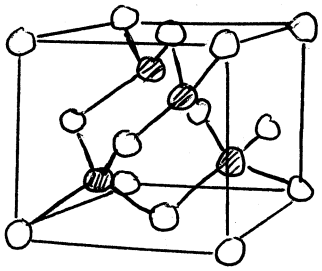
* Semiconductors are a special focus of condensed matter physics

→ technological importance: Complementary metal-oxide-semiconductor (CMOS) process for constructing integrated circuits

→ most common are Ge, Si, and GaAs



→ fcc structure + $a(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ offset copy

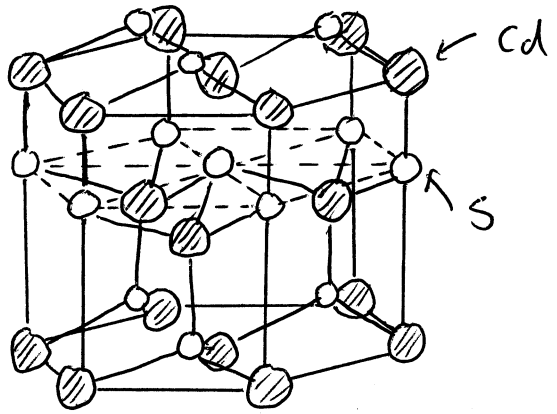
→ diamond (all atoms Si or Ge)

or zincblende (Ga and As on the two interpenetrating fcc lattices)

→ each atom surrounded by 4 equidistant nearest neighbours lying at the corners of a tetrahedron

→ covalent bond formed by two electrons of opposite spin; slightly ionic for III-V and II-VI compounds

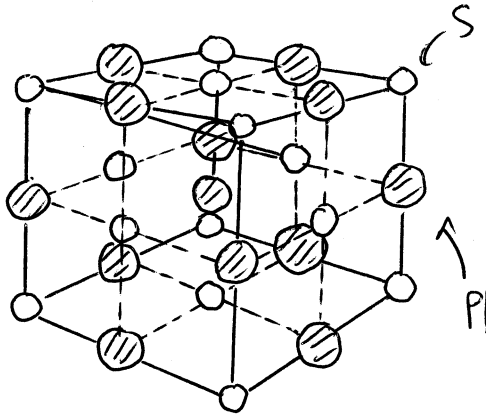
→ Some semiconductors form in the wurtzite or rock-salt structures



Wurtzite (CdS, ZnS, ...)

2 interpenetrating hcp lattices

tetrahedral arrangement with 4 n.n.

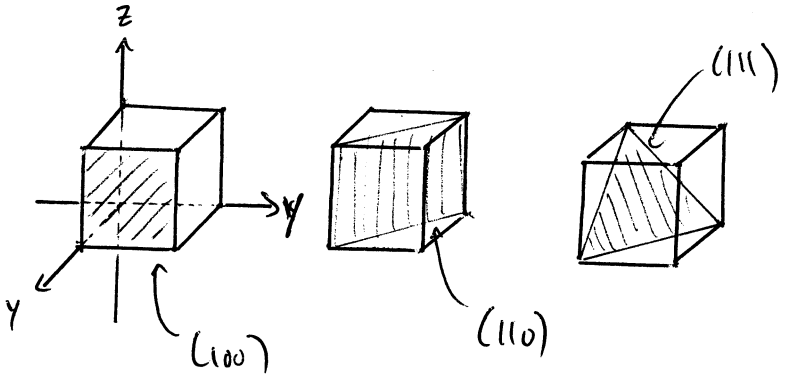


Rock-salt (PbS, PbTe, ...)

2 interpenetrating fcc

cubic arrangement with 6 n.n.

* Reminder about Miller indices in the cubic cell
  → index a plane by its intercepts with the three orthogonal axes



→ usual convention

(hkl) for a plane

$(\bar{h}kl)$ for a plane intercepting the negative x axis

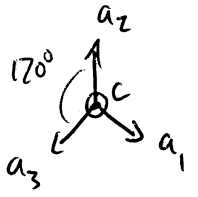
$\{hkl\}$ all planes of equivalent symmetry

e.g. $\{100\}$ for (100), (010), (001),
$(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$

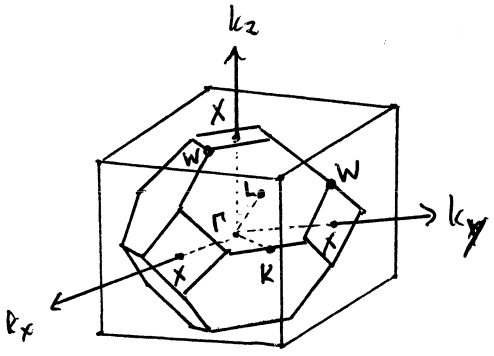
$[hkl]$ for a direction in the crystal

$\langle hkl \rangle$ for all symmetry-equivalent directions

$[a_1 a_2 a_3 c]$ for a direction in the hexagonal lattice



* Notation for "critical points" in the Wigner-Seitz cell



$\Gamma = \frac{2\pi}{a}(0,0,0)$ zone centre

$L = \frac{2\pi}{a}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$

$X = \frac{2\pi}{a}(0,0,1)$

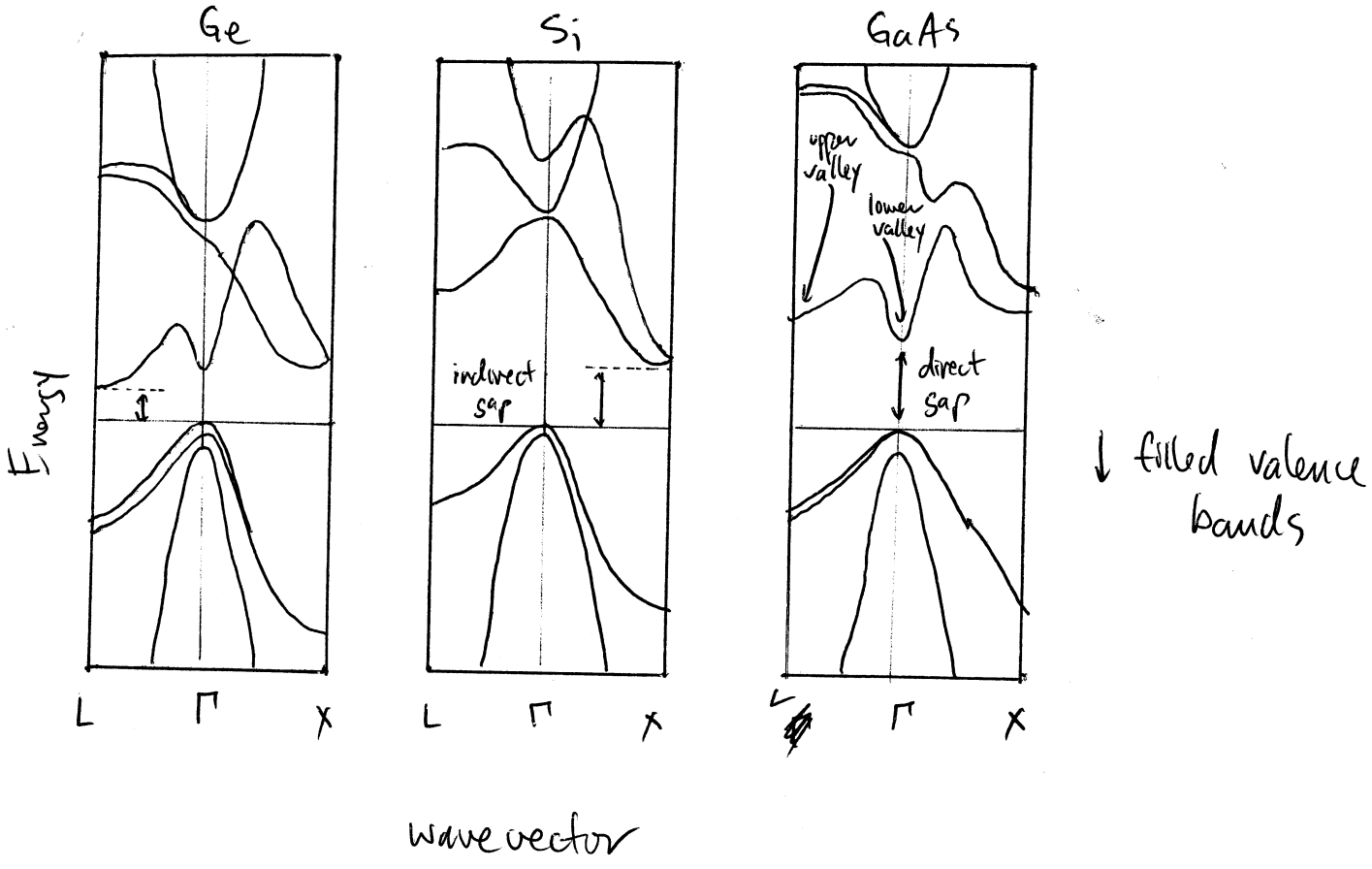
$K = \frac{2\pi}{a}\left(\frac{3}{4},\frac{3}{4},0\right)$

Δ: $\Gamma - X$ along $\langle 100 \rangle$

Σ: $\Gamma - K$ along $\langle 110 \rangle$

Λ: $\Gamma - L$ along $\langle 111 \rangle$

* Band Structure

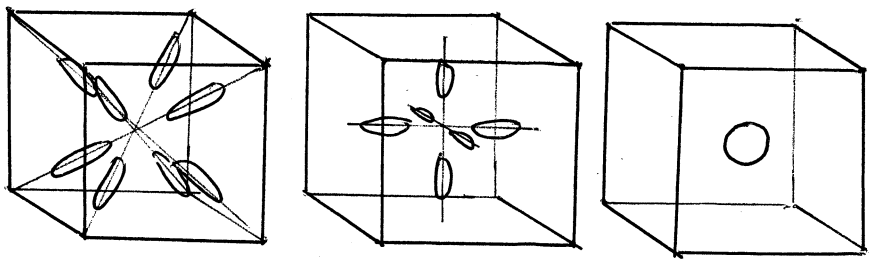


→ the energy gap E_g separating conduction and valence bands is the most important quantity

→ gap is a forbidden region with no dispersing states

→ valence bands can be fit by a parabolic dispersion describing heavy-hole (wider, smaller $\partial^2 E/\partial k^2$) and light-hole (narrower, larger $\partial^2 E/\partial k^2$) bands

→ the bottom of the conduction band can appear along the <111> axes (Δ) or along the <100> axes (Δ) or at $k=0$ (Γ)



Ge Si GaAs

level surfaces (in k-space) of the conduction band

for Ge: 8 half ellipsoids centred on L points
= 4 full ellipsoids

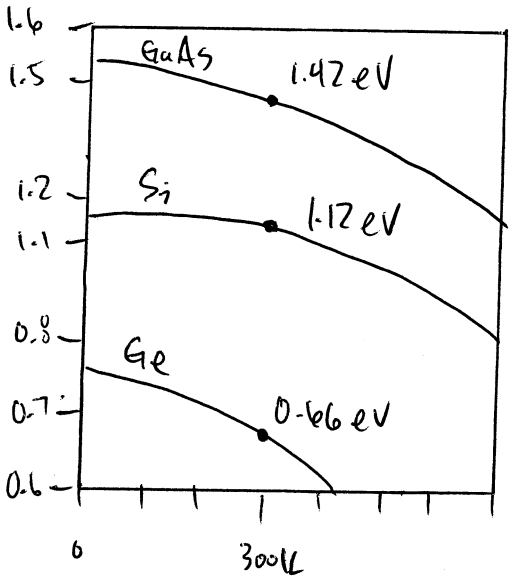
for Si: 6 full ellipsoids centred ≈ 3/4 of the way along the <100> axes

for GaAs: single sphere at zone centre

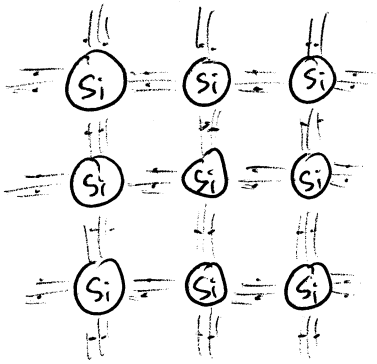
→ implies that there is a single effective mass m^* for GaAs but two for Ge and Si, m^*_ℓ and m^*_t along and transverse to the symmetry axis

* Energy gaps have a weak temperature dependence

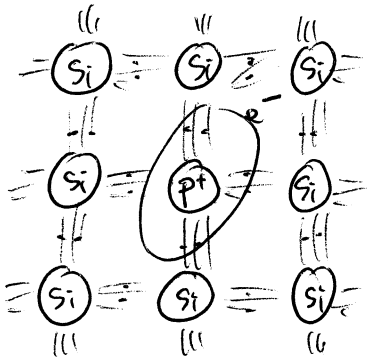
→ these values are appropriate for high-purity materials



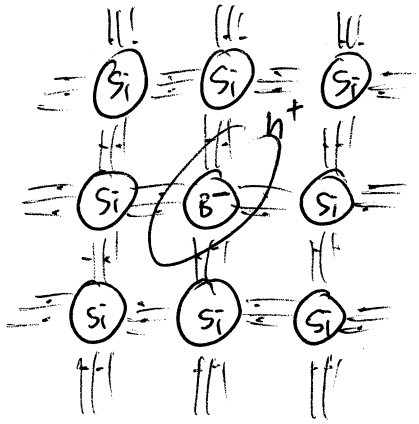
* A certain number of carriers are thermally activated, even in the case of an intrinsic semiconductor



intrinsic Si



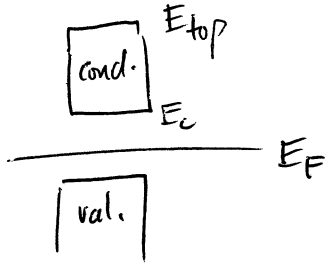
"n-type" Si with phosphorous donor



"p-type" Si with boron donor

→ number of conduction electrons is

$$n_c = \int_{E_c}^{E_{top}} D(\varepsilon) f(\varepsilon - \varepsilon_F) \, d\varepsilon$$



→ at low temperatures and carrier densities, approximate DOS by

$$D(\varepsilon) = M_c \frac{\sqrt{2}}{\pi^2} \frac{(\varepsilon - E_c)^{1/2}}{\hbar^3} (m_{de})^{3/2}$$

where M_c = # of equivalent minima in the conduction band (e.g. 1, 4, 6, ...)

and m_{de} = effective "density-of-states" mass for electrons

$$= (m_1^* m_2^* m_3^*)^{1/3} = (m_l^* m_t^{*2})^{1/3}$$

→ write in terms of the dimensionless Fermi-Dirac integral

$$F_n(x) = \int_0^\infty \frac{t^n \, dt}{e^{t-x} + 1}$$

$$n_c = D_c \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_F - E_C}{k_B T}\right)$$

$$D_c \equiv 2\left(\frac{2\pi m_{de} k_B T}{h^2}\right)^{3/2} N_c$$

→ at temperatures low wrt the gap, the conduction electrons become Boltzmann populated

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

→ equivalent density of holes at the top of the valence band

$$P_v = N_v \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_V - E_F}{k_B T}\right)$$

$$N_v \equiv 2\left(\frac{2\pi m_{dh} k_B T}{h^2}\right)^{3/2}$$

where m_{dh} = effective "density-of-states" mass for holes

$$= \left(m_{lh}^{*\,3/2} + m_{hh}^{*\,3/2}\right)^{2/3}$$ for light and heavy holes

→ again, in the nondegenerate case,

$$p_v = D_v \exp\left(-\frac{E_F - E_V}{k_B T}\right)$$

* In thermal equilibrium, there is a continual random process of electrons getting promoted from V → C band and vice versa

  → rates equilibrate and maintain a steady-state distribution

  → conservation requires that $n = p$ = intrinsic carrier concentration $\equiv n_{intr}$

  → equating $D_c e^{-\frac{(E_c - E_F)}{k_B T}} = D_v e^{-\frac{(E_F - E_V)}{k_B T}}$

  gives

$$E_F = \frac{E_c + E_V}{2} + \frac{k_B T}{2} \log\left(\frac{D_V}{D_c}\right)$$

$$= \frac{E_c + E_V}{2} + \frac{3 k_B T}{4} \log\left(\frac{m_{dh}}{m_{de} M_c^{2/3}}\right)$$

middle of the band gap ↑

↑ plus a small correction

→ also a multiplicative rule

$$np = n_{intr}^2 = D_c D_v \exp\left[-\frac{-E_c + E_F + E_v - E_F}{k_B T} \right]$$

$$= D_c D_v e^{-E_g/k_B T} \quad \text{since } E_g = E_c - E_v$$

→ hence

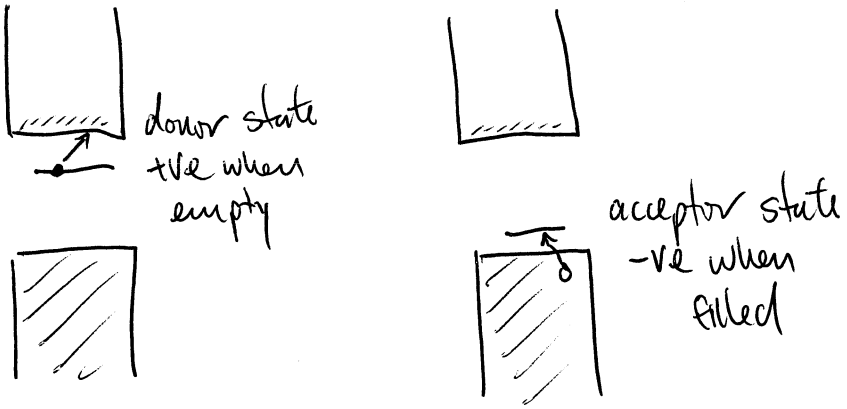
$$n_{intr} = \sqrt{D_c D_v}\, e^{-E_g/2k_B T}$$

$$\simeq 4.9 \times 10^{15}\ cm^{-3} \left(\frac{m_{de}\, m_{dh}}{m_0^2} \right)^{3/4} m_c^{1/2} \left(\frac{T}{K} \right)^{3/2} e^{-E_g/2k_B T}$$

where m_0 = free electron mass

* Donors and acceptors

→ dope semiconductor with impurities to engineer the carrier concentration



→ assume hydrogenic energy levels

$$E^{H}_{ionization} = \frac{m_0 e^4}{32\pi^2 \varepsilon_0^2 \hbar^2} = 13.6\,eV$$

but renormalize for the permittivity in the semiconductor and by the conductivity effective mass:

$$E_{ionization\ (donor)} = \left(\frac{\varepsilon_0}{\varepsilon_s}\right)^2 \left(\frac{m_{ce}}{m_0}\right) E^{H}_{ionization}$$

$\sim$ 0.025 eV for Si

0.006 eV for Ge

0.007 eV for GaAs

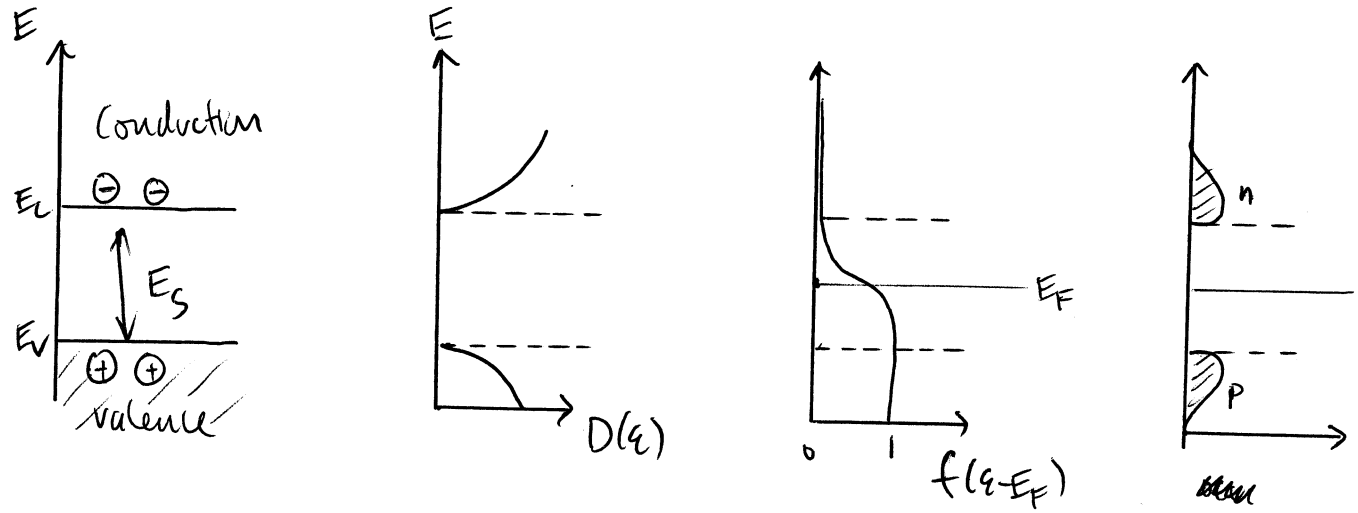
c.f. $k_B T = 0.026\,eV$

* Compute the Fermi level in the presence of impurities

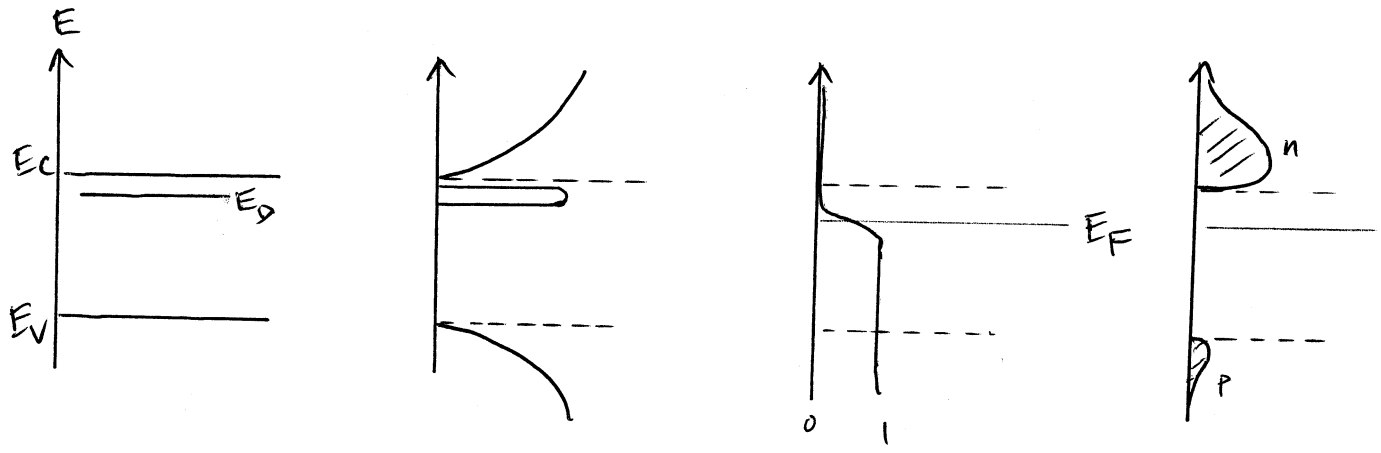
→ no longer pinned to the centre of the band gap

→ must adjust to preserve charge neutrality

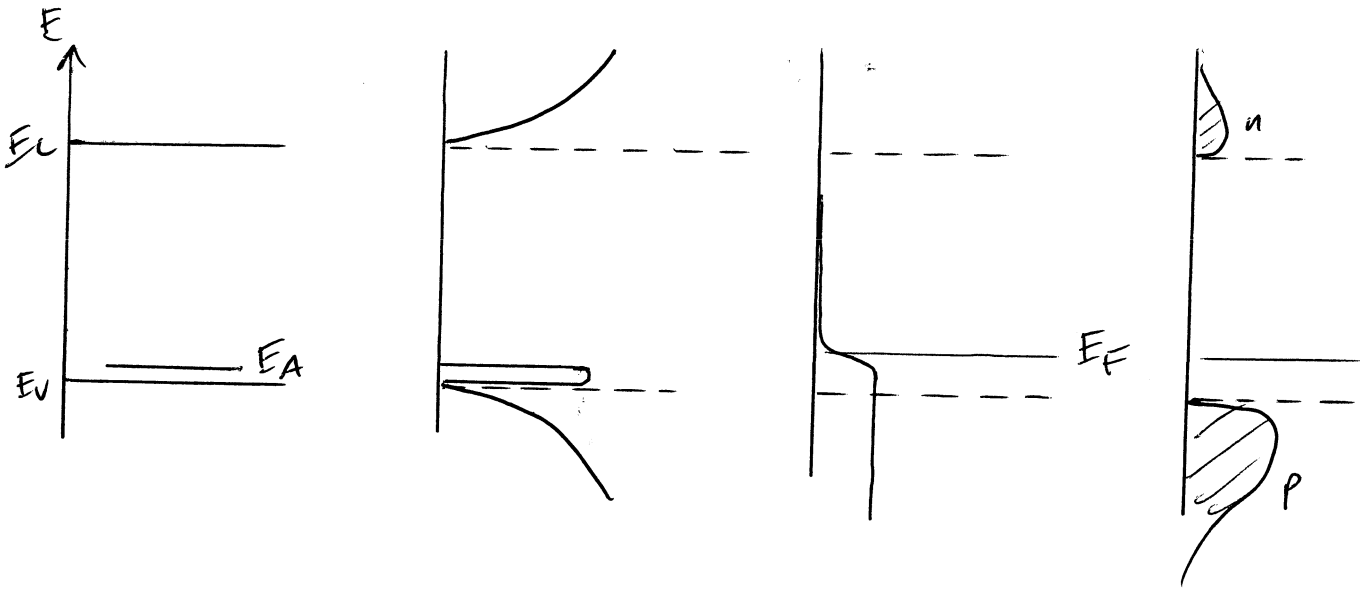
intrinsic



n-type



p-type



Example: donor atoms present with concentration N_D

→ preserve charge neutrality

$$n = N_D^+ + p$$

n: electron density in the conduction band

N_D^+: number of ionized donors

p: hole density in the valence band

$$N_D^+ = N_D \left[1 - \frac{1}{1 + \frac{1}{g} \exp\left(\frac{E_D - E_F}{k_B T}\right)} \right]$$

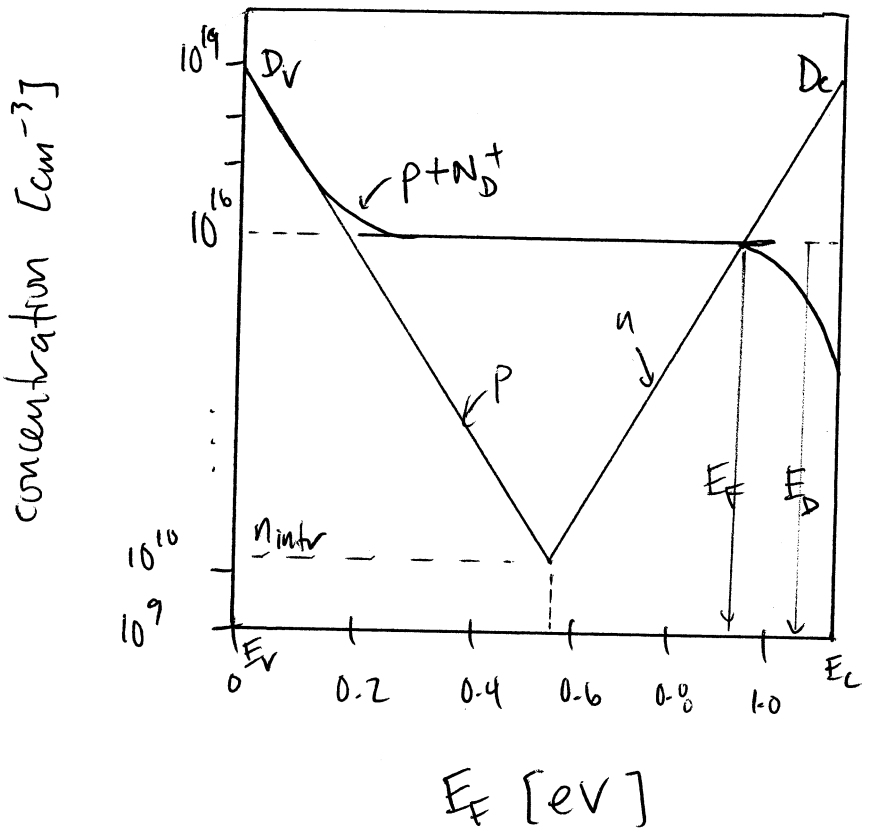
where g = ground-state degeneracy of the donor impurity level ($= 2$)

(similarly $N_A^- = \frac{N_A}{1 + g \exp\left(\frac{E_A - E_F}{k_B T}\right)}$ for the acceptor case)

→ plugging in expressions gives

$$D_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) = N_D \frac{1}{1 + 2\exp\left(\frac{E_F - E_D}{k_B T}\right)} + D_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

which uniquely determines E_F



Si at 300K

n-type with

$N_D = 10^{16}\ cm^{-3}$

→ Fermi level is close to the conduction band edge and is adjusted so that almost all donors are ionized