15.02.10

Surfaces of 3D crystals

Bulk crystal $\xrightarrow{\text{cutting bonds}}$ Surface

- "dangling bonds" $\Rightarrow$ surface reconstruction

- 1D crystal $\Rightarrow$ 0D 'surface' $\Rightarrow$ 0D surface states

  3D —"— $\Rightarrow$ 2D —"— $\Rightarrow$ 2D —"— bands

Density of surface atoms: $n_s = \frac{1}{A_{atom}} \sim \frac{1}{a^2} \sim \frac{1}{(3\text{-}5\,\text{Å})^2}$

$\sim 5 \cdot 10^{18}\ m^{-2}$

Surface density of states pr unit area:

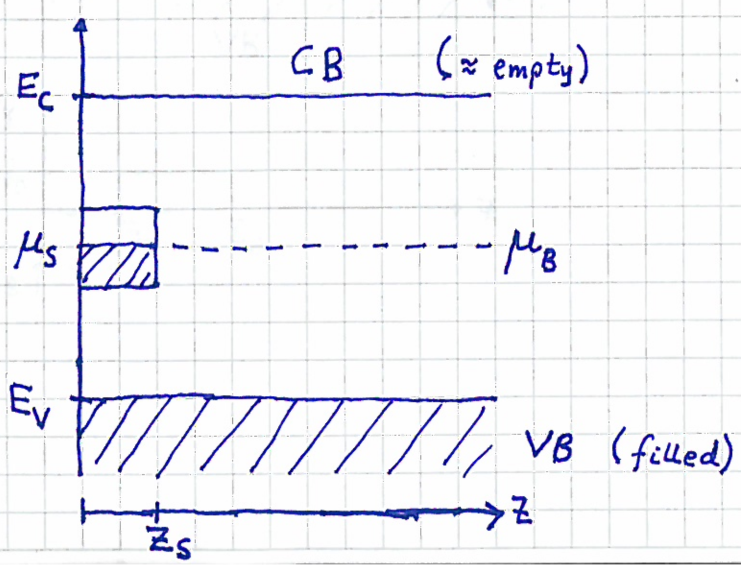
$$\frac{D_2(E)}{A} = \frac{g\, m^*}{2\pi \hbar^2} \sim \frac{2 \cdot 10^{-31}}{2\pi \cdot 10^{-68}}\ J^{-1} \cdot m^{-2} \approx 5 \cdot 10^{17}\ eV^{-1} \cdot m^{-2}$$

Nr. of surface states pr unit area:

$$\frac{N_s}{A} = \frac{D_2(E) \cdot \Delta E_s}{A} \sim \left[5 \cdot 10^{17}\ eV^{-1} \cdot m^{-2}\right] \cdot \Delta E_s$$

Width of surface band: $\Delta E_s \sim 0.1 - 1\ eV$

Intrinsic SC: (surface in $z = 0$) (Assume low T)



Equilibrium: Same value of Fermi level μ throughout crystal

$\Rightarrow \mu_s = \mu_B = \mu$

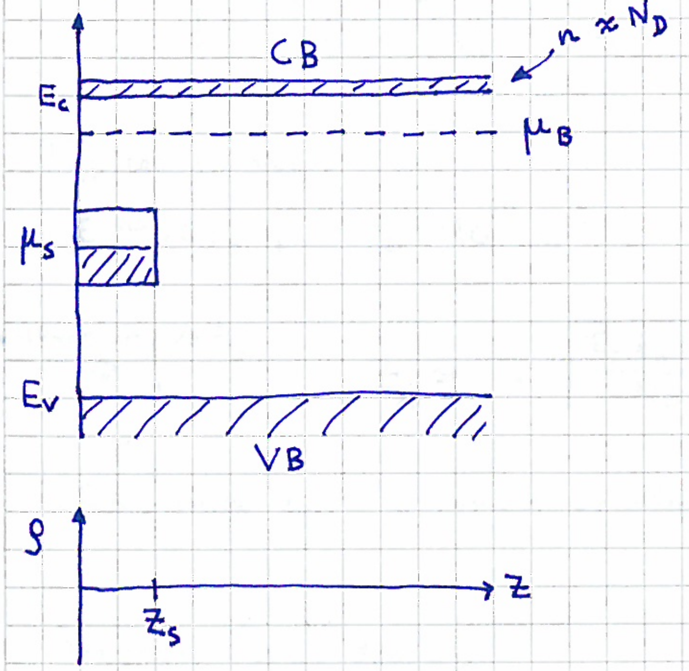
S: surface

B: bulk

(≈ neutral surface)

n-doped SC: (donor conc. N_D, donor level E_D)

Before equilibration:



$\mu_B \approx E_D \neq \mu_s$

Equilibration: CB electrons lower their energy by occupying empty surface states

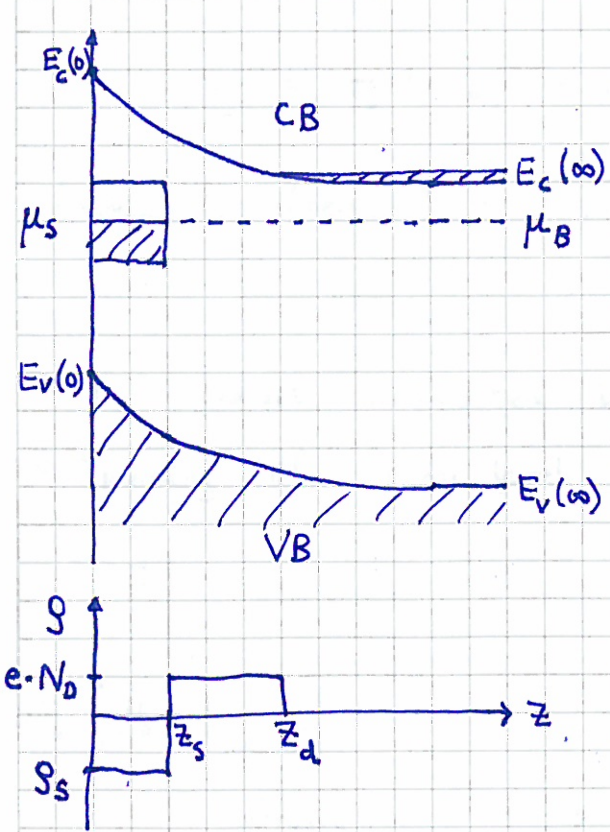
$\Rightarrow$ negative surface $0 < z < z_s$
positive layer $z_s < z < z_d$
("depletion layer")

$\Rightarrow$ build-up of electric field $\vec{E}$ and potential $V(z)$

$\Rightarrow$ $\boxed{\text{Band bending}}$

until $\mu_s = \mu_B$

Equilibrium:



Overall charge neutrality

$$\Rightarrow \rho_s = -eN_D \cdot \frac{z_d - z_s}{z_s}$$

$\vec{E}(z)$ and $V(z)$ from Gauss' Law, $\nabla \cdot \vec{E} = +\rho/\varepsilon$, or from Poisson equation,

$$\nabla^2 V = -\rho/\varepsilon$$

since $\vec{E} = -\nabla V$

Solution (choosing $V(z_d) = 0$):

$$V(z) = \begin{cases} -\dfrac{eN_D}{2\varepsilon}(z-z_d)^2 & z_s < z < z_d \\ -\dfrac{eN_D}{2\varepsilon}\cdot\dfrac{z_d - z_s}{z_s}\left(z_d z_s - z^2\right) & 0 < z < z_s \end{cases}$$

Typical numbers:

$\varepsilon \sim 12\varepsilon_0$; $N_D \sim 10^{24}\,m^{-3}$; $V(0) \approx -\dfrac{E_g}{2e} \sim -0.7\,V$

assume $z_d \gg z_s$ $\Longrightarrow$ $z_d \approx \dfrac{1}{e}\sqrt{\dfrac{\varepsilon_r \varepsilon_0 E_g}{N_D}} \sim 30\,nm$

[OK, since $z_s \sim$ a couple of atomic layers $\sim 1\,nm$]

Surface charge density:

$$\sigma_s \approx \rho_s \cdot z_s = -eN_D\cdot(z_d - z_s) \approx -eN_D z_d$$

$\Rightarrow$ "extra" charge carriers pr unit area at surface:

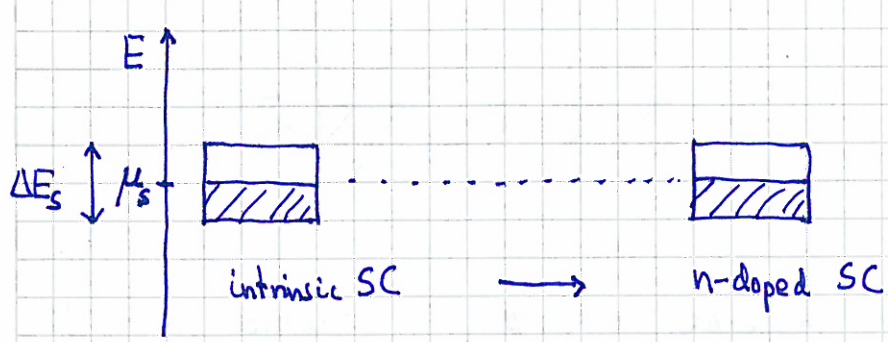
$$n_s = \sigma_s/(-e) \approx N_D \cdot z_d \sim 10^{24}\cdot 30\cdot 10^{-9}\,m^{-2} = 3\cdot 10^{16}\,m^{-2}$$

(which is often ....) $\ll \dfrac{N_s}{A} = \dfrac{D_2 \cdot \Delta E_s}{A} \sim 3\cdot 10^{17}\,m^{-2}$

assuming $\Delta E_s \sim 0.6\,eV$

$\Rightarrow$ μ_s almost unaffected by charge transfer / band bending

$\Rightarrow$ "pinning" of Fermi level μ to μ_s of intrinsic SC

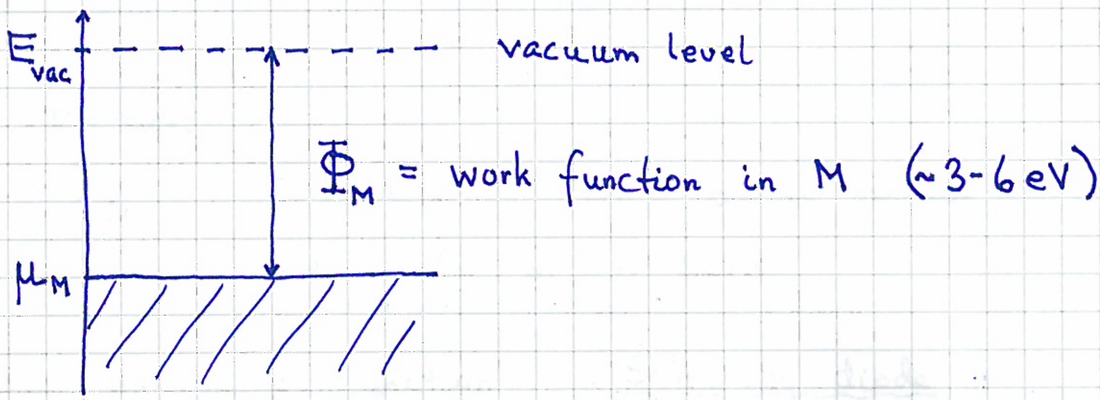


SC - Metal interfaces

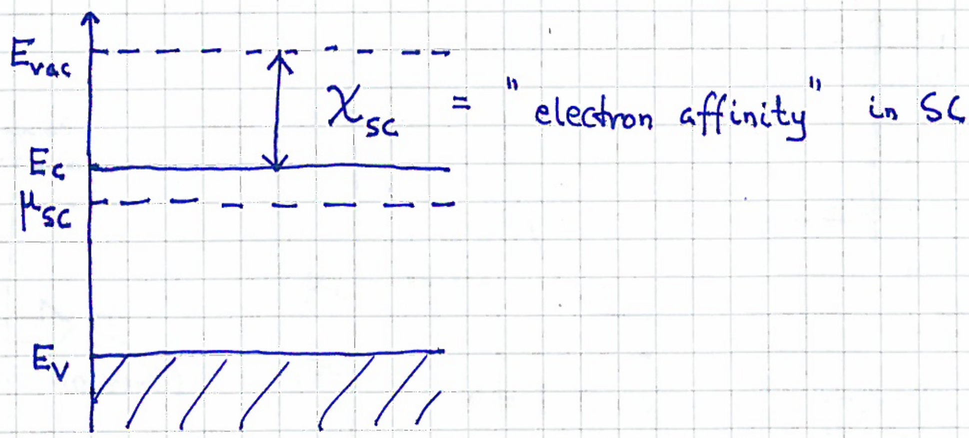
Comments:

- SC device + connecting M wires
  $\Rightarrow$ SC - M interfaces unavoidable
- M and SC surface $\Rightarrow$ surface states
- can discuss M - SC interface without <u>explicitly</u> involving the surface states

Metal:

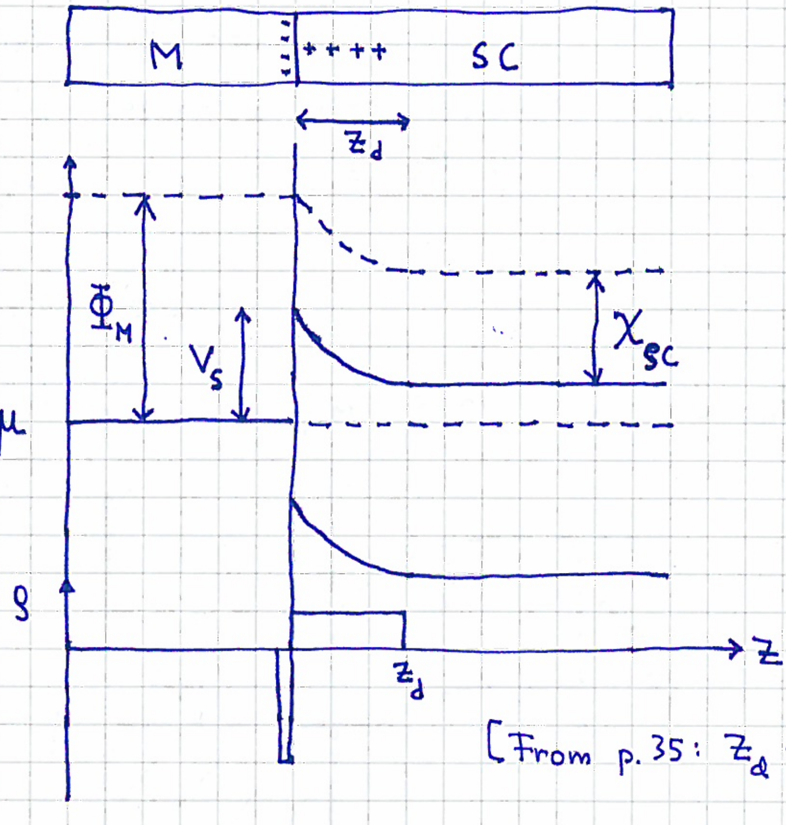


n-doped semiconductor:



M - nSC contact $\Rightarrow$ electron transfer from CB in SC to M (to reduce energy)
$\Rightarrow$ "dipole layer" $\Rightarrow$ band bending until $\mu_M = \mu_{SC}$

Comment:
Large $D(\mu)$ in M $\Rightarrow$ Fermi level "pinned" to $\mu = \mu_M$



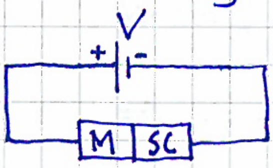
$\boxed{\text{Schottky model}}$

[From p. 35: $z_d \sim \sqrt{V_S/N_D}$]

<u>Schottky barrier:</u>

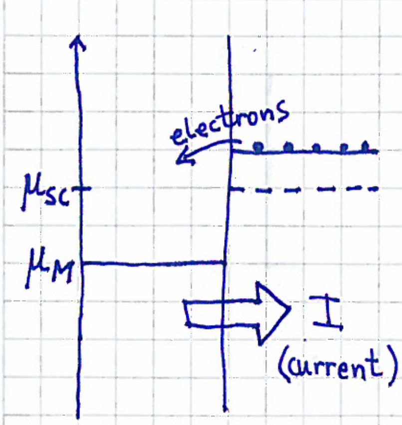
$V_S = \Phi_M - \chi_{SC} \sim 0.4 - 1\ \text{eV}$ for "typical" metals and n-Si or n-GaAs

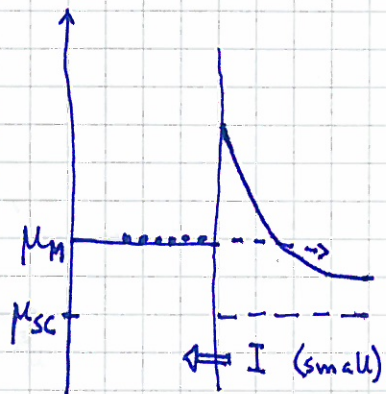
Qualitatively like a pn-junction : <u>Schottky diode</u>



$V > 0 \Rightarrow -e\cdot V < 0 \Rightarrow \mu_M = \mu_{SC} - eV < \mu_{SC}$

$V < 0 \Rightarrow -e\cdot V > 0 \Rightarrow \mu_M > \mu_{SC}$





$\boxed{\text{Diode!}}$

$I = I_0 \{ e^{eV/k_BT} - 1 \}$

$V > 0$

$\Rightarrow$ reduced barrier

$\Rightarrow$ large current I

$V < 0$

$\Rightarrow$ tunneling barrier for electrons at μ_M

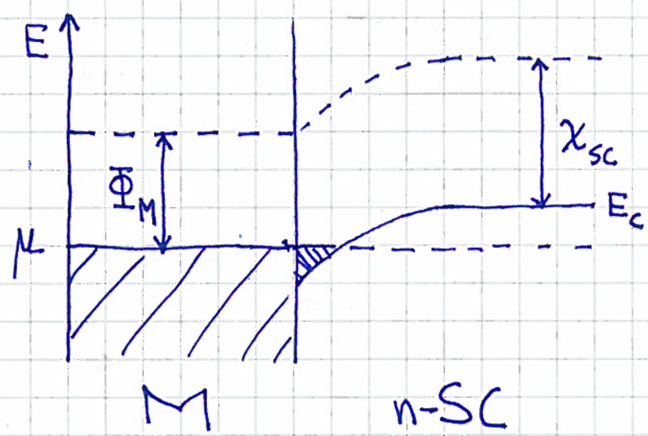
$\Rightarrow$ small current I

Ohmic contact

usually desirable with low-R ohmic M-SC interface, i.e., $I = R^{-1} \cdot V$

"Natural OC"

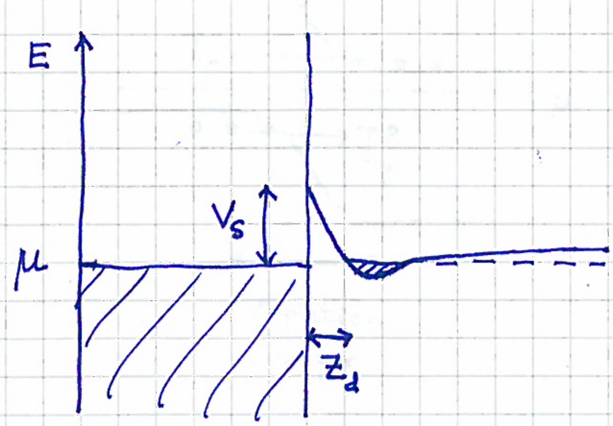
$\Phi_M < \chi_{SC} \Rightarrow \mu_M$ above E_c at interface:



"Designed OC"

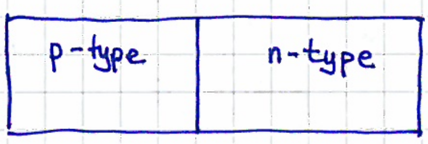
- M-SC combination with small V_s
- heavily doped SC, i.e., large N_D ("n^*-SC")

$\Rightarrow$ small and narrow Schottky barrier ($z_d \sim \sqrt{V_s / N_D}$)

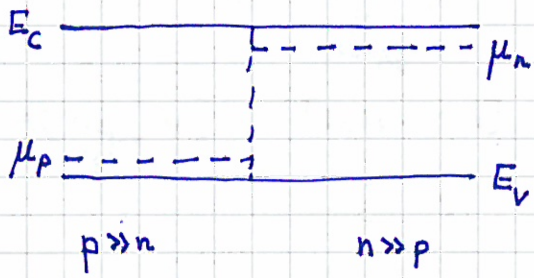


SC – SC interfaces

Example (well known): pn-junction



(same SC on both sides)

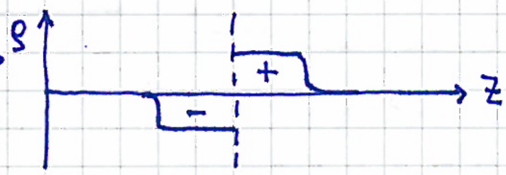


Before equilibration

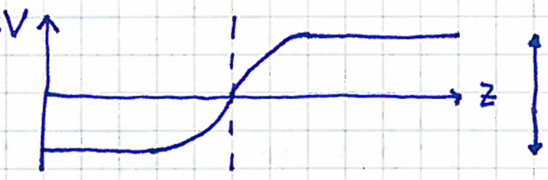
$\Rightarrow$ diffusion: $h \longrightarrow$
$\longleftarrow e$

$\Rightarrow$ recombination on both sides

$\Rightarrow$

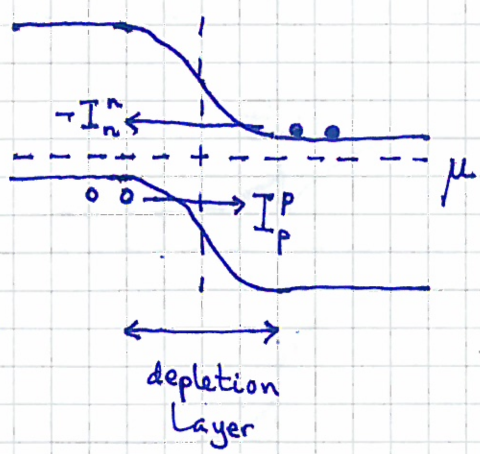


$\Rightarrow$



Built-in potential:
$\Delta V = (\mu_n - \mu_p)/e$

$\Rightarrow$ Equilibrium:

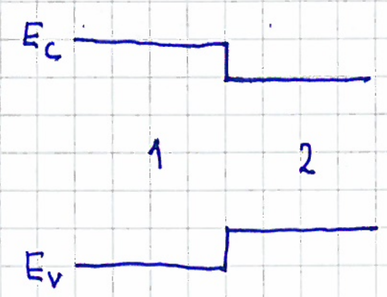


[Dynamic equilibrium:

$$G_n = R_n$$
$$G_p = R_p$$
$$I_n^n + I_n^p = 0$$
$$I_p^p + I_p^n = 0$$
$$\Downarrow$$
$$I(V) = I_0 \{ e^{eV/k_BT} - 1 \} \;]$$

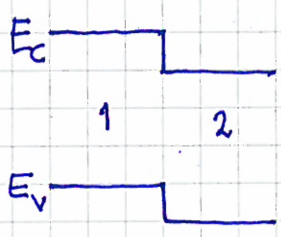
V = applied voltage

SC1 – SC2 heterointerfaces



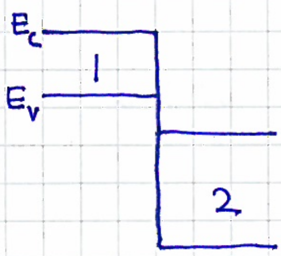
Type I

[GaAs (2) – $Al_x Ga_{1-x} As$ (1)]



Type II staggered

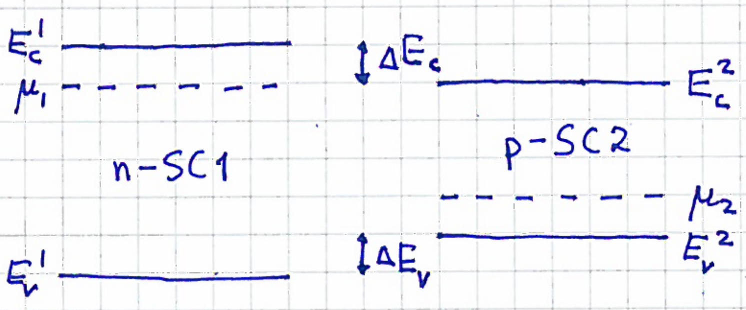
[InAs – AlSb]



Type II misaligned

[InAs – GaSb]

Example: Type I, n-SC1 / p-SC2

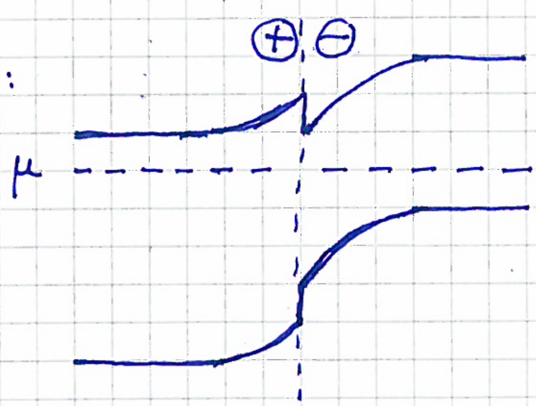


$E_g^1 > E_g^2$

Contact $\Rightarrow$ diffusion of e ($\rightarrow$) and h ($\leftarrow$)

$\Rightarrow$ built-in $\vec{E}$ and V due to charge $\oplus$ on n-side and charge $\ominus$ on p-side of interface

Equilibrium:



Some questions of interest:

- ΔE_c vs ΔE_v ? ($\Delta E_c + \Delta E_v = \Delta E_g$)
- $E_g(x)$ in $Al_x Ga_{1-x} As$?
- .....

Not discussed here.