Physics of Electronics:

5. Electrons in Solids - Intro to Band Theory

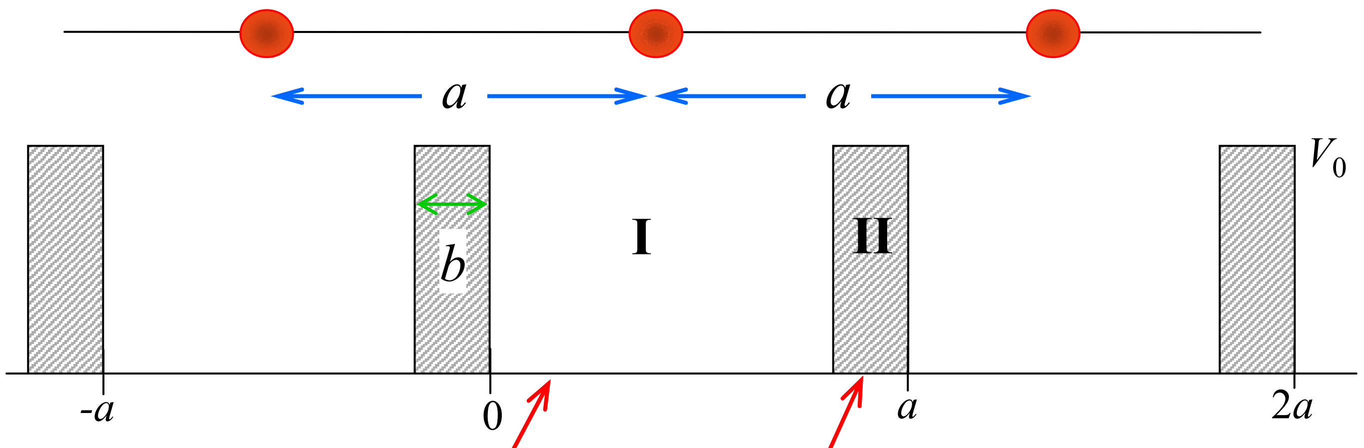
July – December 2008

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.



$$\frac{\partial^2\Psi}{\partial x^2}+\beta^2\Psi=0$$

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

$$\Psi_{\mathrm{I}}=Ae^{j\beta x}+Be^{-j\beta x}$$

$$\frac{\partial^2\Psi}{\partial x^2}-\alpha^2\Psi=0$$

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

we are looking
for bound states

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

Allowed Energy Bands

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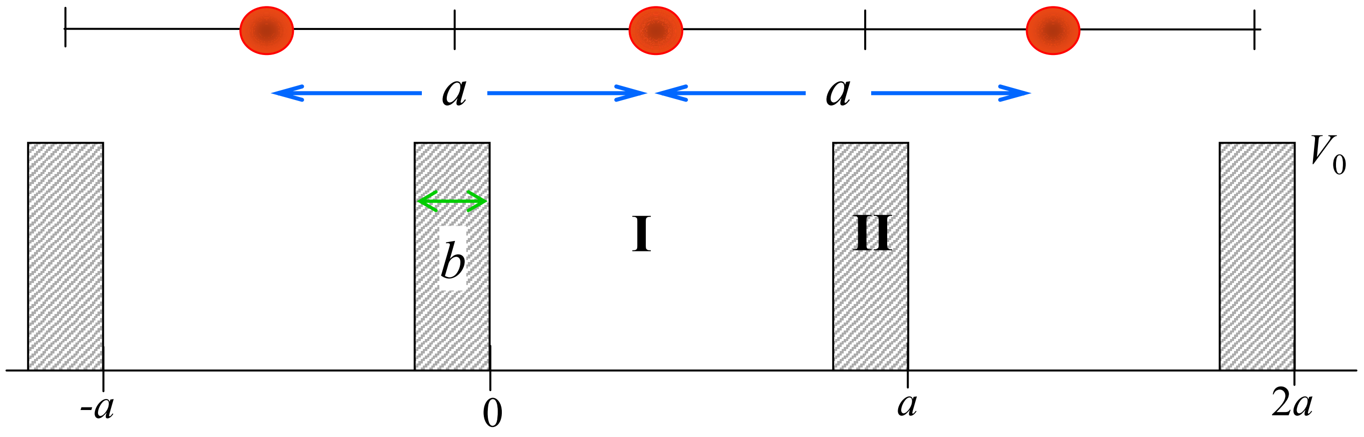


  - From continuity of ψ and $\mathbf{d}\psi/\mathbf{d}x$ at the boundaries:
    - At $x = 0$: $A + B = C + D$; $i\beta(A - B) = \alpha(C - D)$.
  - From Bloch's theorem, $\psi(x + a) = \psi(x)e^{ika}$:
    - At $x = -b$: $Ae^{i\beta(a-b)} + Be^{-i\beta(a-b)} = (Ce^{i\alpha(-b)} + De^{-i\alpha(-b)})\, e^{-ika}$

$$i\beta(Ae^{i\beta(a-b)} - Be^{-i\beta(a-b)}) = \alpha(Ce^{i\alpha(-b)} - De^{-i\alpha(-b)})\, e^{-ika}$$

Allowed Energy Bands

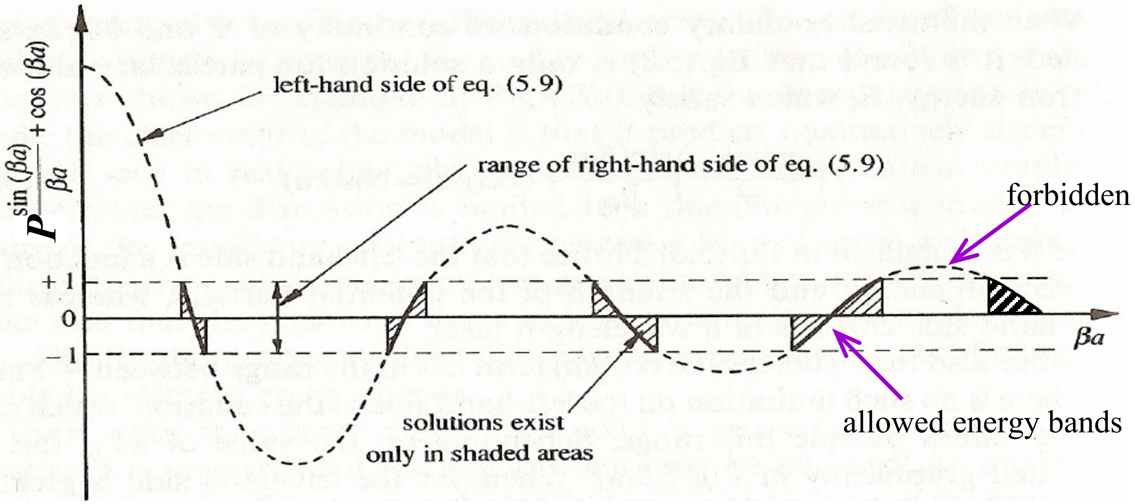
- Kronig-Penney model.
  - A solution only if its determinant is equal to zero giving:

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

  - Consider the case $\boldsymbol{b\rightarrow 0}$ **&** $\boldsymbol{V_0\rightarrow\infty}$ such that $\boldsymbol{\alpha^2 ba/2=P}$ remains constant. In this limit $\boldsymbol{\alpha\gg\beta}$ **&** $\boldsymbol{\alpha b\ll 1}$. Then:

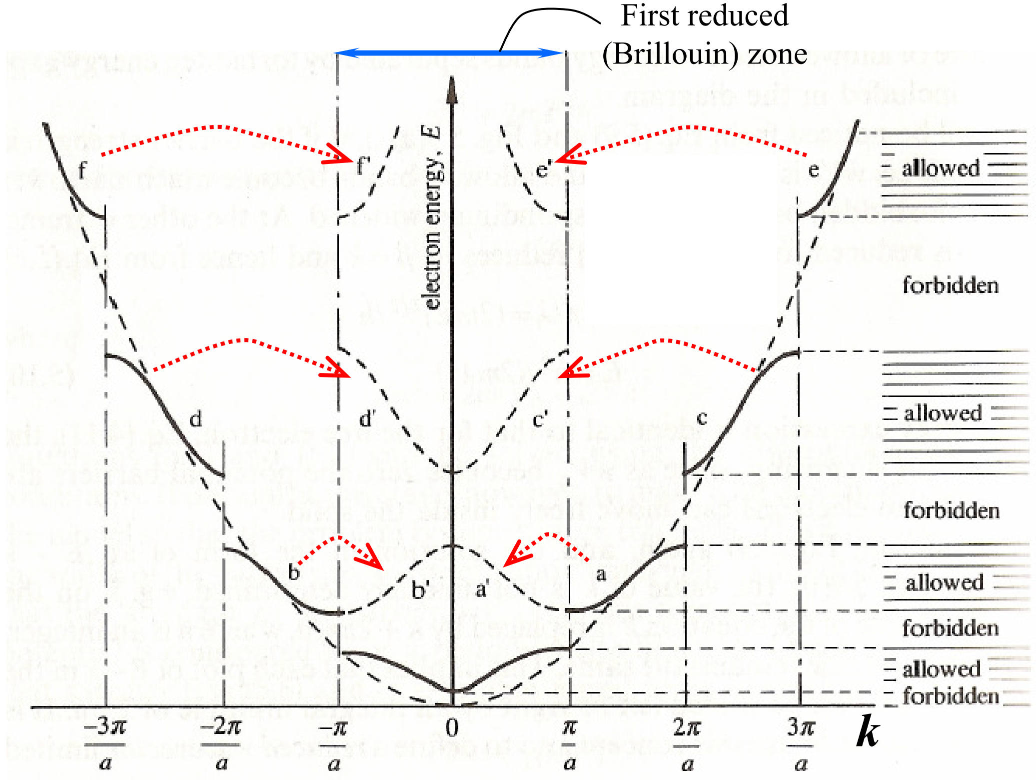
$$(P/\beta a)\sin\beta a+\cos\beta a=\cos ka$$

  - Solving to find allowed electron energies $E=\hbar\beta^2/2\text{m}$:



Allowed Energy Bands

- Kronig-Penney model.
  - Since $(P/\beta a)\sin \beta a + \cos \beta a = \cos ka$
    - The allowed energies are function of the wavenumber ***k***.
    - The solutions have the periodicity of **cos(*ka*)**.



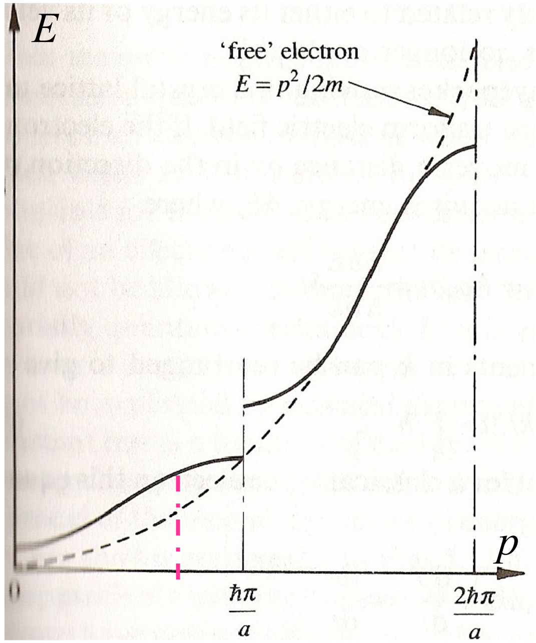
Velocity and Effective Mass

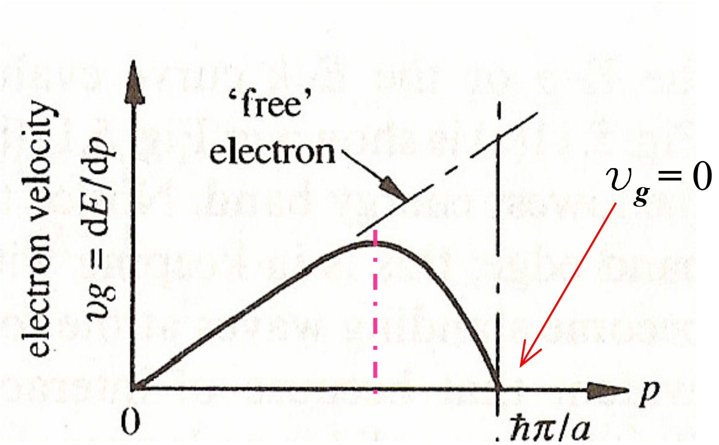
- Group velocity
  - From Bloch's theorem $\psi\,(x,\,t) = \underbrace{u_k(x)}_{\text{spatial modulation}}\,\underbrace{e^{i(kx-Et/\hbar)}}_{\text{plane wave}}$ ← wave packet
  - Therefore, the velocity of the electron is given by the group velocity

$$\upsilon_g = \frac{\partial \omega}{\partial k} = \frac{\partial (E/\hbar)}{\partial k} \Rightarrow \boxed{\upsilon_g = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{\partial E}{\partial p}}$$

← $p = \hbar k$

OBS. $E = f(p)$ is called dispersion relation





Velocity and Effective Mass

- Effective Mass
  - Consider an e^- in a solid moving in an external field that exerts a force F on it. The energy acquired by the e^- is:

$$\delta E = F\delta x = F v_g \delta t = \frac{F\delta E}{\hbar\,\delta k}\delta t \quad \Rightarrow \quad \boxed{F = \hbar\, \mathrm{d}k/\mathrm{d}t = \mathrm{d}p/\mathrm{d}t}$$

      - » External forces and effects of the lattice are included
  - Applied for the case of a free electron (i.e. $p = mv$):

$$F = \frac{\mathrm{d}}{\mathrm{d}t}(\hbar k) = \frac{\mathrm{d}p}{\mathrm{d}t} = m\frac{\mathrm{d}v}{\mathrm{d}t}$$

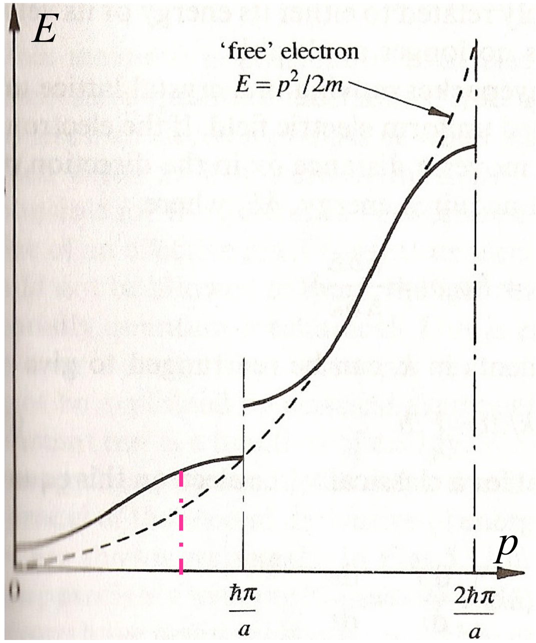
  - Now, in general, differentiating υ_g:

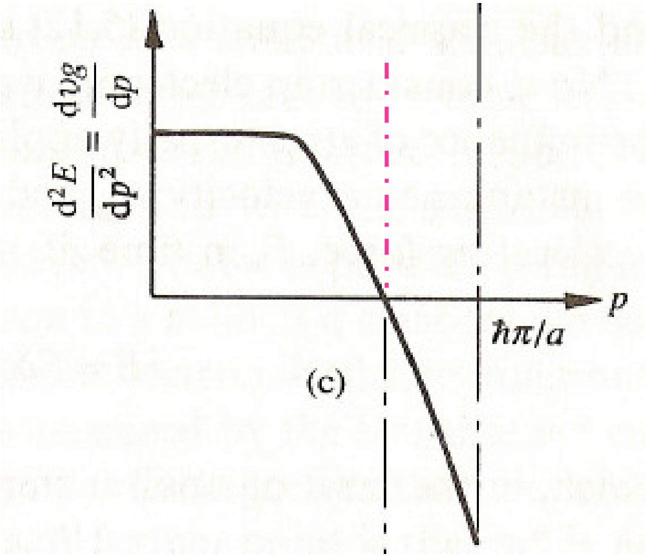
$$\frac{\mathrm{d}v_g}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}E}{\mathrm{d}p}\right) = \frac{\mathrm{d}^2E}{\mathrm{d}t\mathrm{d}p} = \frac{\mathrm{d}p}{\mathrm{d}t}\frac{\mathrm{d}^2E}{\mathrm{d}p^2} = F\frac{\mathrm{d}^2E}{\mathrm{d}p^2} \quad \Rightarrow \quad F = \left(\frac{\mathrm{d}^2E}{\mathrm{d}p^2}\right)^{-1}\frac{\mathrm{d}v_g}{\mathrm{d}t}$$

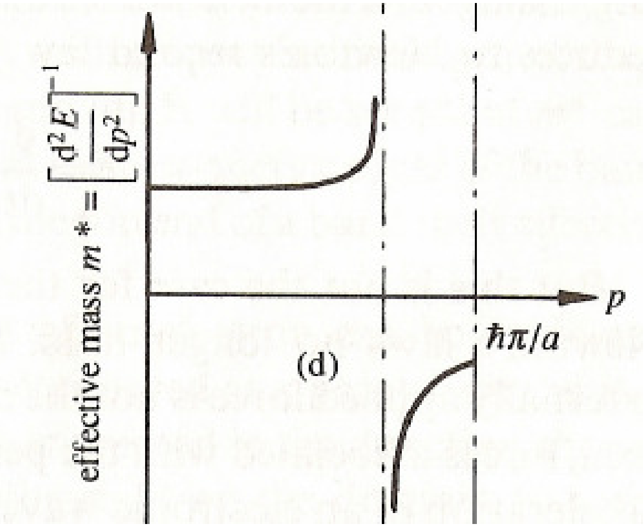
Velocity and Effective Mass

- Effective Mass
  - Comparing both we define:

$$\boxed{m^* = \left(\frac{d^2E}{dp^2}\right)^{-1} = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}} \quad \rightarrow \quad F = m^* dv_g/dt$$







Velocity and Effective Mass

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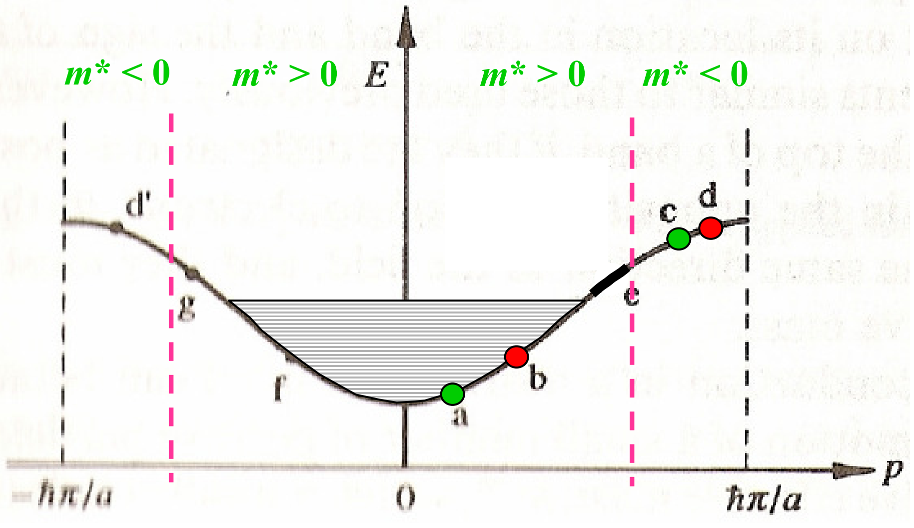

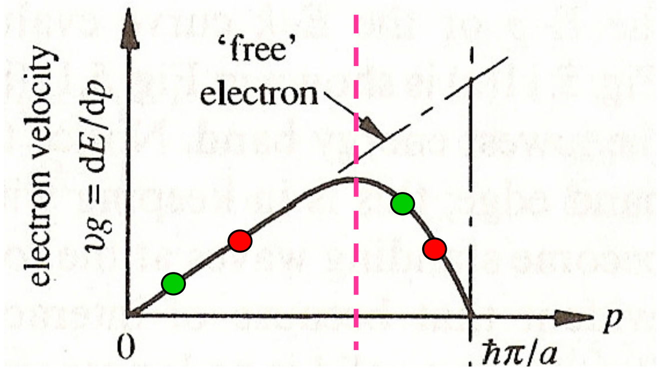

$\mathscr{E} = 0$

$\leftarrow$

$\mathscr{E} \neq 0$

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$\leftarrow$

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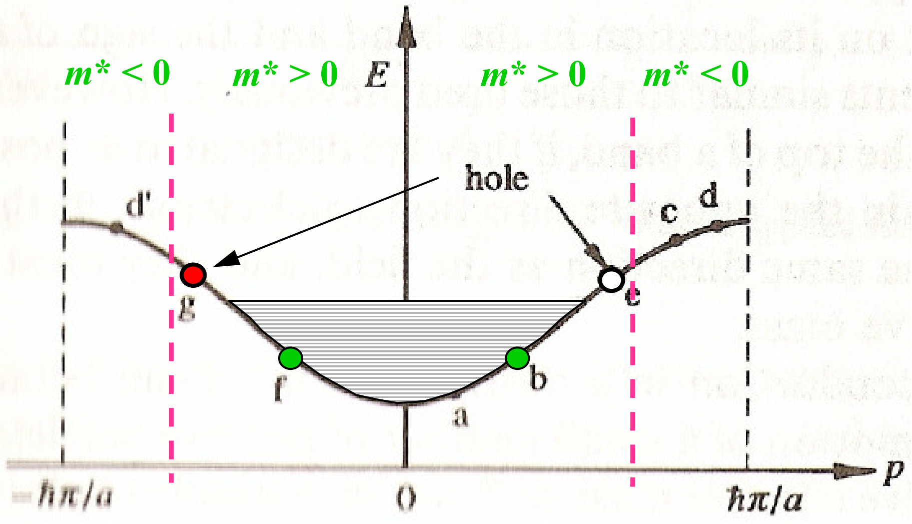
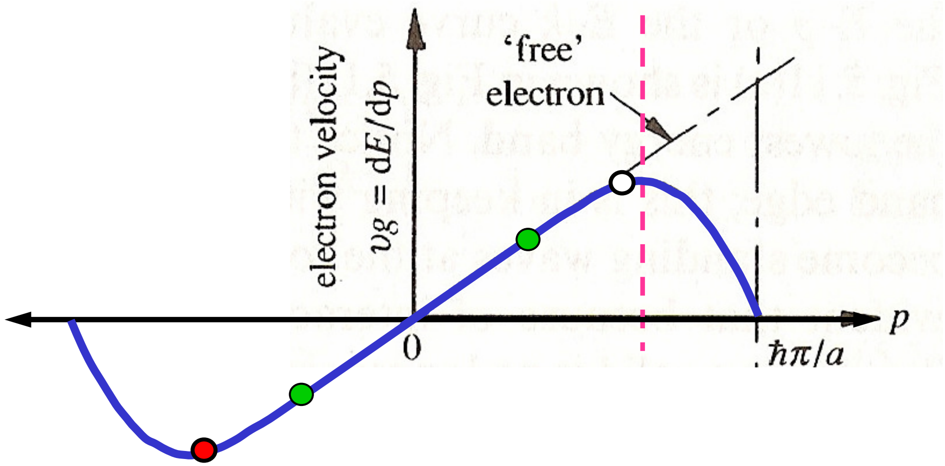
Velocity and Effective Mass

- Effective Mass
  - Comparing both we define:

$$\boxed{m^* = \left(\frac{\mathrm{d}^2 E}{\mathrm{d}p^2}\right)^{-1} = \hbar^2 \left(\frac{\mathrm{d}^2 E}{\mathrm{d}k^2}\right)^{-1}} \Rightarrow F = m^* \mathrm{d}v_g/\mathrm{d}t$$

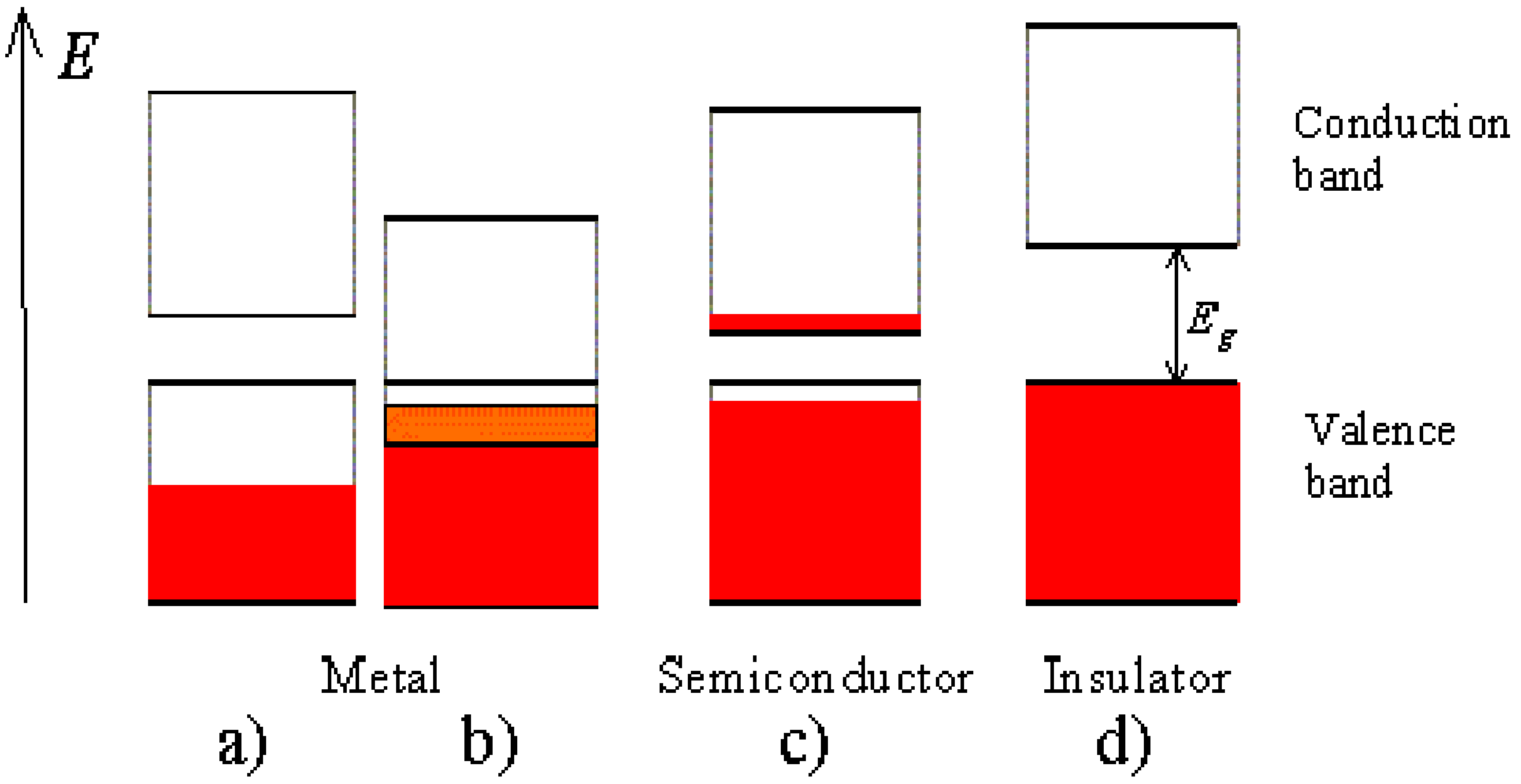




- 🟢 Opposite velocities. No net current,
- 🔴 Not cancelled. Net current.

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)

Physics of Electronics:

6. Semiconductors

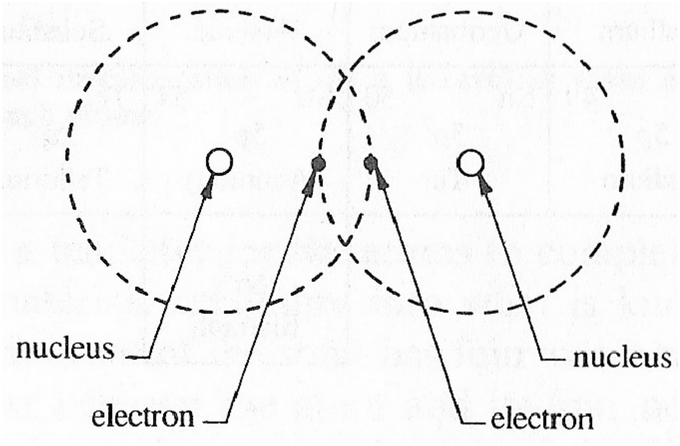
July – December 2008

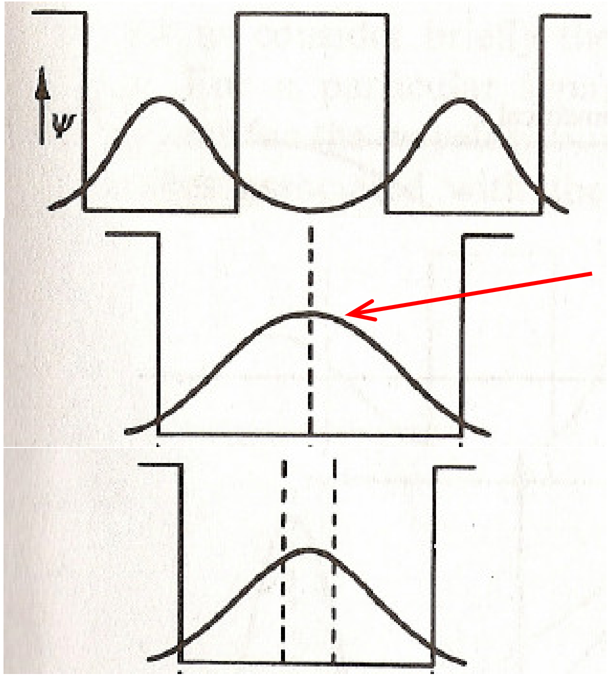
Crystal Binding

- 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





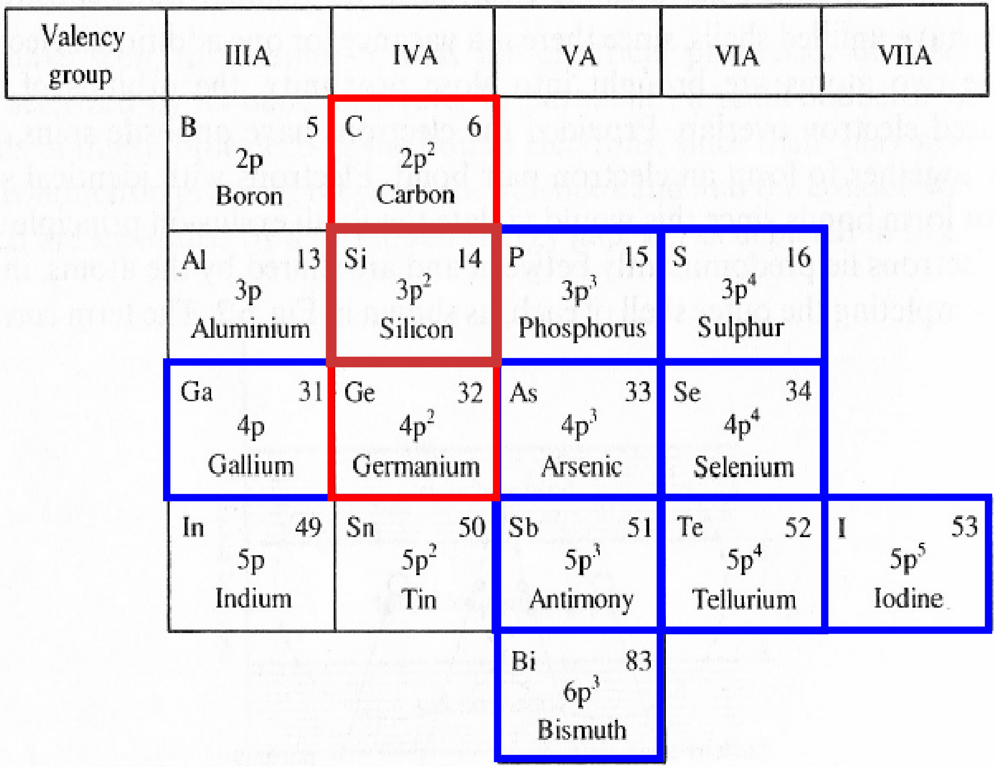
Electron tends to be between the nuclei

  - 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:

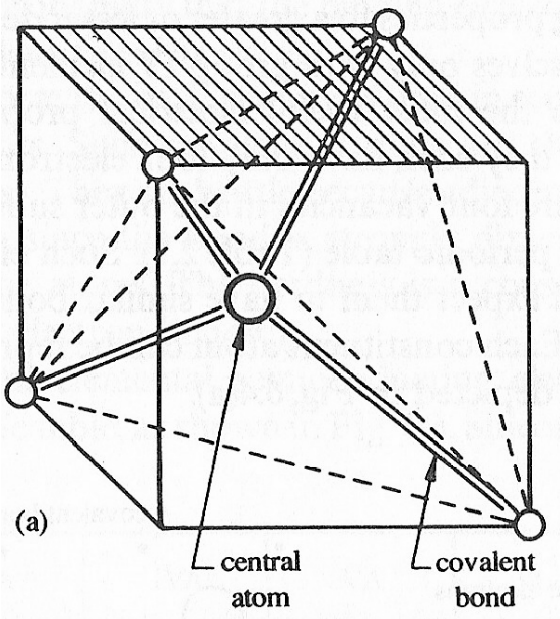


Valency group	IIIA	IVA	VA	VIA	VIIA
	B 5 2p Boron	C 6 $2p^2$ Carbon			
	Al 13 3p Aluminium	Si 14 $3p^2$ Silicon	P 15 $3p^3$ Phosphorus	S 16 $3p^4$ Sulphur	
	Ga 31 4p Gallium	Ge 32 $4p^2$ Germanium	As 33 $4p^3$ Arsenic	Se 34 $4p^4$ Selenium	
	In 49 5p Indium	Sn 50 $5p^2$ Tin	Sb 51 $5p^3$ Antimony	Te 52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

Intermetallic III-V compounds (tetravalent):

GaAs

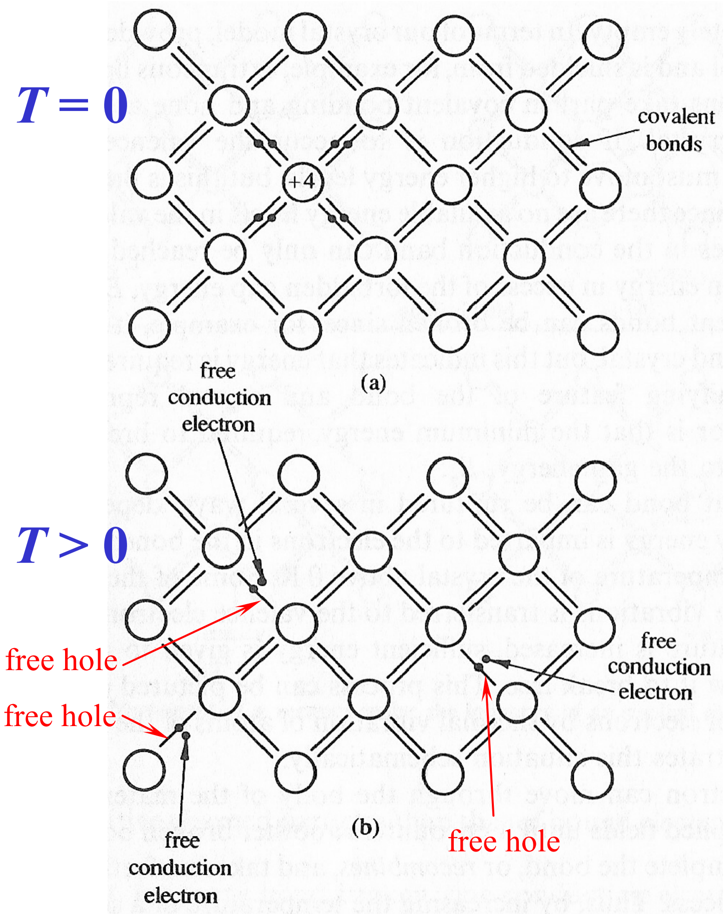
InSb



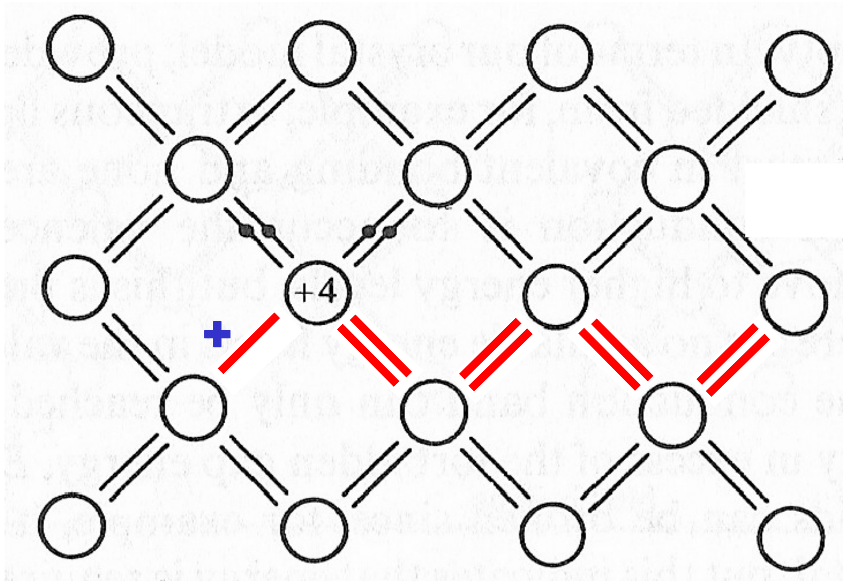
Conduction Processes

- 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:



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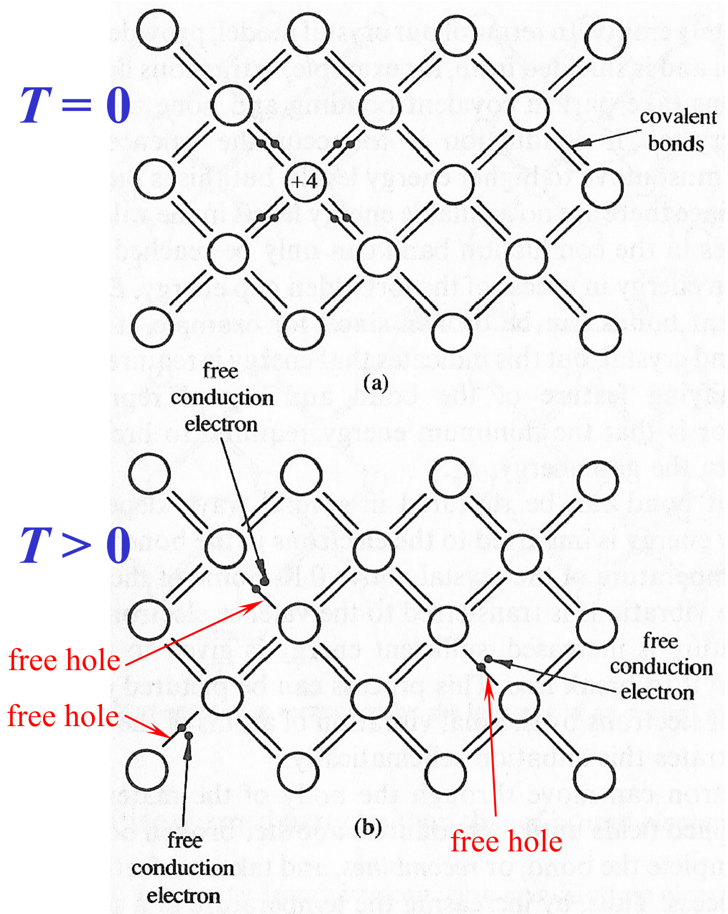

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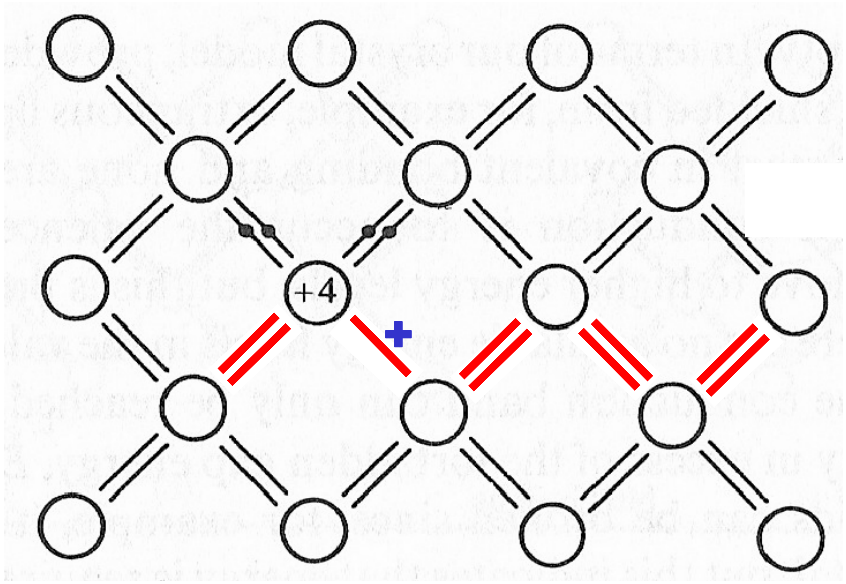

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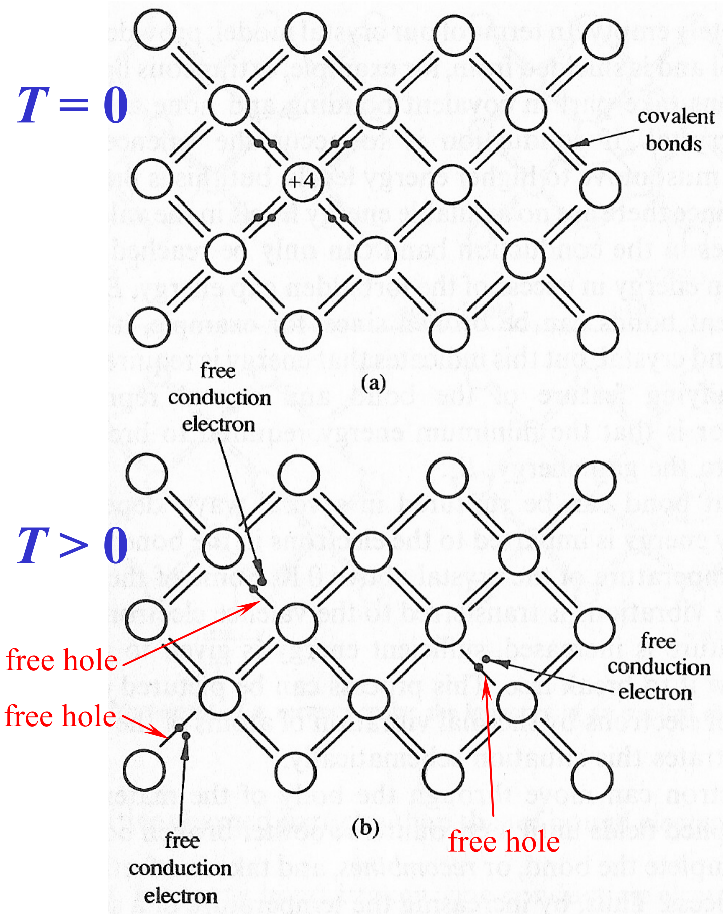

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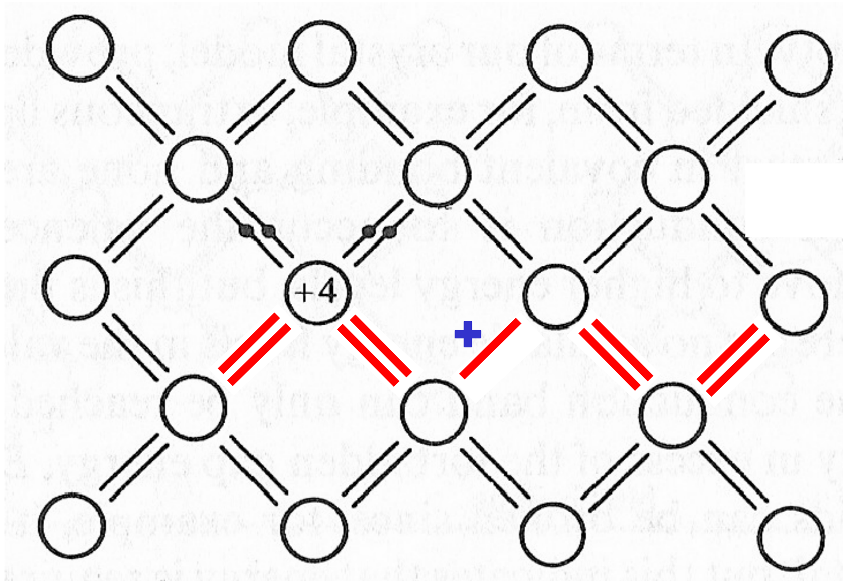

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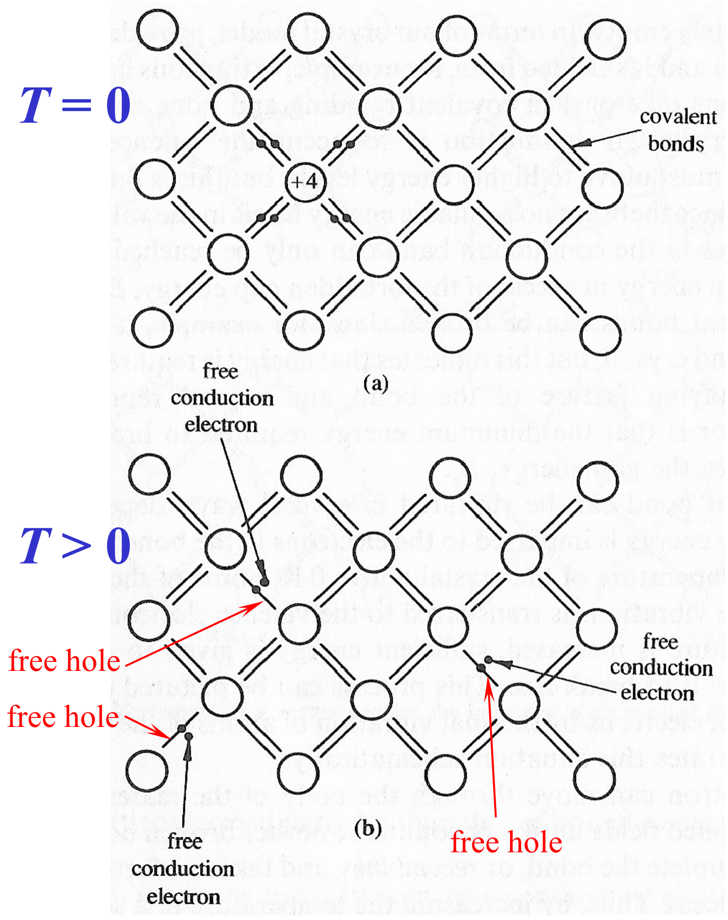

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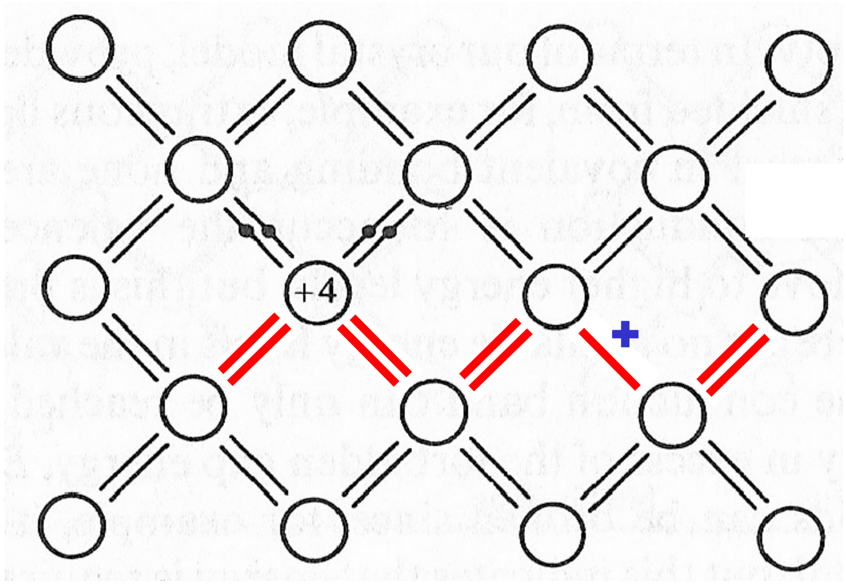

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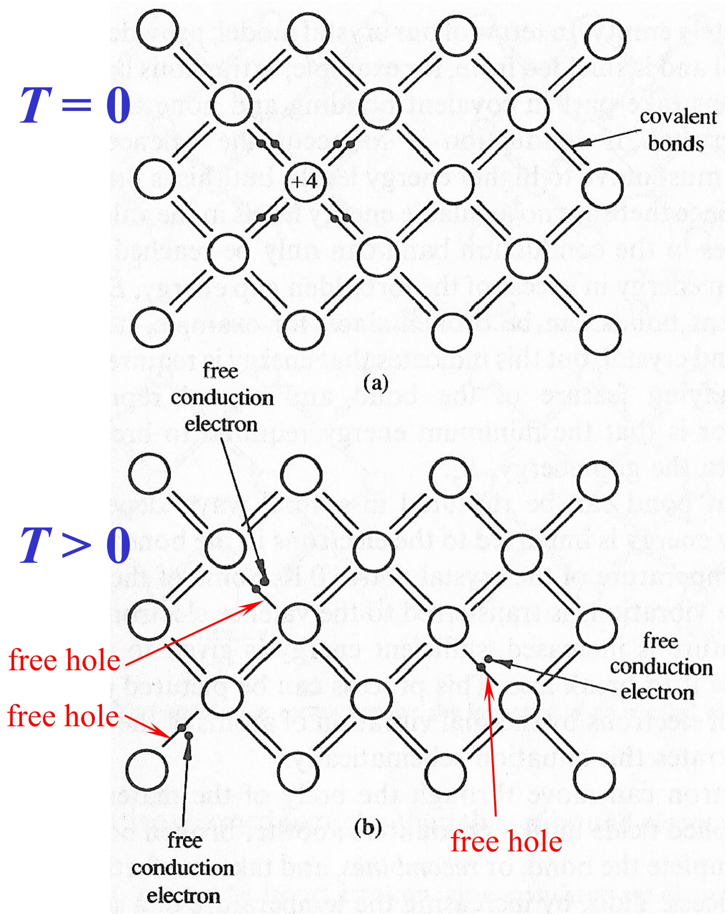

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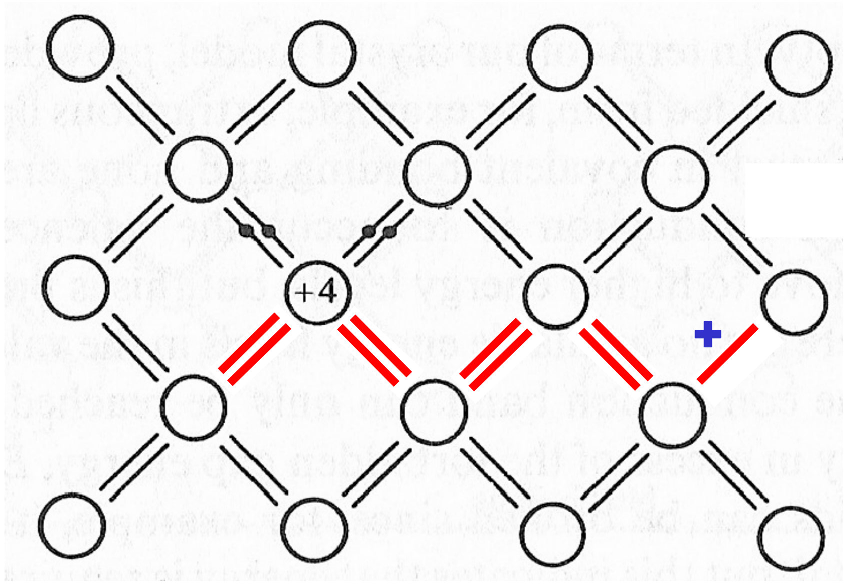
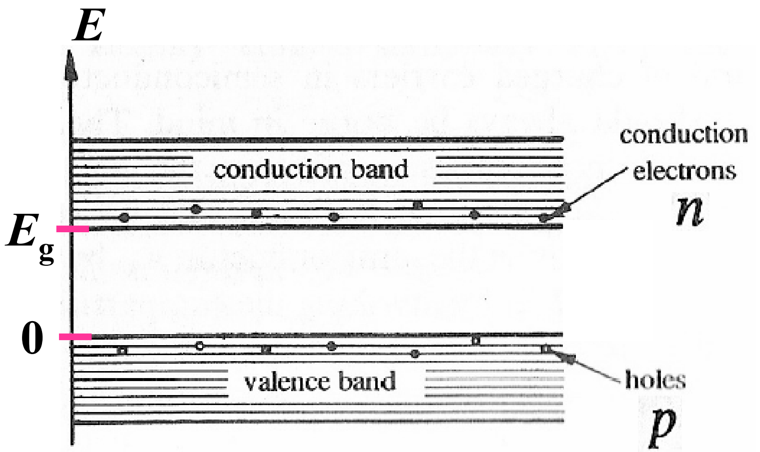


Density of Carriers in Intrinsic sC

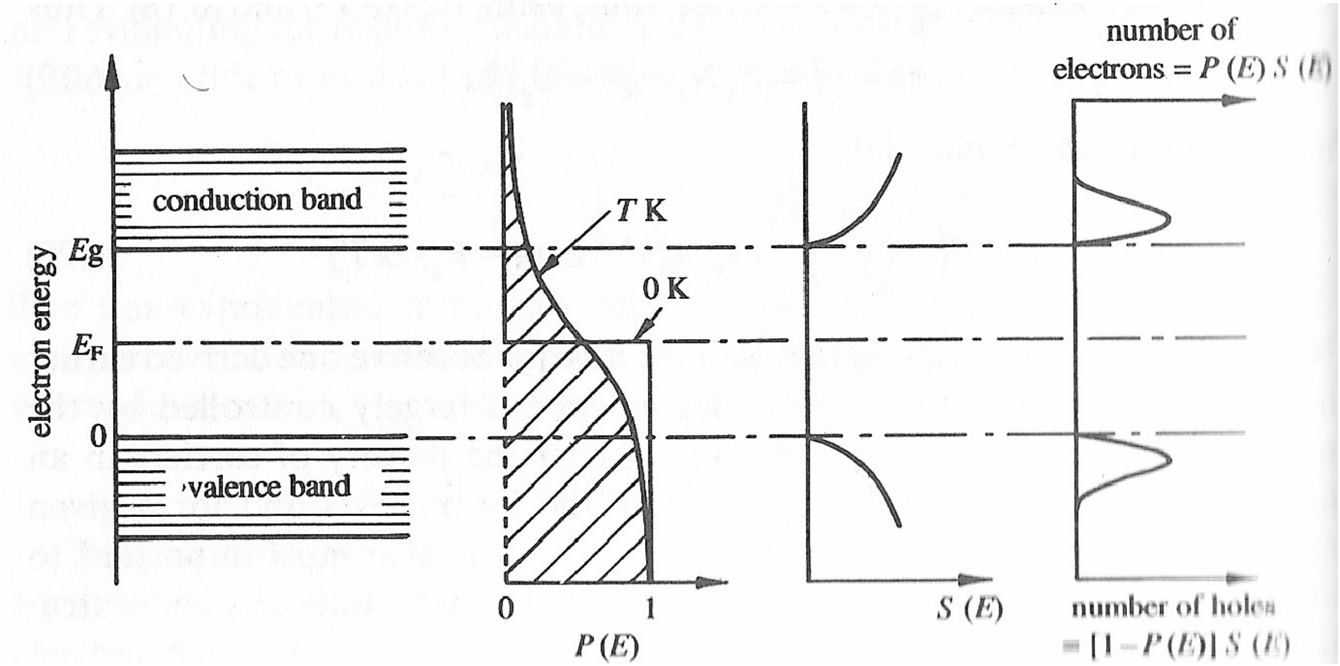
- Concentration of conduction electrons:



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

density of states

probability of occupation



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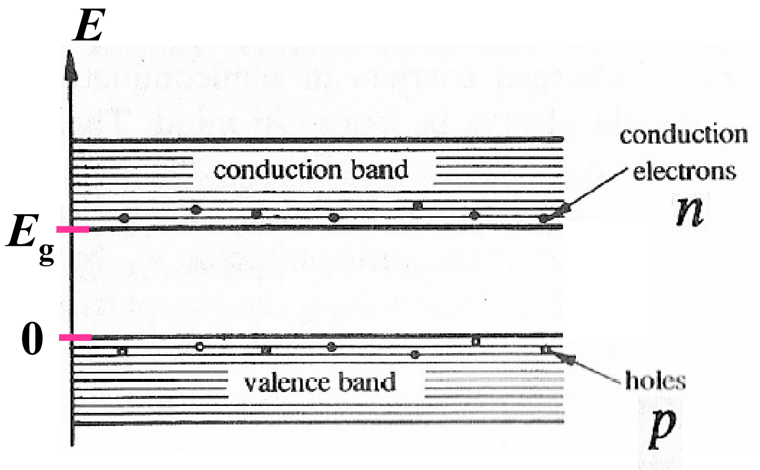


$$n = \int_{\text{conduction band}} S(E) P(E)\, dE$$

density of states

probability of occupation

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

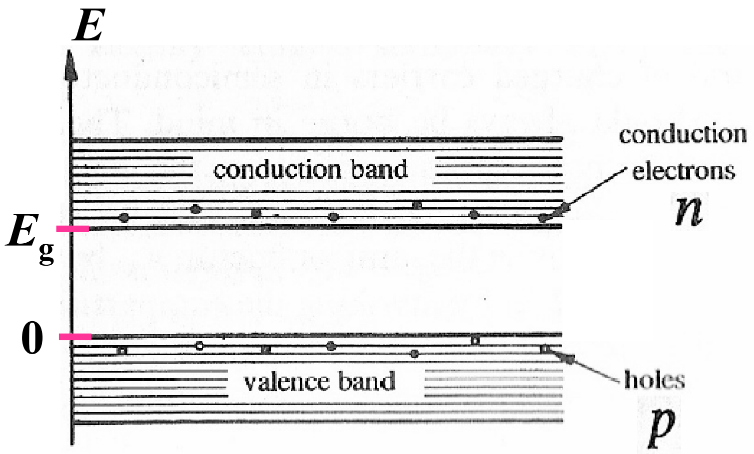
For electrons in a crystal: $S(E) = \frac{(8\sqrt{2})\pi (m_e^*)^{3/2}}{h^3} (E - E_g)^{1/2} = C(E - E_g)^{1/2}$

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

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

Density of Carriers in Intrinsic sC

- Concentration of holes:



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

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

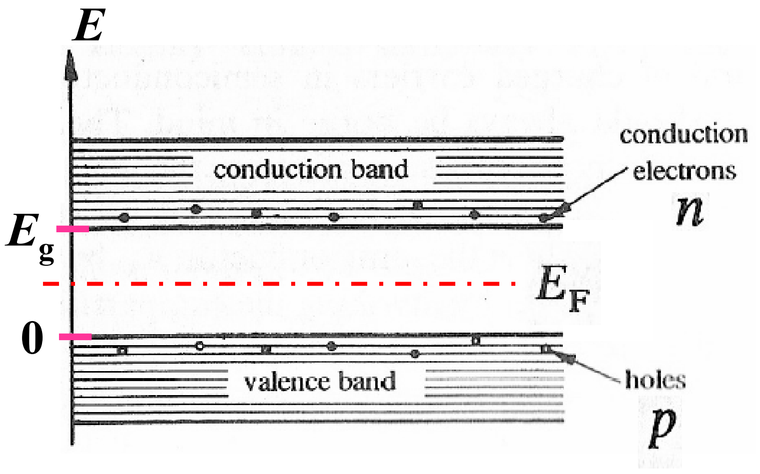
$$S(E)=\frac{(8\sqrt{2})\pi(m_h^*)^{3/2}}{h^3}(-E)^{1/2}$$

E-E_F>>kT ➡

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

Density of Carriers in Intrinsic sC

- Intrinsic density:



$$n = p = n_i$$

From previous results:

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

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

This is also valid for impurity sc's

- Fermi level:

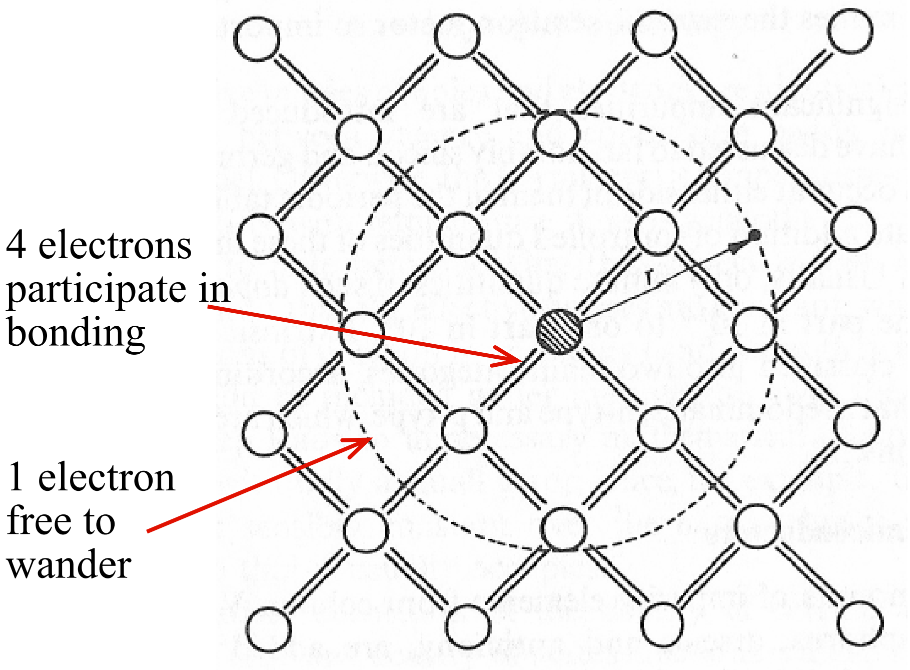
Equating previous results:

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

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

Extrinsic or Impurity sC

- They are obtained by adding tri/pentavalent impurities (1 part in 10^{10} to 1part in 10^{3}).
- n-type semiconductors (pentavalent impurities)



We have a hydrogen type atom:

$$r_h = \frac{h^2\epsilon_0}{\pi e^2 m} \approx 0.05\,\mathrm{nm} \qquad E_h = -\frac{me^4}{8\epsilon_0^2 h^2} = -13.6\,\mathrm{eV}$$

$$\Downarrow$$

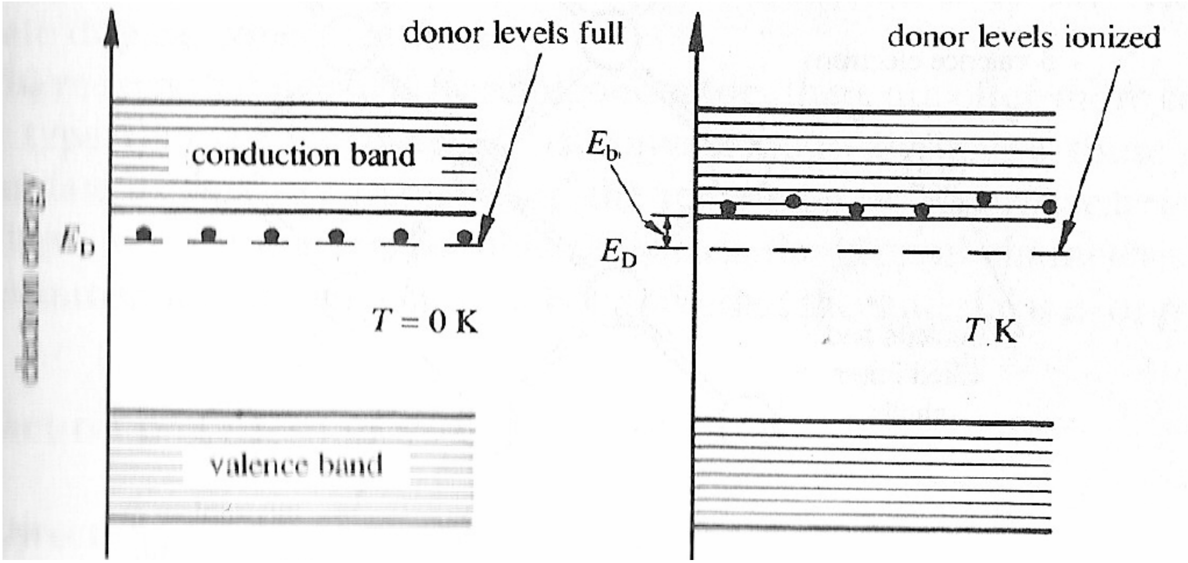
$$r_b = \frac{h^2\epsilon_r\epsilon_0}{\pi e^2 m_e^*} = \epsilon_r\left(\frac{m_e}{m_e^*}\right) r_h \qquad E_b = -\frac{me^4}{8\varepsilon_r^2\varepsilon_0^2 h^2} = -\frac{E_h}{\epsilon_r^2}\left(\frac{m_e^*}{m_e}\right)$$

For germanium: $m_e^* = 0.6 m_e \quad \epsilon_r = 16$

$$r_b = 1.4\,\mathrm{nm} \qquad E_b = -0.03\,\mathrm{eV}$$

Extrinsic or Impurity sC

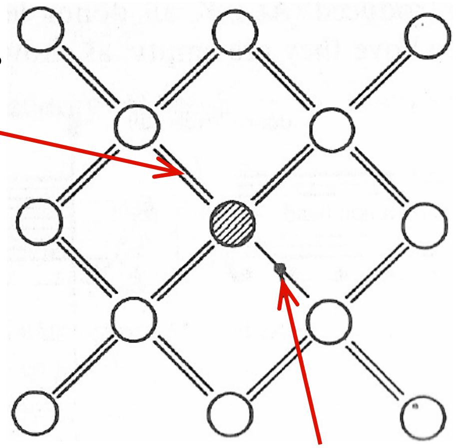
- n-type semiconductors (pentavalent impurities)
  - Band structure



  - Density of conduction electrons. Example: germanium
    - Intrinsic $E_g = 0.75\,\text{eV}$ **T = 300 K** ⇨ $n_i = 2\left(\frac{2\pi kT}{h^2}\right)^{3/2}(m_e^* m_h^*)^{3/4}\exp(-E_g/2kT) = 10^{19}\,\text{m}^{-3}$ minority carriers
    - Extrinsic **density = 10^{28} atom/m3**
      doping = 1 ppm ⇨ **$n_e = 10^{22}$ m^{-3}** majority carriers

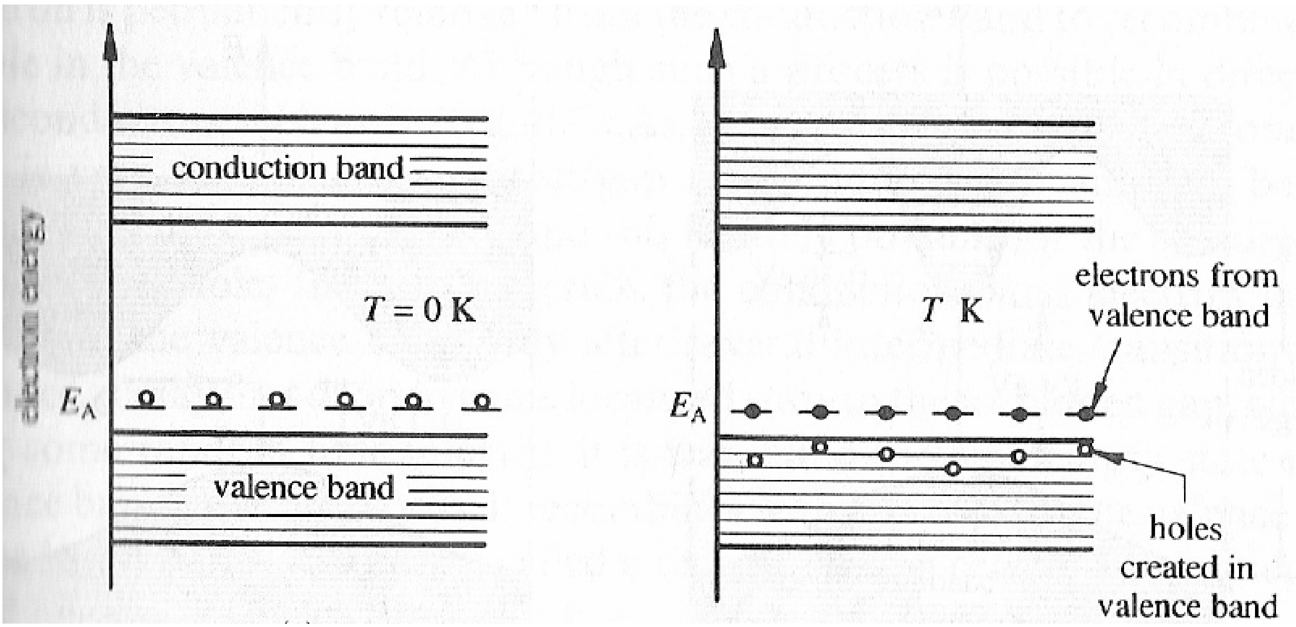
Extrinsic or Impurity sC

- p-type semiconductors (trivalent impurities)



All 3 electrons participate in bonding

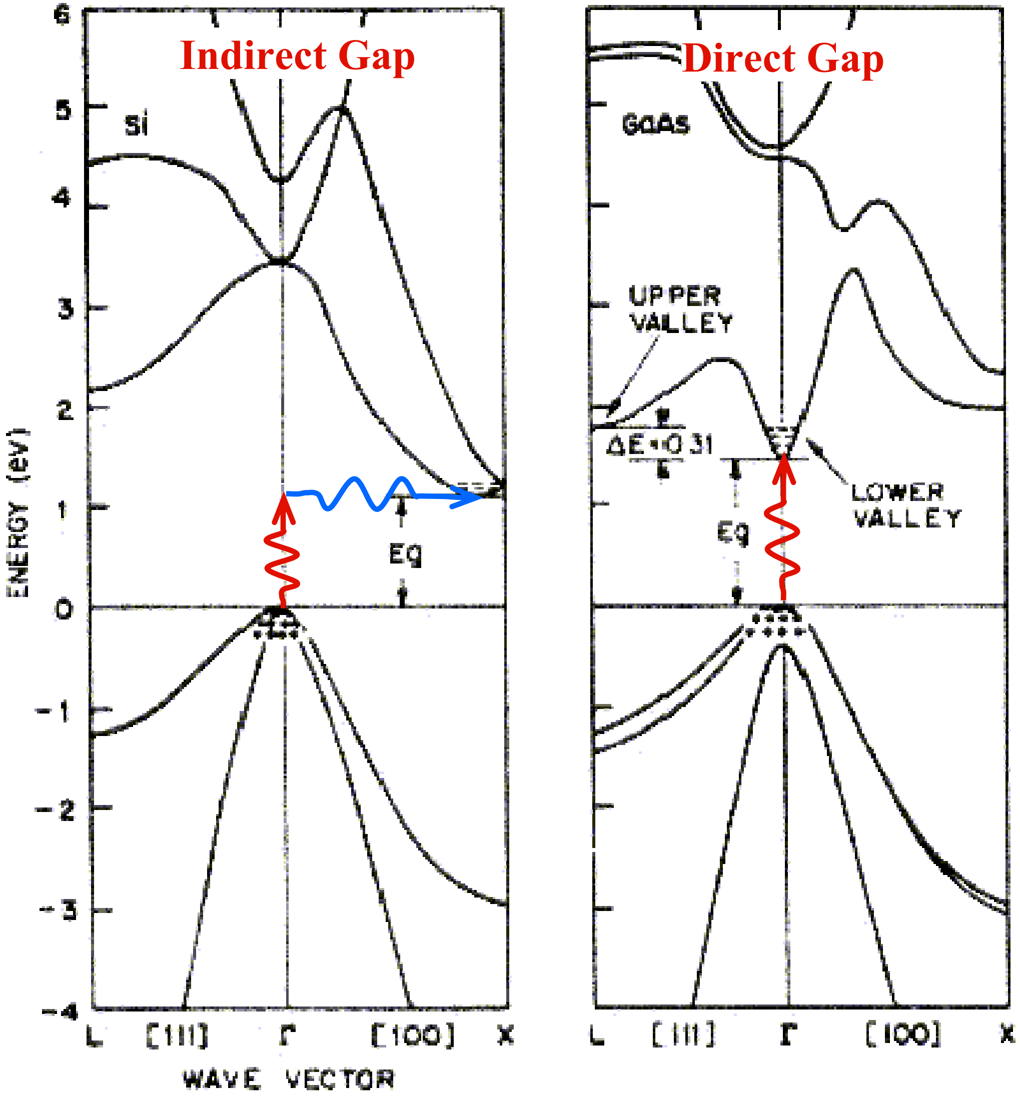
The incomplete bond can, at $T > 0$, be filled creating a hole in the valence band.



Electron Processes in Real sC

- Direct and indirect gap sC

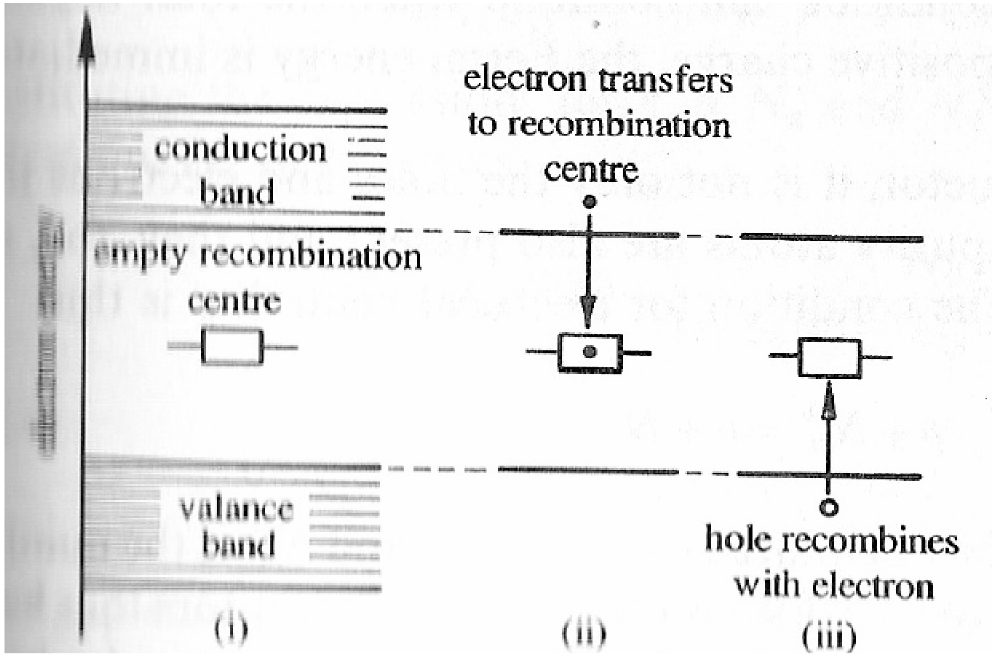
The minimum separation cannot be reached optically.



The minimum separation can be reached optically (by means of a photon).

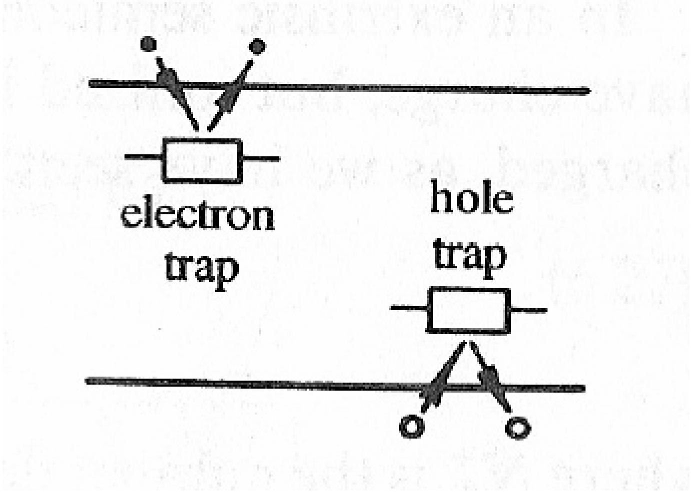
Electron Processes in Real sC

- Recombination
  - Permanent loss of a carrier.
  - Due to conservation of momentum
    - Possible in direct-gap sC's.
    - Marginally probable in indirect-gap sC's. Intermediate steps are required.



Electron Processes in Real sC

- Trapping
  - Temporary removal of a carrier on localized states



- Localized states
  - Lattice defects (dislocations, vacancies).
  - Impurities.

Is an insulator always an insulator?

- Let’s consider the following phase diagram: