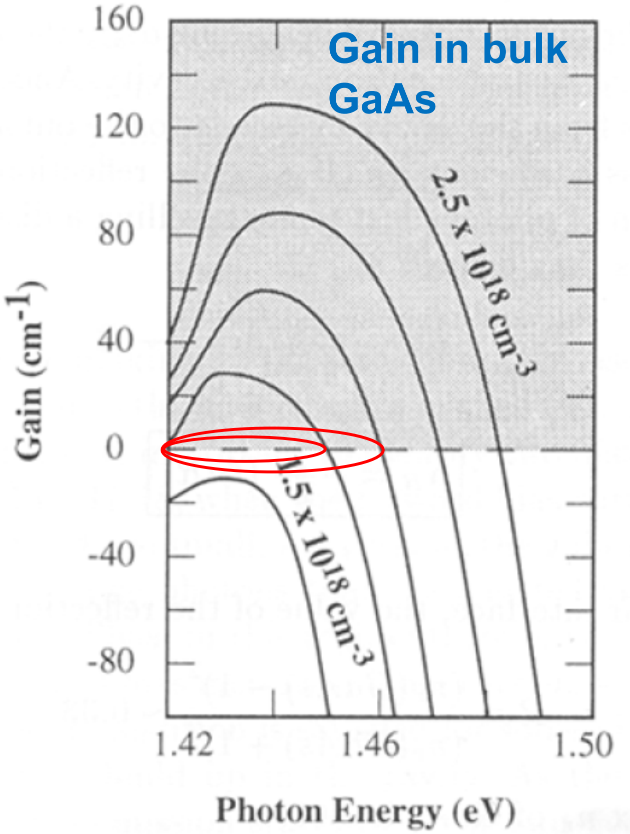
Single-pass device (i.e., no optical feedback)

Gain up to 30 dB

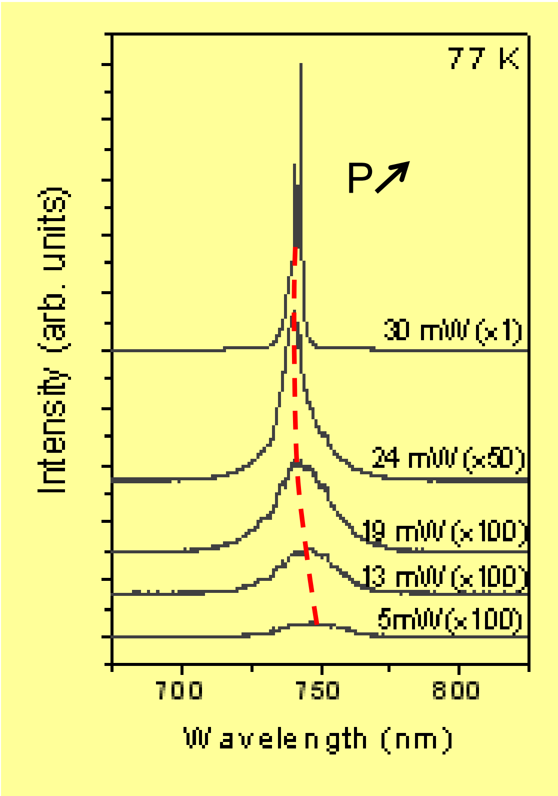
http://en.wikipedia.org/wiki/Wavelength-division_multiplexing

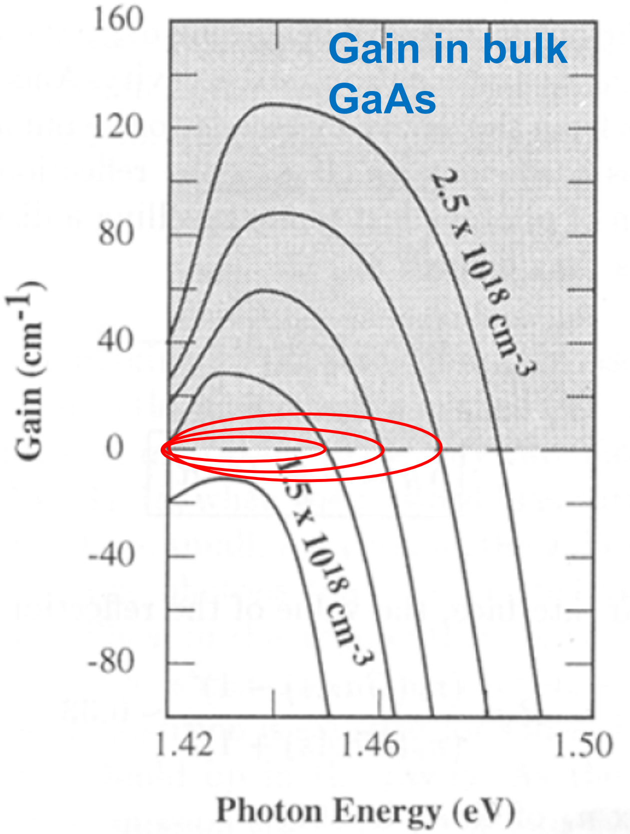
Absorption and gain in semiconductors



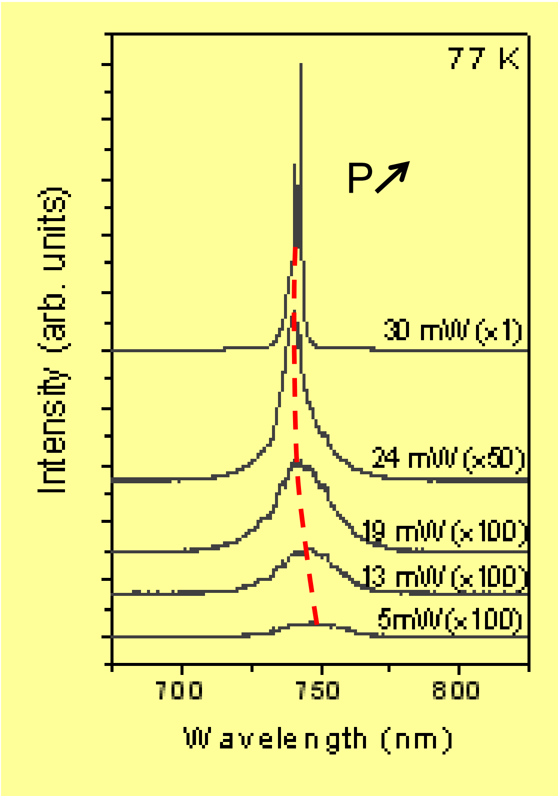


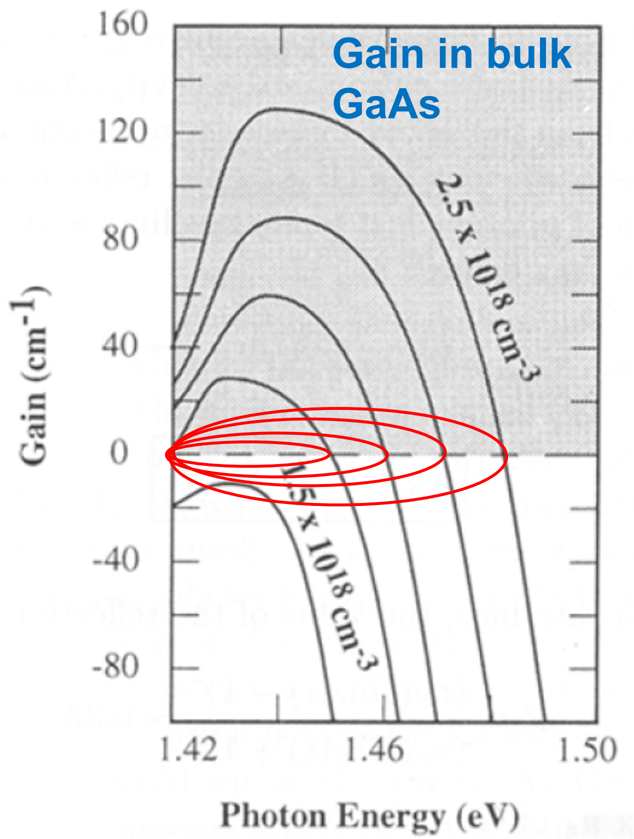
Absorption and gain in semiconductors





Absorption and gain in semiconductors





Absorption and gain in semiconductors