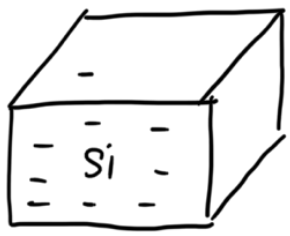
Semiconductor physics

Two major questions

(1) How many charge carriers are there in semiconductors?

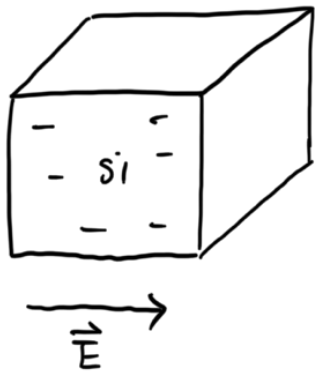


c.f.) # of electrons in metal

$\cong$ # of atoms

But, not quite for semiconductors!

(2) Where are they and how are they moving?



- Charge concentration
- Electric field & potential profiles

⋮

∴ How can engineer these properties and how can I make useful things?
(e.g. MOSFET, diodes, BJTs, ⋯)

- Basic tools to understand semiconductor physics:

  Quantum mechanics & statistical mechanics

- Knowledge needed to answer question (1)

$$\underline{n,p} = \underbrace{\int_{E_A}^{E_B}}_{①} \underbrace{g(E)}_{②} \underbrace{f(E)}_{③} \, dE$$

① Band theory (i.e., E vs. k diagram)
  - * Effective mass
  - * Hole and electron.

② Density of states

③ Fermi-Dirac distribution.

· Knowledge needed to answer question (2)

Maxwell's eqn & Probability theory

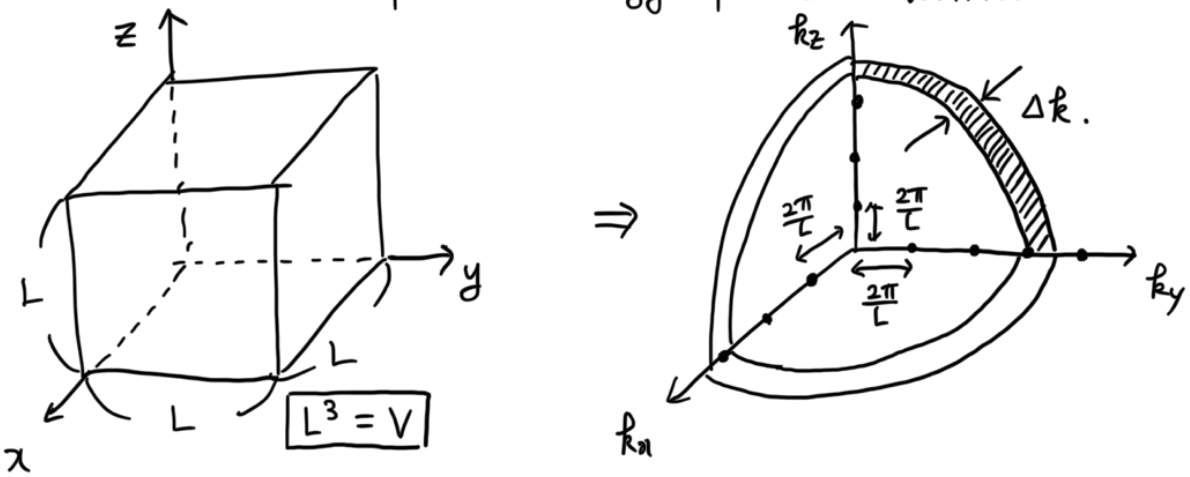
[Carrier drift
Carrier diffusion
Generation & recombination] ⇒ Continuity equation & Ambipolar transport eqn.

· Practical applications (Out of scope) → "반도체 소자" and advanced class at grad level.

P/N junction ⟶ [pn diodes
BJTs
MOSFETs
Optical devices (LEDs, photodiodes, solar cells, ...)]

$$n \text{ or } p = \int_{E_A}^{E_B} \underbrace{g(E)}_{\text{D.O.S.}} f(E)\, dE$$

[1] Density of states : The number of electronic states per unit energy per unit volume.



⟨Real space⟩ ⟨k-space⟩

$$\#\text{ of allowed k-points per unit volume} = \frac{1}{\left(\frac{2\pi}{L}\right)^3}$$

$$\#\text{ of allowed k-points in a thin shell} = (4\pi k^2)\Delta k \cdot \frac{1}{\left(\frac{2\pi}{L}\right)^3}$$

of a radius k and a thickness Δk

# of allowed electronic states in a thin shell $= \Delta N$.

$$= \underset{\uparrow}{\underline{\underline{2}}} \cdot (4\pi k^2)\Delta k \cdot \frac{1}{\left(\frac{2\pi}{L}\right)^3}$$

($\because$ Pauli's exclusion principle)

$$\Delta N = \frac{k^2}{\pi^2}\Delta k L^3 \rightarrow \frac{\Delta N}{V} = \frac{k^2}{\pi^2}\Delta k$$

$$\underbrace{\frac{1}{V}\cdot\frac{\Delta N}{\Delta E}}_{\text{Density of states}} \triangleq g(E) = \frac{k^2}{\pi^2}\frac{\Delta k}{\Delta E} \quad \cdots ①$$

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow dE = \frac{\hbar^2 k}{m}dk \rightarrow \frac{dk}{dE} = \frac{m}{\hbar^2 k}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$g(E) = \frac{k^2}{\pi^2}\cdot\frac{m}{\hbar^2 k} = \frac{m}{\pi^2\hbar^2}k = \frac{m}{\pi^2\hbar^2}\cdot\frac{\sqrt{2mE}}{\hbar}$$

$$\boxed{\therefore g(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}}$$

$$n \text{ or } p = \int_{E_B}^{E_A} g(E)\,\underline{\underline{f(E)}}\,dE$$

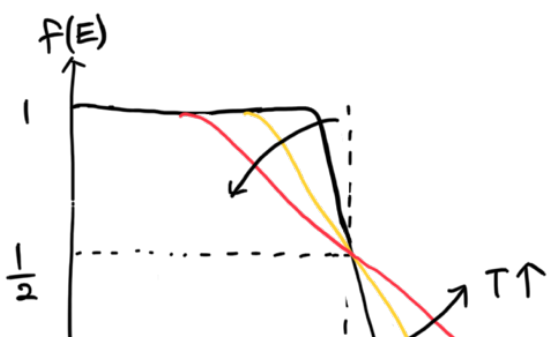
[2] Fermi-Dirac distribution.

$$f(E) = \frac{1}{\exp\left(\frac{E-\mu}{k_B T}\right)+1}$$

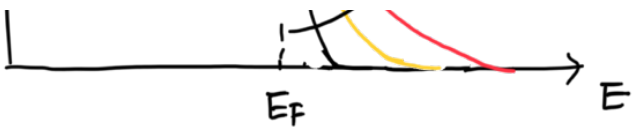
The probability that an electron (Fermion) occupies the energy level E

μ : Chemical potential

$\mu \leftrightarrows E_F$ (The Fermi level).



* $f(E=E_F) = \frac{1}{2}$
* At $T = 300$ (K) (Room temperature) $f(E)$ is nearly <u>a step function!</u>

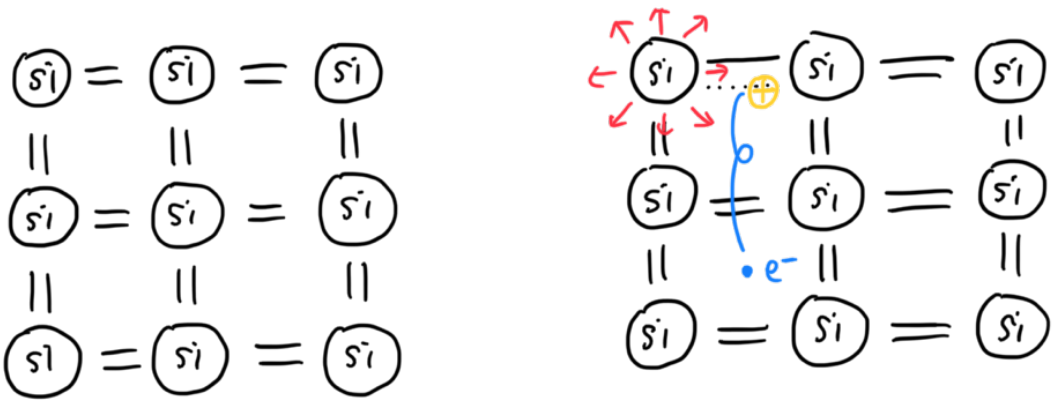


$$n \text{ or } p = \boxed{\int_{E_A}^{E_B}} g(E) f(E)\, dE$$

The range of integration ← Band theory of semiconductors!

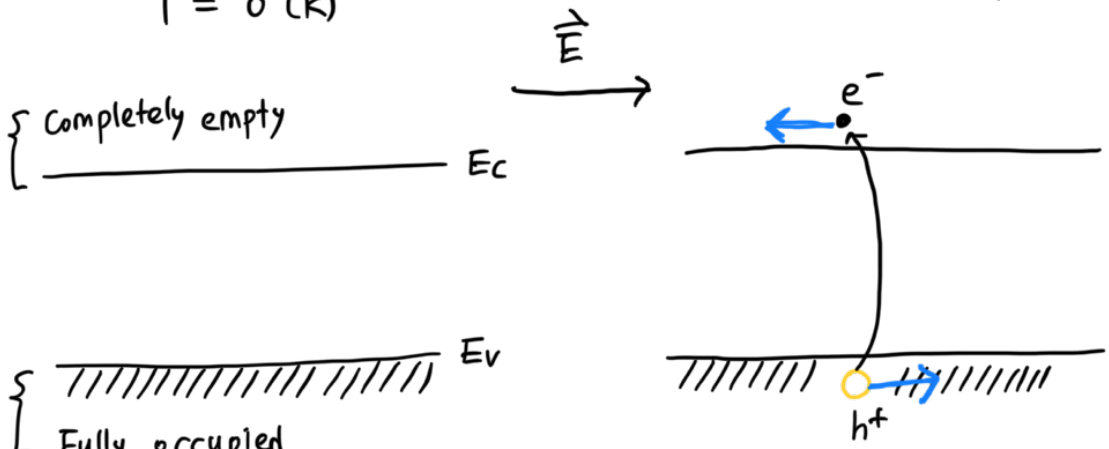
e.g.) Si : 4 valence electrons

lattice vibration → Bond may be broken.



T = 0 (K)

T > 0 (K)



The vacancy of electron in the valence band

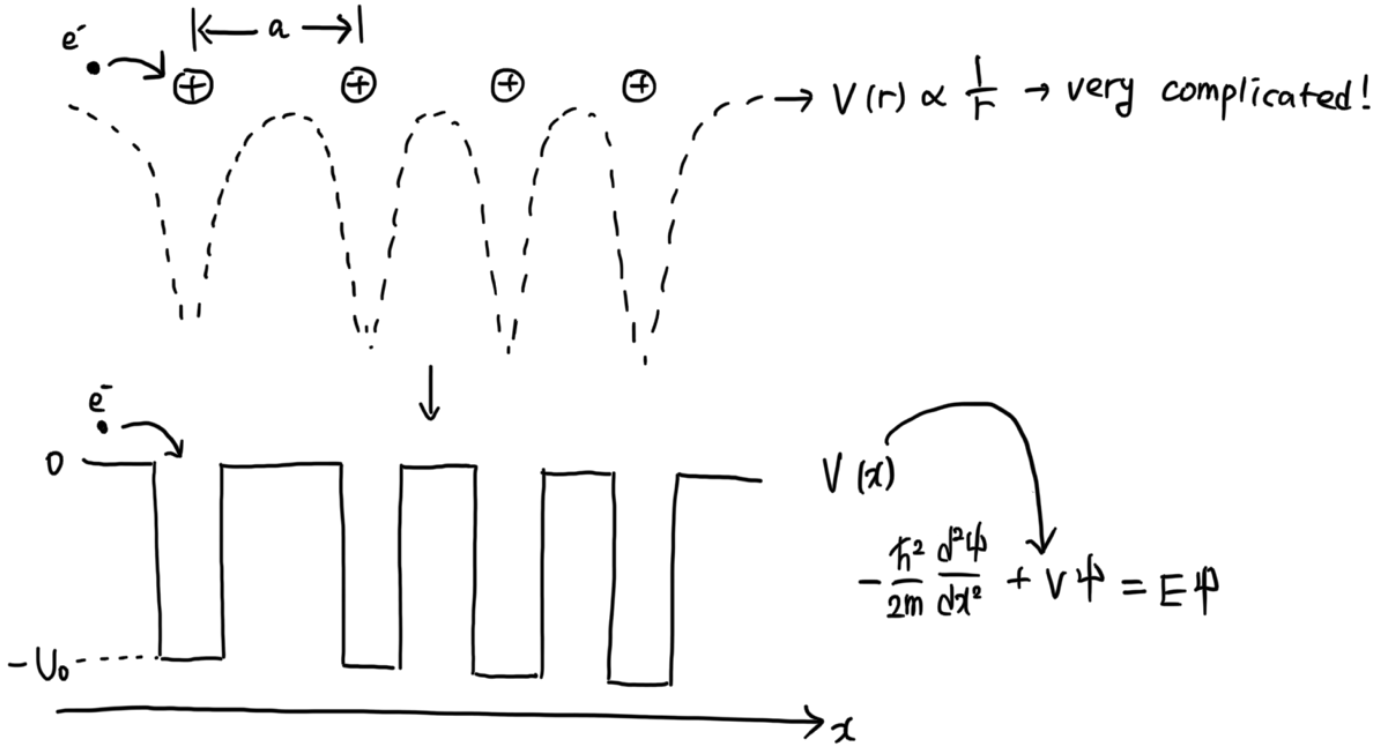
= Mobile particle with a positive charge

= "hole"

$\boxed{\text{Charge carriers in semiconductors : electrons \& holes.}}$

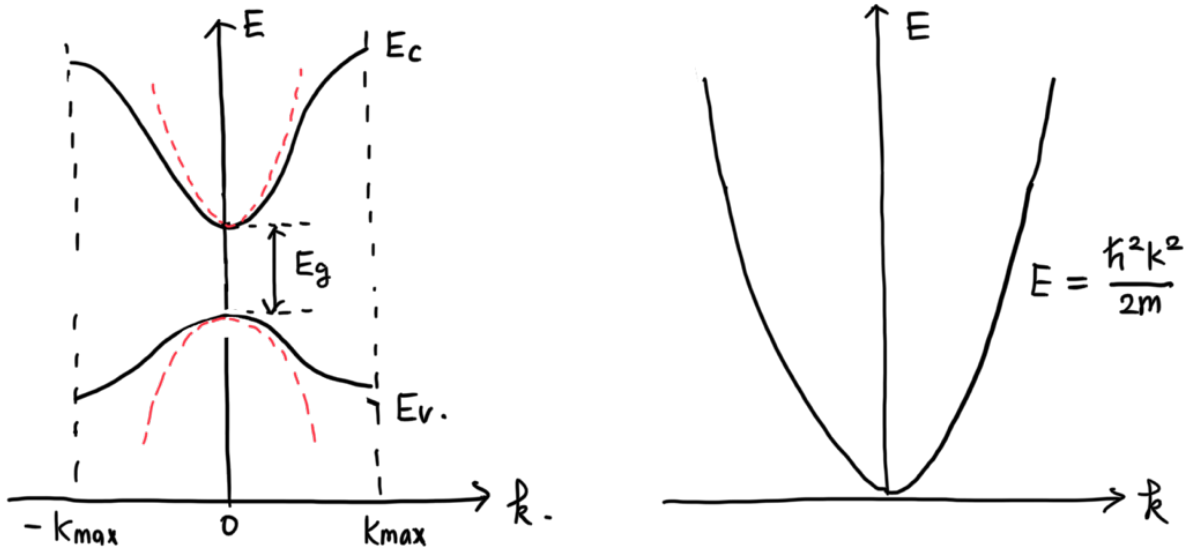
Kronig & Penney model

* More complicated, yet informative one than a Dirac-comb model.



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

The result : E vs. k dispersion relation.



Near $k=0$, $E-k$ can be approximated to be a quadratic function.

$$E = \frac{\hbar^2 k^2}{2m^*} \quad \text{where } \boxed{m^* : \text{Effective mass.}}$$

Definition : An electron (hole) of mass m, when put into a crystal,

responds to the external force "as if" the mass were m^*

Why? The movement of charged particles in a periodic potential can be very different from their motion in a vacuum.

Derivation

- Start with the equation of motion of an electron in an energy band.
- Consider the motion of an "electron wave packet" in an applied E-field. (The wave packet is made up of wavefunctions assembled near a particular k)

$$v_g = \frac{d\omega}{dk} \quad \cdots ①$$

- Since $\varepsilon = \hbar\omega$, $v_g = \frac{1}{\hbar}\frac{d\varepsilon}{dk} \quad \cdots ②$

*** The effects of the crystal on the electron motion determined by $\varepsilon - k$ dispersion!

- The work done on the electron by E-field in the time interval dt:

$$d\varepsilon = (-eE)(v_g\, dt) \quad \cdots ③$$

Also,

$$d\varepsilon = \left(\frac{d\varepsilon}{dk}\right) dk = \hbar v_g\, dk \quad \cdots ④ \quad (\because ②)$$

- ③ = ④ $\rightarrow$ $-eE v_g\, dt = \hbar v_g\, dk \rightarrow -eE = \hbar\frac{dk}{dt}$

$$\boxed{\therefore F = \hbar\frac{dk}{dt}} \quad \cdots ⑤$$

(consistent with the Newton's law of motion!)

c.f.) $F = \frac{dp}{dt} = \frac{d(mv)}{dt}$ for a free particle

- To obtain acceleration, take a time derivative of v_g:

$$\frac{dv_g}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{d\varepsilon}{dk}\right) = \frac{d}{dk}\left(\frac{1}{\hbar}\frac{d\varepsilon}{dk}\right)\cdot\frac{dk}{dt} = \frac{1}{\hbar}\left(\frac{d^2\varepsilon}{dk^2}\right)\frac{dk}{dt}$$

$\left(\because v_g = \frac{1}{\hbar}\frac{d\varepsilon}{dt} \cdots ② \right)$ From $F = \hbar \frac{dk}{dt}$, $\frac{dk}{dt} = \frac{F}{\hbar}$

$$\frac{dv_g}{dt} = \frac{F}{\hbar^2}\frac{d^2\varepsilon}{dk^2} \rightarrow F = \frac{\hbar^2}{\left(\frac{d^2\varepsilon}{dk^2}\right)} \cdot \frac{dv_g}{dt} \triangleq m^* \cdot a$$

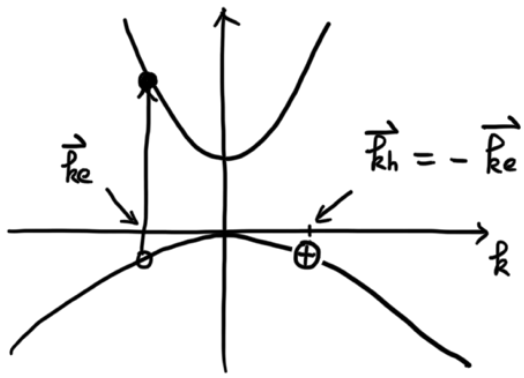
$$\therefore \boxed{\frac{1}{m^*} = \frac{1}{\hbar^2}\left(\frac{d^2\varepsilon}{dk^2}\right)}$$

Near $k=0$, $E-k$ is approximated to be a quadratic function,

$$\frac{d^2\varepsilon}{dk^2} = \frac{\hbar^2}{m^*} \rightarrow \boxed{\varepsilon = \frac{\hbar^2 k^2}{2m^*} + C}$$

· Hole.

- Total wavevector of the electrons in a filled band is zero
  $\sum \vec{k} = 0$
- If an electron is missing from an orbital of wavevector $\vec{k}_e$, the total wavevector of the system is $-\vec{k}_e$, which is attributed to the hole.



· Absorption of a photon ($\hbar\omega$) promotes an electron ($\vec{k}_e$) in the valence band to the conduction band.

· The total wavevector of the valence band after the absorption is $-\vec{k}_e$.

· This is the wavevector for the hole as $\vec{k}_h = -\vec{k}_e$

* The equation of motion for electron and hole.

$$e^-: \hbar\frac{d\vec{k}_e}{dt} = -e\left(\vec{E} + \frac{1}{c}\vec{v}_e \times \vec{B}\right)$$

$$h^+: \hbar\frac{d\vec{k}_h}{dt} = -\hbar\frac{d\vec{k}_e}{dt} = +e\left(\vec{E} + \frac{1}{c}\vec{v}_h \times \vec{B}\right)$$

The equation of motion for a particle of a positive charge

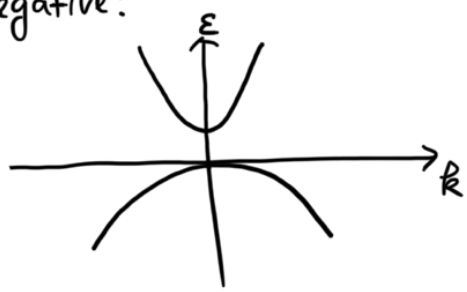
The equation of motion for a particle of a positive charge

* The effective mass for holes.

The effective mass for holes (missing electrons) in the valence band :

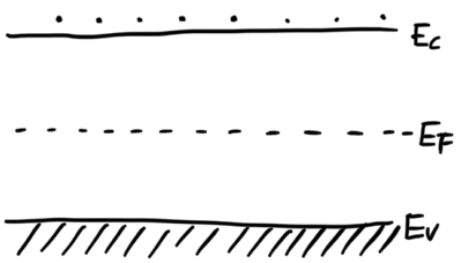
$$m_h^* = -m_e^* = -\frac{1}{\hbar^2}\left(\frac{d^2\varepsilon}{dk^2}\right)^{-1}$$

∵ The curvature of the hole band is "negative!"



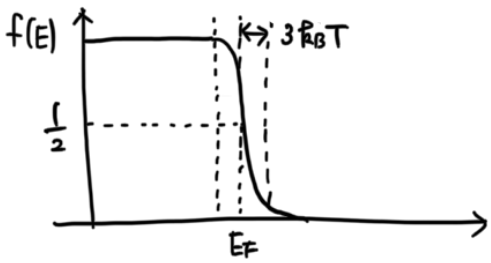
Electron concentration

$$n = \int_{E_c}^{E_{c,max}} g(E)\, f(E)\, dE$$



If $E \gg E_F + 3k_BT$,

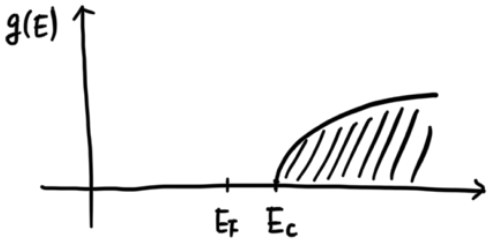
- $f(E) = \dfrac{1}{1+e^{(E-E_F)/k_BT}} \cong e^{-(E-E_F)/k_BT}$



- $E_{c,max} \to \infty$ since $f(E) \cong 0$

$$n = \int_{E_c}^{\infty} \frac{4\pi (m_e^*)^{3/2}}{h^3} \sqrt{E-E_c}\; e^{(E_F-E)/k_BT}\, dE$$

$$= 2\left(\frac{2\pi m_e^* k_BT}{h^2}\right)^{\frac{3}{2}} e^{-\frac{E_c-E_F}{k_BT}}$$



$$\therefore \boxed{n = N_c\, e^{-\frac{E_c-E_F}{k_BT}}, \quad \text{where } N_c = 2\left(\frac{2\pi m_e^* k_BT}{h^2}\right)^{\frac{3}{2}}}$$

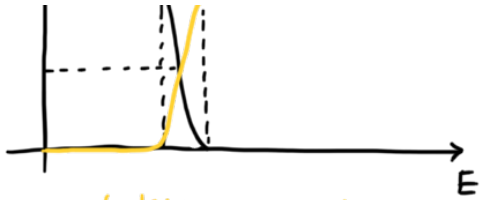
Hole concentration.

$f_p(E) = 1 - f(E)$

$$p = \int_{E_v}^{-\infty} g_v(E) f_p(E)\, dE$$

$$= \int_{E_v}^{-\infty} \frac{4\pi (2m_p^*)^{\frac{3}{2}}}{h^2} \sqrt{E_v - E}\,\left(1 - f(E)\right) dE$$

$$= 2\left(\frac{2\pi m_p^* k_B T}{h^2}\right) e^{-\frac{E_F - E_v}{k_B T}}$$



- probability that a hole is occupied
- probability that an electron is NOT occupied

$$\therefore \boxed{p = N_v e^{-\frac{E_F - E_v}{k_B T}}, \quad N_v = 2\left(\frac{2\pi m_p^* k_B T}{h^2}\right)^{\frac{3}{2}}}$$

$$\left\{\begin{array}{l} n = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) \\ p = N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right) \end{array}\right] \rightarrow np = N_c N_v \exp\left(\frac{E_v - E_c}{k_B T}\right) = N_c N_v \exp\left(\frac{-E_G}{k_B T}\right)$$

$$\boxed{np = \text{constant!}}$$

- In an intrinsic semiconductor, by definition, $\boxed{n = p}$
  (non-doped)

$$\left[n = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right)\right] = \left[p = N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right)\right] \rightarrow E_F \rightarrow E_i$$

$$\rightarrow \boxed{E_i = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right) = \frac{E_c + E_v}{2} + \frac{3}{4} k_B T \left(\frac{m_p^*}{m_n^*}\right)} \quad \left(\because \frac{N_v}{N_c} = \left(\frac{m_p^*}{m_n^*}\right)^{\frac{3}{2}}\right)$$

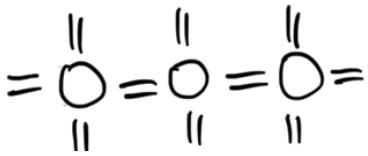
≈ -0.0073 (eV) for Si.

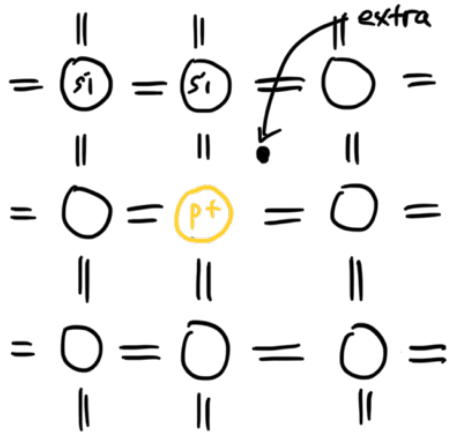
$$n = p = n_i \qquad \boxed{np = n_i^2}$$

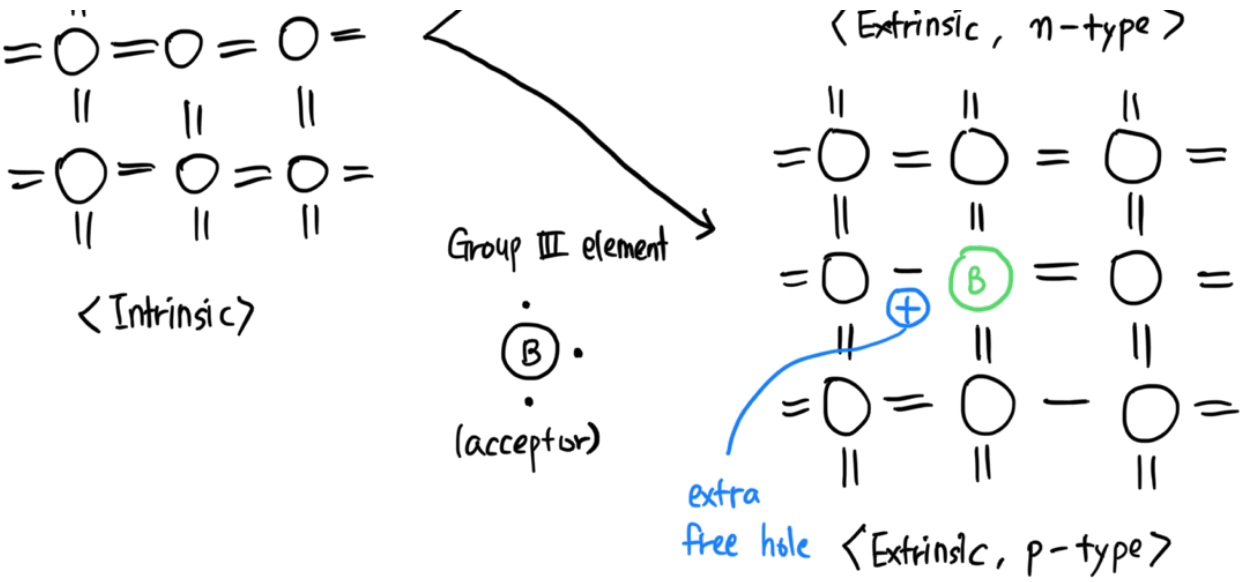
Semiconductor doping

Group V element

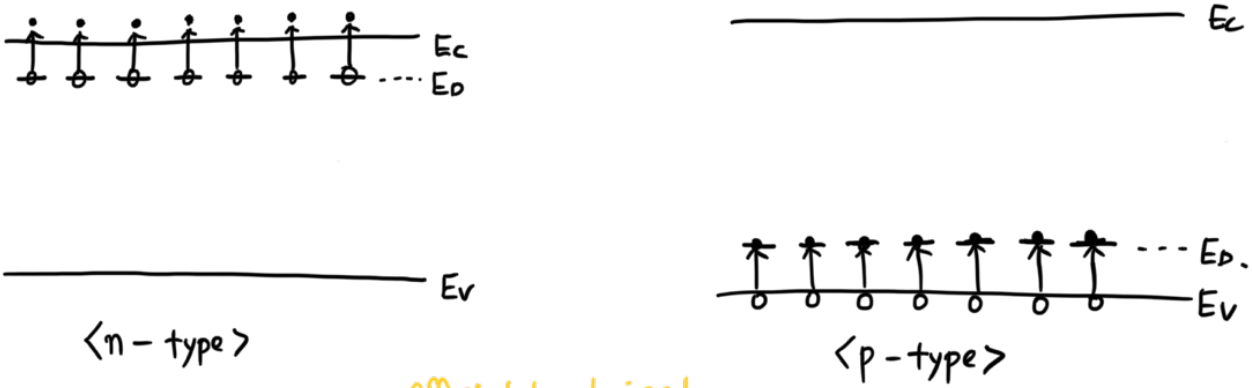
(Donor)







Band diagram for n, p-type semiconductors.



affected by doping!

$$n = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) \qquad p = N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right)$$

- Charge neutrality.

$$p - n + N_D - N_A = 0$$

where N_D : # of ionized donor, N_A : # of ionized acceptor.

since $pn = n_i^2 \rightarrow p = \frac{n_i^2}{n}$,

$$\frac{n_i^2}{n} - n + N_D - N_A = 0 \longrightarrow n^2 - (N_D - N_A)n - n_i^2 = 0.$$

$$\boxed{\begin{aligned} \therefore n &= \frac{N_D - N_A}{2} + \left[\left(\frac{N_D - N_A}{2}\right)^2 + n_i^2\right]^{\frac{1}{2}} \\ p &= \frac{N_A - N_D}{2} + \left[\left(\frac{N_A - N_D}{2}\right)^2 + n_i^2\right]^{\frac{1}{2}} \end{aligned}}$$

- n-type semiconductor ($N_D \gg N_A$, $N_D \gg n_i$)

$$\boxed{n \cong N_D \ , \quad p \cong \frac{n_i^2}{N_D}}$$

- p-type semiconductor ($N_A \gg N_D$, $N_A \gg n_i$)

$$\boxed{p \cong N_A \ , \quad n \cong \frac{n_i^2}{N_A}}$$

• Fermi level change

$$n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

$$p = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

For intrinsic semicond.

$$n_i = N_c \exp\left(\frac{E_i - E_c}{k_B T}\right)$$

$$n_i = N_v \exp\left(\frac{E_v - E_i}{k_B T}\right)$$

Solving for N_c, N_v

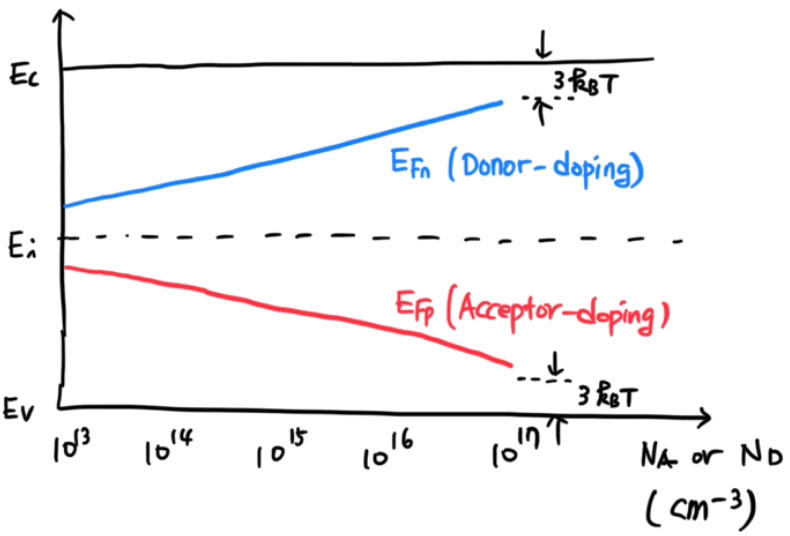
$$N_c = n_i \exp\left(\frac{E_c - E_i}{k_B T}\right)$$

$$N_v = n_i \exp\left(\frac{E_i - E_v}{k_B T}\right)$$

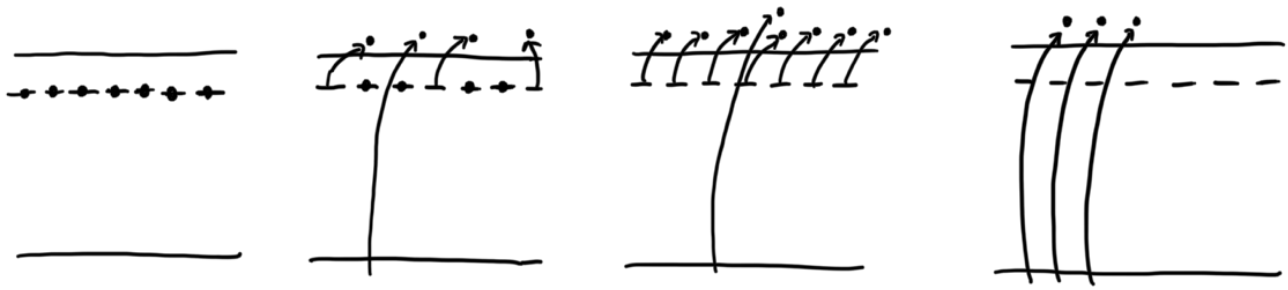
substitution

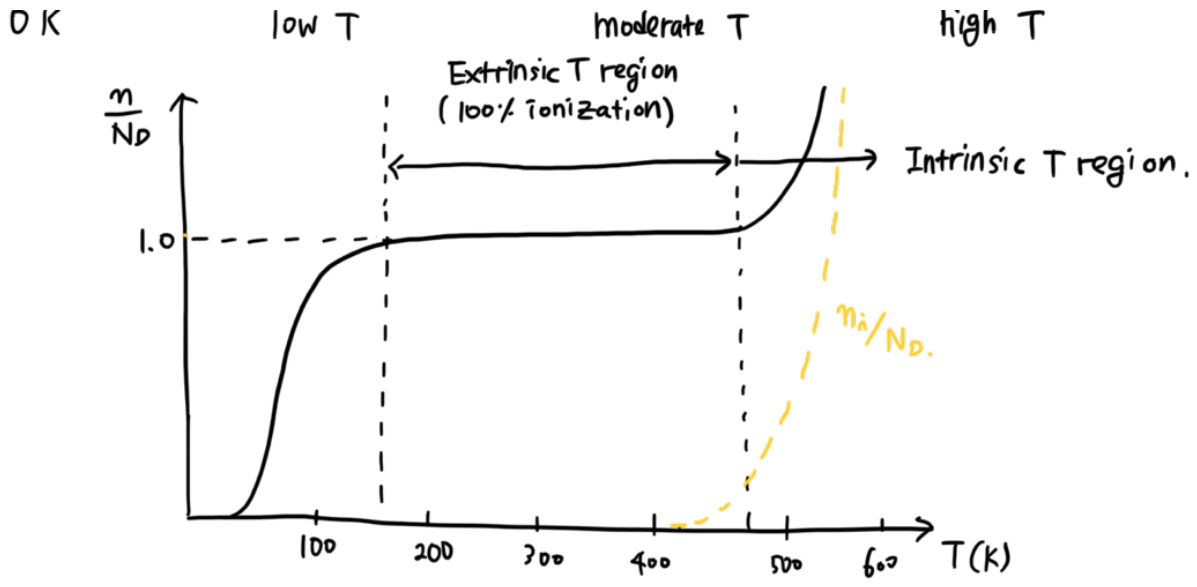
$$\boxed{\begin{aligned} n &= n_i \exp\left(\frac{E_F - E_i}{k_B T}\right) \\ p &= n_i \exp\left(\frac{E_i - E_F}{k_B T}\right) \end{aligned}}$$

$$\boxed{\begin{aligned} E_F - E_i &= k_B T \ln \frac{n}{n_i} \\ E_i - E_F &= k_B T \ln \frac{p}{n_i} \end{aligned}}$$



• Temperature-dependence of doped semiconductors.





Carrier dynamics

How are charges generated / recombined and how are they moving?

① Drift
② Diffusion
$\boxed{\text{Current}}$

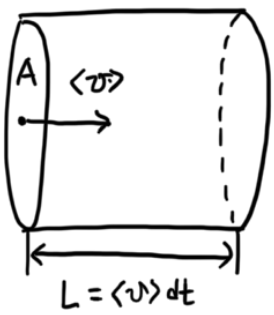
③ Generation
- Direct thermal
- Indirect thermal
- Optical

④ Recombination

Continuity equation!

① Drift current

Electrical current due to electrons moving with an average speed $\langle v \rangle$ with a volume density n



▷ Average speed : $\langle v \rangle = \frac{1}{N} \sum_j v_j$

▷ Volume swept by electrons in dt : $dV = A \langle v \rangle dt$

▷ # of electrons in the volume : $dN = n\,dV = nA\langle v \rangle dt$