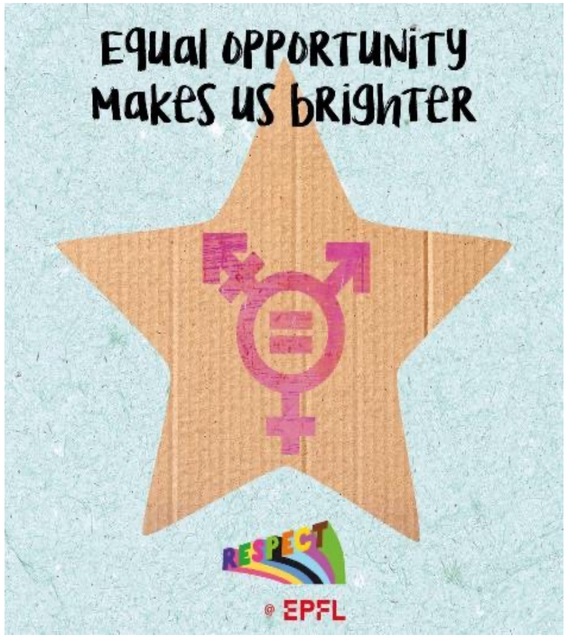
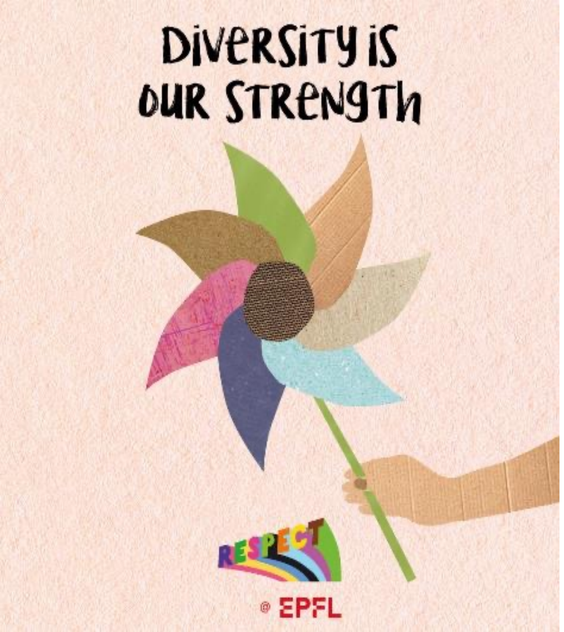
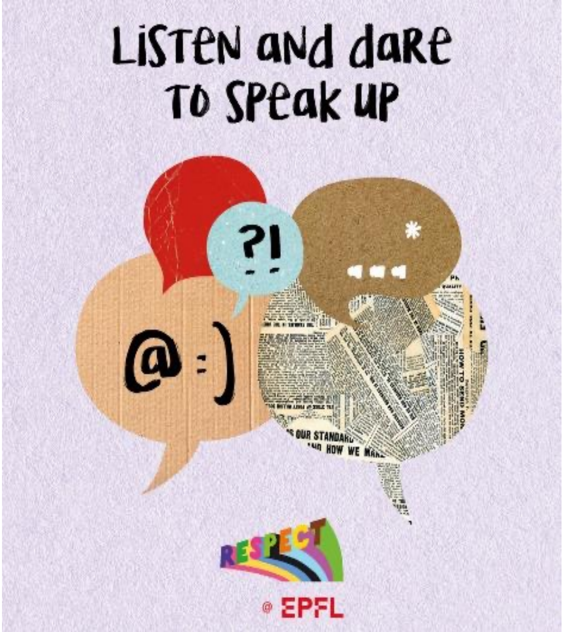
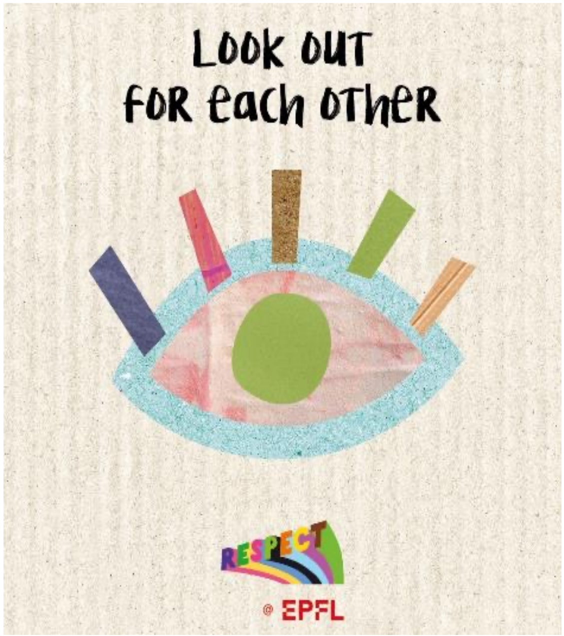
EPFL


Equal opportunity makes us brighter
RESPECT
@ EPFL


Diversity is our strength
RESPECT
@ EPFL


Listen and dare to speak up
?!
@ :)
RESPECT
@ EPFL


Look out for each other
RESPECT
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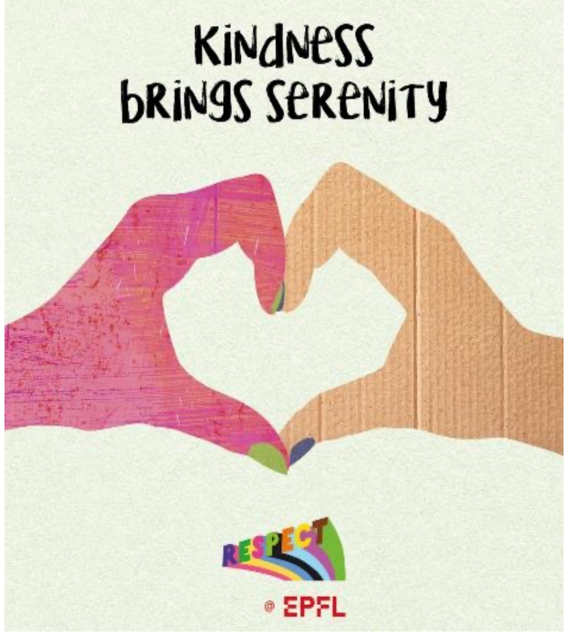
Kindness brings serenity
RESPECT
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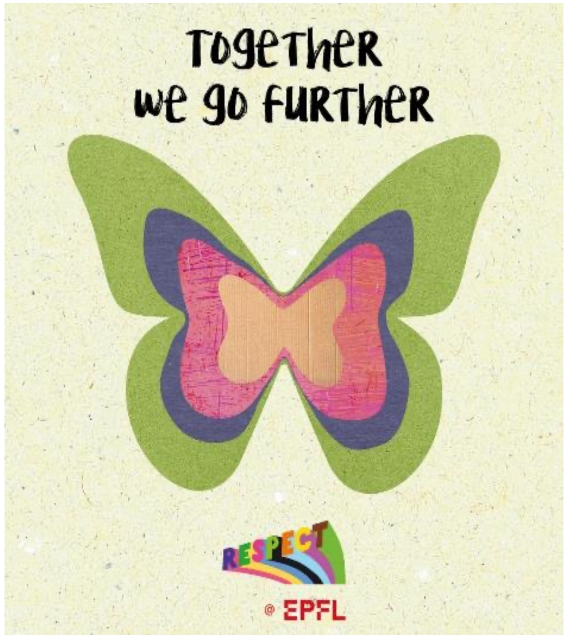
Together we go further
RESPECT
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EE-557
Semiconductor devices I

Doping and carrier concentration

Génie Electrique et Electronique
Master program
Prof. Elison Matioli

Outline of the lecture

1. Energy Bands
2. Carrier concentration

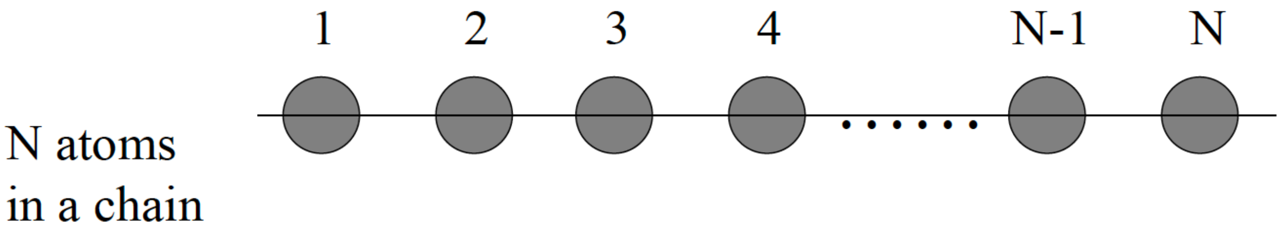
Read Chapter 2 of the reference book (on moodle)

References:

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

How Energy Bands and Energy Gap are calculated?

In 1D – simple case



$$\psi = c_1\varphi_1 + c_2\varphi_2 + c_3\varphi_3 + c_4\varphi_4 + \ldots + c_N\varphi_N$$

One keeps nearest neighbours interactions only:

$$\langle \varphi_n | V_n | \varphi_m \rangle = \langle \varphi_m | V_m | \varphi_n \rangle = \delta_{n,m\pm 1} \times V$$

V<0

Again, we use:

orthogonality $\langle \varphi_n | \varphi_m \rangle = \delta_{nm}$

renormalization $E_n = E_{n0} + \sum_m \langle \varphi_n | V_m | \varphi_n \rangle$

Identical atoms, $E_n = E_0$

$$\Rightarrow \begin{vmatrix} E_0 - E & V & 0 & 0 \\ V & E_0 - E & V & 0 \\ 0 & V & E_0 - E & V \\ 0 & 0 & V & E_0 - E \end{vmatrix} = 0$$

Courtesy J. Y. Duboz

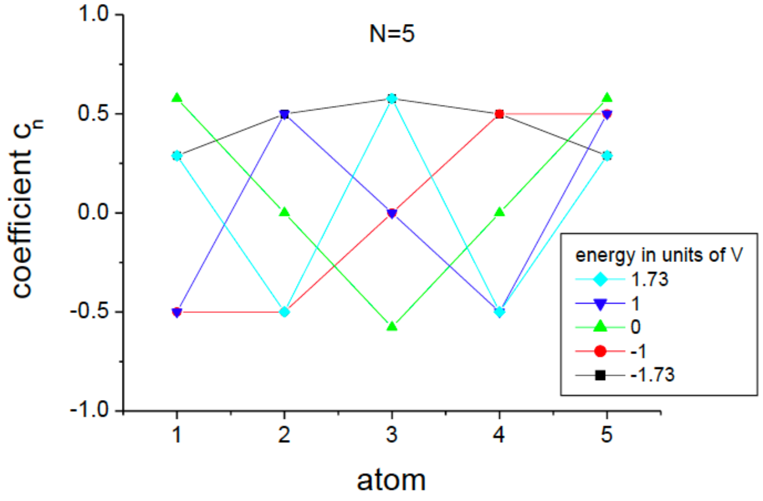
How Energy Bands and Energy Gap are calculated?

what are the new eigen states associated with the energy eigenvalues ?

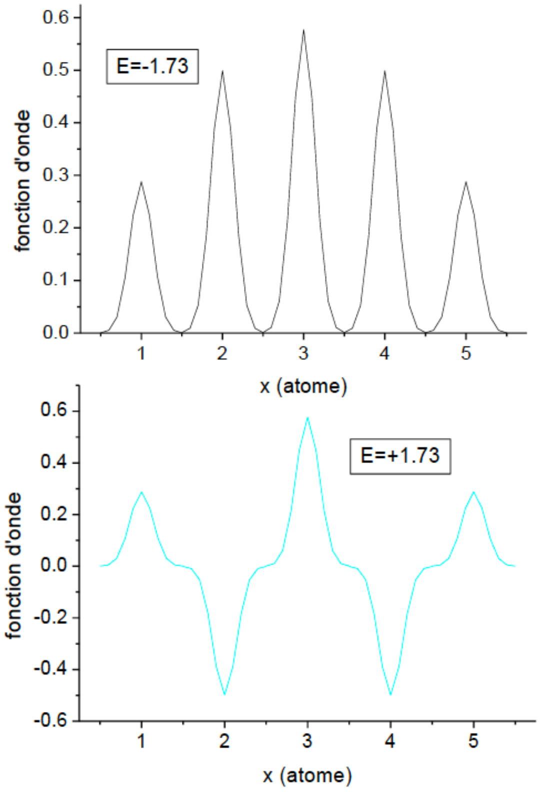
$$\Phi = \sum c_n \varphi_n$$

For each energy, one calculates the c_n coefficient and the wavefunction :

For 5 atoms:



we take φ_n=gaussian centered on each atom n

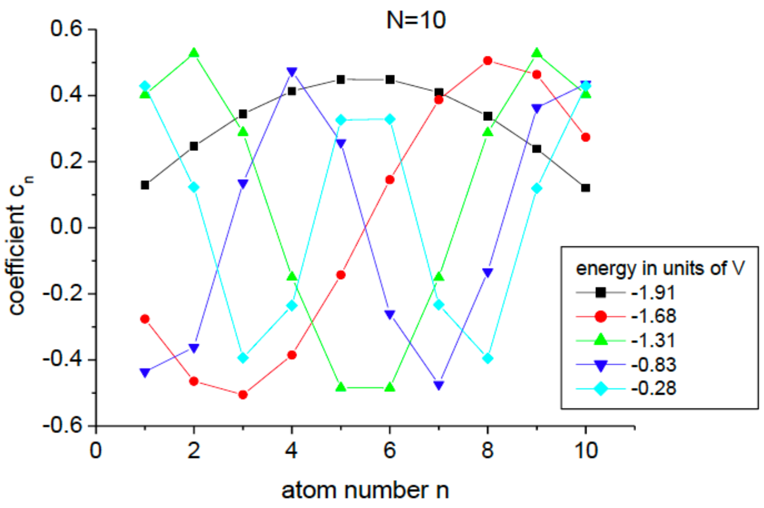


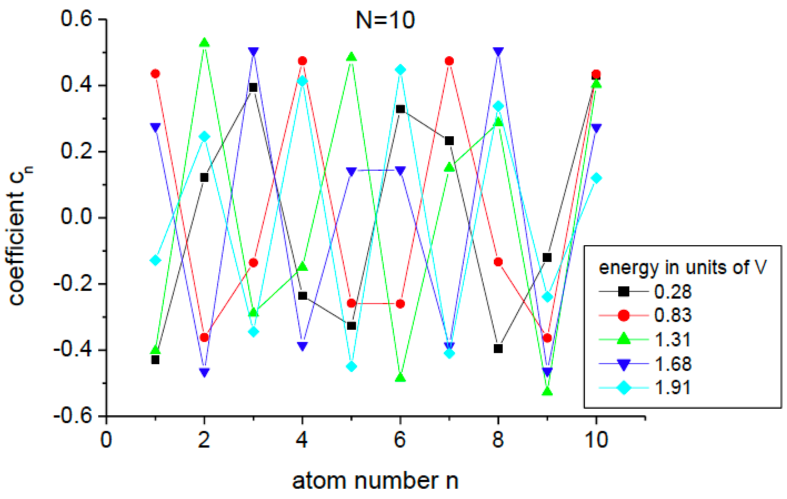
The wavefunction spacially oscillates more when energy increases

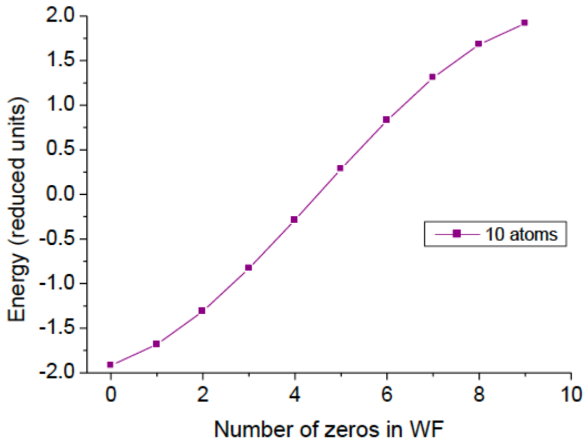
Courtesy J. Y. Duboz

How Energy Bands and Energy Gap are calculated?

For 10 atoms:







wavefunction amplitude becomes more uniform

Wavefunction oscillates more in space when energy increases

Courtesy J. Y. Duboz

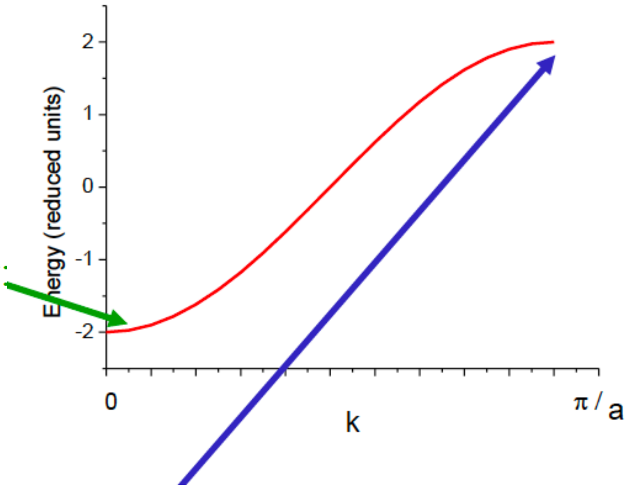
How Energy Bands and Energy Gap are calculated?

For large N, the system is periodic(all atoms identical), **period= a**

$$c_{n-2}V + c_{n-1}(E_0 - E) + c_n V = 0$$

$$c_{n-1}V + c_n(E_0 - E) + c_{n+1}V = 0$$

Lowest energy:



Highest energy

General solution : $c_n = Ae^{in\theta} = Ae^{inka}$

$$\Rightarrow \quad e^{-ika}V + (E_0 - E) + e^{ika}V = 0 \qquad \Rightarrow \quad E = E_0 + 2V\cos(ka)$$

V<0

NB: one initial level per atom ⇒ one band

M levels ⇒ M bands

Courtesy J. Y. Duboz

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: - π/a, π/a
- Entire band structures need only to be calculated within the brillouin zone.

How Energy Bands and Energy Gap are calculated?

In 3D

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 many states are in a 1D material of length L, with atomic spacing a, and N atoms?

Crystal structure: Definitions

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

Bravais lattices: describe the geometric arrangement of the lattice points

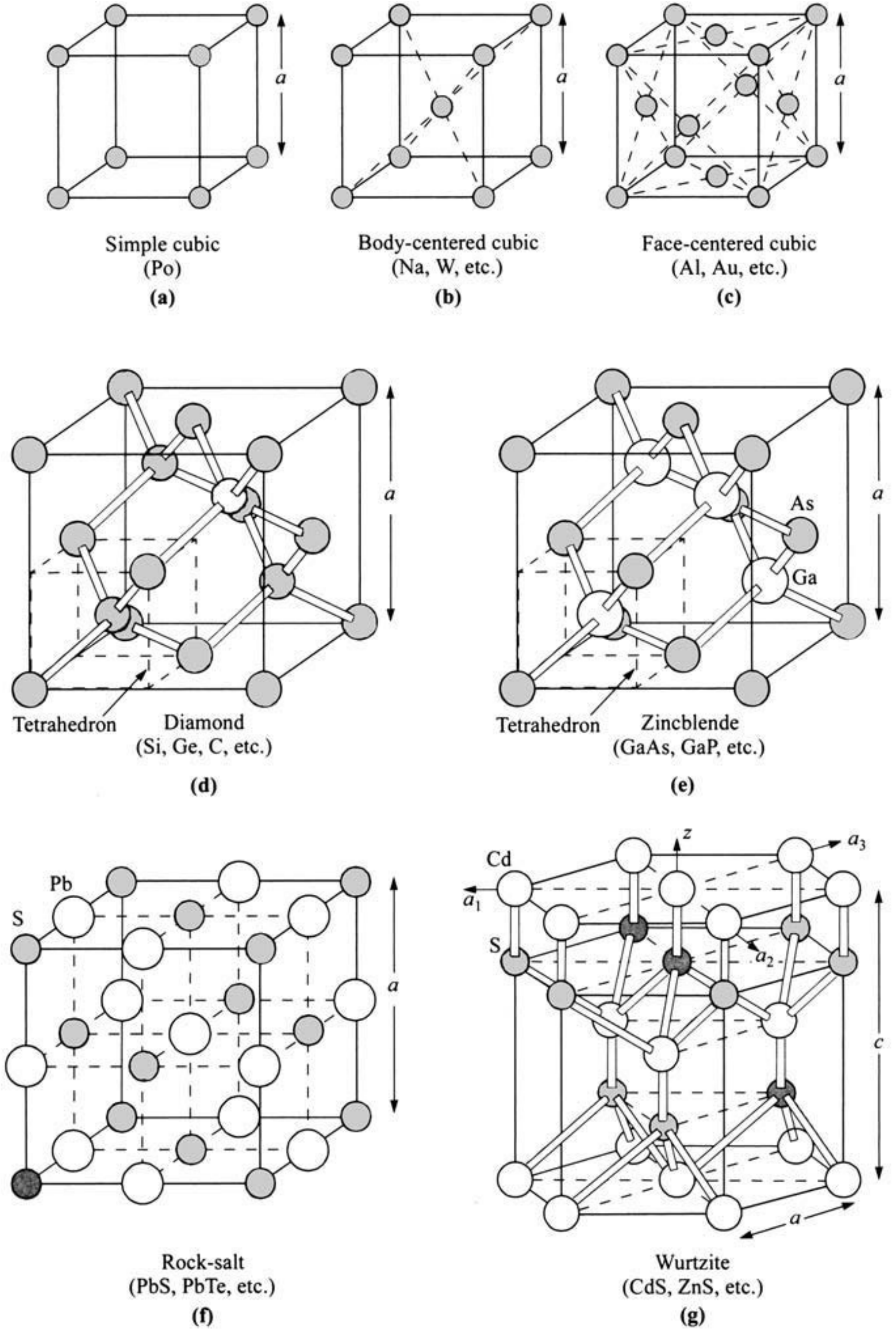
a is the lattice constant.

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



Simple cubic
(Po)
(a)

Body-centered cubic
(Na, W, etc.)
(b)

Face-centered cubic
(Al, Au, etc.)
(c)

Diamond
(Si, Ge, C, etc.)
(d)

Zincblende
(GaAs, GaP, etc.)
(e)

Rock-salt
(PbS, PbTe, etc.)
(f)

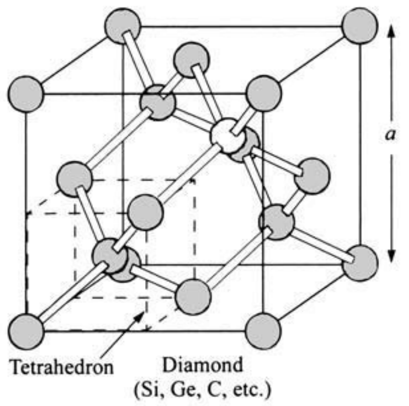
Wurtzite
(CdS, ZnS, etc.)
(g)

Crystallographic Notation

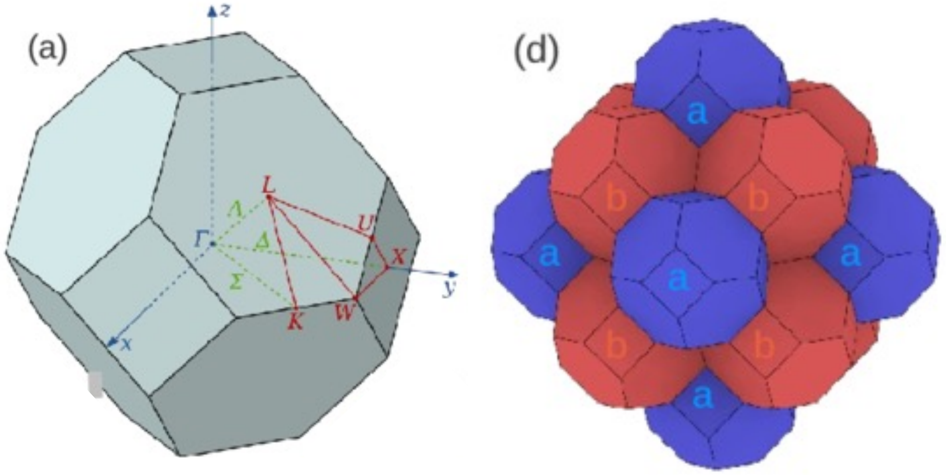
In 3D - Reciprocal space

Defines the principal symmetry points :

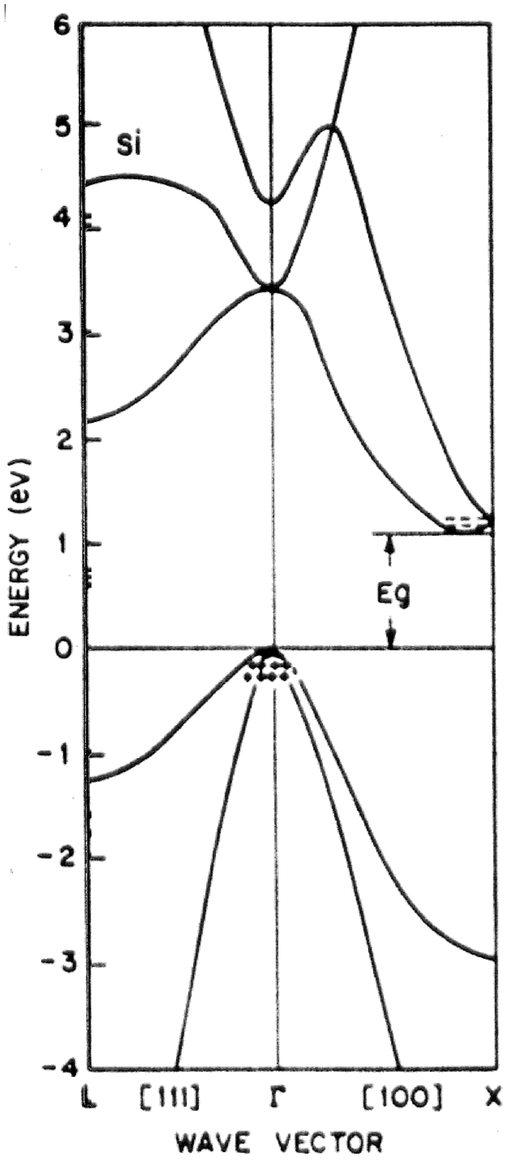
Gamma = (0; 0; 0) is the origin
X = (1; 0; 0) + 6 equivalent points,
L = (1; 1; 1) + 8 equivalent points



Real space



Reciprocal space



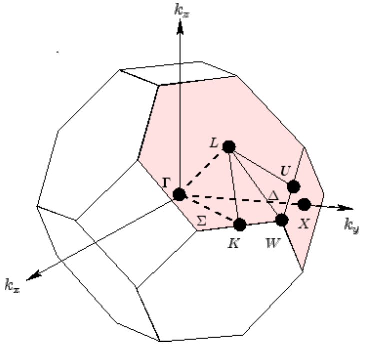
Fundamental to define the band structure of a semiconductor

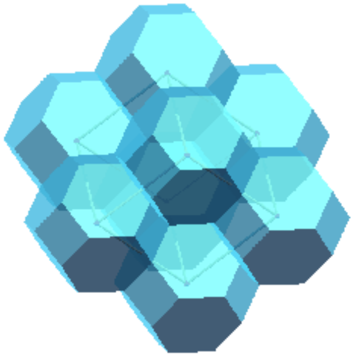
The reciprocal lattice plays a fundamental role in most analytic studies (properties related to momentum) of periodic structures:

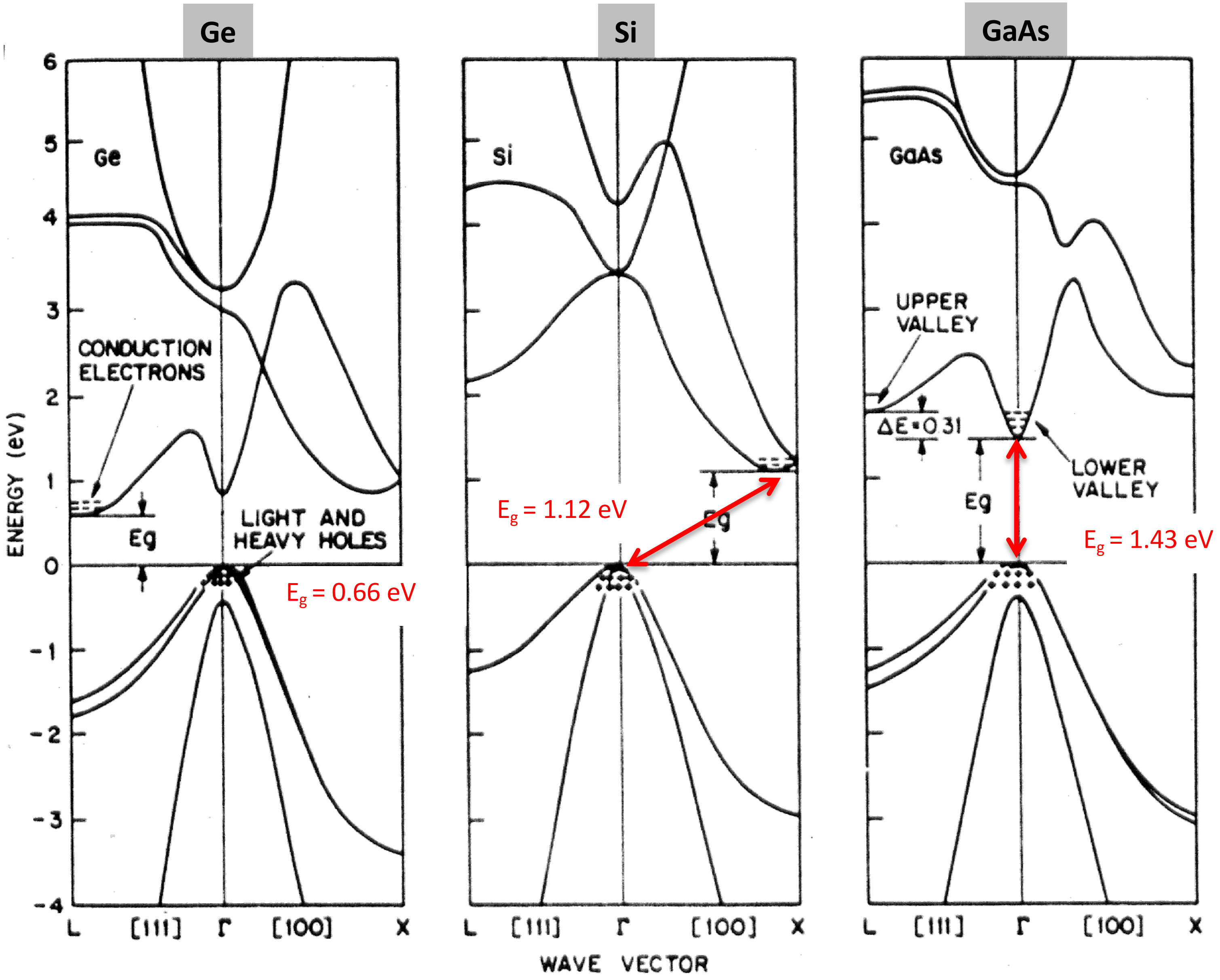
- Energy-momentum relationship
- Theory of diffraction: X-Ray diffraction

Energy band-gap

Reciprocal space directions:



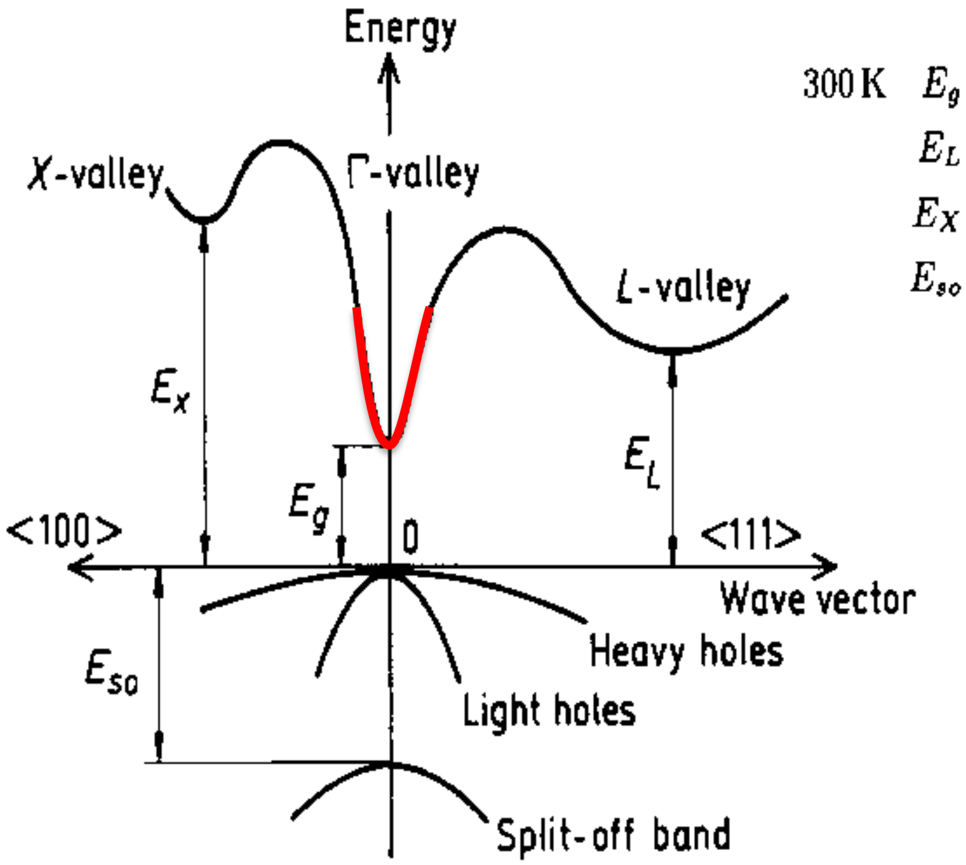




What do we learn from band diagrams

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

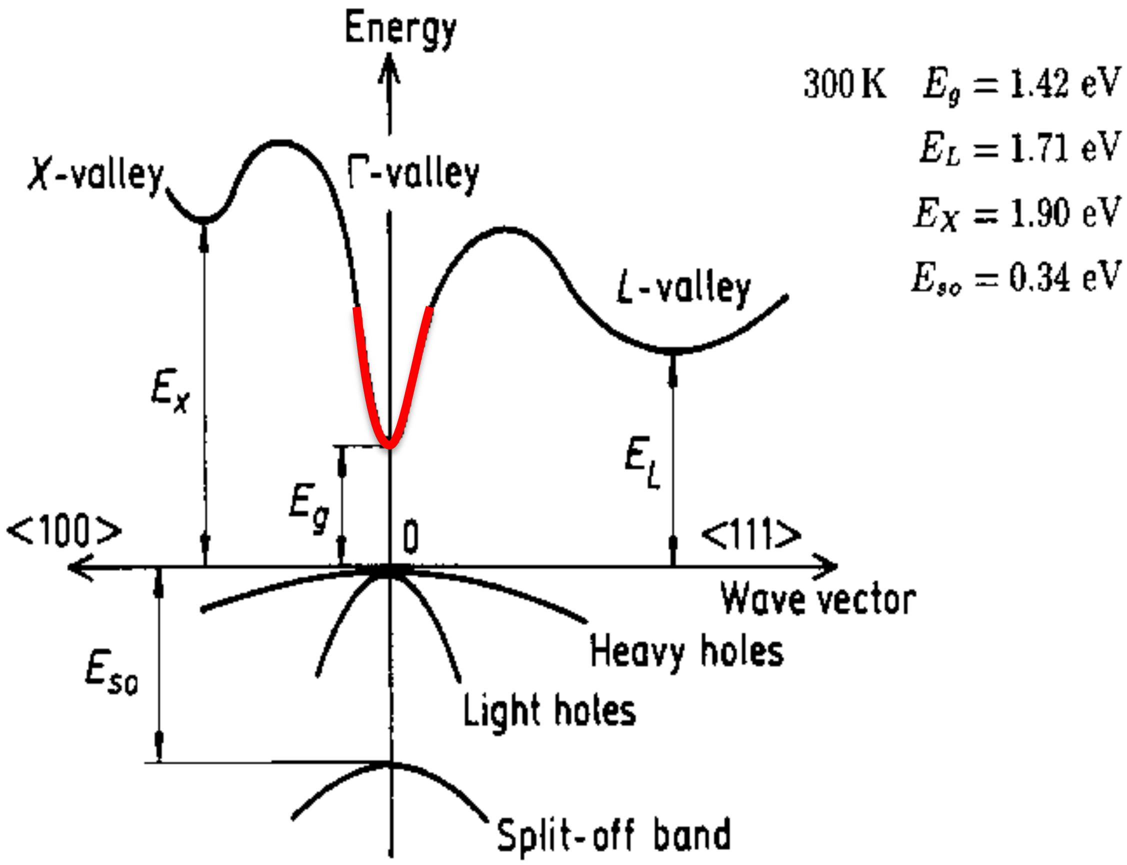
1. Allowed and forbidden states
2. Group velocity: slope of the bands
3. Electron/hole mass: curvature of bands

What do we learn from band diagrams

Effective mass

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

GaAs



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 $p = \hbar\, k$

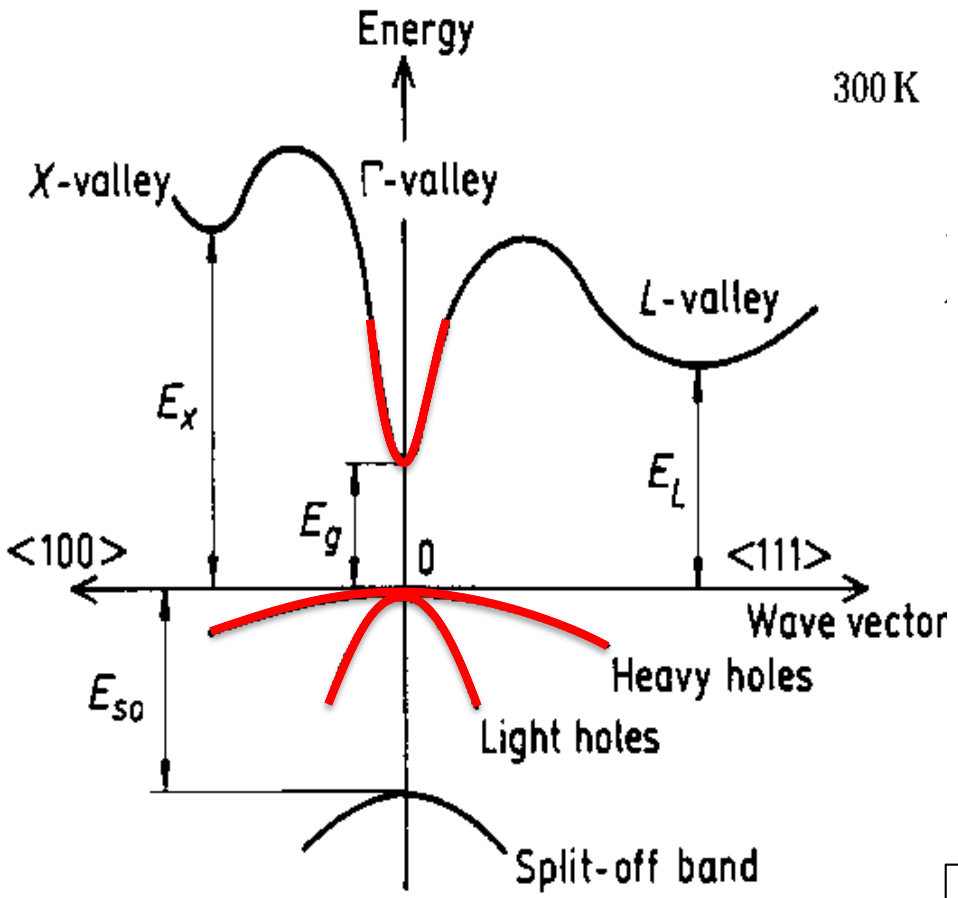
Key questions

- 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



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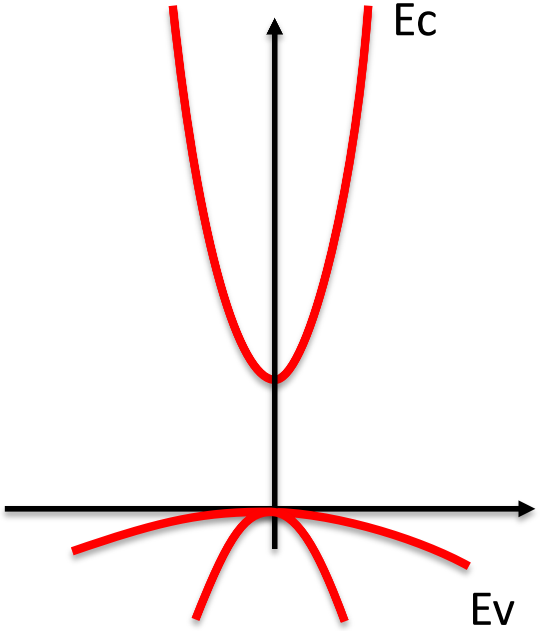


Available electrons in the conduction band:

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

density of electrons

Probability of occupation

A few important concepts

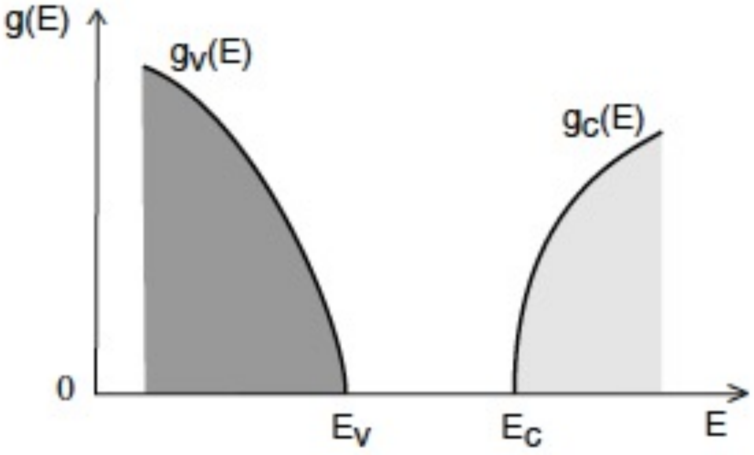
What is the density of electrons $g_c(E)$?

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



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

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

$m_{de}^* \equiv$ 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

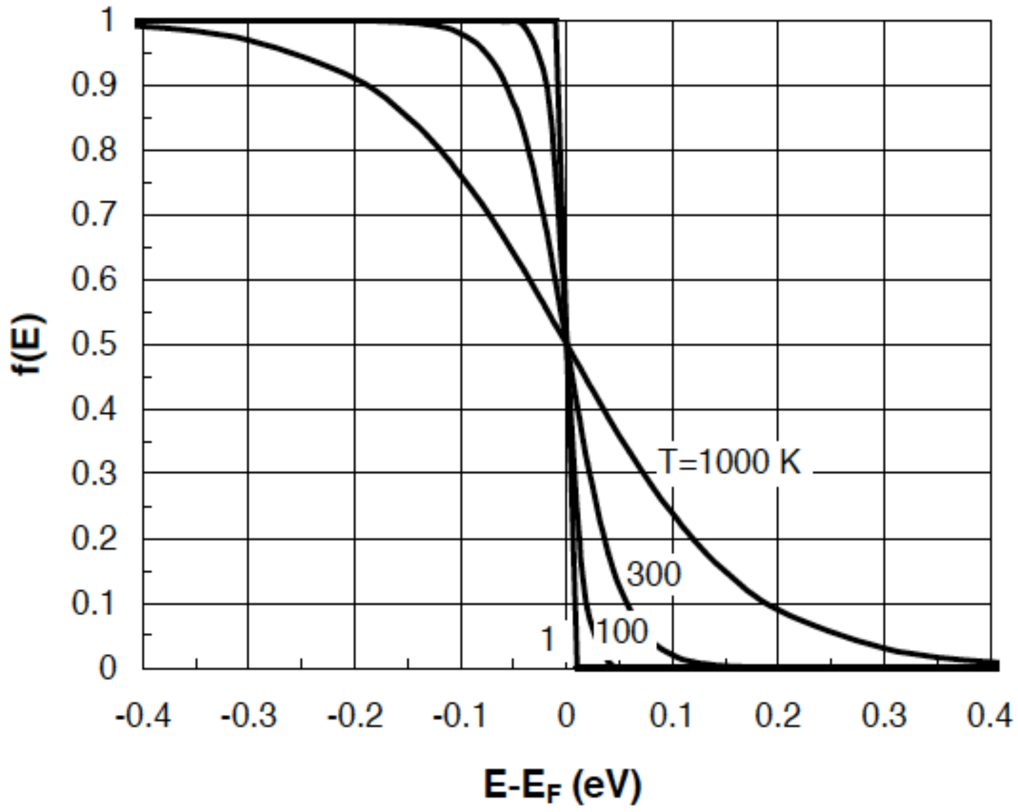
Density of states

A few important concepts

Electron statistics

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

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



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*

A few important concepts

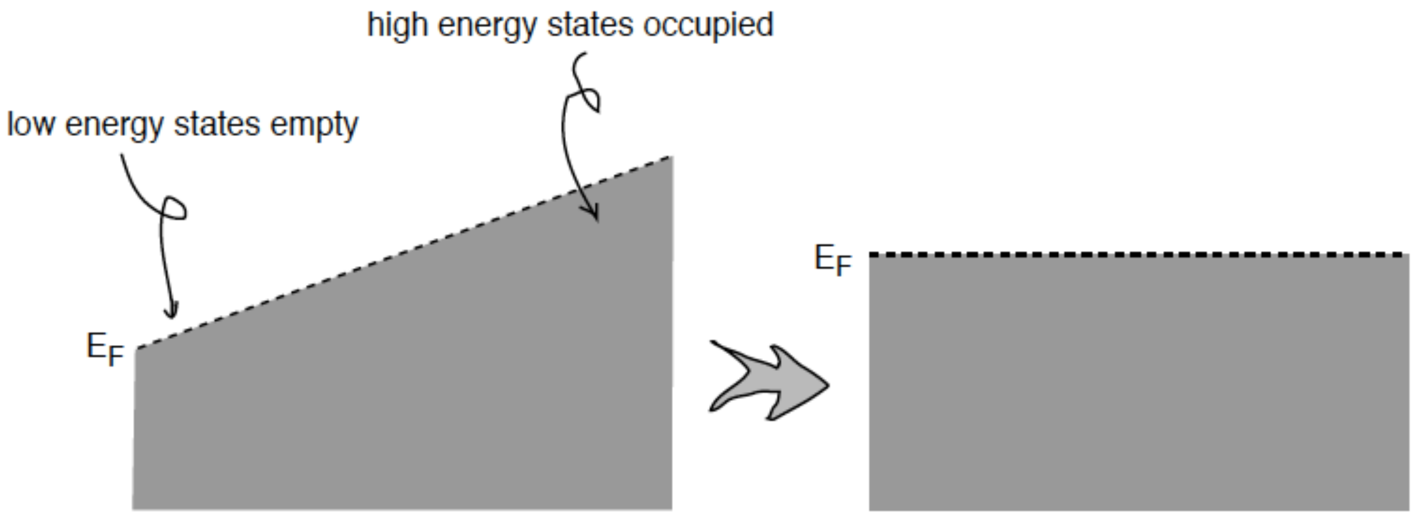
Notion of thermal equilibrium

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

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

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

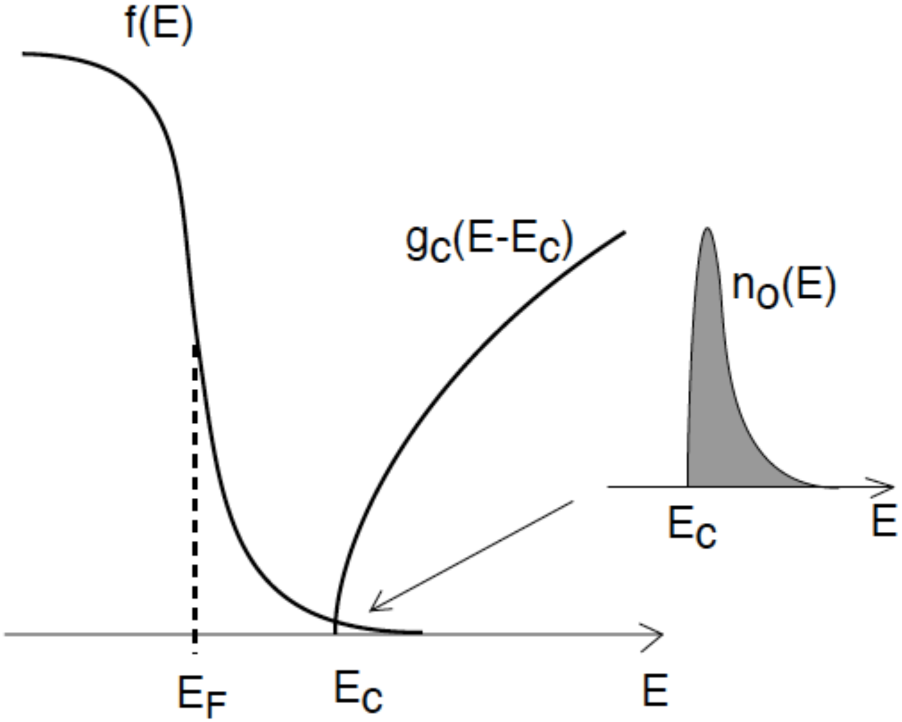
X

Probability of a state to be occupied

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

Integrated for all energies

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



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: $n \sim 5\times10^{22}\ \mathrm{cm}^{-3}$

– 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

Appendix – Supplementary Material

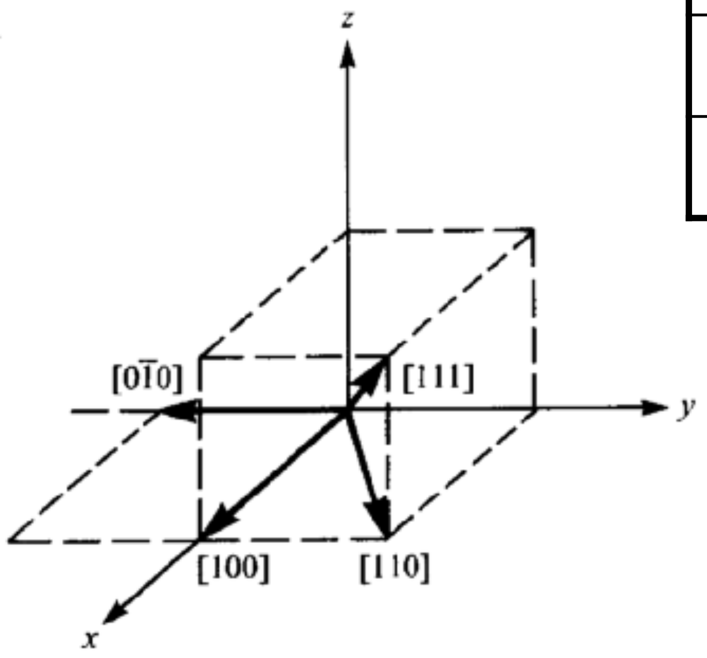
Crystallographic Notation

Miller Indices:

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

_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.)

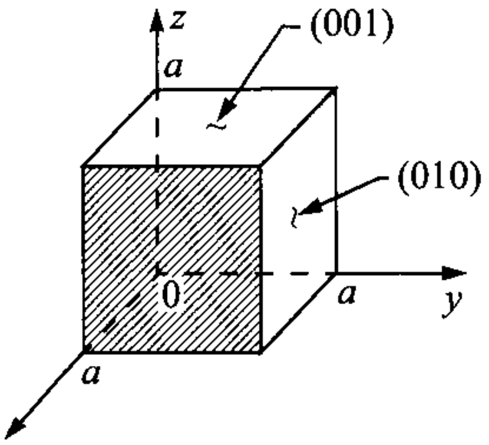


Sample direction vectors and their corresponding Miller indices.

** 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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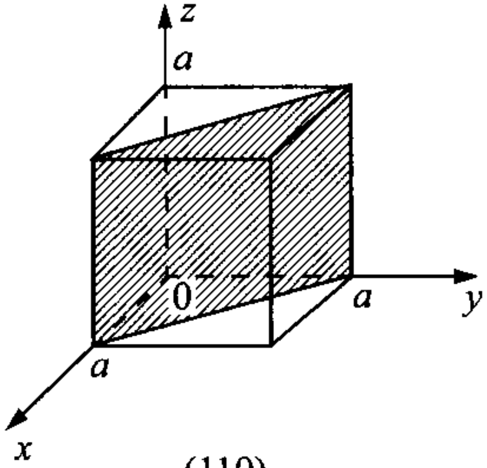

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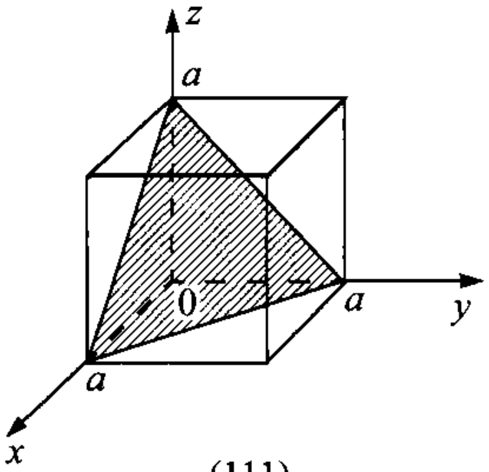

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Reciprocal space is also called **Fourier space, k- space, or momentum space**

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

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

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

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

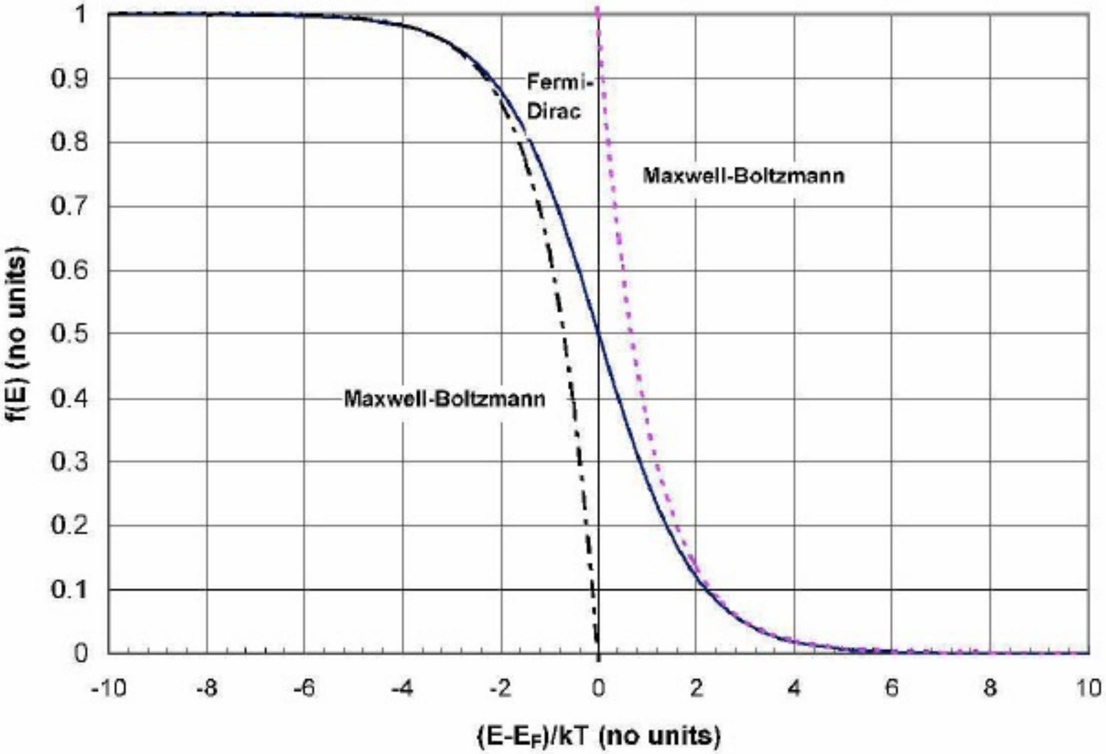
Interesting video: https://www.youtube.com/watch?v=DFFU39A3fPY

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 $E - E_F \ll kT$:

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