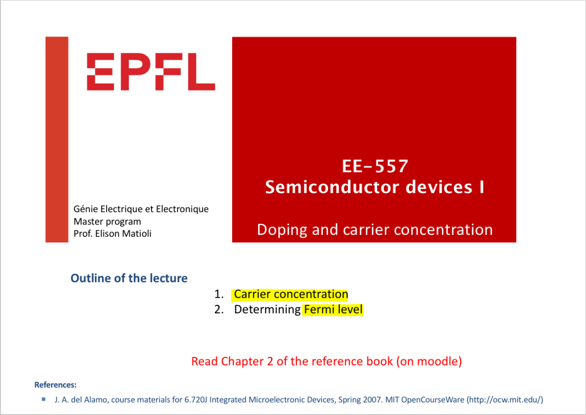
Course 3

Wednesday, 18 September 2024 09:57

EE557Cours 3 - Carrier...

Equal opportunity makes us brighter
Diversity is our strength
Listen and dare to speak up
Look out for each other
Kindness brings serenity
Together we go further
EPFL



EE-557
Semiconductor devices I

Doping and carrier concentration

Génie Electrique et Electronique
Master program
Prof. Elison Matioli

Outline of the lecture

1. Carrier concentration
2. Determining Fermi level

Read Chapter 2 of the reference book (on moodle)

References:

- J. A. del Alamo, course materials for 6.720J Integrated Microelectronic Devices, Spring 2007. MIT OpenCourseWare (http://ocw.mit.edu/)

Crystal structure: Definitions

Unit cell: Defines the symmetry and structure of the entire lattice

Bravais lattices: describe the geometric arrangement of the lattice points

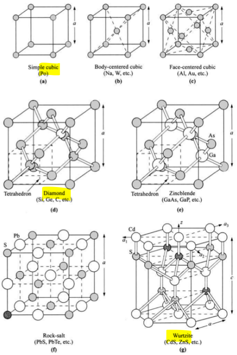
a is the lattice constant.

Crystal structure and symmetry play a critical role in determining many physical properties, such as:

- **Cleavage:**
  Check out this video:
  https://www.youtube.com/watch?v=IRoIXjxIcBQ
- **Mechanical properties** (elastic compliance, stiffness)
- **Electronic band structure**: Band gap
- **Optical transparency**
- **Thermal properties**
- **Polarization fields**

GaN: most common in wurtzite structure

Zincblende structure: III-V compound semiconductors: GaAs, GaP, *etc:*
Important for optoelectronics and high-speed Ics


a
Simple cubic (Po)
(a)
Body-centered cubic (Na, W, etc.)
(b)
Face-centered cubic (Al, Au, etc.)
(c)
Tetrahedron
Diamond (Si, Ge, C, etc.)
(d)
As
Ga
Tetrahedron
Zincblende (GaAs, GaP, etc.)
(e)
Pb
S
Rock-salt (PbS, PbTe, etc.)
(f)
Cd
S
z
a_1
a_2
a_3
c
Wurtzite (CdS, ZnS, etc.)
(g)

How Energy Bands and Energy Gap are calculated?

Energy-momentum relationship: characterizes the band structure

- Important for the interactions with photons and phonons

Schrödinger's equation: $$\underbrace{\left[-\frac{\hbar^2}{2m^*}\nabla^2\right.}_{}+\underbrace{V(\boldsymbol{r})}_{}\Big]\psi(\boldsymbol{r},\boldsymbol{k}) = E(\boldsymbol{k})\psi(\boldsymbol{r},\boldsymbol{k})$$

Bloch function $$\psi(\boldsymbol{r},\boldsymbol{k}) = \underbrace{\exp(j\boldsymbol{k}\cdot\boldsymbol{r})}_{}\underbrace{U_b(\boldsymbol{r},\boldsymbol{k})}_{}$$

$\psi(\boldsymbol{r},\boldsymbol{k})$ and $U_b(\boldsymbol{r},\boldsymbol{k})$ are periodic in R in real space

$$\psi(x+R) = \psi(R)$$

$$= e^{jkx} \cdot e^{jk.R} \cdot U_b(x+R,k)$$

$$U_b(x+R,k) = U_b(x,k)$$

$$= \underbrace{e^{ikx} \cdot U_b(x,k)}_{\psi(R)} \cdot e^{ikR}$$

Thus:

$$e^{ik.R} = 1$$

$$k.R = n.2\pi$$

$$\psi(\boldsymbol{r}+\boldsymbol{R},\boldsymbol{k}) = \exp[j\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{R})]U_b(\boldsymbol{r}+\boldsymbol{R},\boldsymbol{k})$$
$$= \exp(j\boldsymbol{k}\cdot\boldsymbol{r})\exp(j\boldsymbol{k}\cdot\boldsymbol{R})U_b(\boldsymbol{r},\boldsymbol{k})$$

$\boldsymbol{k}\cdot\boldsymbol{R}$ is a multiple of 2π.

How Energy Bands and Energy Gap are calculated?

In 1D – simple case

$$\psi(x) = \underset{\text{plane wave}}{e^{ik.x}} \cdot \underset{\text{periodicity of crystal}}{u_k(x)}$$: bloch function

real space

N atoms = L = N.a

$$u(x+a) = u(x)$$

$$\psi(x+L) = \psi(x)$$

$$\psi(x+L) = e^{ikx} \cdot \underset{u_k(x+L)}{\overset{}{u_k(x)}} \cdot e^{ik.L} = \psi(x) \Rightarrow k.L = p.2\pi$$

$$\boxed{k = p.\frac{2\pi}{L}}$$

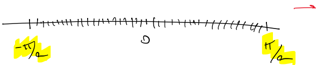
$$k = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \ldots, \overset{+}{\cancel{-}}\frac{N\pi}{L} = \pi/a$$

$-\frac{N\pi}{L} = -\pi/a$ is not counted as it was already counted in $+\pi/a$

Consequences:

- In 1D: only *k* = 2**π**/*L* are allowed (where *a* is the real space period)
- E(*k*) is periodic in k-space: E(*k*) = E(*k*+G)
- It is sufficient to define *k* in a primitive cell, which is defined by the Brillouin zone: - **π**/*a*, **π**/*a*
- Entire band structures need only to be calculated within the brillouin zone.

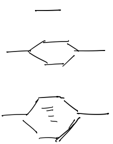
Brillouin Zone



How many states are there:

$$\underbrace{2}_{\text{spins}} \times \frac{2\pi/a}{2\pi/L} = 2.\frac{L}{a} = \boxed{2N}$$

$$\frac{L}{a} = \underbrace{N}_{\#\text{ atoms or unit cells}}$$



1 atom : 1 state

2 atoms : 2 states

N atoms : N states

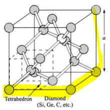
Crystallographic Notation

solutions: $E(k)$, $\psi(x,k)$

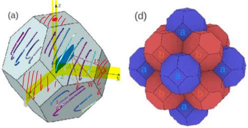
In 3D - Reciprocal space

Defines the principal symmetry points :

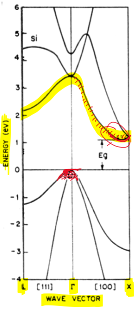
Gamma = (0; 0; 0) is the origin
X = (1; 0; 0) + 6 equivalent points,
L = (1; 1; 1) + 8 equivalent points

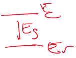


Real space



Reciprocal space





Fundamental to define the band structure of a semiconductor

The reciprocal lattice plays a fundamental role in most analytic studies (properties related to momentum) of periodic structures:

- Energy-momentum relationship
- Theory of diffraction: X-Ray diffraction

Energy band-gap

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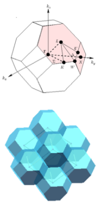
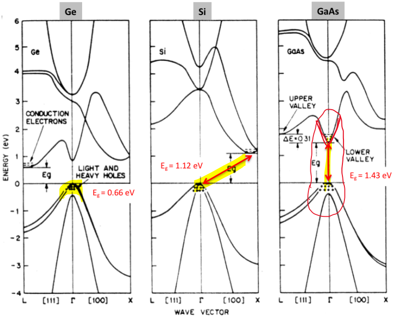
Reciprocal space directions:





Indirect band gap

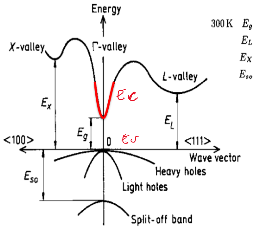
direct band gap

What do we learn from band diagrams

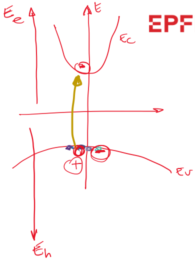
EPFL

Band diagram: We focus on minimum of the bands (quadratic region)

GaAs



$$300\,\text{K} \quad E_g = 1.42\ \text{eV}$$
$$E_L = 1.71\ \text{eV}$$
$$E_X = 1.90\ \text{eV}$$
$$E_{so} = 0.34\ \text{eV}$$



What do we learn from it:

Energy-momentum relationship near band edges

1. Allowed and forbidden states
2. Group velocity: slope of the bands
3. Electron/hole mass: curvature of bands

What do we learn from band diagrams

EPFL

Effective mass

Band diagram: We focus on minimum of the bands (quadratic region)

GaAs

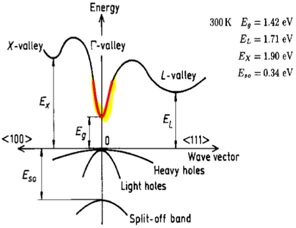
Energy-momentum relationship near band edges

$$\boxed{E(k) = \frac{p^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*}}$$

Effective mass in 1D

electron in free space

$$E = \frac{\hbar^2 k^2}{2m_e}$$



$$m_j^* = \hbar^2 \left(\frac{\partial^2 E_j}{\partial k_y^2} \right)^{-1}$$

$\hbar = h/2\pi$: planck's constant = 6.58 eV.s

For example:

Si: $m^* = 1.09\ m_0$

GaN: $m^* = 0.2\ m_0$

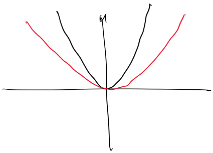
GaAs: $m^* = 0.06\ m_0$

Group velocity:

$$v_n(k) = \frac{1}{\hbar} \nabla_k\, E_n(k)$$

$$v_n(k) = \frac{\hbar k}{m^*} = \frac{p}{m^*}$$

Momentum $p = \hbar\, k$



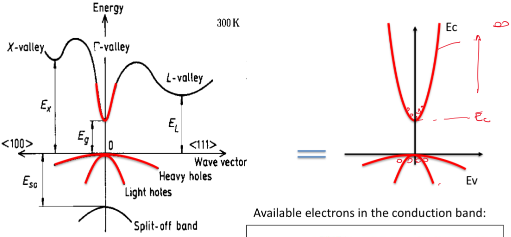
Key questions

- How many carriers are available for conduction?
- How can we increase and control the conductivity in semiconductors?

A few important concepts

How many carriers are available for conduction?

We are interested in analyzing the minimum of the conduction and valence bands



Available electrons in the conduction band:

$$\boxed{n_o = \int_{E_c}^{\infty} g_c(E)\ f(E)\, dE}$$

density of electrons   Probability of occupation

A few important concepts

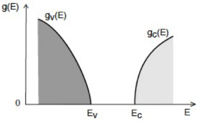
What is the density of electrons $g_c(E)$?

What law regulates the electron occupation of states *f*(E) as a function of energy and temperature?

$$\boxed{n_o = \int_{E_c}^{\infty} g_c(E)\ f(E)\, dE}$$

A few important concepts

Density of states



$$g_c(E) = 4\pi\underbrace{\left(\frac{2m_{de}^*}{h^2}\right)^{3/2}}\underbrace{\sqrt{E-E_c}}\qquad E \ge E_c$$

$$g_v(E) = 4\pi\left(\frac{2m_{dh}^*}{h^2}\right)^{3/2}\sqrt{E_v-E}\qquad E \le E_v$$

$m_{de}^{*} \equiv$ density of states electron effective mass
$m_{dh}^{*} \equiv$ density of states hole effective mass

Attention: this is the density of states for a 3D system. 2D, 1D and 0D systems have different energy dependencies

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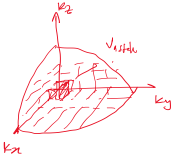
A few important concepts

Density of states

$K_x = n \frac{2\pi}{L_x}$ $\quad K_y = m \cdot \frac{2\pi}{L_y}$ $\quad K_z = \ell \cdot \frac{2\pi}{L_z}$

each (n, m, ℓ) represents one available state ⇒ that can be occupied by 2 electrons ↑↓



$V_{sphere}\, dk = 4\pi |K|^2 dk$

$V_{1\,state} = \left(\frac{2\pi}{L}\right)^3$, considering $L_x = L_y = L_z$

$$g(k)\,dk = \underbrace{2}_{spin} \times \frac{4\pi |k|^2 dk}{(2\pi)^3} \cdot L^3 = \frac{|k|^2}{\pi^2} \cdot dk \cdot L^2$$

change in variable : $E = \frac{\hbar^2 k^2}{2m^*} \Rightarrow g(E) \Rightarrow dE = \frac{\hbar^2 k\, dk}{m^*}$

$$g(E)\,dE = \frac{m^* dE}{\hbar^2} \cdot \frac{\sqrt{2m^* E}}{\hbar^2} \cdot \frac{1}{\pi^2} = 4\pi \left(\frac{2m^*}{h^2}\right)^{3/2} \cdot \sqrt{E - E_c}\, dE$$

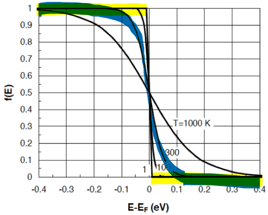
A few important concepts

Electron statistics

At finite temperature, state occupation probability by electron determined by **Fermi-Dirac distribution function:**

$$f(E) = \frac{1}{1 + \exp \frac{E - E_F}{\underbrace{kT}}}$$

$\frac{26\,meV}{at\ 30K}$



E_F: *Fermi energy* -energy for which occupation probability is 50%
k: Boltzmann constant = 8.62x 10^{-5} *eV/K*
kT -thermal energy = 25.9*meV at* 300 *K*

A few important concepts

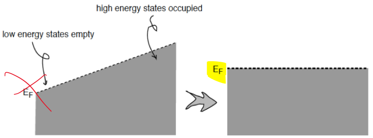
Notion of thermal equilibrium

A particle system is in thermal equilibrium (TE) if:

- it is closed: no energy flows through boundaries of system
- it is in steady-state: time derivatives of all ensemble averages (global and local) are zero

Thermal equilibrium important because all systems evolve towards TE after having been perturbed.

In thermal equilibrium, E_F constant throughout system



Carrier concentration

How to calculate the carrier concentration? (which is related to the current)

Density of states

$$\boxed{g_c(E) = 4\pi \left(\frac{2m_{de}^*}{h^2}\right)^{3/2} \sqrt{E - E_c}} \quad E \geq E_c$$

$$m_{de} = (m_1^* m_2^* m_3^*)^{1/3}$$

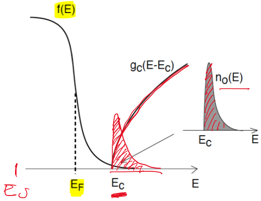
X

Probability of a state to be occupied

$$\boxed{f(E) = \frac{1}{1 + \exp\frac{E-E_F}{kT}}}$$

Integrated for all energies

$$n_o = \int_{E_c}^{\infty} g_c(E)\, f(E)\, dE$$



Questions

1. What is a simplified expression for the number of electrons n and holes p?
2. What is the position of the Fermi level?
3. What is the np product?

Carrier concentration

EPFL

$$f(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{kT}\right)}$$

$$g(E) = 4\pi \cdot \left(\frac{2m^*}{h^2}\right)^{3/2} \sqrt{E-E_c}$$

$$n = \int_{E_c}^{\infty} f(E) \cdot g(E)\, dE = N_c \cdot \frac{2}{\sqrt{\pi}} \cdot \mathcal{F}_{1/2}\left(\frac{E-E_c}{kT}\right)$$

effective density of states

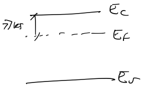
$$N_c = 2 \cdot \left(\frac{2\pi m_e^* \cdot kT}{h^2}\right)^{3/2}$$

Fermi-Dirac integral

$$\mathcal{F}_{1/2}(x) = \int_{E_c}^{\infty} \frac{x^{1/2}}{1+\exp^{x-x_f}} dx$$

Simplification: non-degenerate semiconductor

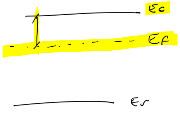
- Doping << N_c
- $E_c - E_f \gg$ a few kT



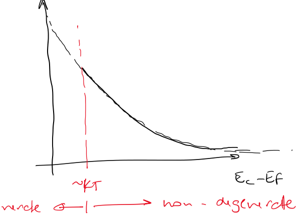
$$f_{1/2}\left(\frac{E-E_c}{kT}\right) \simeq \frac{\sqrt{\pi}}{2} \cdot \exp\left(-\frac{E_c-E_f}{kT}\right)$$

thus:

$$\boxed{n = N_c \cdot \exp\left(-\frac{E_c-E_f}{kT}\right)}$$



#e/cm³



for Silicon at 300K

$$N_C = 2\left(\frac{2\pi m_e^* \cdot kT}{h^2}\right)^{3/2}$$

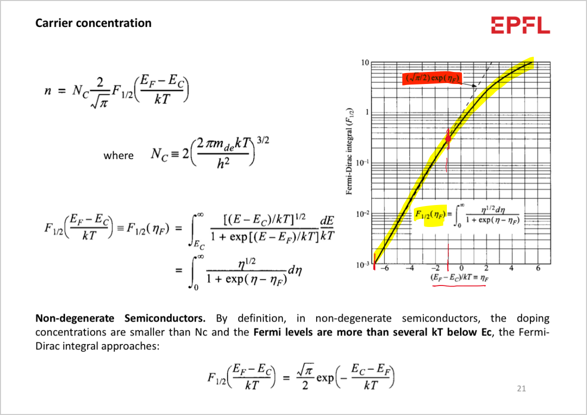
$$= 2\left(\frac{2\pi \times 5.69\times10^{-16}\, eV\, s^2/cm^2 \times 0.0259\, eV}{(4.14\times10^{-15}\, eV\, s)^2}\right)^{3/2} = \boxed{2.9\times10^{19}\, cm^{-3}}$$

$$N_C^* = \frac{N_C}{(300K)^{1.5}} \cdot (kT)^{1.5}$$

For holes:

$$\boxed{p = N_V \cdot \exp\left(-\frac{E_F - E_V}{kT}\right)}$$

$$\boxed{N_V = 3.1\times10^{19}\, cm^{-3}}$$



Carrier concentration

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_F - E_C}{kT}\right)$$

where $N_C \equiv 2\left(\frac{2\pi m_{de} kT}{h^2}\right)^{3/2}$

$$F_{1/2}\left(\frac{E_F - E_C}{kT}\right) \equiv F_{1/2}(\eta_F) = \int_{E_C}^{\infty} \frac{[(E-E_C)/kT]^{1/2}}{1+\exp[(E-E_F)/kT]}\frac{dE}{kT} = \int_0^{\infty} \frac{\eta^{1/2}}{1+\exp(\eta-\eta_F)}d\eta$$

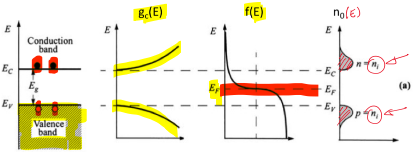
10
1
10⁻¹
10⁻²
10⁻³
Fermi-Dirac integral ($F_{1/2}$)
$(\sqrt{\pi}/2)\exp(\eta_F)$
$F_{1/2}(\eta_F) \equiv \int_0^{\infty} \frac{\eta^{1/2} d\eta}{1+\exp(\eta-\eta_F)}$
−6
−4
−2
0
2
4
6
$(E_F - E_C)/kT \equiv \eta_F$

Non-degenerate Semiconductors. By definition, in non-degenerate semiconductors, the doping concentrations are smaller than Nc and the **Fermi levels are more than several kT below Ec**, the Fermi-Dirac integral approaches:

$$F_{1/2}\left(\frac{E_F - E_C}{kT}\right) = \frac{\sqrt{\pi}}{2}\exp\left(-\frac{E_C - E_F}{kT}\right)$$

Carrier concentration

Intrinsic semiconductor (undoped)

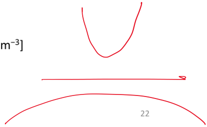


n_o ≡ equilibrium (free) electron concentration in conduction band [cm^{-3}]
p_o ≡ equilibrium hole concentration in valence band [cm^{-3}]

In intrinsic semiconductors:

$n_o = p_o = ni$ $\qquad$ n_i ≡ intrinsic carrier concentration [cm^{-3}]

$$\begin{cases} n = N_c \exp\left(-\frac{E_c - E_F}{kT}\right) \\ p = N_v \exp\left(-\frac{E_F - E_v}{kT}\right) \end{cases}$$



where is the position of E_F ?

[1] $E_c - E_f = kT \ln(N_c/n)$

[2] $E_f - E_v = kT \ln(N_v/p)$

[2] − [1] :

$$E_f - E_v - E_c + E_f = kT \ln(N_v/p) - kT \ln(N_c/p)$$

$$\boxed{E_f = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln\left(\frac{N_v}{N_c} \cdot \overset{1}{\cancel{\frac{n}{p}}}\right) = E_i}$$

very close to the center of the gap

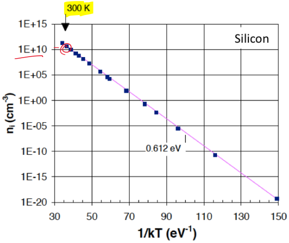
Carrier concentration

Intrinsic semiconductor (undoped)

First important result:

$n_o = p_o = n_i = 10^{10}\ cm^{-3}$

n_i ≡ intrinsic carrier concentration [cm^{-3}]



A second important result:

$$n_o p_o = n_i^2$$

E_C

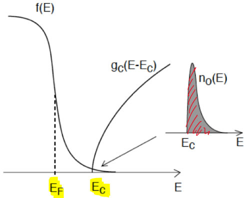
$E_g = 1.12\ eV$

E_V

Equilibrium ***np* product** in a semiconductor at a certain temperature is a **constant specific to the semiconductor**.

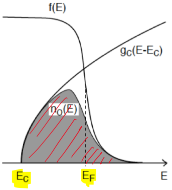
$kT = 26\ meV$

Carrier concentration



Non degenerate

$n = N_C \exp\left(\frac{-(E_C - E_F)}{kT}\right)$

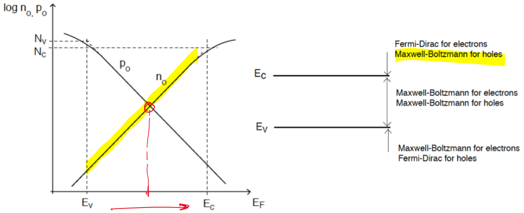


degenerate

n^{++}

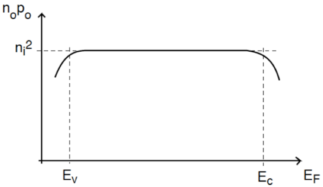
Carrier concentration

Summary of carrier statistics depending on E_F location


log n_o, p_o
N_V
N_C
p_o
n_o
E_V
E_C
E_F
E_C
E_V
Fermi-Dirac for electrons
Maxwell-Boltzmann for holes
Maxwell-Boltzmann for electrons
Maxwell-Boltzmann for holes
Maxwell-Boltzmann for electrons
Fermi-Dirac for holes

Carrier concentration

Summary of carrier statistics depending on E_F location



If E_F is inside bandgap:

$$n_o p_o \simeq N_c N_v \exp -\frac{E_g}{kT} = n_i^2$$

For a given semiconductor, $n_o p_o$ depends only on T and is independent of precise location of EF . But only if semiconductor is non-degenerate.

Carrier concentration

In intrinsic semiconductor, $n_o = p_o$ and usually fairly small ⇒semiconductor non-degenerate.

$$n_i = \sqrt{n_o p_o} = \sqrt{N_c N_v} \exp -\frac{E_g}{2kT}$$

Key conclusions

In solids, electron states cluster in bands separated by bandgaps.

Band structure:

- Depends on the atomic and crystal structure
- Dependent on the momentum of electrons
- Band gaps can be direct or indirect

E(*k*) is periodic in **k-space**: E(*k*) = E(*k*+G)

Entire band structures need only to be calculated within the brillouin zone.

Order of magnitude of key parameters:

– Atomic density of Si: $n \sim 5\times10^{22}$ cm^{-3}

– Bandgaps at 300K	Si:	E_g = 1.12 eV
	GaAs:	E_g = 1.43 eV
	GaN:	E_g = 3.39 eV

thermal energy: kT ~26 meV @300K

Key conclusions

Distinct feature of semiconductors: at 0 K, quantum state filling ends up with full band separated from next empty band by ~1-3eV bandgap at around 300 K, some electrons populate next band above bandgap.

System in thermal equilibrium:

- isolated from outside world and in steady state.
- In thermal equilibrium, E_F is independent of position: it is constant!

Occupation probability of quantum systems in thermal equilibrium governed by Fermi-Dirac distribution function:

$$f(E) = \frac{1}{1 + \exp\frac{E-E_F}{kT}}$$

Density of states give us the number of states per volume available at a give energy

In 3D:

$$g_c(E) = 4\pi \left(\frac{2m_{de}^*}{h^2}\right)^{3/2} \sqrt{E - E_c} \qquad E \geq E_c$$

$$g_v(E) = 4\pi \left(\frac{2m_{dh}^*}{h^2}\right)^{3/2} \sqrt{E_v - E} \qquad E \leq E_v$$

Key conclusions

Non-degenerate semiconductor:

$$n_o = N_c \exp\frac{E_F - E_c}{kT}, \qquad p_o = N_v \exp\frac{E_v - E_F}{kT}$$

Intrinsic semiconductor: ideally pure semiconductor.

$$n_o = p_o = n_i = \sqrt{N_c N_v} \exp -\frac{E_g}{2kT}$$

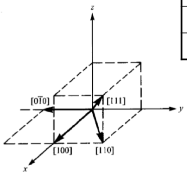
In non-degenerate semiconductor $n_o p_o$ $\quad n_o p_o = n_i^2$

Appendix – Supplementary Material

Crystallographic Notation

Miller Indices:

Notation	Interpretation
$(h\ k\ l)$	crystal plane
$\{h\ k\ l\}$	equivalent planes
$[h\ k\ l]$	crystal direction
$<h\ k\ l>$	equivalent directions



Sample direction vectors and their corresponding Miller indices.

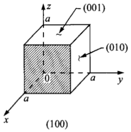
h: **inverse *x*-intercept of plane**
k: **inverse *y*-intercept of plane**
l: **inverse *z*-intercept of plane**

(Intercept values are in multiples of the lattice constant; *h*, *k* and *l* are reduced to 3 integers having the same ratio.)

** Wurtzite materials have an hexagonal crystal structure:
4 Miller indices are used to represent it more easily (see appendix for more information)

Crystallographic Notation

Real space or direct space (represented by Miller indices)



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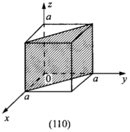

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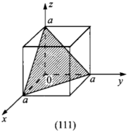

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Reciprocal space is also called **Fourier space, k- space, or momentum space**

$$\boldsymbol{a}^* \equiv 2\pi \frac{\boldsymbol{b} \times \boldsymbol{c}}{\boldsymbol{a} \cdot \boldsymbol{b} \times \boldsymbol{c}}$$

$$\boldsymbol{b}^* \equiv 2\pi \frac{\boldsymbol{c} \times \boldsymbol{a}}{\boldsymbol{a} \cdot \boldsymbol{b} \times \boldsymbol{c}}$$

$$\boldsymbol{c}^* \equiv 2\pi \frac{\boldsymbol{a} \times \boldsymbol{b}}{\boldsymbol{a} \cdot \boldsymbol{b} \times \boldsymbol{c}}$$

The reciprocal lattice plays a fundamental role in most analytic studies (properties related to momentum) of periodic structures:

- Energy-momentum relationship
- Theory of diffraction: X-Ray diffraction

This is not covered in this course (solid-state physics classes will cover this in details)

Reciprocal lattice vector:

$\boldsymbol{G} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$ for which: $\boldsymbol{G} \cdot \boldsymbol{R} = 2\pi \times \text{Integer}$

Crystallographic Notation

Reciprocal space is also called **Fourier space, k- space, or momentum space**

For instance, X-ray diffraction reveals the reciprocal space

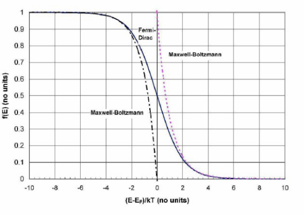
Interesting video: https://www.youtube.com/watch?v=DFFU39A3fPY

Electronic structure of semiconductors

Electron statistics

Approximation

$$f(E) = \frac{1}{1 + \exp \frac{E - E_F}{kT}}$$



- Maxwell-Boltzmann approximation:

  For $E - E_F \gg kT$:

$$f(E) \simeq \exp -\frac{E - E_F}{kT}$$

  For $E - E_F \ll kT$:

$$f(E) \simeq 1 - \exp \frac{E - E_F}{kT}$$