Physics of Electronics:

5. Electrons in Solids - Intro to Band Theory

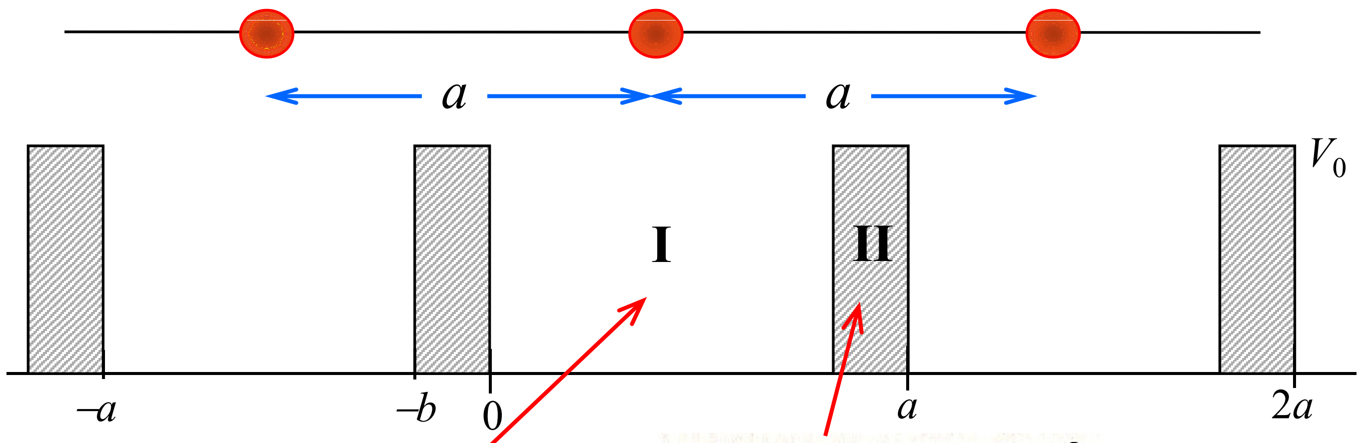
July – December 2009

Contents overview

- Allowed energy bands.
- Velocity and effective mass of electrons in solids.
- Conductors, semiconductors, and insulators.
- Electrical resistance in solids
- Crystal structure of semiconductors.
- Conduction processes in semiconductors.
- Density of carriers in intrinsic semiconductors.
- Extrinsic semiconductors.
- Electron processes in real semiconductors.

Allowed Energy Bands

- Kronig-Penney model.
  - Let's consider a 1D chain of N atoms of period a.



$\beta^2 = 2mE/\hbar^2$

$\Psi_I = Ae^{j\beta x} + Be^{-j\beta x}$

$\alpha^2 = 2m(V_0 - E)/\hbar^2$

$\Psi_{II} = C\exp(\alpha x) + D\exp(-\alpha x)$

ψ and dψ/dx at $x=0$

ψ, dψ/dx and Bloch's theorem at $x=–b$

$$[(\alpha^2 - \beta^2)/2\alpha\beta]\sinh \alpha b \sin \beta(\boldsymbol{a–b}) + \cosh \alpha b \cos \beta(\boldsymbol{a–b}) = \cos k\boldsymbol{a}$$

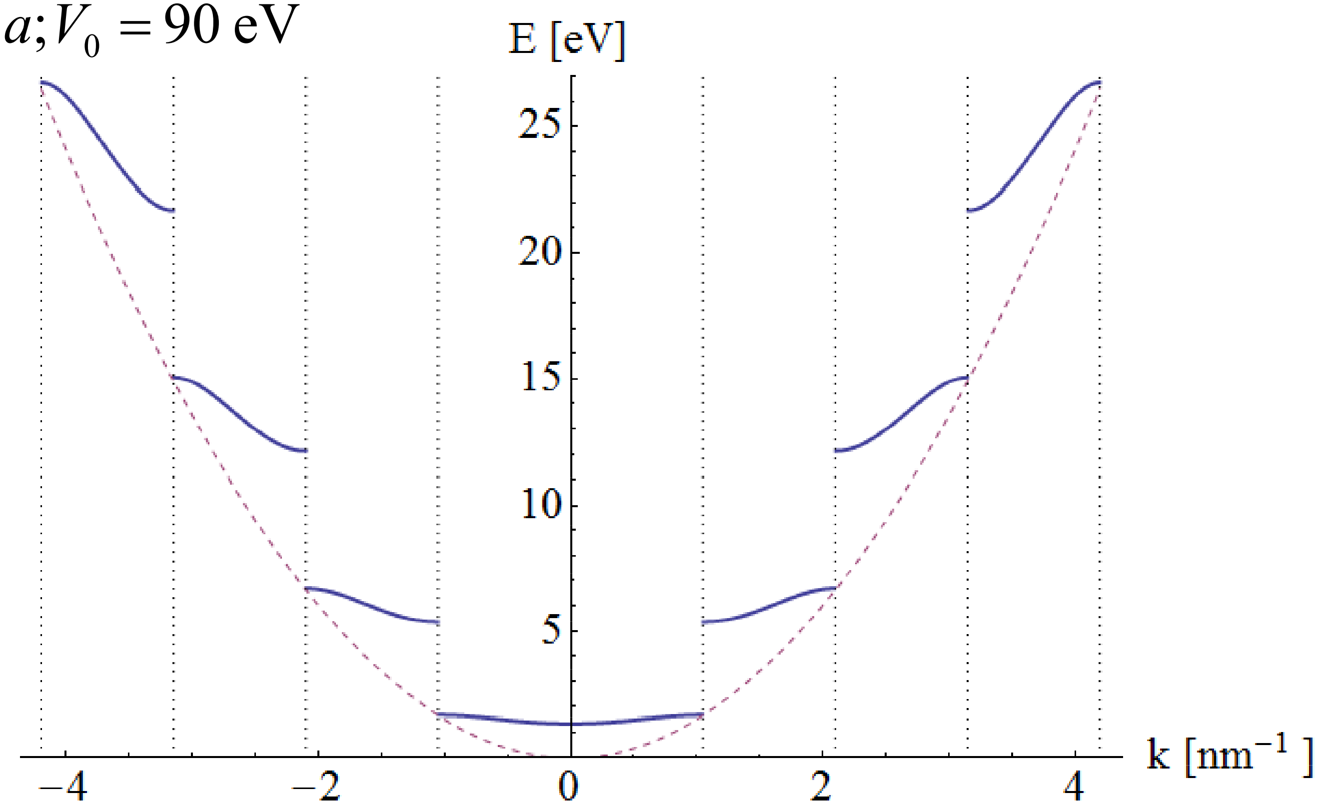
Allowed Energy Bands

- Kronig-Penney model.

$$[(\alpha^2 - \beta^2)/2\alpha\beta]\sinh \alpha b \sin \beta(a-b) + \cosh \alpha b \cos \beta(a-b) = \cos ka$$

  - The allowed energies are function of the wavenumber ***k***.
  - The solutions have the periodicity of **cos(*ka*)**.

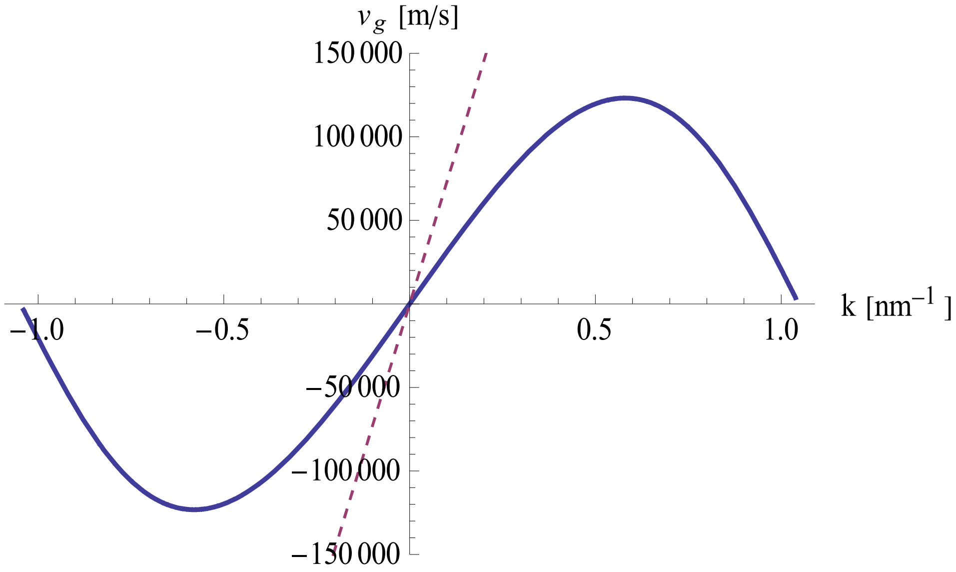
$a = 3\text{ nm}; b = 0.05\,a; V_0 = 90\text{ eV}$

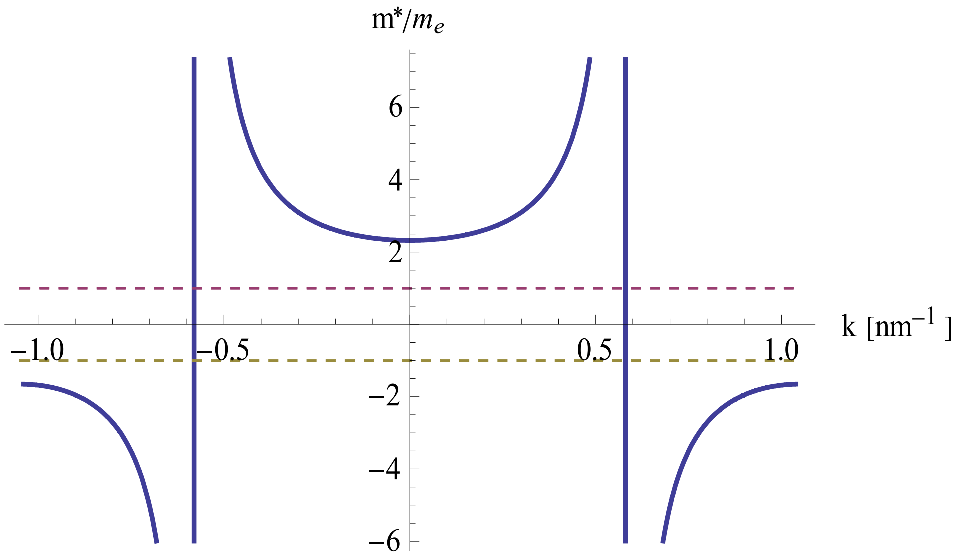


Velocity and Effective Mass

- Wavepacket (Bloch theorem): $\psi\ (x,\ t) = u_k(x)\ e^{i(kx\text{-}Et/\hbar)}$
  - Group velocity $v_g = \frac{\partial\omega}{\partial k} = \frac{\partial(E/\hbar)}{\partial k}$ ➡ $\boxed{v_g = \frac{1\partial E}{\hbar\partial k} = \frac{\partial E}{\partial p}}$ ← $p = \hbar\, k$
  - Effective mass $F = \left(\frac{d^2E}{dp^2}\right)^{-1}\frac{dv_g}{dt}$ ➡ $\boxed{m^* = \left(\frac{d^2E}{dp^2}\right)^{-1} = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}}$

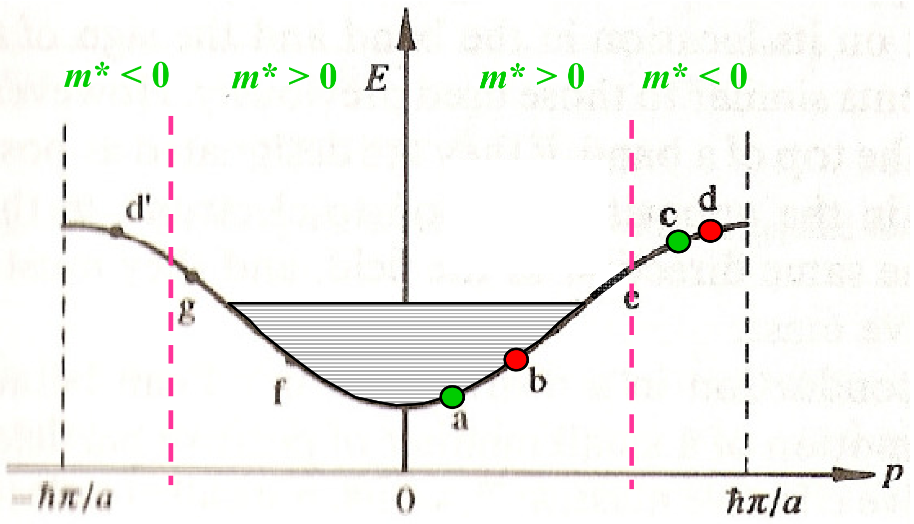
$$a = 3\ \text{nm}; b = 0.05\, a; V_0 = 90\ \text{eV}$$





Velocity and Effective Mass

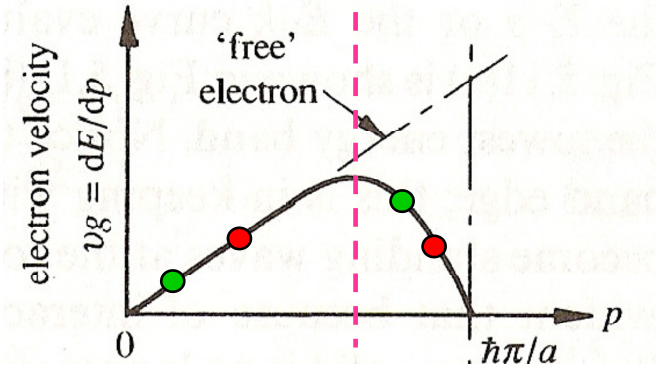
- Wavepacket (Bloch theorem): $\psi\,(x,\,t) = u_k(x)\ e^{i(kx-Et/\hbar)}$
  - Group velocity $v_g = \dfrac{\partial \omega}{\partial k} = \dfrac{\partial(E/\hbar)}{\partial k}$ ⇨ $\boxed{\upsilon_g = \dfrac{1\partial E}{\hbar \partial k} = \dfrac{\partial E}{\partial p}}$



$\mathscr{E} = 0$

←

$\mathscr{E} \neq 0$



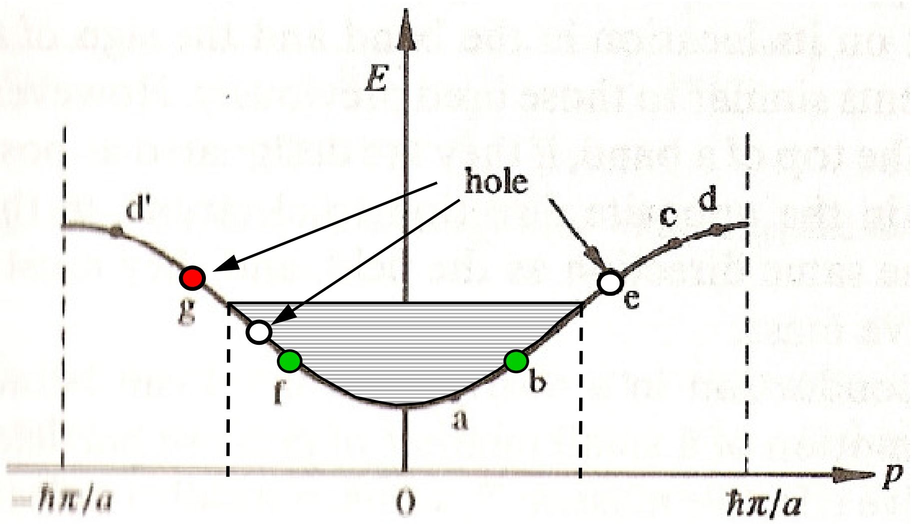
$\mathscr{E} = 0$

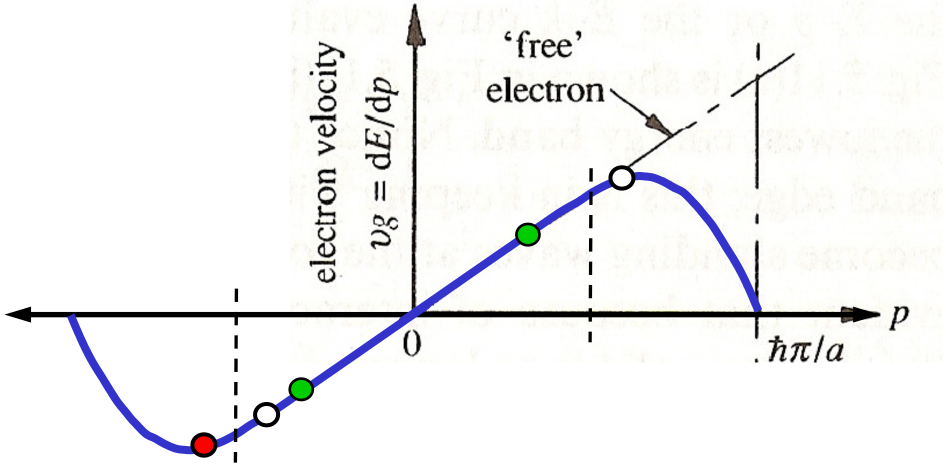
←

$\mathscr{E} \neq 0$

Velocity and Effective Mass

- Wavepacket (Bloch theorem): $\psi\ (x,\ t) = u_k(x)\ e^{i(kx\text{-}Et/\hbar)}$
  - Group velocity $v_g = \dfrac{\partial \omega}{\partial k} = \dfrac{\partial (E/\hbar)}{\partial k}$ ⇨ $\boxed{\upsilon_g = \dfrac{1}{\hbar}\dfrac{\partial E}{\partial k} = \dfrac{\partial E}{\partial p}}$

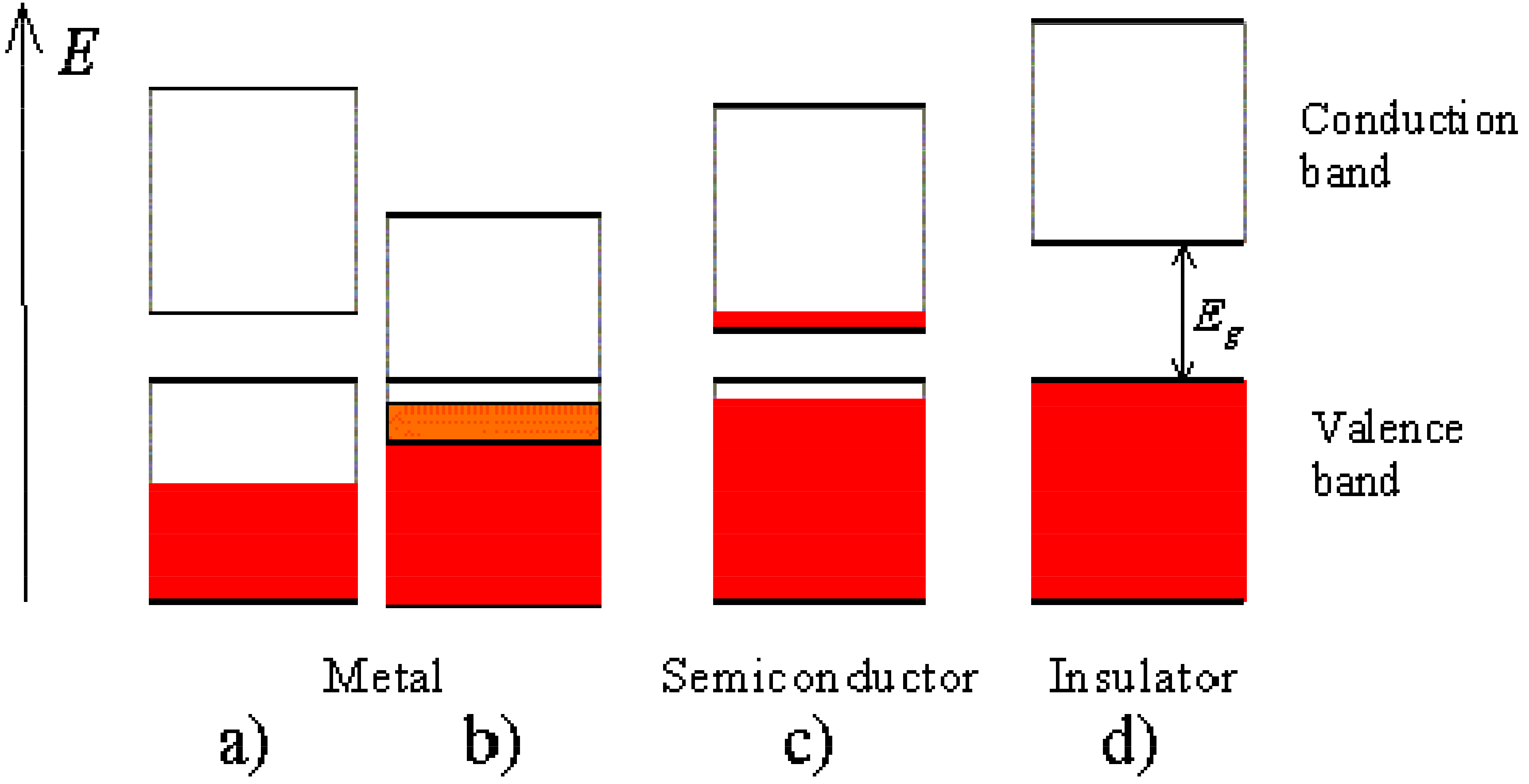




- 🟢 Opposite velocities. No net current,
- 🔴 Not cancelled. Net current.

Conductors, Semiconductors & Insulators

- Classification according to the filling of the gaps

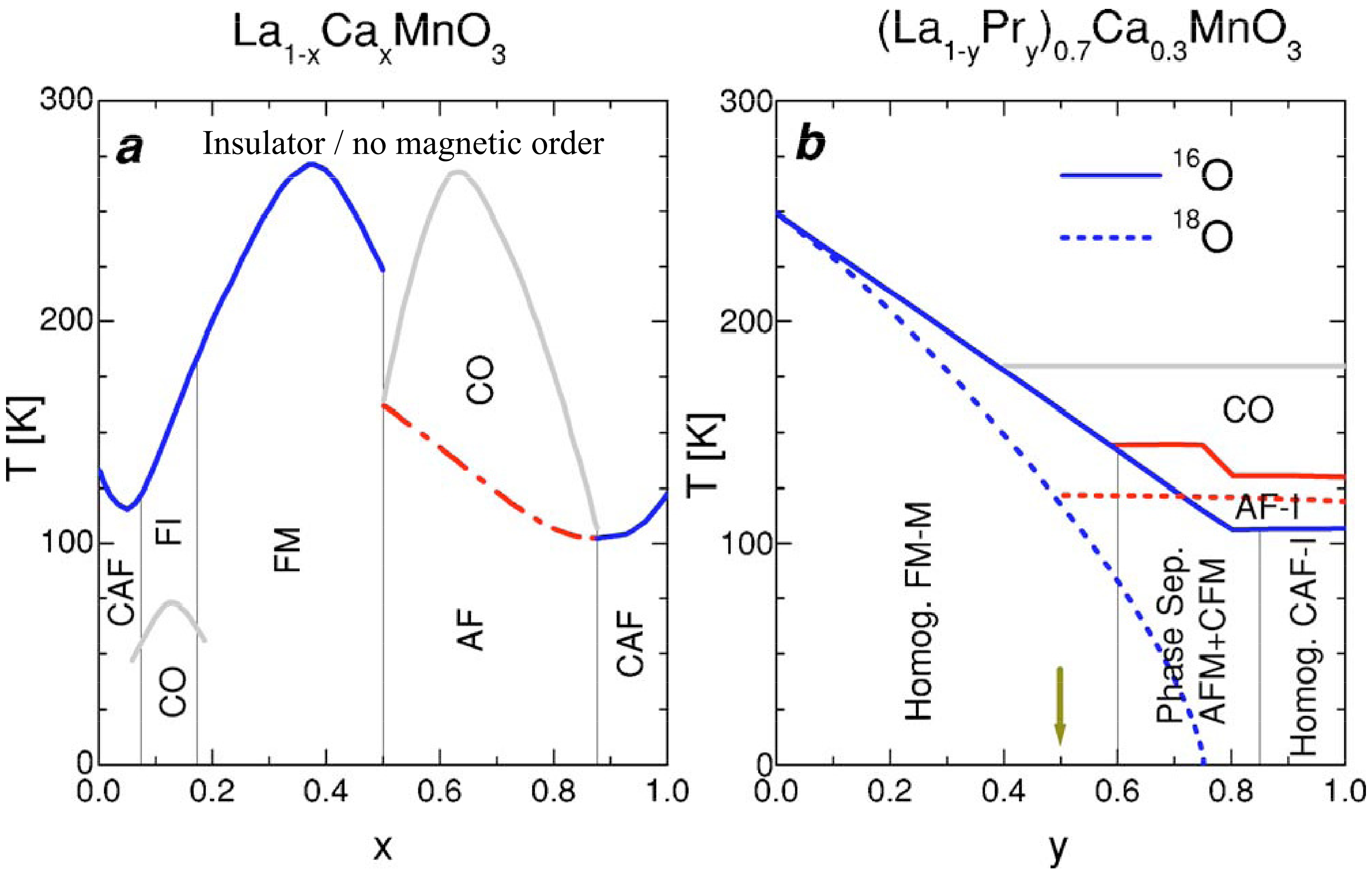


Electrical Resistance

- Electrons scattered on ion cores DO NOT account for measured electrical resistivities.
- Scattering processes:
  - On phonons (thermal vibrations of the lattice)
  - On impurity atoms
  - Lattice imperfections (vacancies, dislocations)

Is an insulator always an insulator?

- Let's consider the following phase diagram:



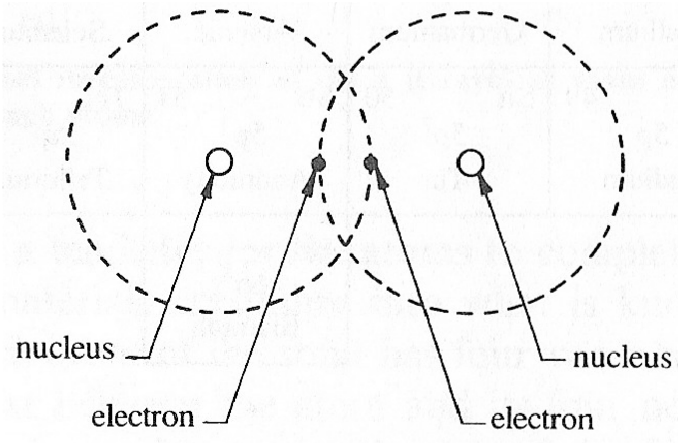
6. Semiconductors

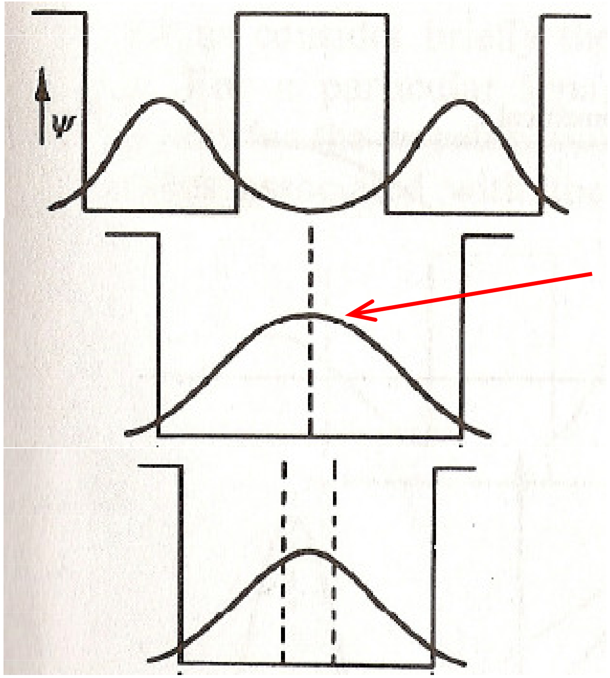
Crystal Binding

- Bonding between atoms.
  - Crystals of inert gases (Van der Waals forces).
  - Ionic crystals (electrostatic interaction).
  - Covalent crystals (electron sharing).
  - Metals (interaction ion cores with conduction e^-'s).
  - Hydrogen bonds.

Covalent Bond

- Valence electrons are shared
  - Among atoms that have unfilled shells
  - Example: hydrogen molecule





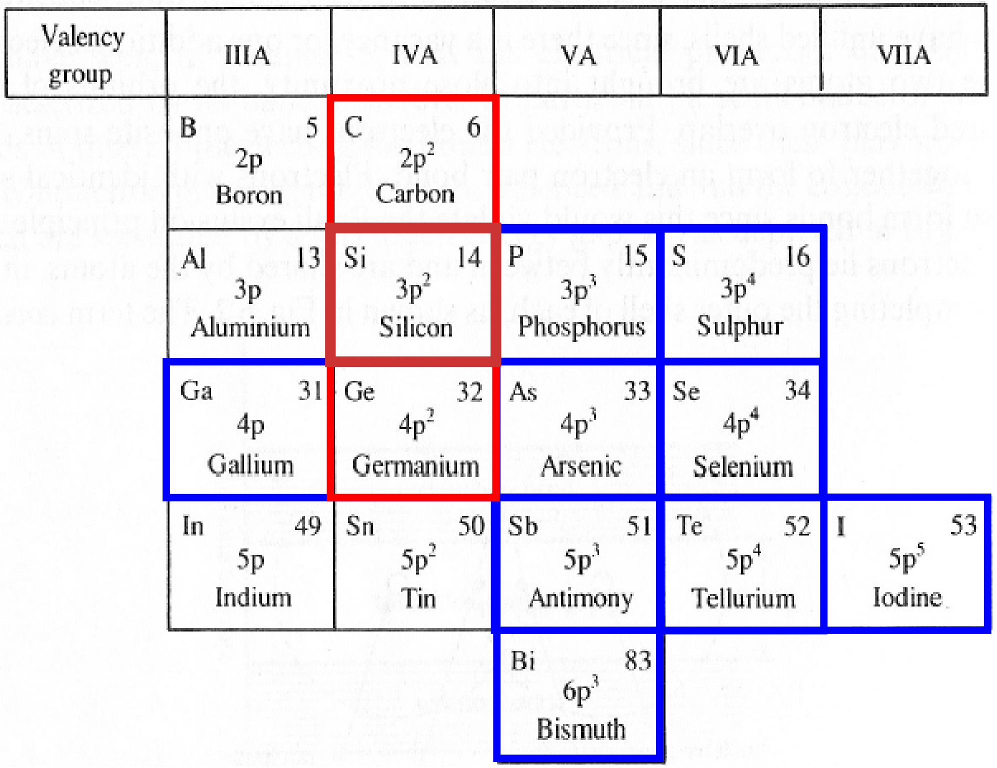
Electron tends to be between the nuclei

  - The bonding is strong and extremely directional.
  - Therefore materials are hard and brittle.

Covalent Bond

- Valence electrons are shared
  - Materials having sc properties

Single Elements:

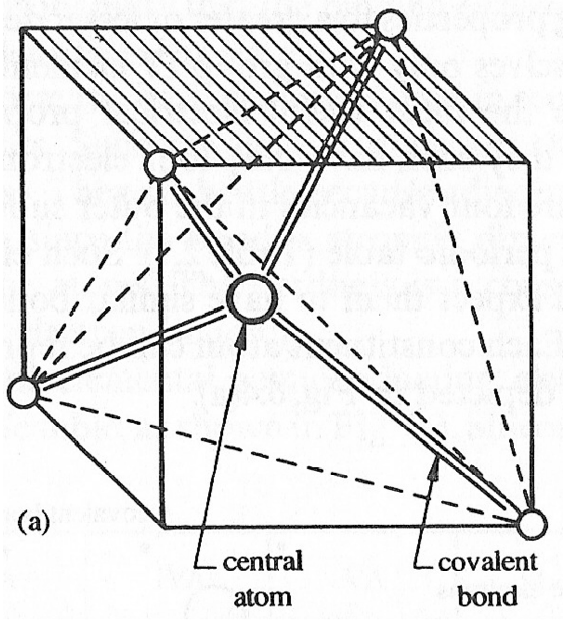


Valency group	IIIA	IVA	VA	VIA	VIIA
	B 5 2p Boron	C 6 $2p^2$ Carbon			
	Al 13 3p Aluminium	Si 14 $3p^2$ Silicon	P 15 $3p^3$ Phosphorus	S 16 $3p^4$ Sulphur	
	Ga 31 4p Gallium	Ge 32 $4p^2$ Germanium	As 33 $4p^3$ Arsenic	Se 34 $4p^4$ Selenium	
	In 49 5p Indium	Sn 50 $5p^2$ Tin	Sb 51 $5p^3$ Antimony	Te 52 $5p^4$ Tellurium	I 53 $5p^5$ Iodine
			Bi 83 $6p^3$ Bismuth		

Intermetallic III-V compounds (tetravalent):

GaAs

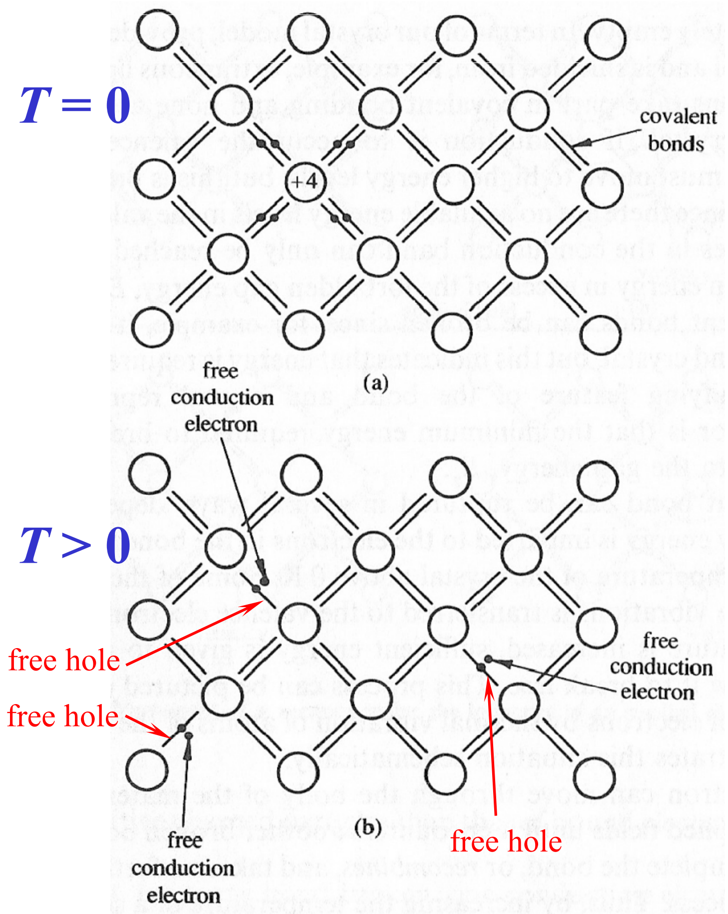
InSb



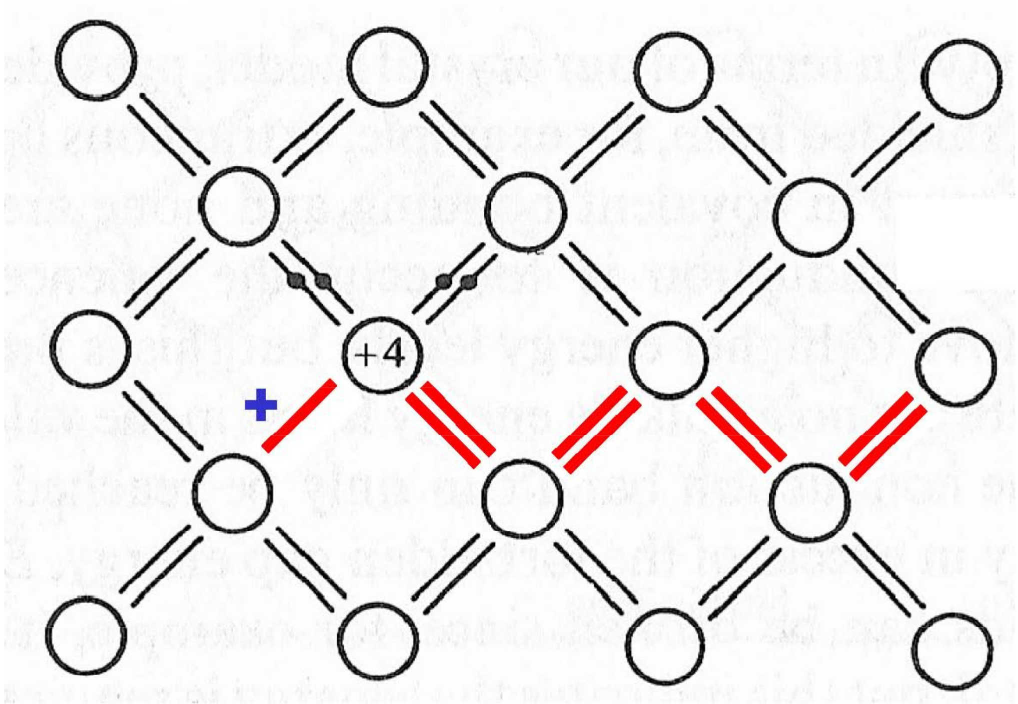
Conduction Processes

- Vacancies:

Electrons and holes are created at $T > 0$:

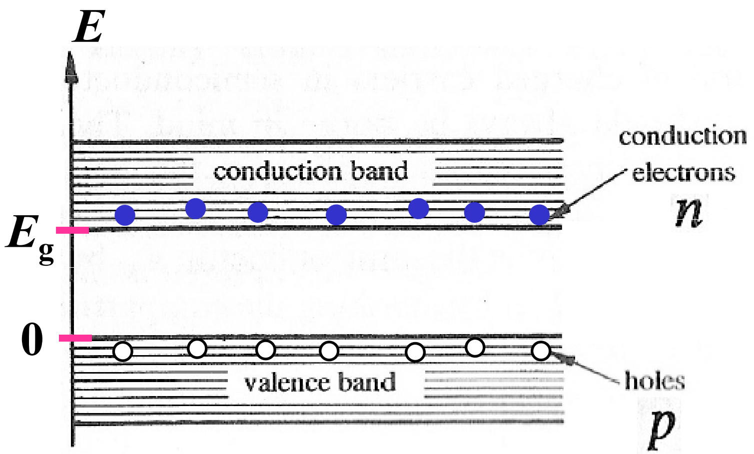


Electrons (m_e^*) and holes (m_h^*) move independently in an external field. Pictorially for holes we have:



Density of Carriers in Intrinsic sC

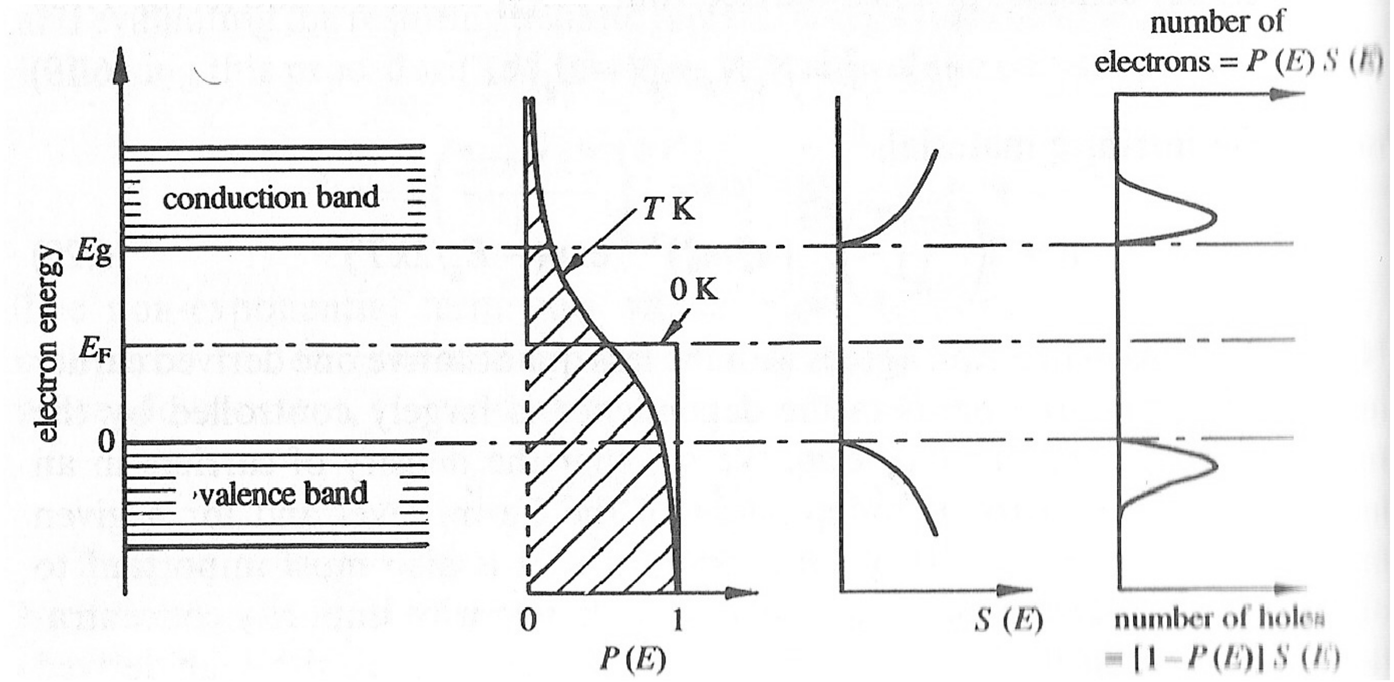
- Concentration of conduction electrons:



$$n = \int_{\text{conduction band}} S(E)P(E)\,\mathrm{d}E$$

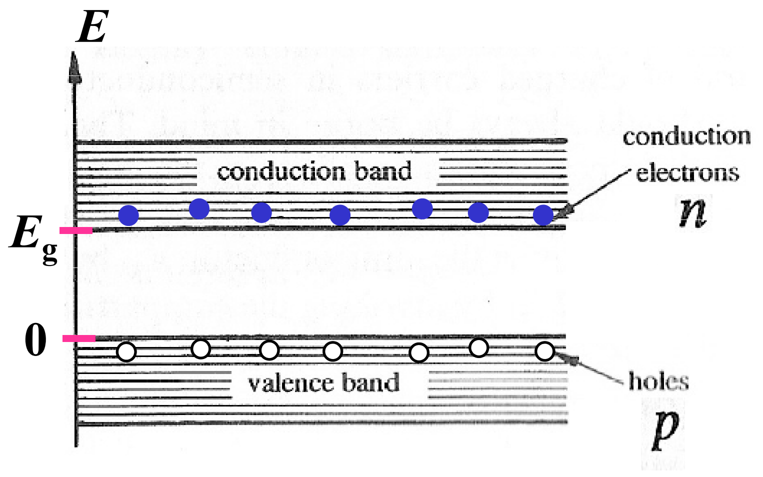
density of states

probability of occupation



Density of Carriers in Intrinsic sC

- Concentration of conduction electrons:



$$n = \int_{\substack{\text{conduction}\\ \text{band}}} \underset{\substack{\uparrow\\ \text{density}\\ \text{of states}}}{S(E)}\,\underset{\substack{\uparrow\\ \text{probability of}\\ \text{occupation}}}{P(E)}\,\mathrm{d}E$$

Density of states for free electrons: $S(E) = \dfrac{\left(8\sqrt{2}\right)\pi m^{2/2}}{h^3} E^{1/2}$

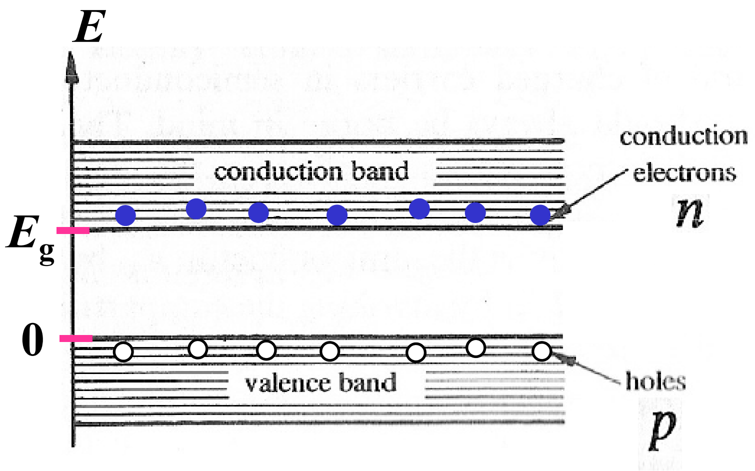
For conduction electrons in a crystal: $S(E) = \dfrac{\left(8\sqrt{2}\right)\pi m^{2/2}}{h^3} \left(E - E_g\right)^{1/2} = C\left(E - E_g\right)^{1/2}$

$$\Rightarrow \quad n = C\int_{E_g}^{\boxed{\infty}} \frac{(E-E_g)^{1/2}\mathrm{d}E}{1+\exp[(E-E_F)/kT]} \quad \xrightarrow{E\text{-}E_F>>kT} \quad n \simeq C\int_{E_g}^{\infty} (E-E_g)^{1/2}\exp[-(E-E_F)/kT]\,\mathrm{d}E$$

$$\Rightarrow \quad n = \underbrace{2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{3/2}}_{N_c} \exp[-(E_g - E_F)/kT]$$

Density of Carriers in Intrinsic sC

- Concentration of holes:



$$p = \int_{\text{valence band}} S_h(E) P_h(E) \mathrm{d}E$$

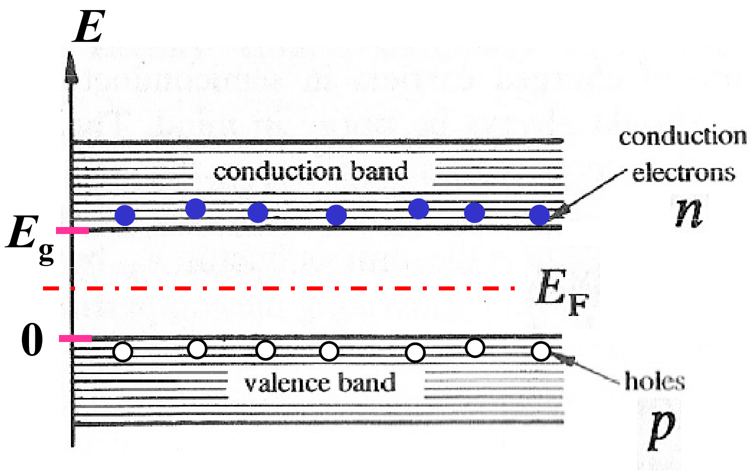
$$P_h(E) = 1 - P(E) = 1 - \frac{1}{1 + \exp[(E - E_F)/kT]} = \frac{\exp[-(E_F - E)/kT]}{1 + \exp[-(E_F - E)/kT]}$$

$$S(E) = \frac{(8\sqrt{2})\pi(m_h^*)^{3/2}}{h^3}(-E)^{1/2}$$

$$\xrightarrow{E\text{-}E_F >> kT} \quad p = 2\underbrace{\left(\frac{2\pi m_h^* kT}{h^2}\right)^{3/2}}_{N_v} \exp(-E_F/kT)$$

Density of Carriers in Intrinsic sC

- Intrinsic density:



$$n = p = n_i$$

From previous results:

$$np = n_i^2 = N_c N_v \exp(-E_g/kT)$$

$$\boxed{n_i = 2\left(\frac{2\pi kT}{h^2}\right)^{3/2} (m_e^* m_h^*)^{3/4} \exp(-E_g/2kT)}$$

This is also valid for impurity sc’s

- Fermi level:

Equating previous results:

$$(m_e^*)^{3/2}\exp[-(E_g - E_F)/kT] = (m_h^*)^{3/2}\exp(-E_F/kT)$$

$$\Rightarrow \boxed{E_F = \tfrac{1}{2}E_g - \tfrac{3}{4}kT\log(m_e^*/m_h^*)} \xrightarrow{m_e^* = m_h^*} E_F = E_g/2$$

Conclusions

- An crystal model for sC was introduced:
  - Electron form the covalent bonds.
  - Once broken, those electron are free to conduct.
  - Behind the electron, a hole is formed.
  - The energy necessary to break the bond is E_g.
- We have started studying intrinsic sC:
  - The density of electrons and holes was calculated.