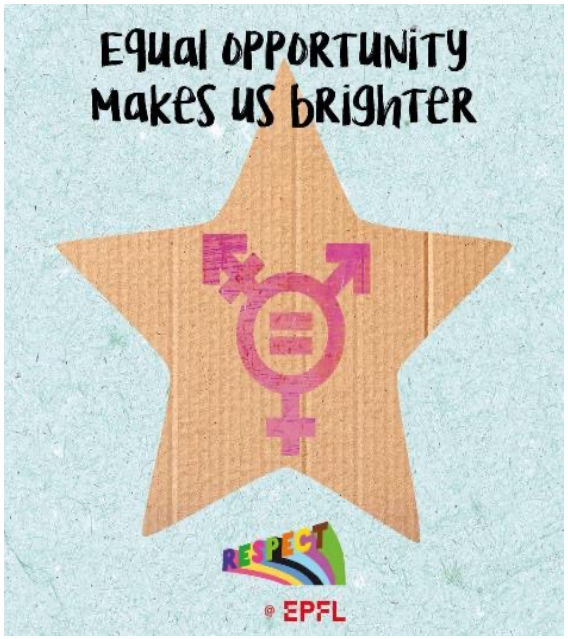
Equal opportunity
makes us brighter
RESPECT
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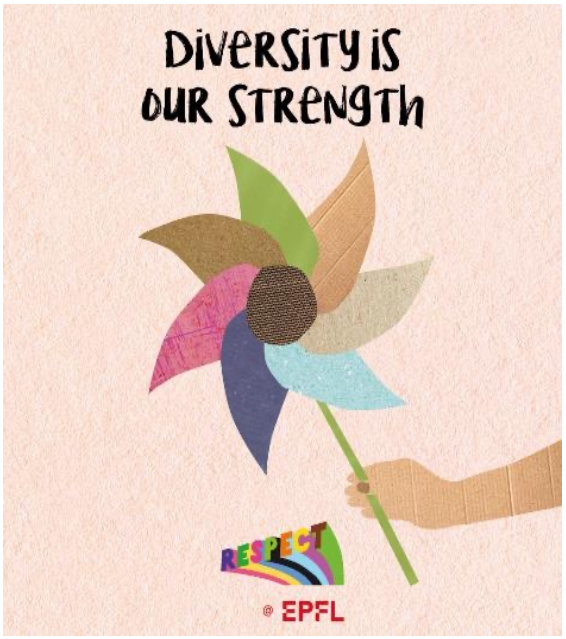
Diversity is
our strength
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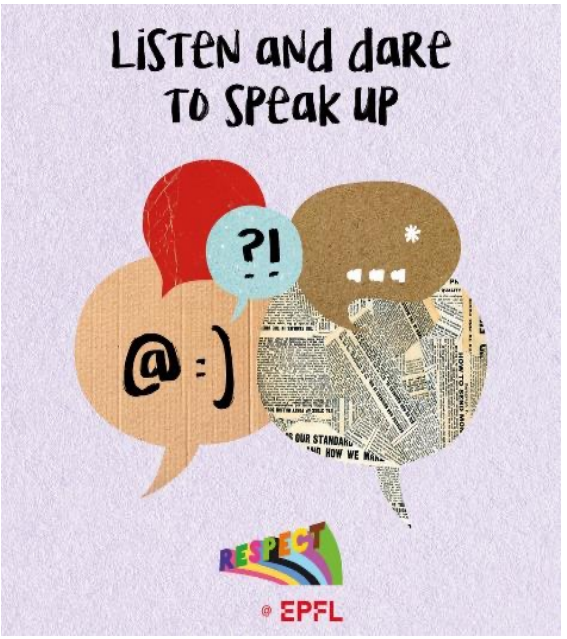
Listen and dare
to speak up
?!
@ :)
RESPECT
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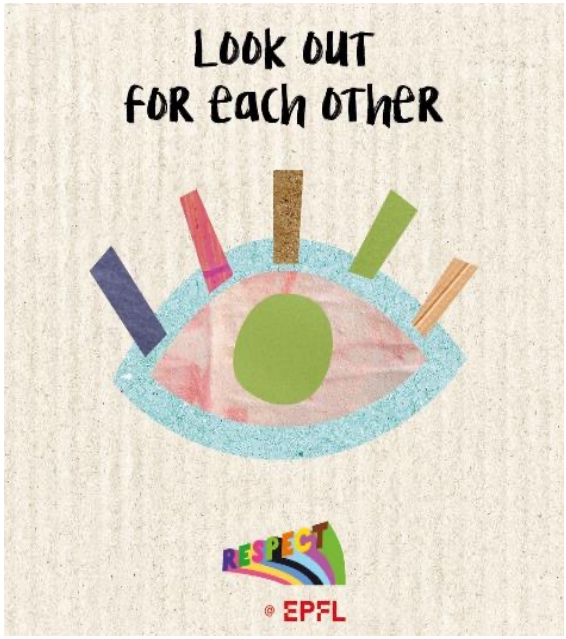
Look out
for each other
RESPECT
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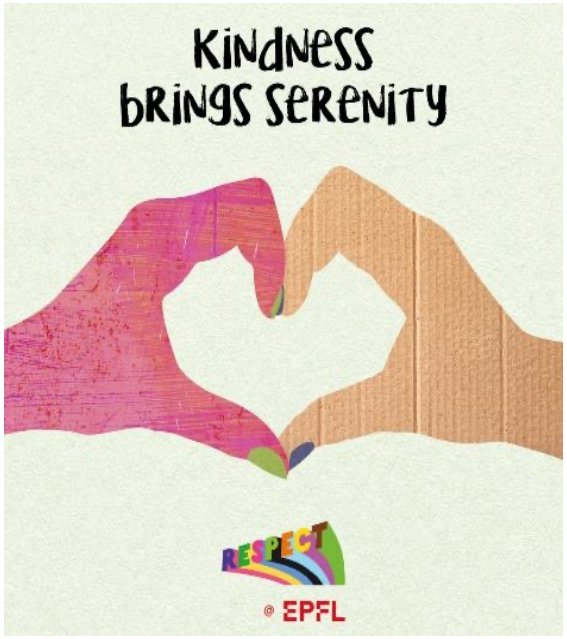
Kindness
brings serenity
RESPECT
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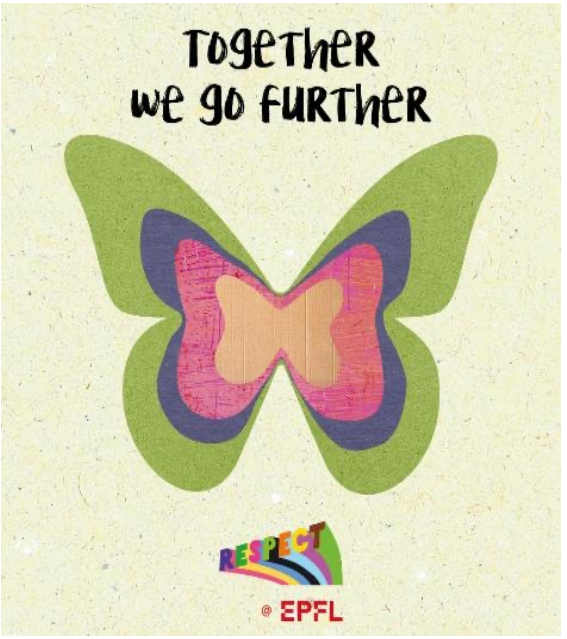
Together
we go further
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EE-557
Semiconductor devices I

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

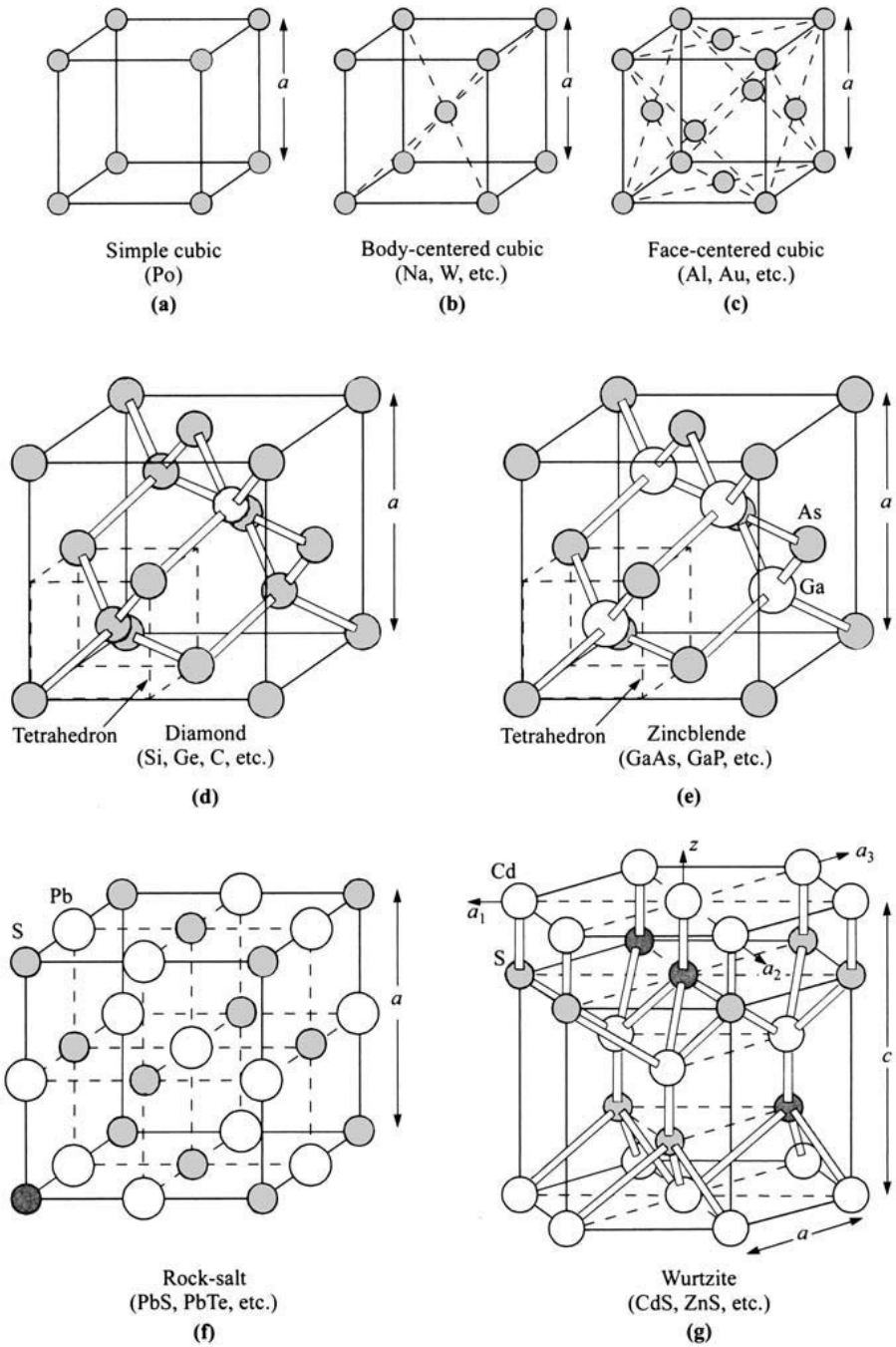
a is the lattice constant.

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



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: $$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r},\boldsymbol{k}) = E(\boldsymbol{k})\psi(\boldsymbol{r},\boldsymbol{k})$$

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

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

Thus:

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

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

How Energy Bands and Energy Gap are calculated?

In 1D – simple case

Consequences:

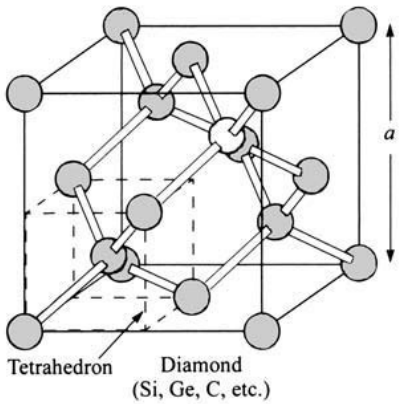
- In 1D: only $k = 2\pi/L$ are allowed (where a is the real space period)
- E(k) is periodic in k-space: E(k) = E(k+G)
- It is sufficient to define k in a primitive cell, which is defined by the Brillouin zone: $-\pi/a$, π/a
- Entire band structures need only to be calculated within the brillouin zone.

Crystallographic Notation

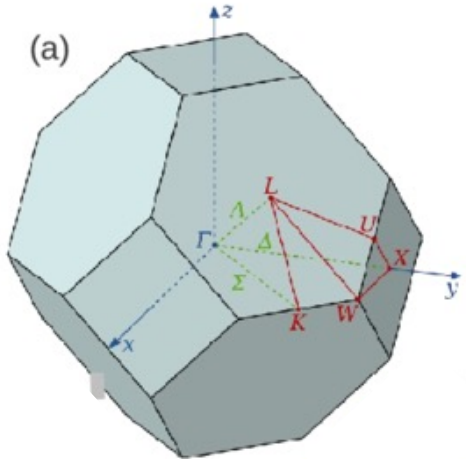
In 3D - Reciprocal space

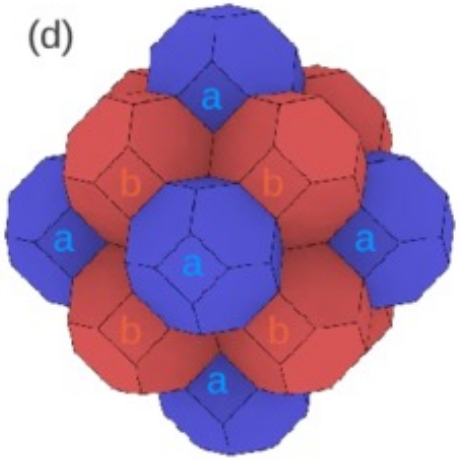
Defines the principal symmetry points :

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

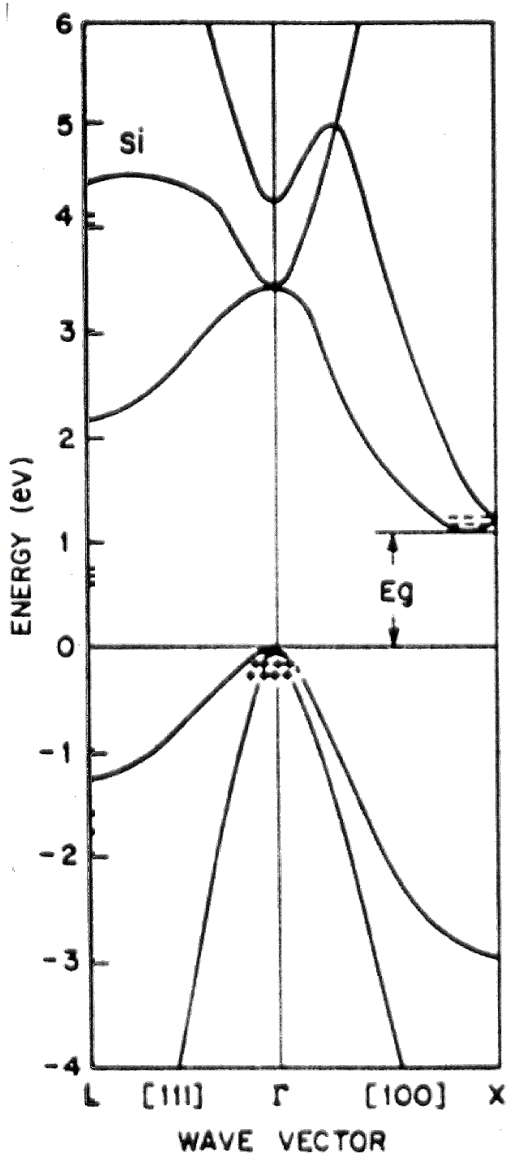


Real space





Reciprocal space



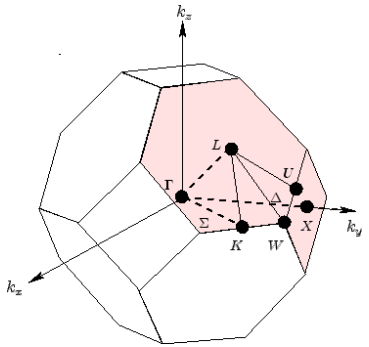
Fundamental to define the band structure of a semiconductor

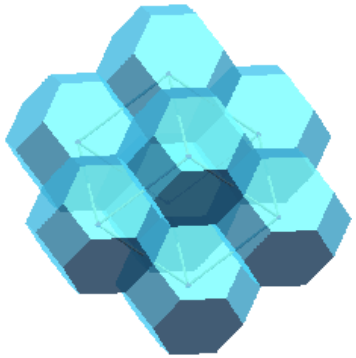
The reciprocal lattice plays a fundamental role in most analytic studies (properties related to momentum) of periodic structures:

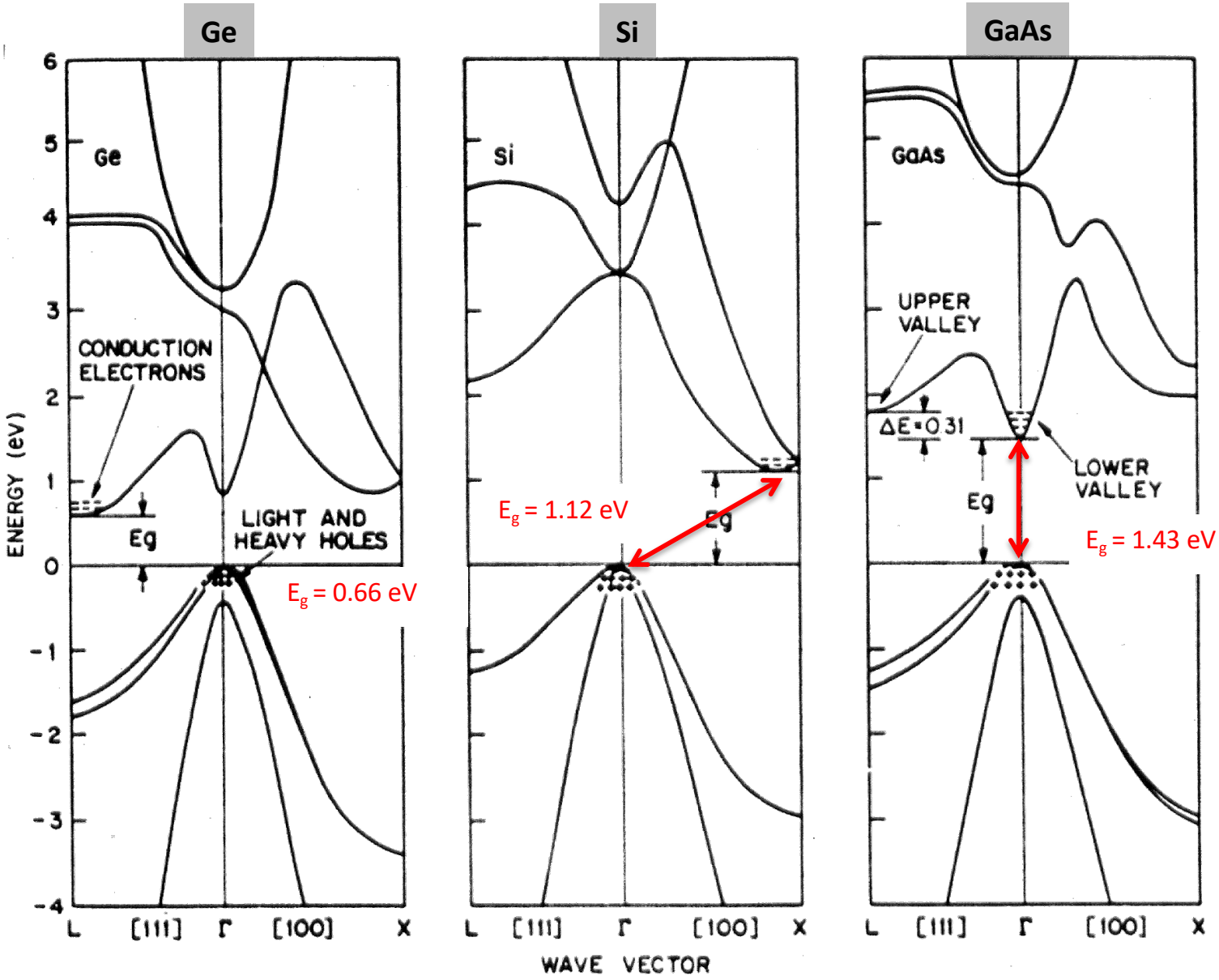
- Energy-momentum relationship
- Theory of diffraction: X-Ray diffraction

Energy band-gap

Reciprocal space directions:







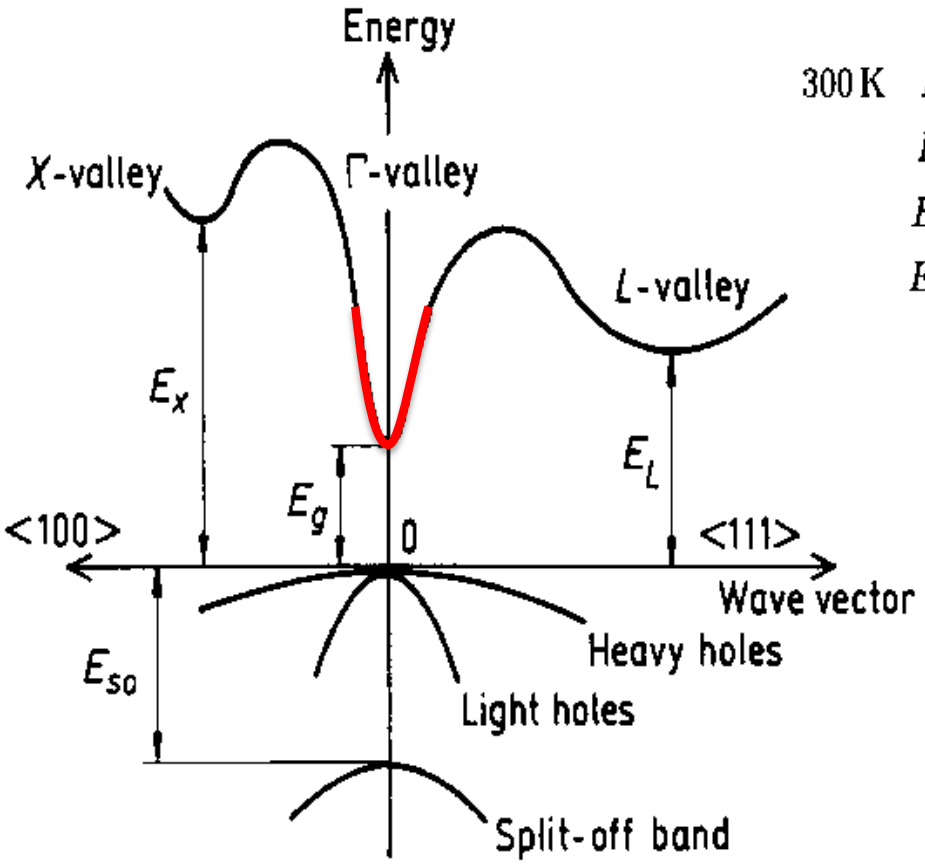
Indirect band gap

direct band gap

What do we learn from band diagrams

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

GaAs



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

What do we learn from it:

Energy-momentum relationship near band edges

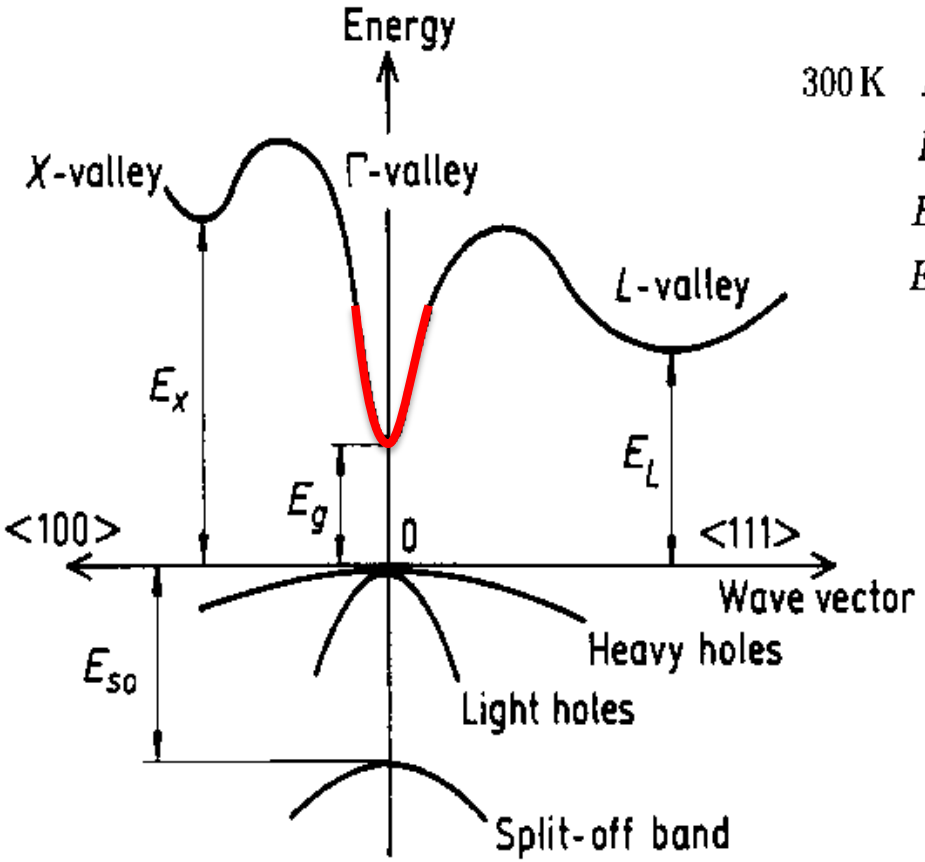
1. Allowed and forbidden states
2. Group velocity: slope of the bands
3. Electron/hole mass: curvature of bands

What do we learn from band diagrams

Effective mass

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

GaAs



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

Energy-momentum relationship near band edges

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

Effective mass in 1D

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

$\hbar = h/2\pi$: 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 $p = \hbar k$

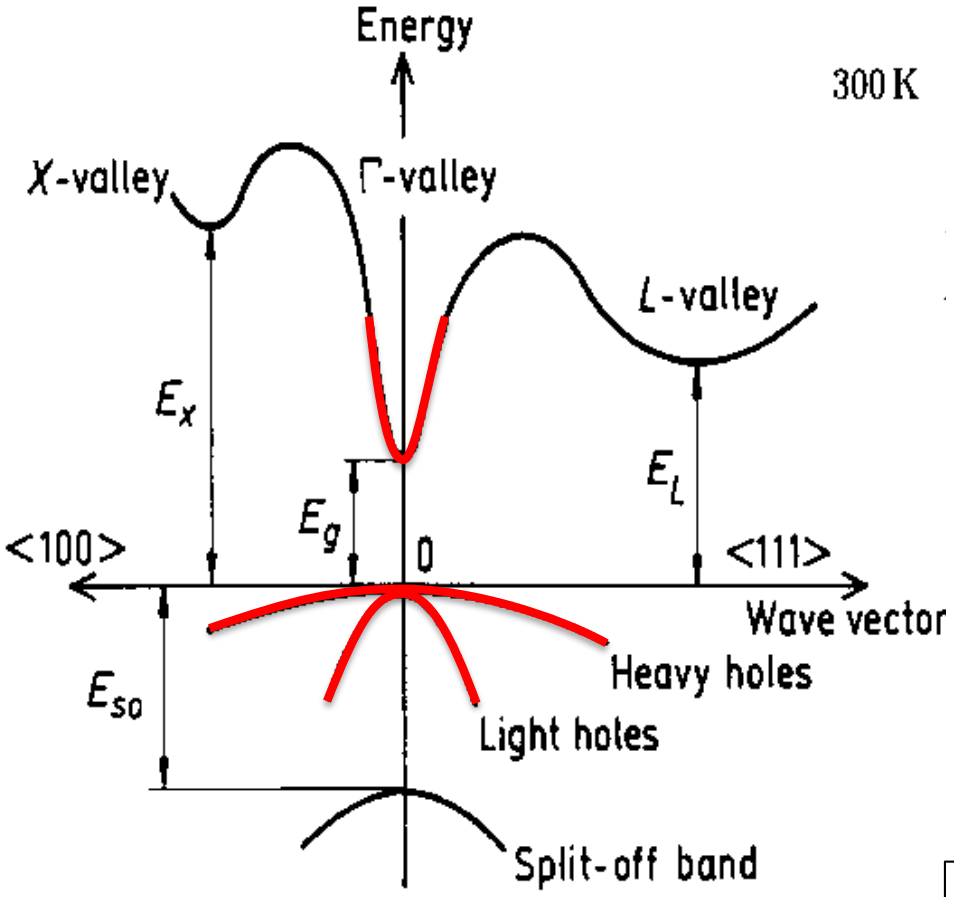
Key questions

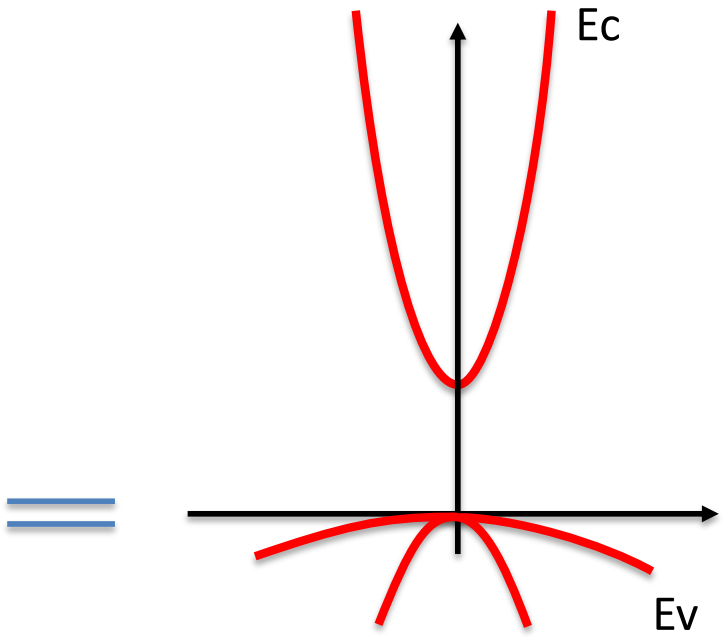
- How many carriers are available for conduction?
- How can we increase and control the conductivity in semiconductors?

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:

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

density of electrons — Probability of occupation

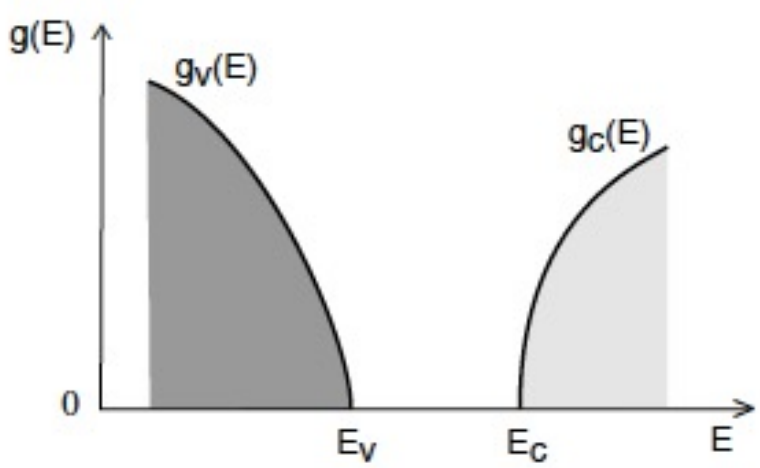
What is the density of electrons $g_c(E)$?

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

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

A few important concepts

Density of states



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

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

$m^*_{de} \equiv$ 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

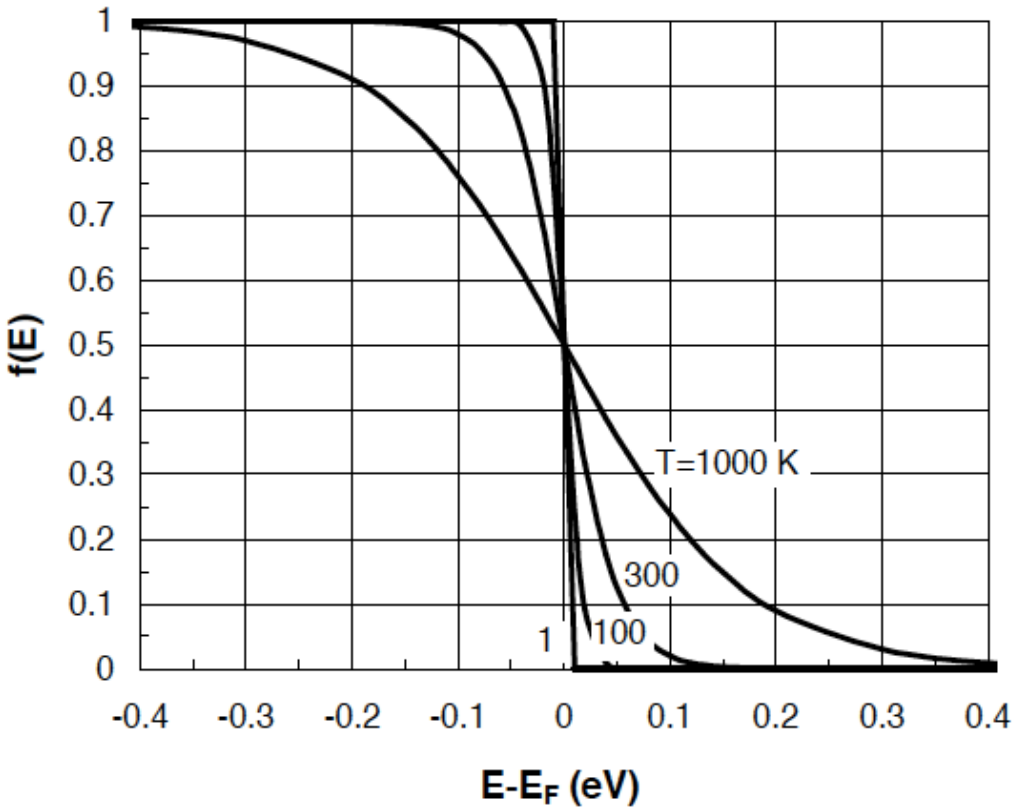
A few important concepts

Density of states

Electron statistics

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

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



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

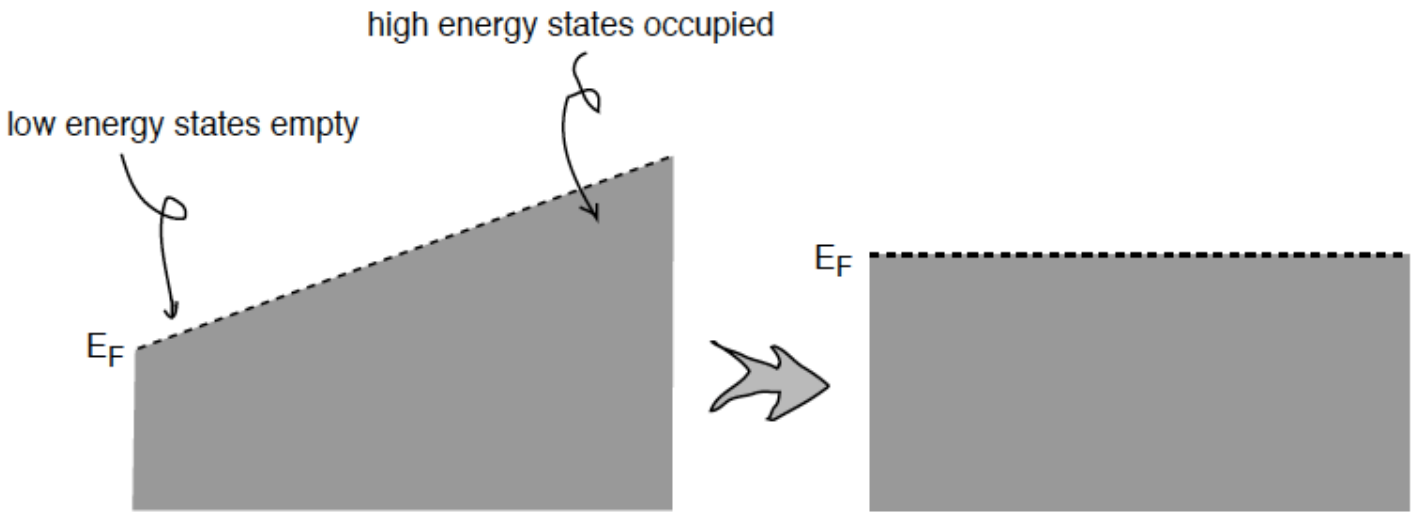
Notion of thermal equilibrium

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

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

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

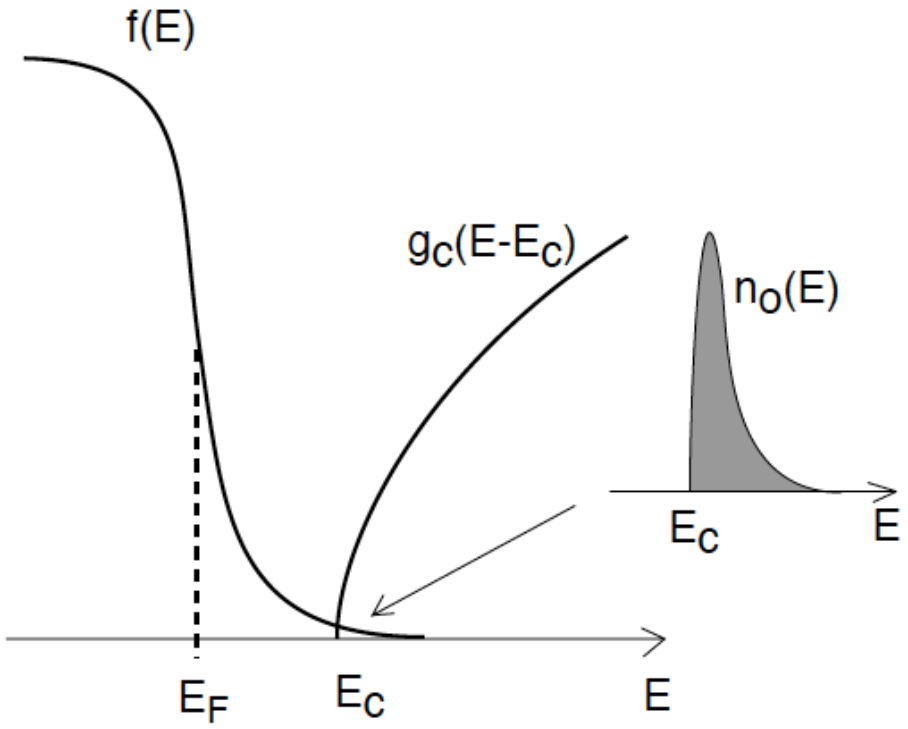
X

Probability of a state to be occupied

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

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

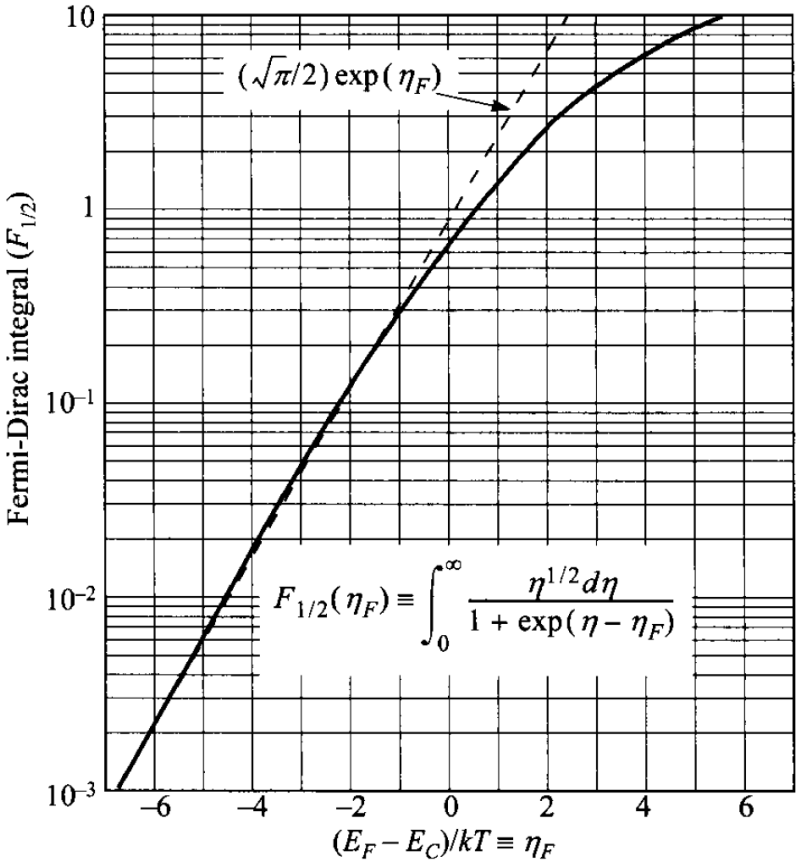
Carrier concentration

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

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

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

$$= \int_0^{\infty} \frac{\eta^{1/2}}{1 + \exp(\eta - \eta_F)} d\eta$$

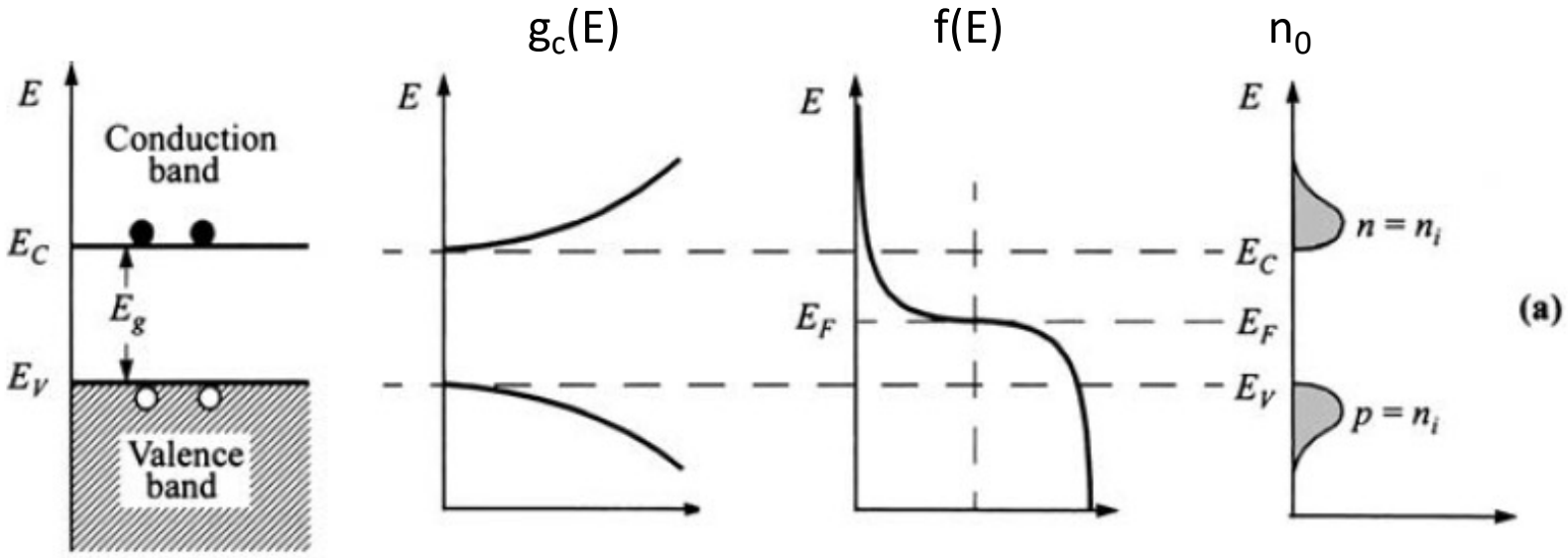


Non-degenerate Semiconductors. By definition, in non-degenerate semiconductors, the doping concentrations are smaller than Nc and the **Fermi levels are more than several kT below Ec**, the Fermi-Dirac integral approaches:

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

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

Carrier concentration

Intrinsic semiconductor (undoped)

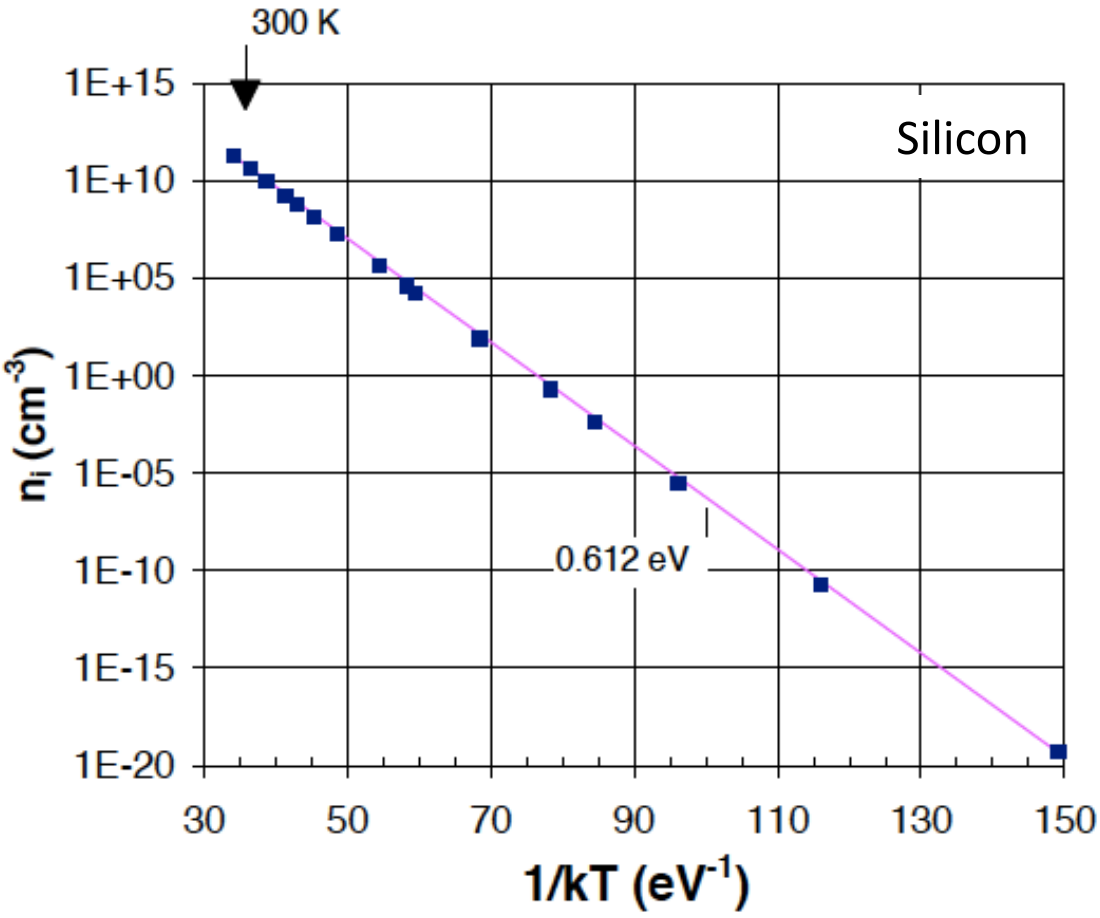
First important result:

$$n_o = p_o = ni$$

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

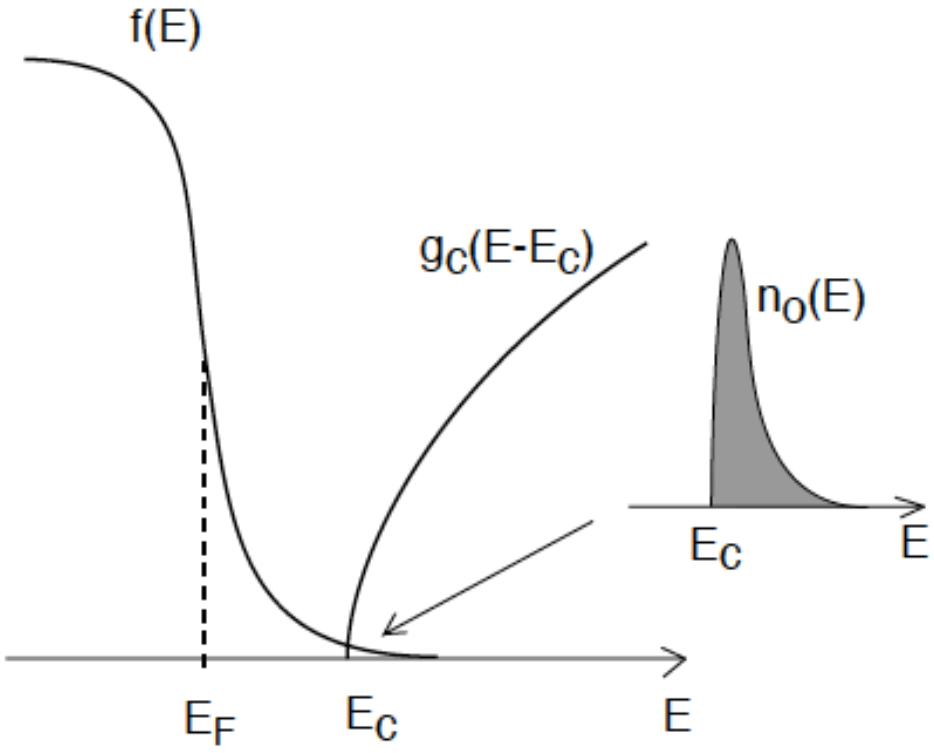
A second important result:

$$n_o p_o = n_i^2$$

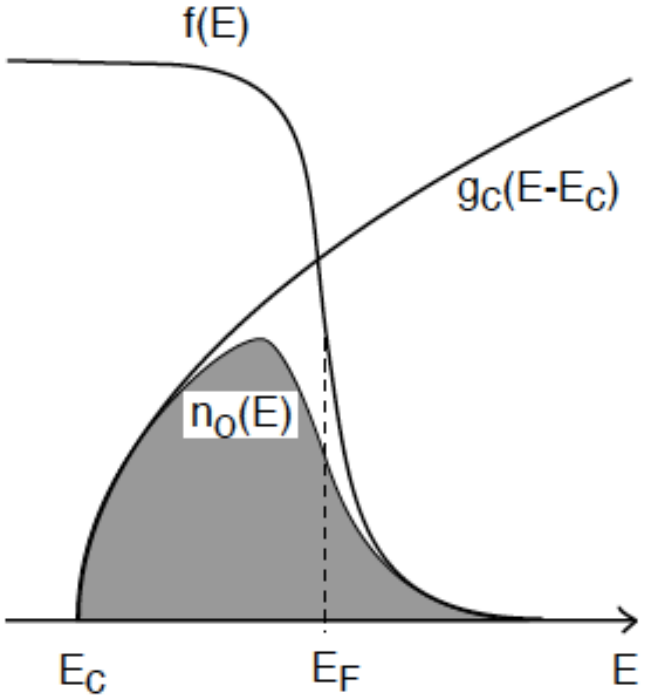


Equilibrium ***np* product** in a semiconductor at a certain temperature is a **constant specific to the semiconductor**.

Carrier concentration



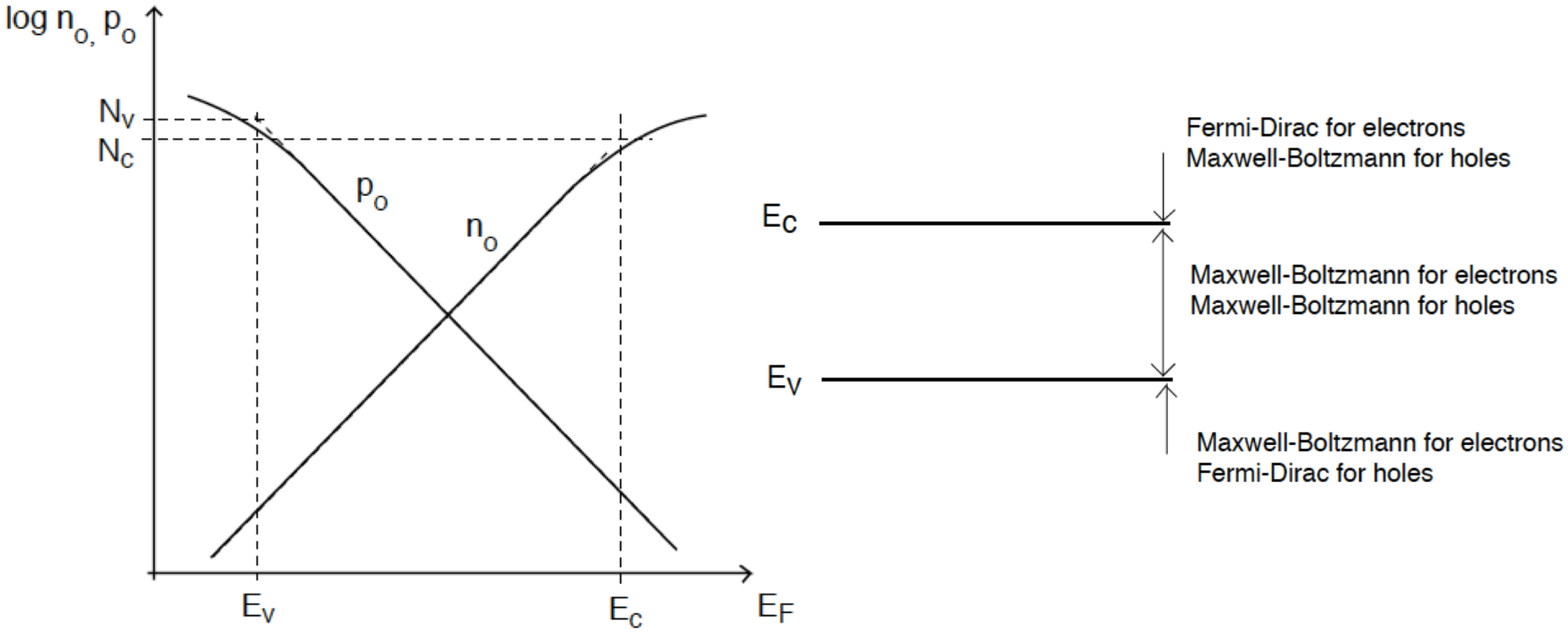
Non degenerate



degenerate

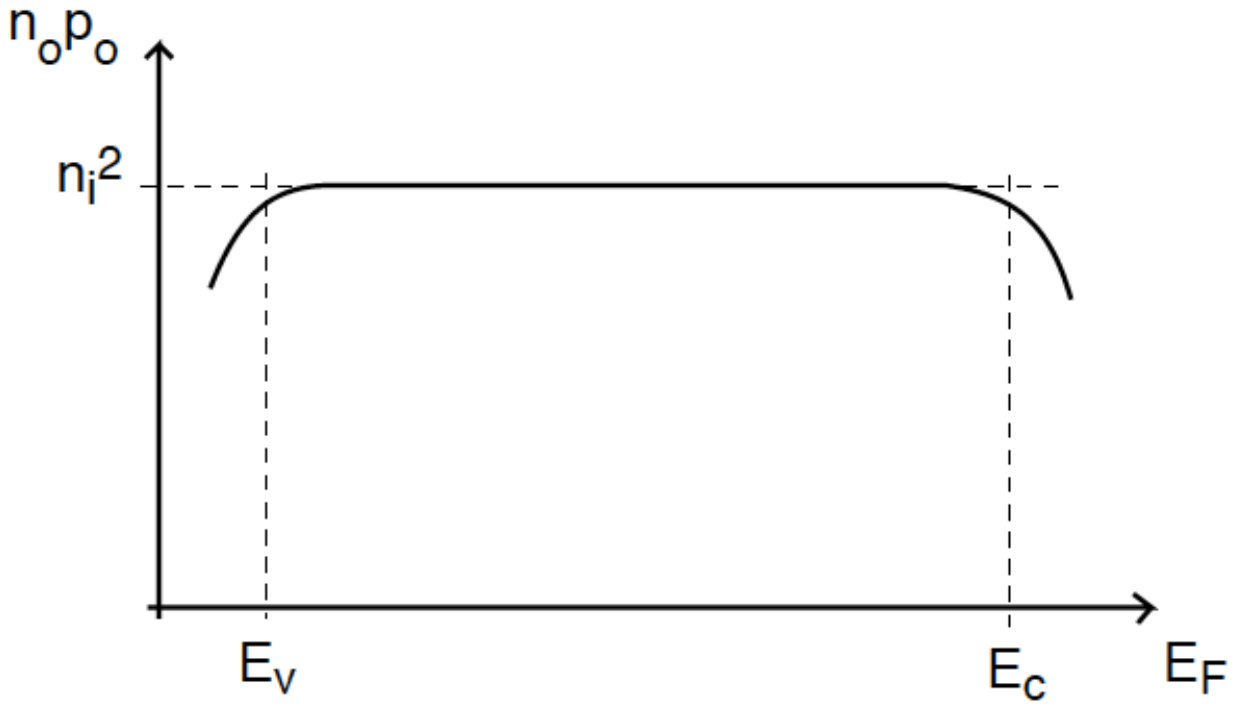
Carrier concentration

Summary of carrier statistics depending on E_F location



Carrier concentration

Summary of carrier statistics depending on E_F location



If E_F is inside bandgap:

$$n_o p_o \simeq N_c N_v \exp -\frac{E_g}{kT}$$

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.

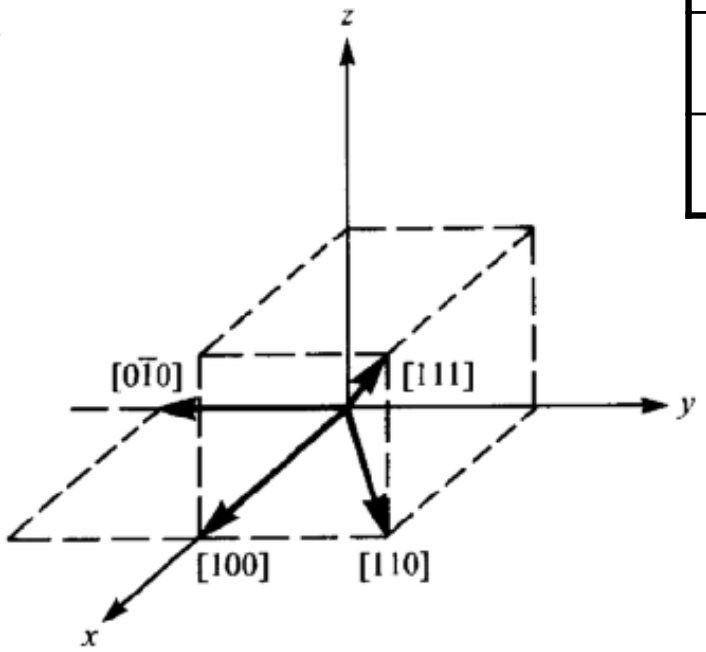
$$n_o = p_o = n_i = \sqrt{N_c N_v} \exp -\frac{E_g}{2kT}$$

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

Appendix – Supplementary Material

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.

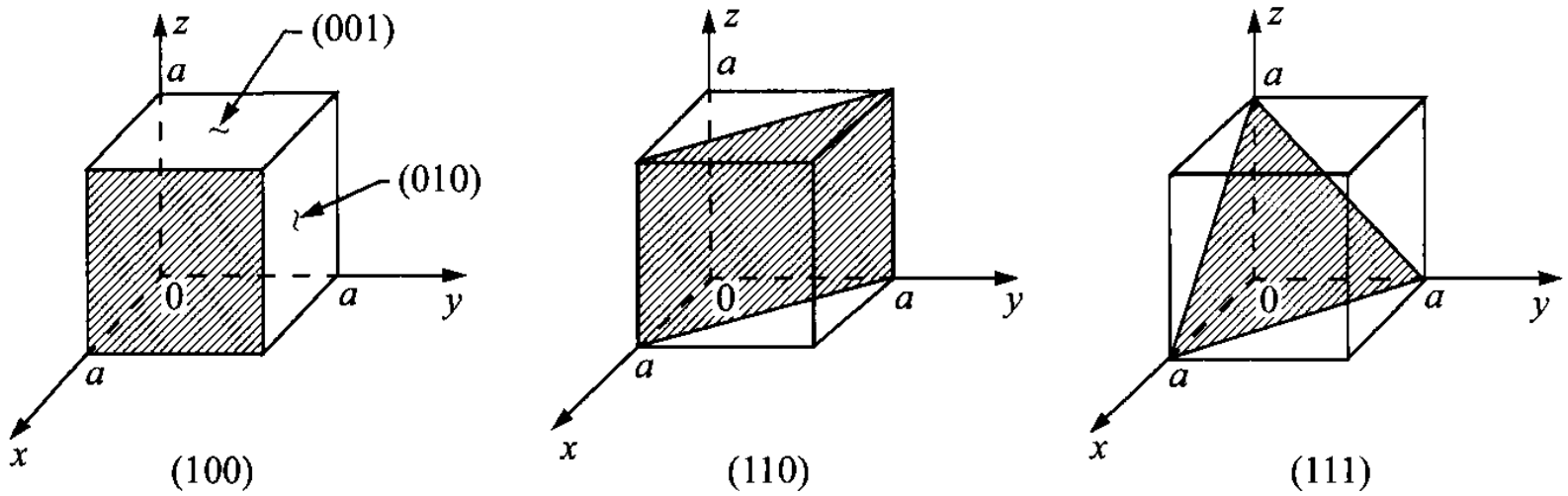
***h*: inverse *x*-intercept of plane**
***k*: inverse *y*-intercept of plane**
***l*: inverse *z*-intercept of plane**

(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)



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**

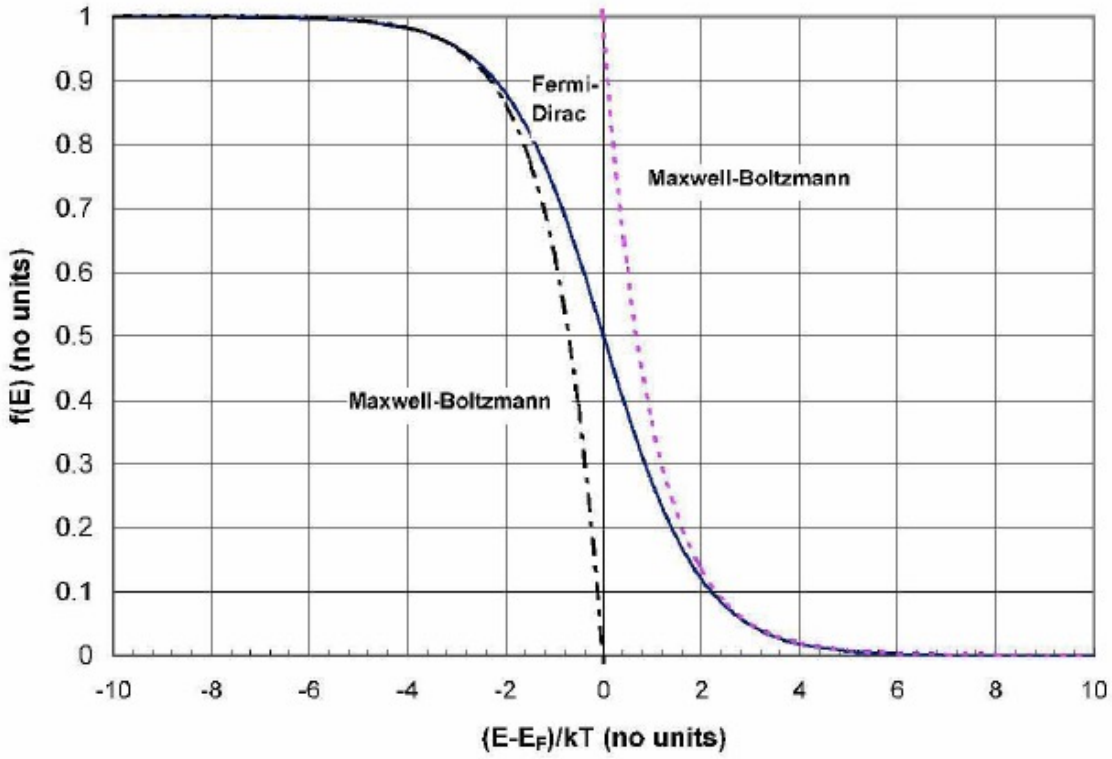
For instance, X-ray diffraction reveals the reciprocal space

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

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 $E - E_F \ll kT$:

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