Lecture 1: Energy Bands, Fermi Energy and doping
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Reading guide:
Liu: 1-40 (First 20 pages are an overview)
Jena: 50-53 (46-50 for some background on Fermi-Dirac)
Effective mass approximation:

Kinetic Energy:

\[ E - E_c = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2 + k_z^2) \]

Effective Mass:

\[ m^* = \frac{\hbar^2}{\frac{d^2 E}{dk^2}} \]

Group Velocity:

\[ v_x = \frac{1}{\hbar} \frac{dE_k}{dk_x} = \frac{\hbar}{m^*} k_x \]

Density of states:

\[ D_{3D} = \frac{(2m^*)^{1.5}}{2\pi^2 \hbar^3} \sqrt{E - E_c} \]
Energy Bands – $E(k)$ and $E(x)$

The bottom of the conduction band ($E_C$) corresponds to the *potential energy* of an electron.

$E_k = E - E_c$ corresponds to the kinetic energy
2D Energy Bands – Quantum Wells

For a very thin slab of semiconductor material – the electrons are confined in the z direction

Infinite quantum well energies

\[ E_n \approx \frac{\hbar^2 n^2 \pi^2}{2m^*W^2} \]

Sub-band energy dispersion

\[ E_k = \frac{\hbar}{2m^*} (k_x^2 + k_y^2) + E_n + E_C \]

Density of states:

\[ D_{2D} = \sum_n \frac{m^*}{\pi \hbar^2} \Theta(E - E_n) \]

Carriers are free to move in the x-y plane!
Semiconductor Bandgaps

Semiconductors with different bandgaps.

Binarys (III-V): GaAs, InP, InAs..

Ternaries: \( \text{In}_{1-x}\text{Ga}_x\text{As}, \text{In}_{1-x}\text{Al}_x\text{As}, \text{GaAs}_{1-x}\text{Sb}_x \).  

Materials with similar lattice constants can easily be combined.

- GaAs-Al\(_x\)Ga\(_{1-x}\)As
- InP-In\(_{0.53}\)Ga\(_{0.47}\)As-In\(_{0.52}\)Al\(_{0.48}\)As
- InAs-AlSb-GaSb

*Fig. 18*  Energy bandgap and lattice constant for three III-V compound solid alloy systems.
Semiconductor heterostructures

• Different materials have different affinities and different band gaps.

• When forming heterostructures – different materials obtain conduction and valence band offsets to each other.

\[ \Delta E_C - \text{conduction band offsets} \]
\[ \Delta E_V - \text{valence band offsets} \]

Note: This is a simplistic explanation!
Tabulated affinities and bandgaps cannot be used to accurately calculate \( \Delta E_C \) and \( \Delta E_V \) between materials.
Semiconductor Bandgaps

Common (almost) lattice matched semiconductors:

- **GaAs** – Al$_{1-x}$Ga$_x$As
- **InP-In$_{0.53}$Ga$_{0.47}$As-In$_{0.52}$Ga$_{0.48}$As
- **InAs-GaSb-AlSb**
- The materials have different $E_g$ and $m^*$
- $\Delta E_C$ and $\Delta E_V$ characterize the heterojunctions

Not lattice matched, but technologically important:

- **Si (SiGe)**
- **GaN-AlN-InGaN-AlGaN**
- **InP-InAs**
Crystal Growth: Lattice Matching III - Strain

\[ a \approx 5.95\text{Å} \]

\[ \text{In}_{0.7}\text{Ga}_{0.3}\text{As} \]

\[ a = 5.87\text{Å} \]

\[ \text{InP} \]

\[ f = \frac{\Delta a}{a} - 0.014 \]

Lattice Mismatch:

Small lattice-mismatch: \textit{Large} critical thickness before relaxation

Large lattice mismatch: \textit{Small} critical thickness before relaxation

\[ \text{In}_{1-x}\text{Ga}_x\text{As on InP} \]
Fermi Level and F/D Statistics

Electrons obey Fermi-Dirac statistics:

\[ f_0(E, E_F) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}} \]

Total concentration of free electrons:

\[ n = \int_{E_c}^{\infty} D_{3D}(E)f_0(E - E_F)dE \]

Effective density of states:

\[ N_c = 2 \left( \frac{2\pi m^* kT}{h^2} \right)^{1.5} \]

\[ \frac{n}{N_c} = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} dx \frac{\sqrt{x}}{1 + \exp\left[x - \frac{E_F - E_c}{kT}\right]} = F_{1/2}(\frac{(E_f - E_c)}{kT}) \]

For InAs:

\[ N_c = 8.7 \times 10^{16}\text{cm}^{-3} \]
\[ N_v = 6.6 \times 10^{18}\text{cm}^{-3} \]
Fermi Level and F/D Statistics

Integral for electron concentration:

\[ \frac{n}{N_c} = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{\eta}}{1 + e^{\eta - \eta_F}} d\eta = F_{1/2}(\eta_F) \]

\[ N_c = 2 \left( \frac{2\pi m^* kT}{\hbar^2} \right)^{1.5} \]

\[ n \approx N_c e^{(E_f - E_c)/kT} \]

Maxwell-Boltzmann statistics, valid if \( n < 0.05 N_c \), or \( E_c - E_f >> 3kT \)

\[ \frac{E_f - E_c}{kT} \approx \ln \left( \frac{n}{N_c} \right) + \frac{n}{N_c} \cdot \frac{1}{\left( 64 + \frac{3.6n}{N_c} \right)^{1/4}} \]

\[ \frac{E_f - E_c}{kT} \approx \ln \left( \frac{n}{N_c} \right) + \frac{1}{\sqrt{8}} \left( \frac{n}{N_c} \right) - 0.00495 \left( \frac{n}{N_c} \right)^2 + \ldots \]

(Joyce-Dixon approximation)

For InAs:

\( N_c = 8.7 \times 10^{16} \text{cm}^{-3} \)

\( N_v = 6.6 \times 10^{18} \text{cm}^{-3} \)
\[
\frac{E_f - E_c}{kT} \approx \ln \left( \frac{n}{N_c} \right) + \frac{1}{\sqrt{8}} \left( \frac{n}{N_c} \right) - 0.00495 \left( \frac{n}{N_c} \right)^2
\]

\[
\frac{n}{N_c} = F_{1/2}(E_f - E_c)
\]

Exact! (within the EMA)

Very easy to calculate \(E_f - E_c\) if \(n\) is known!
(reverse is usually not true – numerical calculations needed.)
Intrinsic Semiconductor – Thermally excited charges

Intrinsic semiconductor (Boltzmann approx.) has thermally excited charges:

\[ n = p = n_i = \sqrt{N_V N_C} e^{-\frac{E_G}{2kT}} \]

\[ E_F - E_C \approx \frac{E_G}{2} + kT \ln \left( \frac{N_C}{N_V} \right) \]

Only strongly valid if \( n<N_C \) and \( p<N_V \)! (Boltzmann approx.)

Ex:
InAs: \( n_i=7\times10^{15} \) cm\(^{-2}\)
GaAs: \( n_i=1.8\times10^6 \) cm\(^{-2}\)

An intrinsic semiconductor has \( E_F \) in close to the middle of the bandgap.
Semiconductor Crystals - doping

- Introduction of donor atoms into the semiconductor creates free electrons
  - Each ionized donor atom – one free electron (e-) and one fixed donor ion. \((N_D^+)\)

- Introduction of acceptor atoms into the semiconductor captures an electron from the valence band
  - Each ionized acceptor atom – one free hole \((h^+)\) and one fixed acceptor ion. \((N_A^-)\)

Doping Range \(\approx 10^{14} – 10^{20} \text{ cm}^{-3}\)

Most semiconductors are never intrinsic!
Carrier Concentration – Doped Semiconductors

N-doping

\[ n = \sqrt{\frac{N_d^2 + 4n_i^2 + N_d}{2}} \approx N_d \]

\[ N_d \gg n_i \]

p-doping

\[ p = \sqrt{\frac{N_a^2 + 4n_i^2 + N_a}{2}} \approx N_a \]

\[ np = n_i^2 \quad \text{Mass action law (Boltzmann approx)} \]

N-type material:

\[ n_n \approx \frac{N_d}{N_d} \gg n_i \quad \text{Majority Carriers} \]

\[ p_n \approx \frac{n_i^2}{N_d} \ll n_i \quad \text{Minority Carriers} \]
Semiconductor Crystals – high doping

*Low doping* – isolated states

*High doping* – ionized dopant atoms interact with band edge – donor atoms inside above $E_c$.

*No freezeout!*

This is usually the case for most small bandgap III-Vs.