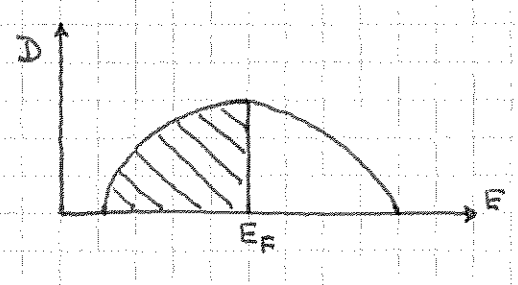
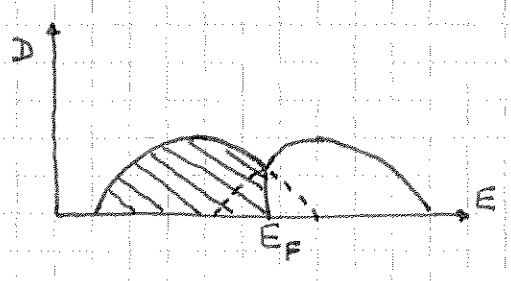
Normal metal:



Half-filled CB

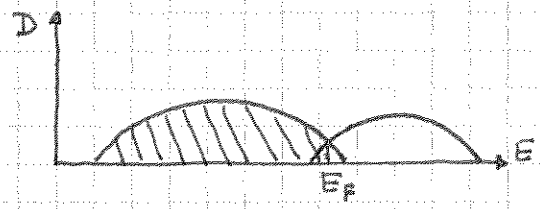
or



Large band overlap

$\Rightarrow$ Large $D(E_F)$ $\Rightarrow$ Large conductivity σ

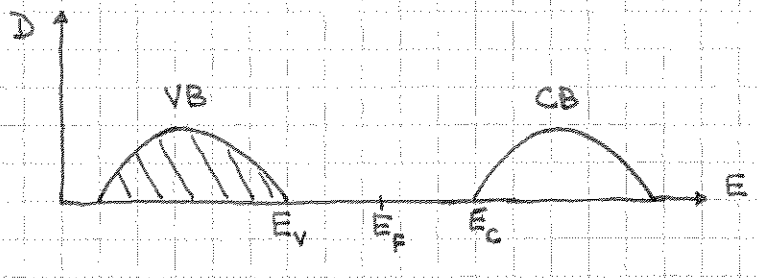
Semimetal:



Small band overlap $\Rightarrow$ Small $D(E_F)$

$\Rightarrow$ Small σ

Insulator:

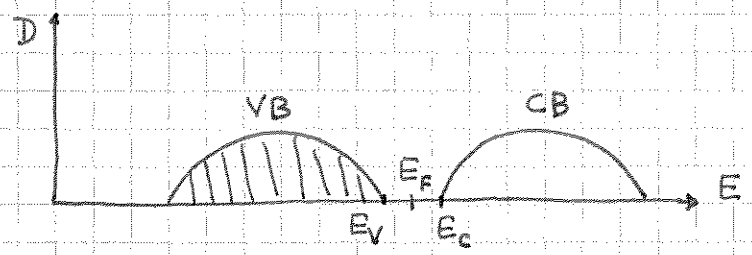


$E_g = E_c - E_v > 2\text{-}3$ eV

Large gap E_g $\Rightarrow$ No thermal activation of electrons from VB to CB

$\Rightarrow$ $\sigma \approx 0$

Semiconductor:



$E_g < 2\text{-}3$ eV

Small gap E_g $\Rightarrow$ Many electrons thermally activated from VB to CB

$\Rightarrow$ $\sigma > 0$

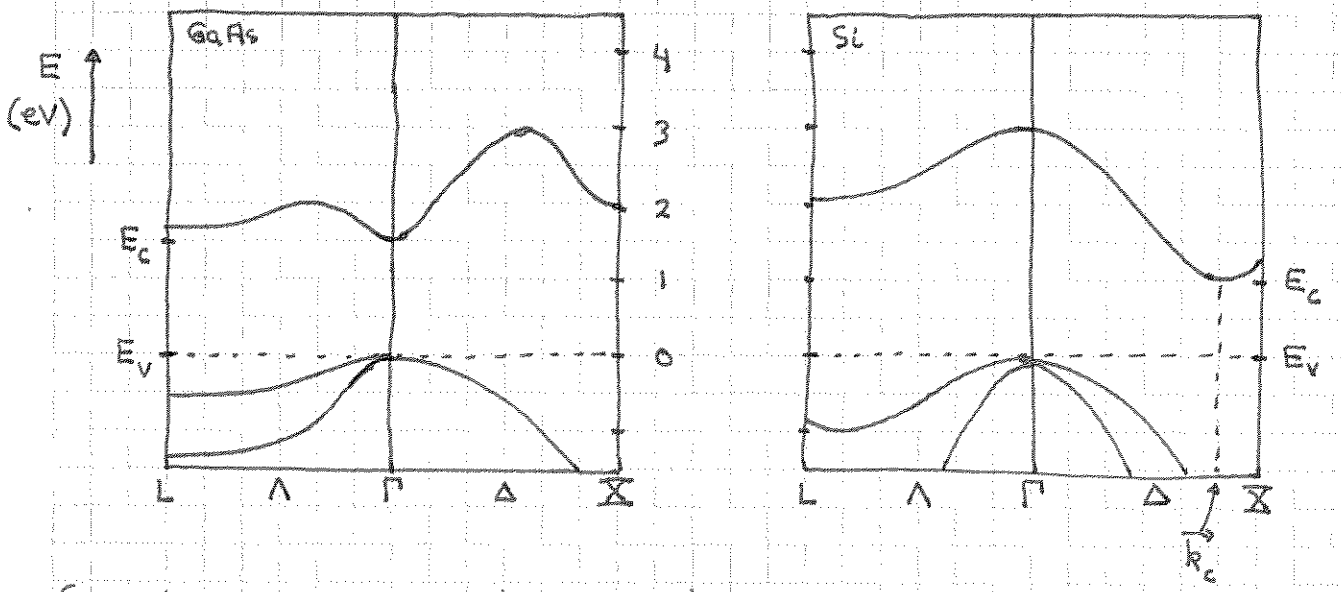
Semiconductors

Group IV : Si, Ge

III - V : GaAs, AlAs, GaSb, ..., $Al_x Ga_{1-x} As$, ...

II - VI : CdSe, ZnTe

Band structure of GaAs and Si:



Special points and directions in k-space:

Γ: k = 0

X: on surface of 1BZ along $(\pm1,0,0)$, $(0,\pm1,0)$, $(0,0,\pm1)$

L: ——— " ——— $(1,1,1)$ etc

K: ——— " ——— $(1,1,0)$ etc

Δ: along lines between Γ and X

Λ: ——— " ——— Γ and L

Σ: ——— " ——— Γ and K

GaAs:

- Direct gap; $\vec{k}_c = \vec{k}_v = 0$
- $E_g = 1.42$ eV at 300 K
- $m_c^* = 0.067\, m_e$
- $g_v = 1$ (= valley degeneracy; only one Γ-point)

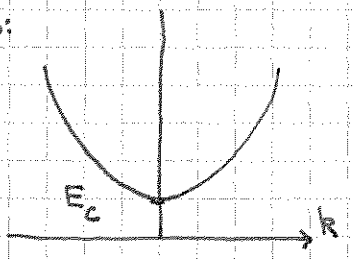
Si:

- Indirect gap; $\vec{k}_v = 0$, $\vec{k}_c = 0.85\,\vec{k}_X$
- $E_g = 1.12$ eV at 300 K
- $m_t^* = 0.19\, m_e$, $m_l^* = 0.92\, m_e$
  (t = transverse, $\vec{k} - \vec{k}_c \perp \vec{k}_X$,
  l = longitudinal, $\vec{k} - \vec{k}_c \parallel \vec{k}_X$)
- $g_v = 6$ (six X points in 3D)

Carrier concentration

Assume direct gap SC and parabolic bands ("effective mass approx.")

CB:



$$E(k) = E_c + \frac{\hbar^2 k^2}{2 m_c^*}$$

$$D_c(E) = \frac{V}{2\pi^2}\left(\frac{2 m_c^*}{\hbar^2}\right)^{3/2}(E - E_c)^{1/2} \qquad \text{(see p.7)}$$

Density of electrons in CB (thermally excited from VB, or from impurity states with energy level(s) within gap, more later):

$$n = \frac{N}{V} = \frac{1}{V}\int_{E_c}^{\infty} D_c(E)\, f(E)\, dE \qquad \text{(see p. 9)}$$

$$= \frac{1}{2\pi^2}\left(\frac{2 m_c^*}{\hbar^2}\right)^{3/2} \int_{E_c}^{\infty} \frac{\sqrt{E - E_c}\, dE}{e^{(E-\mu)/k_B T} + 1}$$

Assume $E_c - \mu \gg k_B T$, substitute $x^2 = (E - E_c)/k_B T$, and use

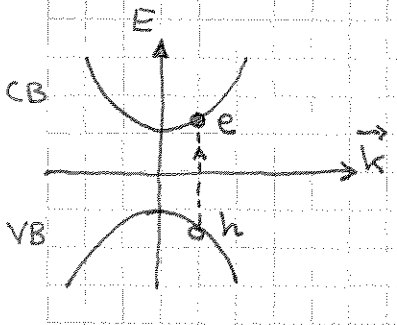
$$\int_0^\infty x^2 e^{-x^2} dx = \frac{1}{2}\left\{-\frac{d}{d\alpha}\int_{-\infty}^{\infty} e^{-\alpha x^2} dx\right\}_{\alpha=1} = \frac{1}{2}\left\{-\frac{d}{d\alpha}\sqrt{\frac{\pi}{\alpha}}\right\}_{\alpha=1} = \left\{\frac{\sqrt{\pi}}{4\alpha^{3/2}}\right\}_{\alpha=1} = \frac{\sqrt{\pi}}{4}$$

$$\Rightarrow n = N_c\, e^{-(E_c - \mu)/k_B T} \quad ; \quad N_c = 2\left(\frac{m_c^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$

Holes

Excitation of electron from VB to CB (or to impurity level in gap)

$\Rightarrow$ Empty state in VB = Hole



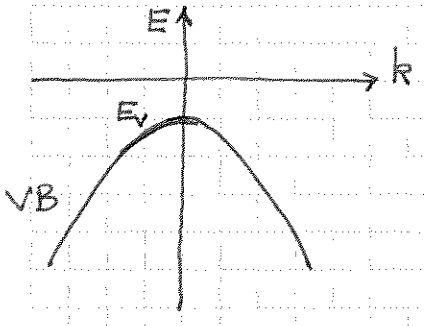
$\Delta\vec{k} = 0$ in excitation

$\Rightarrow \vec{k}_h = -\vec{k}_e$

E = electron energy, positive up

E_h = hole energy, positive down

Relative to top of VB: $E_h(\vec{k}_h) = -E(\vec{k}_e) = -E(-\vec{k}_h)$



$$E(k) = E_V + \frac{\hbar^2 k^2}{2 m_e^*} \qquad \text{(electron energy)}$$

$$\Rightarrow m_e^* < 0 \quad \text{in VB}$$

$$\frac{1}{m_h^*} = \frac{1}{\hbar^2}\frac{\partial^2 E_h}{\partial k_h^2} = \frac{1}{\hbar^2}\frac{\partial^2(-E)}{\partial k_e^2} = -\frac{1}{m_e^*} \quad \Rightarrow \quad m_h^* > 0$$

$$D_V(E) = \frac{V}{2\pi^2}\left(\frac{2m_V^*}{\hbar^2}\right)^{3/2}\sqrt{E_V - E} \qquad (m_V^* = m_h^* > 0) \qquad \text{(p. 7)}$$

Density of holes in VB (= absence of electrons, thermally excited to CB, or to impurity levels in the gap):

$$p = \frac{1}{V}\int_{-\infty}^{E_V} D_V(E)\underbrace{\{1 - f(E)\}}_{\text{= prob. of empty state (hole) at energy E}} dE$$

Assume $\mu - E_V \gg k_B T$, substitute $x^2 = (E_V - E)/k_B T$ etc.

$$\Rightarrow \quad p = N_V\, e^{-(\mu - E_V)/k_B T} \quad ; \quad N_V = 2\left(\frac{m_V^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$

$\Rightarrow$ Law of mass action:

$$n \cdot p = 4\left(m_c^* m_V^*\right)^{3/2}\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 e^{-E_g/k_B T} \quad ; \quad E_g = E_c - E_V$$

- independent of Fermi level μ
- valid for both <u>intrinsic</u> and <u>doped</u> semiconductors

Intrinsic semiconductors

no impurities

$$\Rightarrow n = p = n_i = 2 \left(m_c^* m_v^*\right)^{3/4} \left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-E_g/2k_BT}$$

$$\Rightarrow \mu = \underbrace{\frac{1}{2}(E_c + E_v)}_{\text{center of gap}} + \underbrace{\frac{3}{4} k_B T \ln \frac{m_v^*}{m_c^*}}_{\text{small correction } \sim T \; (=0 \text{ if } m_v^* = m_c^*)}$$

E_c ——————

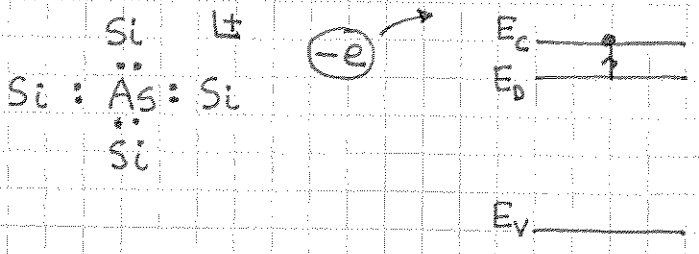
μ - - - - - - -

E_v ——————

$\Rightarrow$ assumptions $E_c - \mu \gg k_B T$ (p 22) and $\mu - E_v \gg k_B T$ (p 23) were OK, since $E_g/2 \gtrsim 1\,eV$ and $k_B T \sim 25\,meV$

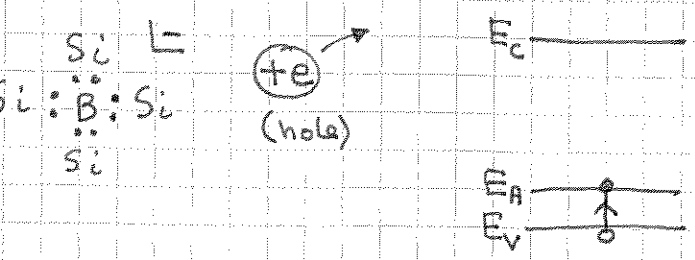
Doped semiconductors

Example: As (5 valence el.) in Si crystal (4 valence el.)



E_D = highest occupied level in As atom (in Si crystal environment) = Donor level

Example: B (3 valence el.) in Si



E_A = lowest unoccupied level in B atom (in Si crystal) = Acceptor level

Impurity ionization:

$As \rightarrow As^+ + e$, $\Delta E = E_{ion} \approx E_C - E_D$

$B \rightarrow B^- + h$, $\Delta E = E_{ion} \approx E_A - E_V$

Use H-atom knowledge for rough estimate:

$$E_{ion}^H = \frac{m_e e^4}{32\pi^2\hbar^2\varepsilon_0^2} = 13.6\,eV = \text{binding energy of electron in H}$$

$$a^H = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 0.53\,\text{Å} = \text{Bohr radius} = \text{average distance between electron and nucleus}$$

In Si crystal:

$m_c^* \sim m_e/3$ $\quad \left[(m_t^* m_t^* m_\ell^*)^{1/3} = 0.32\, m_e \right]$

$\varepsilon \sim 12\,\varepsilon_0$ $\quad$ [= permittivity]

$$\Rightarrow E_{ion}\,(As \text{ in } Si) \approx 13.6\,eV \cdot \frac{m_c^*}{m_e} \cdot \left(\frac{\varepsilon_0}{\varepsilon}\right)^2 \sim 30\,meV$$

$$a\,(As \text{ in } Si) \approx 0.53\,\text{Å} \cdot \frac{\varepsilon}{\varepsilon_0} \cdot \frac{m_e}{m_c^*} \sim 20\,\text{Å}$$

$\Rightarrow$ "extra" electron is <u>loosely bound</u> to As in Si crystal

<u>Carrier concentration in doped semiconductors</u>

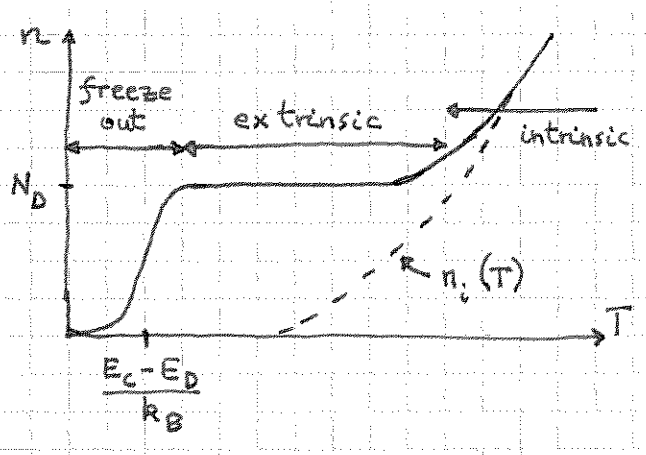
N_D donors pr unit volume, donor level E_D at 10-50 meV below E_C $\quad (E_g \gtrsim 1\,eV)$

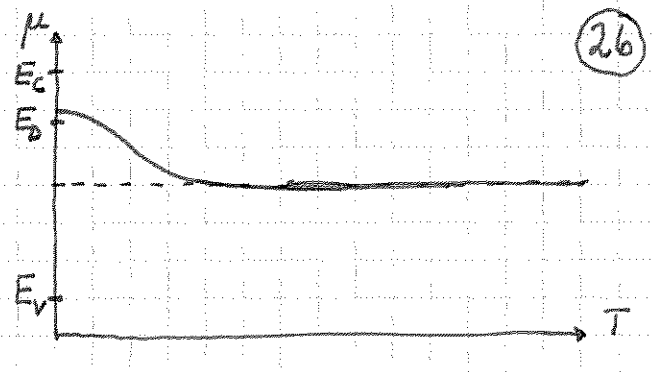
First, <u>qualitatively</u>, for $n(T)$ = electron density in CB:

$T = 0$: $n = 0$, E_D occupied by 1 e $\Rightarrow$ $E_D < \mu < E_C$

$T \gtrsim (E_C - E_D)/k_B$: $n \approx N_D$, E_D empty, $\mu \approx (E_C + E_V)/2$

$T \gg (E_C - E_D)/k_B$: $n_i(T) \gg N_D \Rightarrow n(T) \approx n_i(T)$, $\mu \approx (E_C + E_V)/2$





Next, quantitatively for freeze-out and extrinsic region:

j = donor occupancy: $j=0 \;\hat{=}$ Ionized donor

$j=1 \;\hat{=}$ Neutral donor (2 states, $s = \pm 1/2$)

($E(j=2) \gg E_D$ due to Coulomb repulsion)

$$P(j,s) = \frac{1}{Z} e^{-j(E_D-\mu)/k_BT}$$

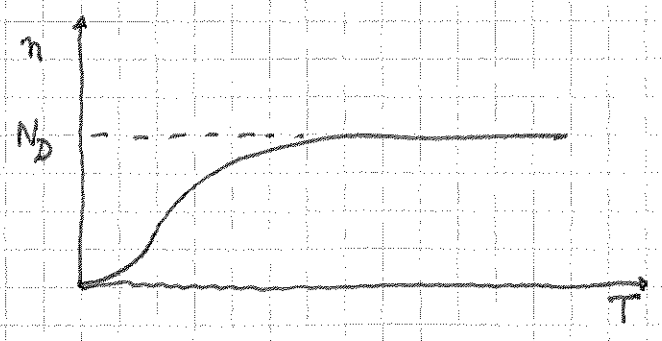
$$Z = \sum_{j,s} e^{-j(E_D-\mu)/k_BT} = 1 + 2e^{-(E_D-\mu)/k_BT}$$

$$n \approx n_D = N_D \cdot P(j=0) = N_D \cdot \frac{e^0}{Z} = N_D \left\{ 1 + 2 e^{\mu/k_BT} e^{-E_D/k_BT} \right\}^{-1}$$

From p. 22: $n = N_c e^{\mu/k_BT} e^{-E_c/k_BT}$

Two eqns. for e^{μ/k_BT} → 2. order eqn. for n ⇒ .... ⇒

$$n(T) = \frac{2N_D}{1 + \left\{ 1 + \frac{8N_D}{N_c} e^{(E_c-E_D)/k_BT} \right\}^{1/2}} \quad ; \quad N_c = 2 \left\{ \frac{m_c^* k_B T}{2\pi\hbar^2} \right\}^{3/2}$$



$T \to 0 \Rightarrow n \to 0$

$T \to \infty \Rightarrow N_c^{-1} \to 0$

$\Rightarrow n \to N_D$

$n \gg n_i$ in extrinsic region $\Rightarrow p = n_i^2/n \ll n_i \ll n$ for n-type SC

Similarly: $n \ll p$ for p-type SC in extrinsic region (p = hole conc. in VB)

End 31.01.12