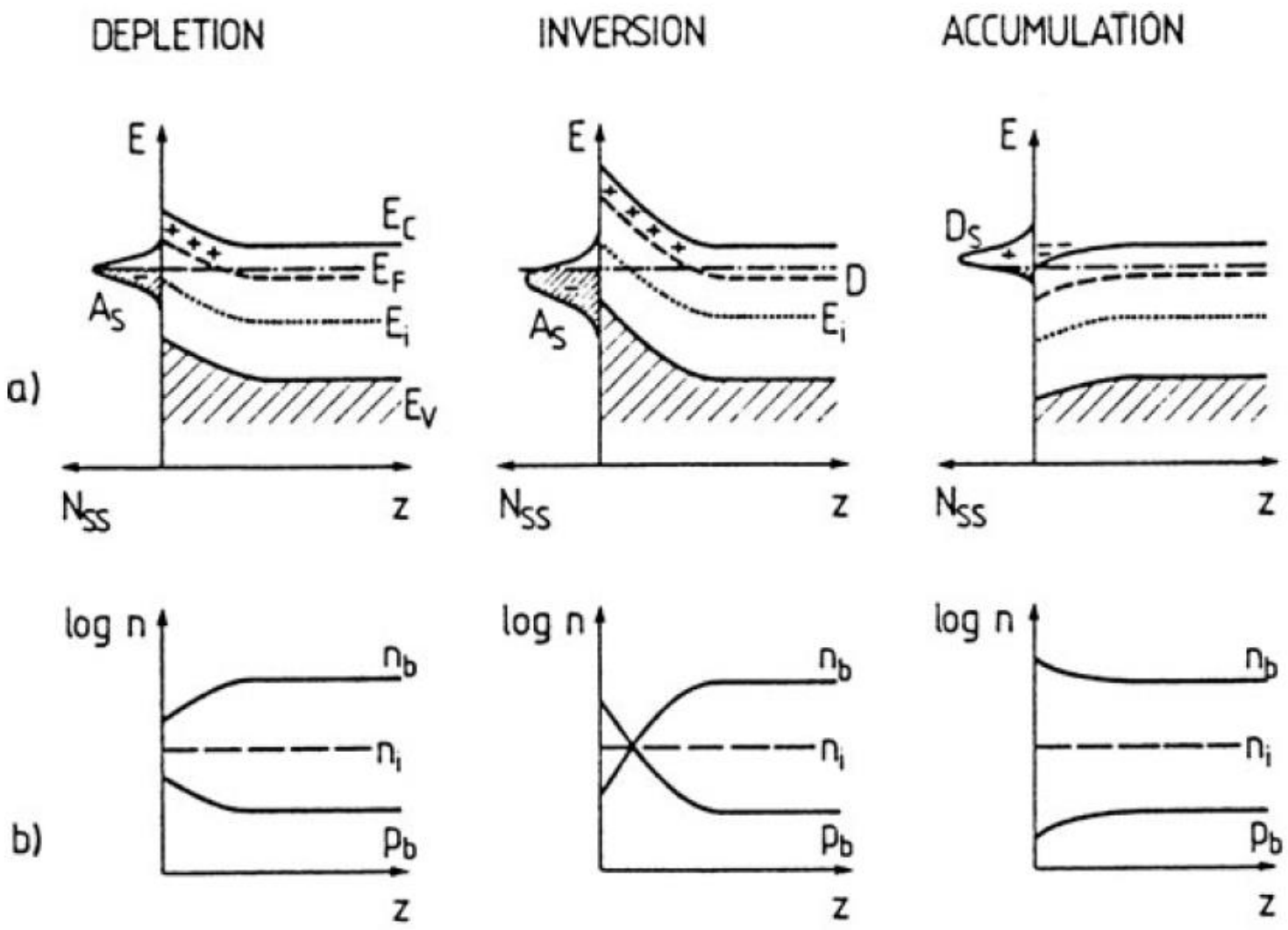
Class 09
Homojunction and Heterostructures

31.03.2025

- ❑ pn junction
  - Space charge region and doping
  - Electrical characteristic
- ❑ Heterostructures
  - Anderson's rule
  - Band alignments
- ❑ Lattice mismatch

Surface band bending

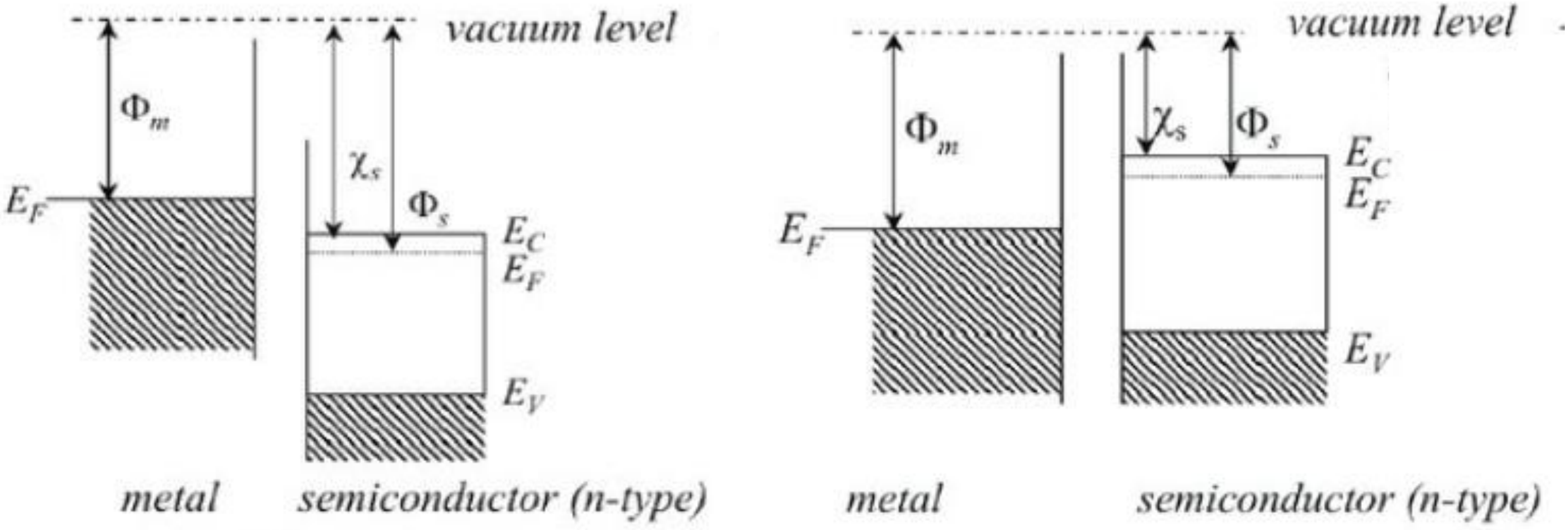


The energetic position of surface states with respect to conduction and valence band induces:

- Charge accumulation at the surface
- Conduction and valence band bending
- Modifications to the carrier concentration close to the surface

Exercise (10 minutes):

Sketch the band profile of these material once they are placed in contact.
What is the difference between the two cases? Which parameters define the band bending?



<u>workfunction ϕ</u>: energy difference between E_F and E_{vac}
<u>electron affinity χ</u>: energy difference between E_C and E_{vac}

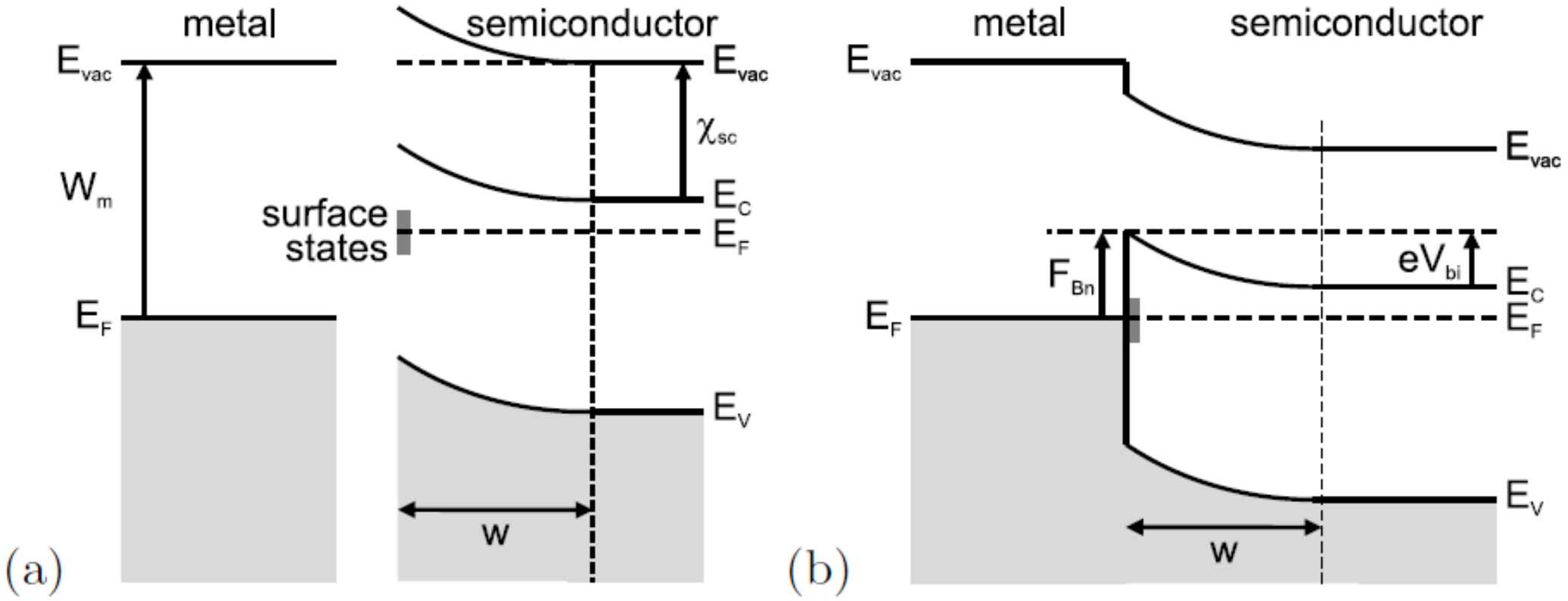
Ohmic contact

To be discussed in class

Schottky contact

To be discussed in class

Metal-Semiconductor contact with surface states

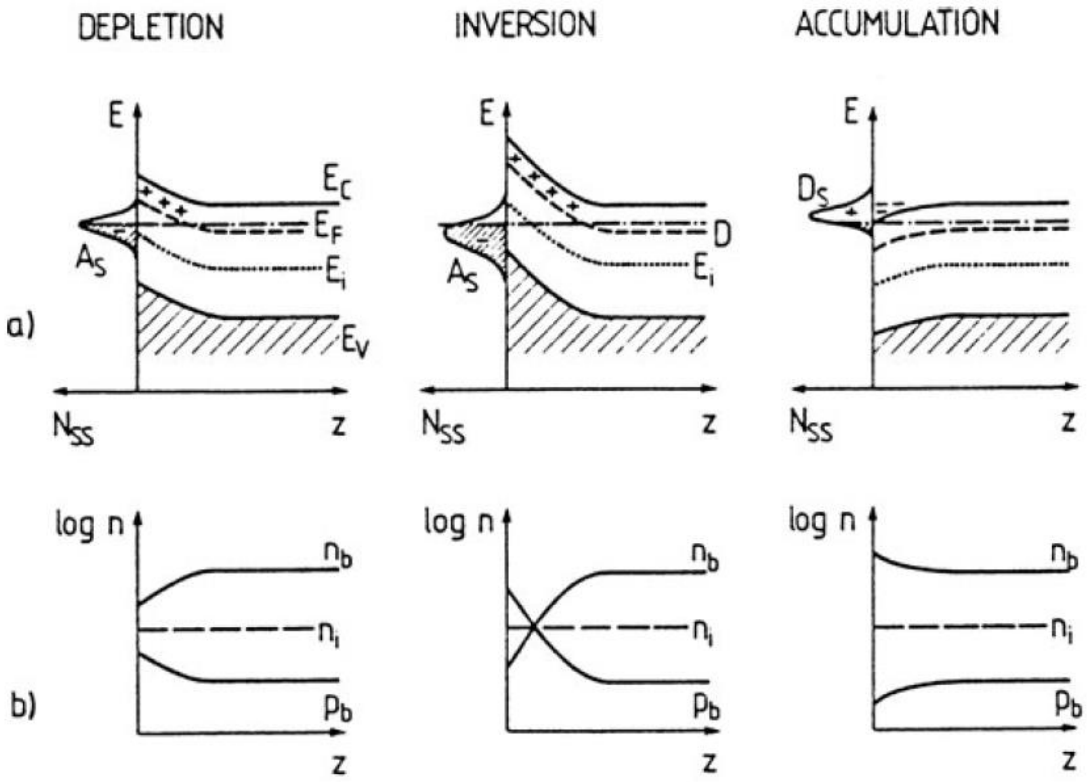


Bardeen model

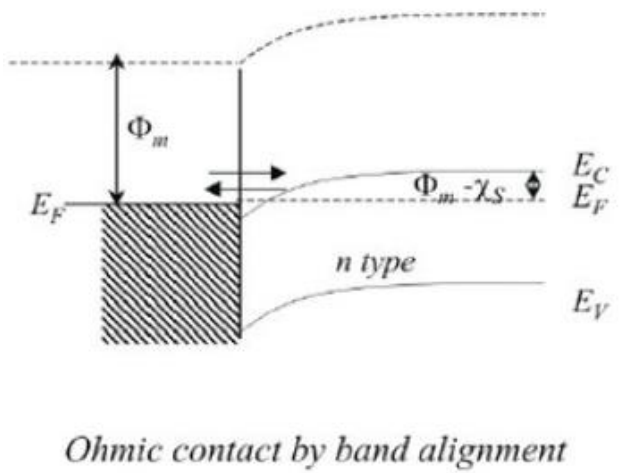
Due to Fermi energy pinning, a band bending is present in the semiconductor even before the contact with the metal. Thus, this barrier at the interface does not depend on the workfunction.

Band bending at surface and interfaces

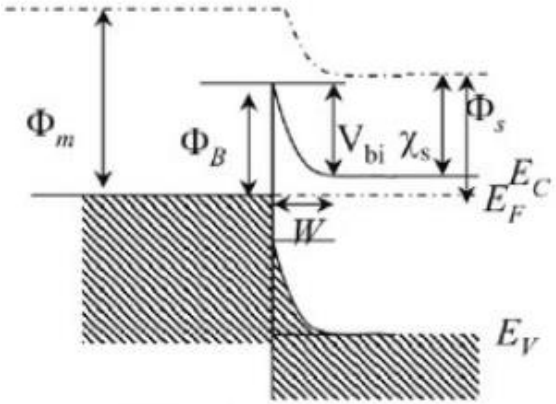
Surface states



Metal-semiconductor interface

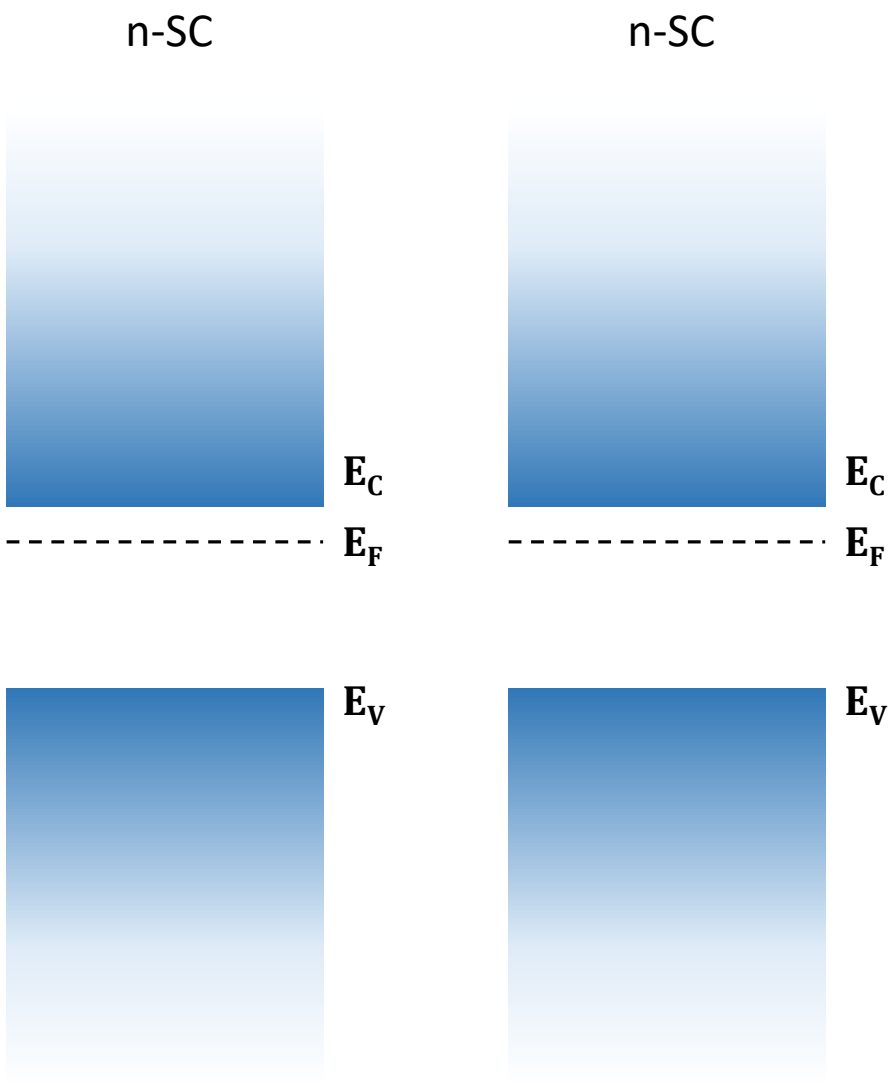


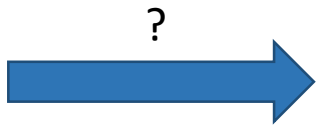
Ohmic contact by band alignment



Schottky contact

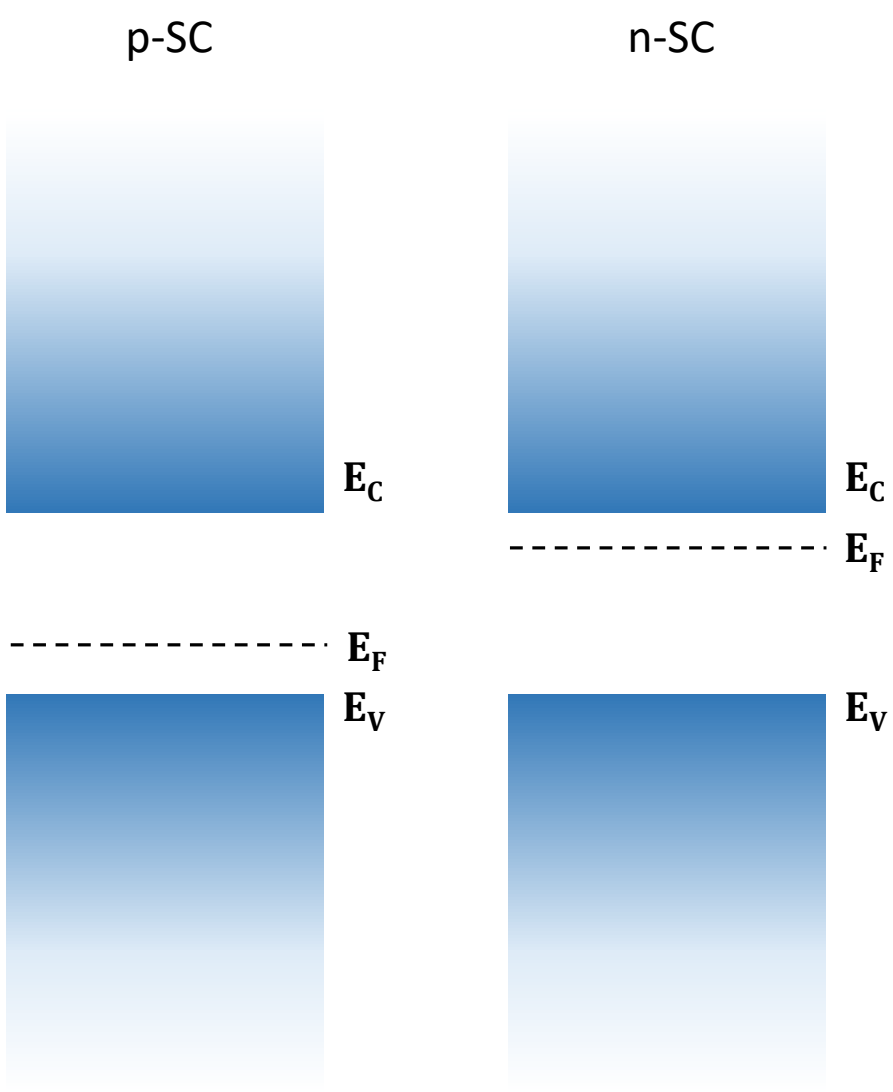
Semiconductor – semiconductor interface





To be discussed in class

Semiconductor – semiconductor interface



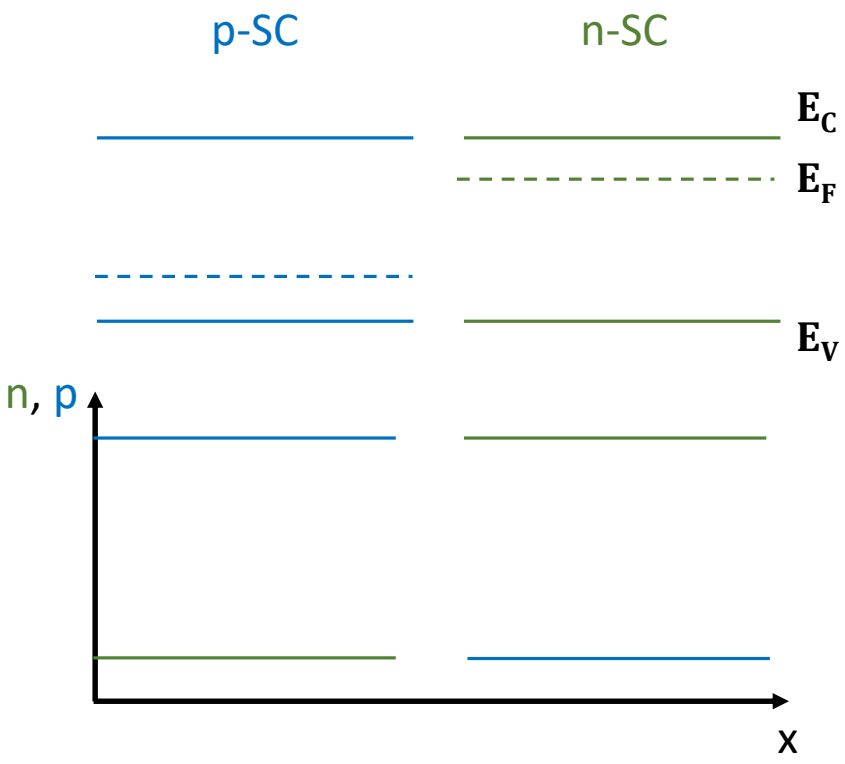
?

To be discussed in class

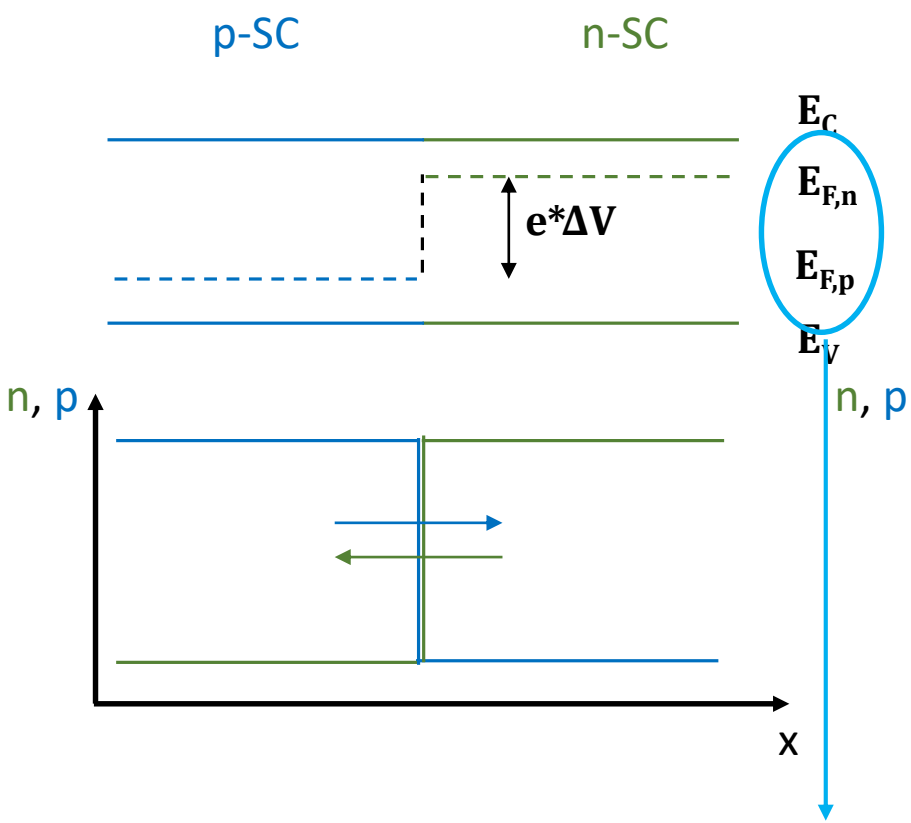
pn (homo)junction

Ch. 21.4, Grundmann

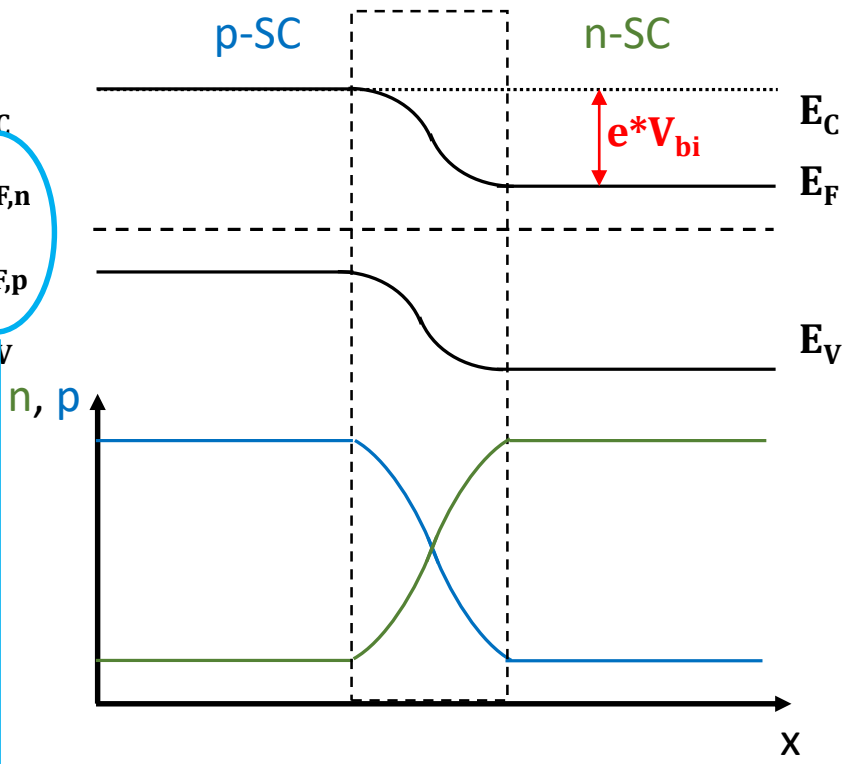
No contact



Contact – out of equilibrium



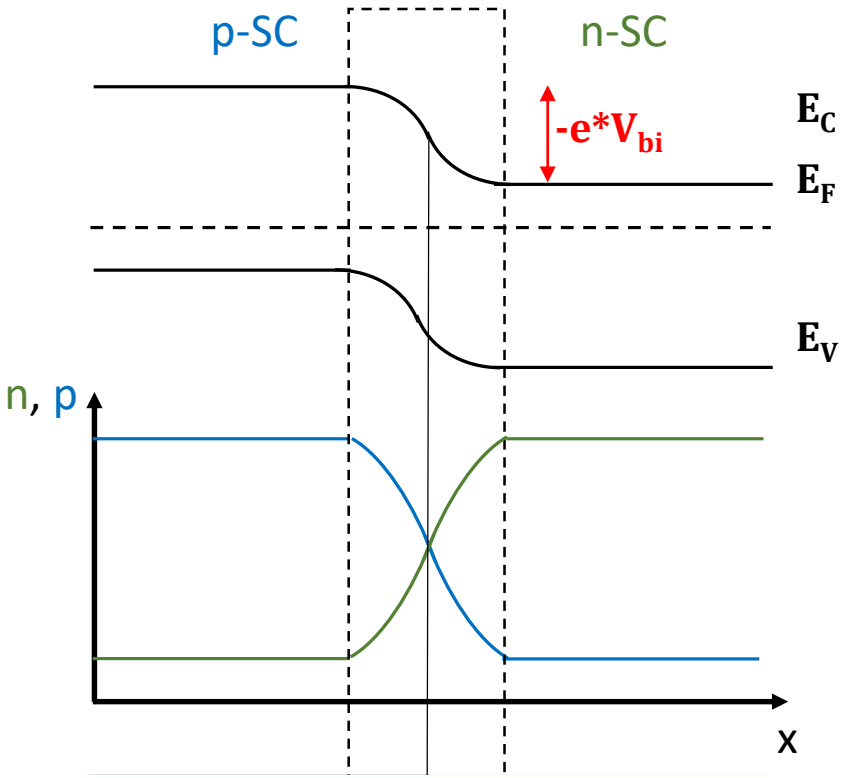
Contact – Equilibrium



Quasi-Fermi Energies (describing carrier concentration out of equilibrium)

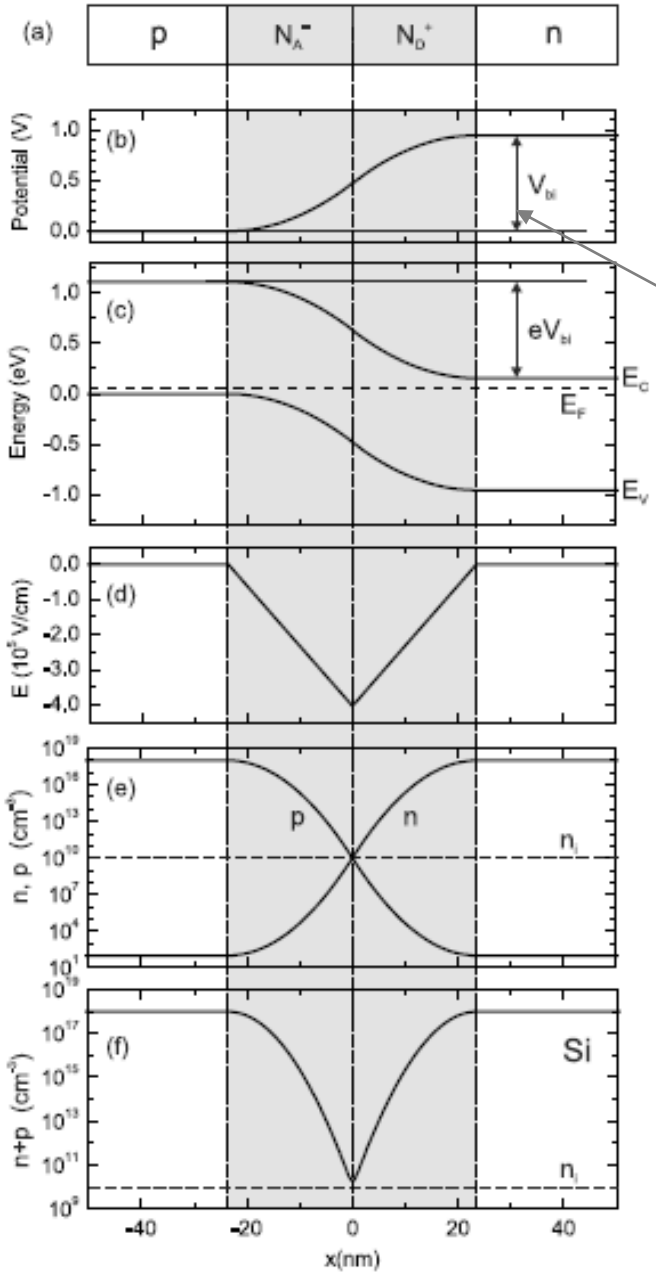
$$\Delta V = \frac{E_{F,n} - E_{F,p}}{e}$$

pn (homo)junction



Built-in electric field

Ch. 21.4, Grundmann



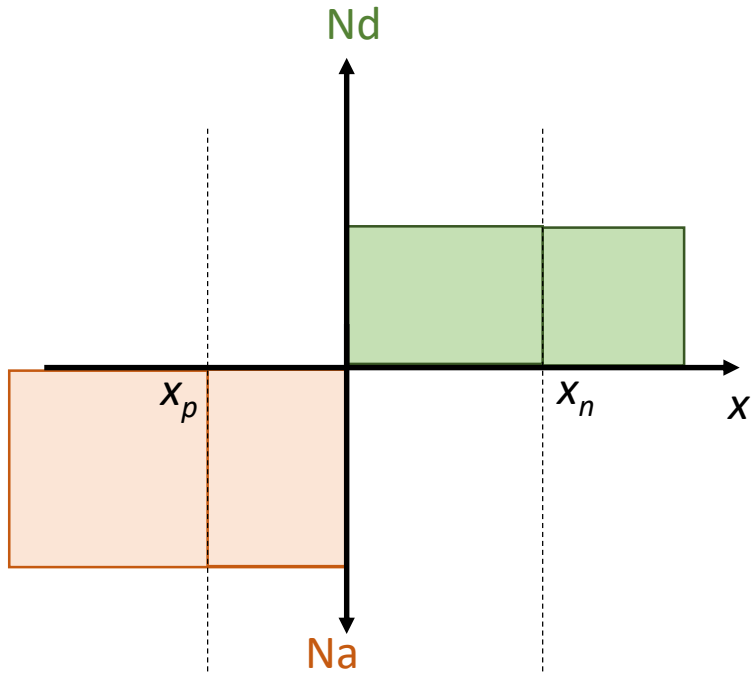
Space charge region or depletion region

Fig. 21.41 pn junction (abrupt approximation) in thermal equilibrium (zero bias) for Si at room temperature and $N_A = N_D = 10^{18}\,cm^{-3}$. **a** Schematic representation of p-doped and n-doped region with depletion layer (*grey area*) and fixed space charges, **b** diffusion potential, **c** band diagram with Fermi level (*dashed line*), **d** electric field, **e** free-carrier concentrations n and p and **f** total free-carrier density $n + p$

Space charge region in the abrupt approximation

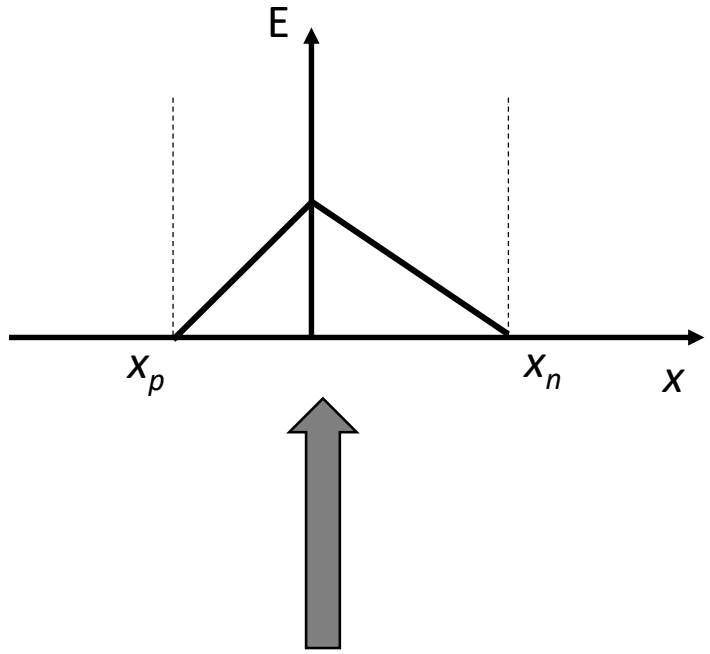
Abrupt approximation:

- pn interface is a pure surface
- Charge concentration at the pn interface equals n_i
- Squared N_D and N_A profiles
- Electric field does not extend beyond the SCR
- 1D model



Maximum electric field at the interface

$$E_m = -\frac{e\,N_D\,x_n}{\epsilon_s} = -\frac{e\,N_A\,x_p}{\epsilon_s}\,.$$



CHARGE NEUTRALITY: $N_a \mid x_p \mid = N_d \mid x_n \mid$

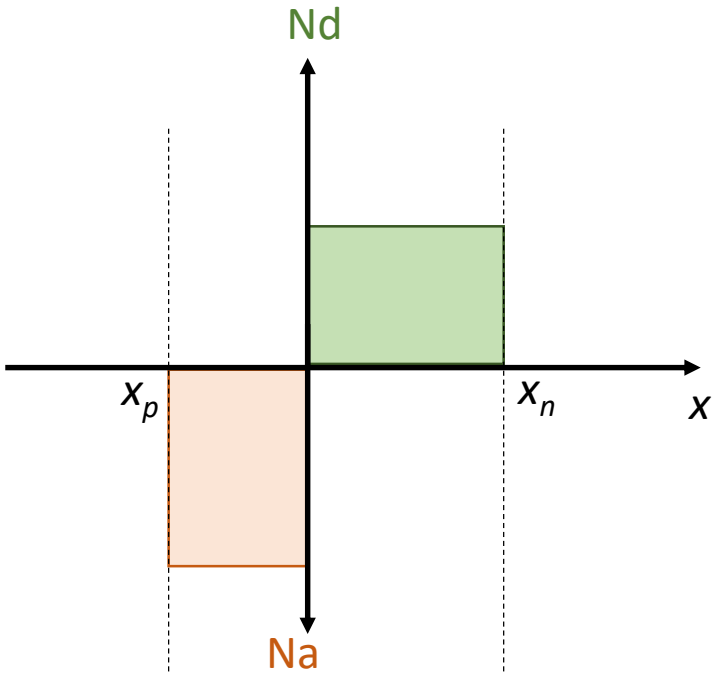
$$E(x) = \frac{e}{\epsilon_s} N_D\,(x - x_n),\ \ 0 \le x \le x_n$$

$$E(x) = -\frac{e}{\epsilon_s} N_A\,(x + x_p),\ \ -x_p \le x \le 0$$

Space charge region in the abrupt approximation

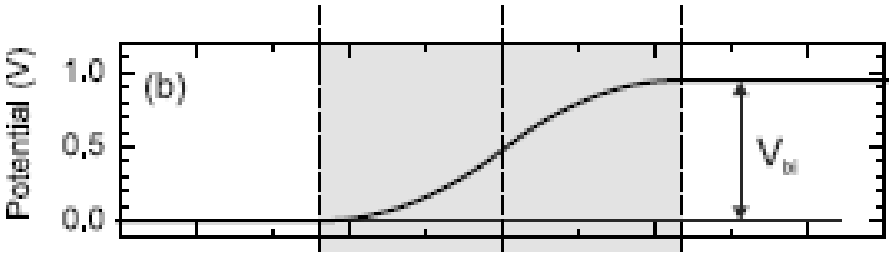
Abrupt approximation:

- pn interface is a pure surface
- Charge concentration at the pn interface equals ni
- Squared N_D and N_A profiles
- Electric field does not extend beyond the SCR
- 1D model



Built-in field

$$V_{bi} = \frac{e}{2\varepsilon}(N_D x_n^2 + N_A x_p^2)$$



$$V(x) = -E_m\left(x - \frac{x^2}{2x_n}\right), \quad 0 \le x \le x_n$$

$$V(x) = -E_m\left(x + \frac{x^2}{2x_p}\right), \quad -x_p \le x \le 0$$

$$V(x) = \int E(x)dx$$

CHARGE NEUTRALITY: $N_a \mid x_p \mid = N_d \mid x_n \mid$

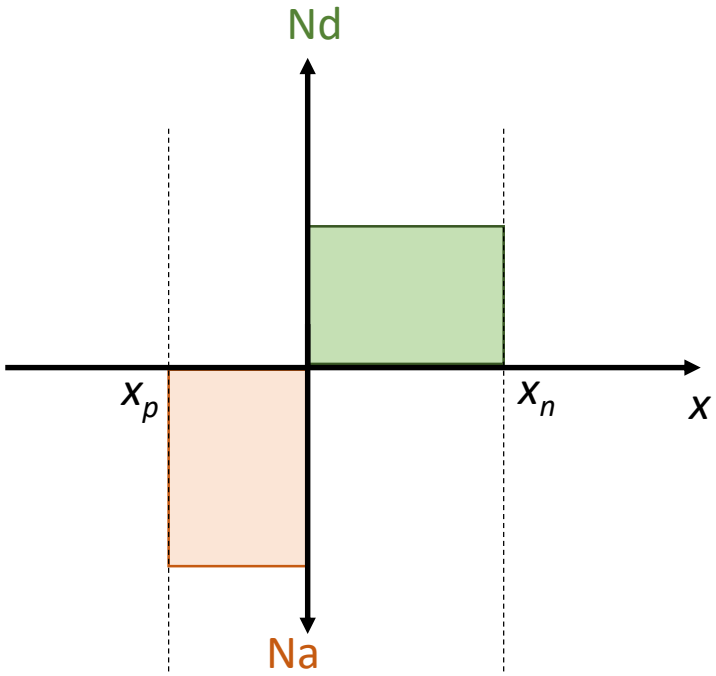
$$E(x) = \frac{e}{\epsilon_s} N_D (x - x_n), \quad 0 \le x \le x_n$$

$$E(x) = -\frac{e}{\epsilon_s} N_A (x + x_p), \quad -x_p \le x \le 0$$

Space charge region in the abrupt approximation

Abrupt approximation:

- pn interface is a pure surface
- Charge concentration at the pn interface equals ni
- Squared N_D and N_A profiles
- Electric field does not extend beyond the SCR
- 1D model



Charge neutrality

$$N_a \mid x_p \mid = N_d \mid x_n \mid$$

Built-in field

$$V_{bi} = \frac{e}{2\varepsilon}(N_D x_n^2 + N_A x_p^2)$$

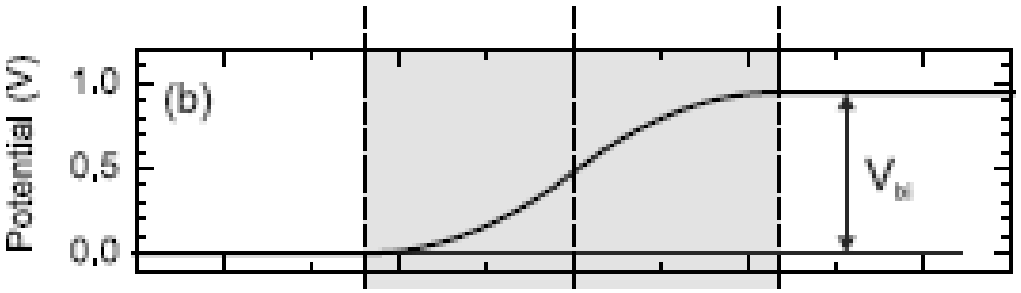
From E_F alignment between n-SC and p-SC, the built-in field is commonly expressed as:

$$V_{bi} = \frac{k_b T}{e} * ln \frac{N_D N_A}{{n_i}^2}$$

Space charge region extension

$$x_n + x_p = W_{SCR} = \sqrt{\frac{2\varepsilon V_{bi}}{e}\left(\frac{1}{N_A} + \frac{1}{N_D}\right)}$$

Exercise



The general formulation of depletion region width includes the impact of a voltage bias (V) as following:

$$x_n + x_p = W_{SCR} = \sqrt{\frac{2\varepsilon(V_{bi} - V)}{e}\left(\frac{1}{N_A} + \frac{1}{N_D}\right)}$$

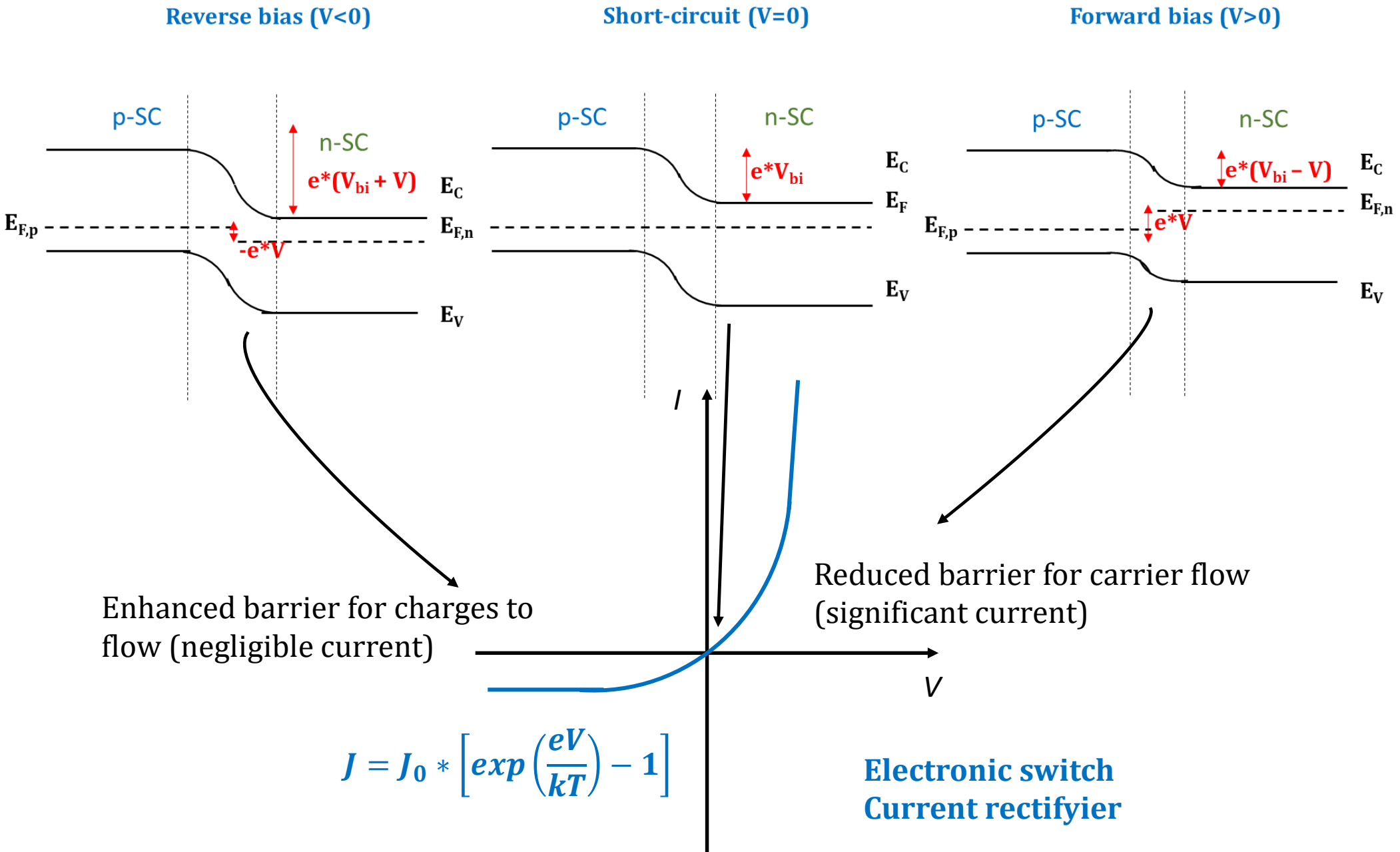
Questions:

1. How the SCR changes with the dopant concentrations?
2. How the bias impact the SCR? What are the implications of applying a bias?

15 minutes

To be solved in Class

Current characteristic of a pn junction

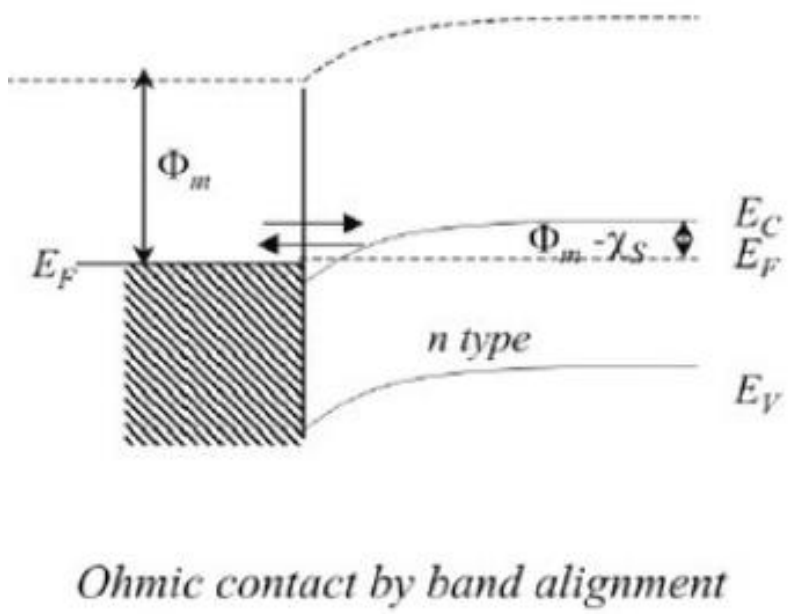


$$J = J_0 * \left[exp\left(\frac{eV}{kT}\right) - 1 \right]$$

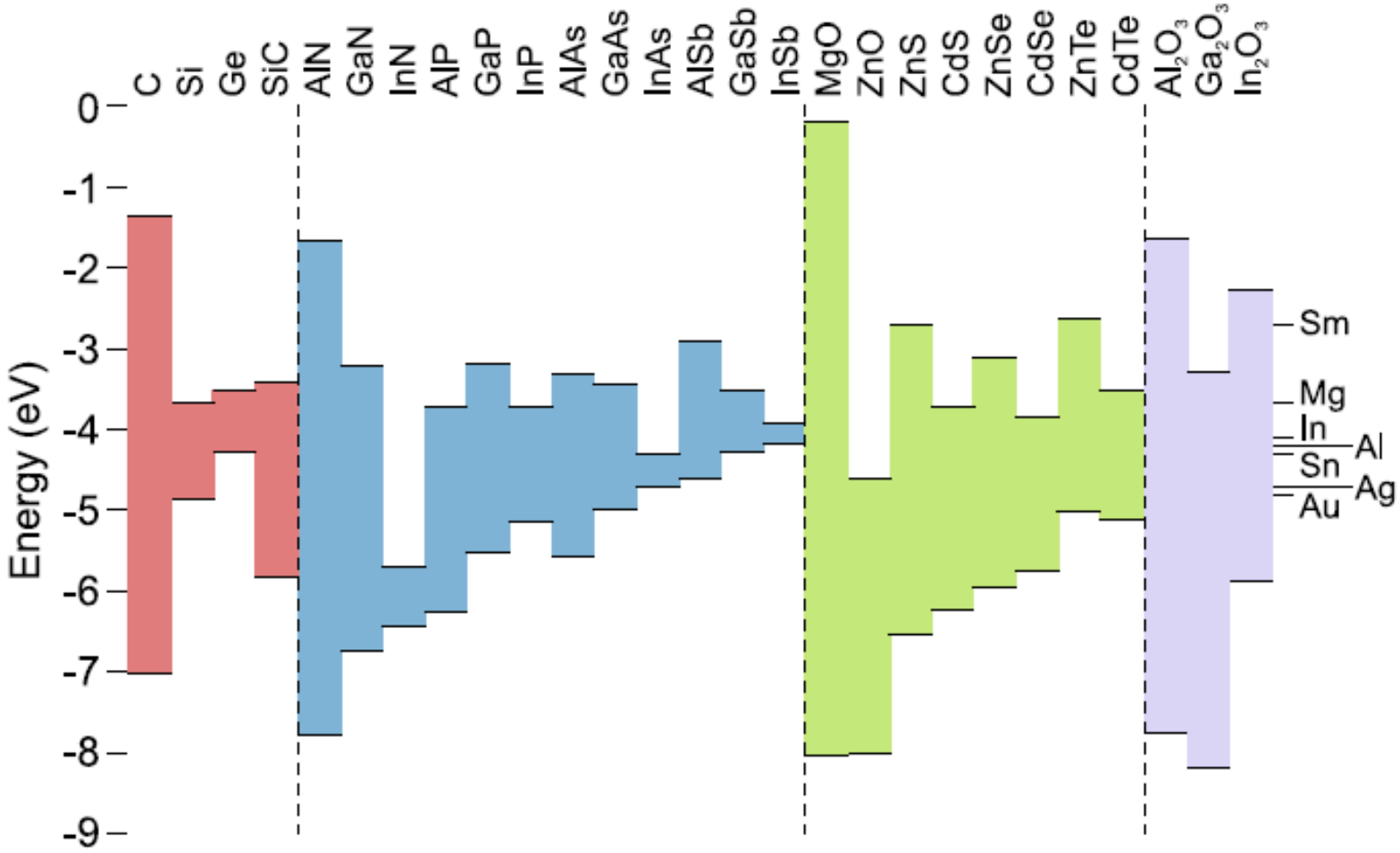
Electronic switch
Current rectifyier

Heterostructures

Metal-semiconductor interface

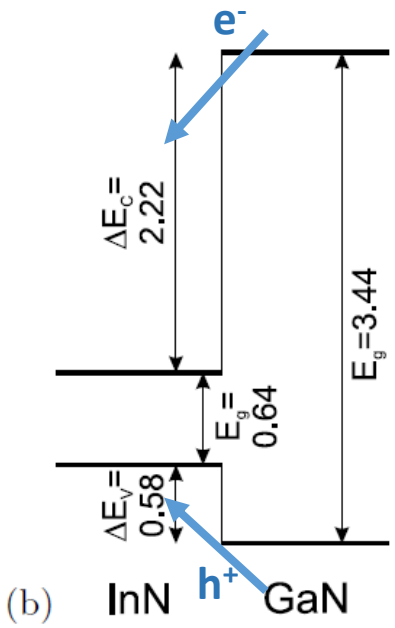


Ohmic contact by band alignment

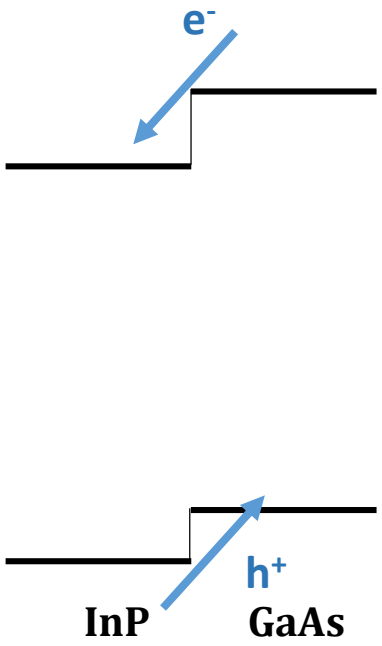


Band alignments

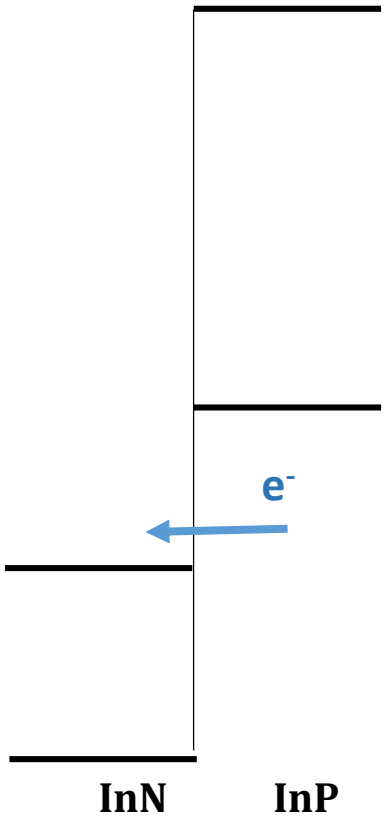
Type I – Straddling alignment

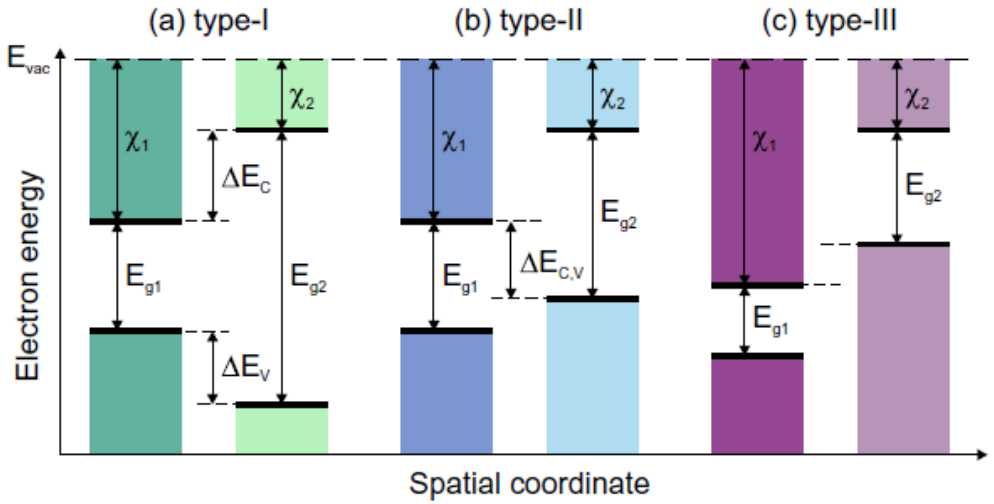


Type II – Staggered alignment

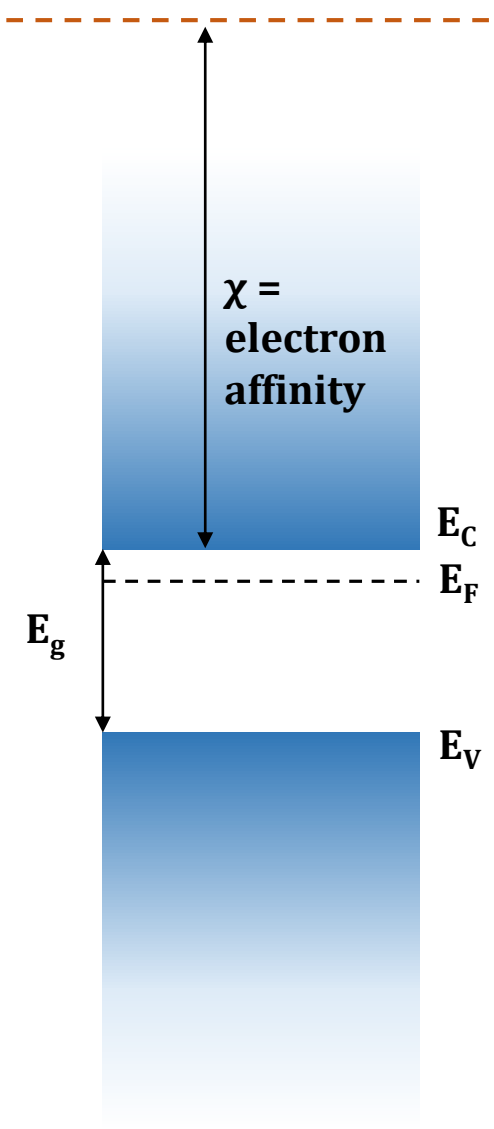


Type III – Broken alignment





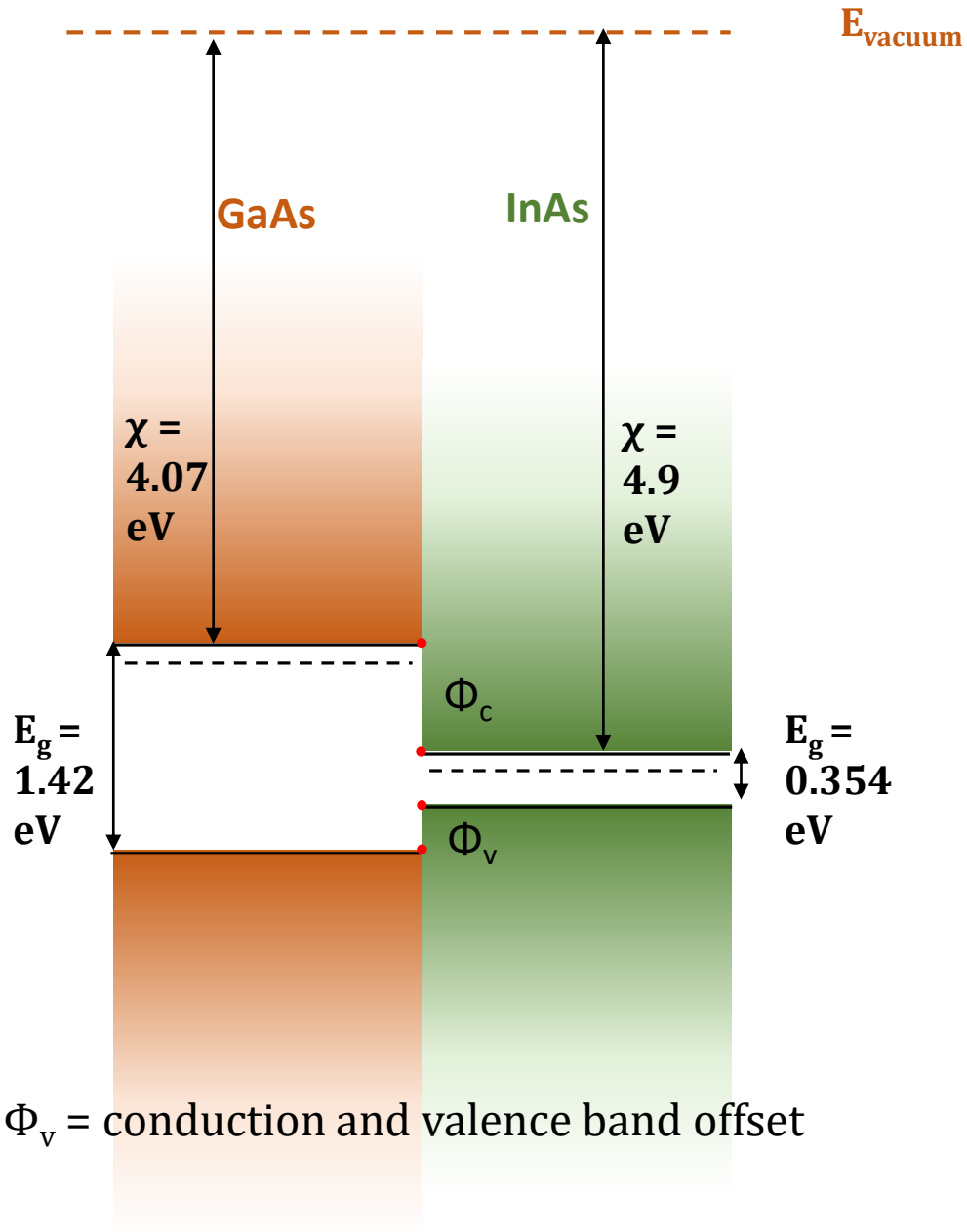
Anderson's rule for heterostructures



Anderson's rule:

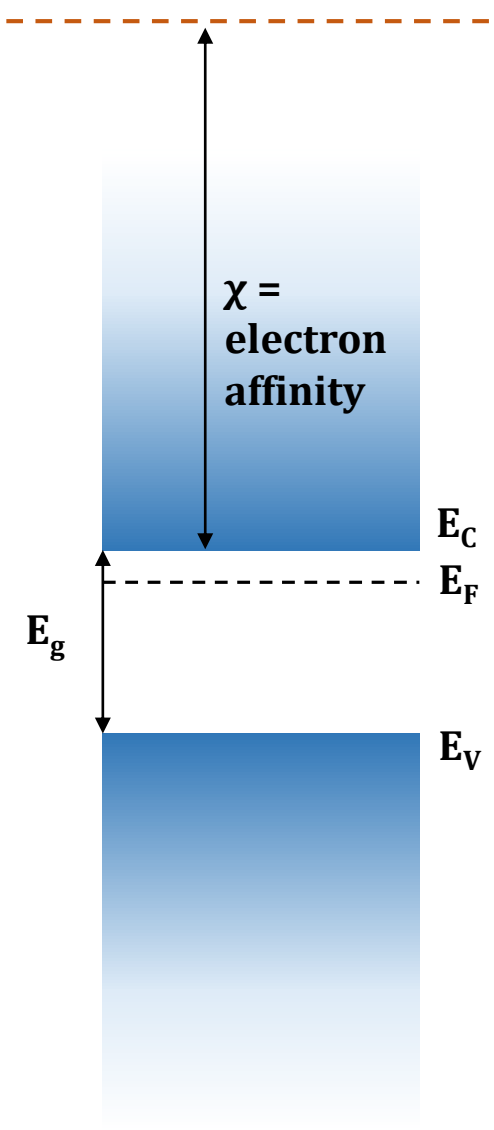
- Align the vacuum energy at the interface
- Align the Fermi energy far from the interface

EXAMPLE	n-GaAs	n-InAs
E_g	1.42 eV	0.354 eV
χ	4.07 eV	4.9 eV
E_C-E_F	0.3 eV	0.1 eV



Φ_c, Φ_v = conduction and valence band offset

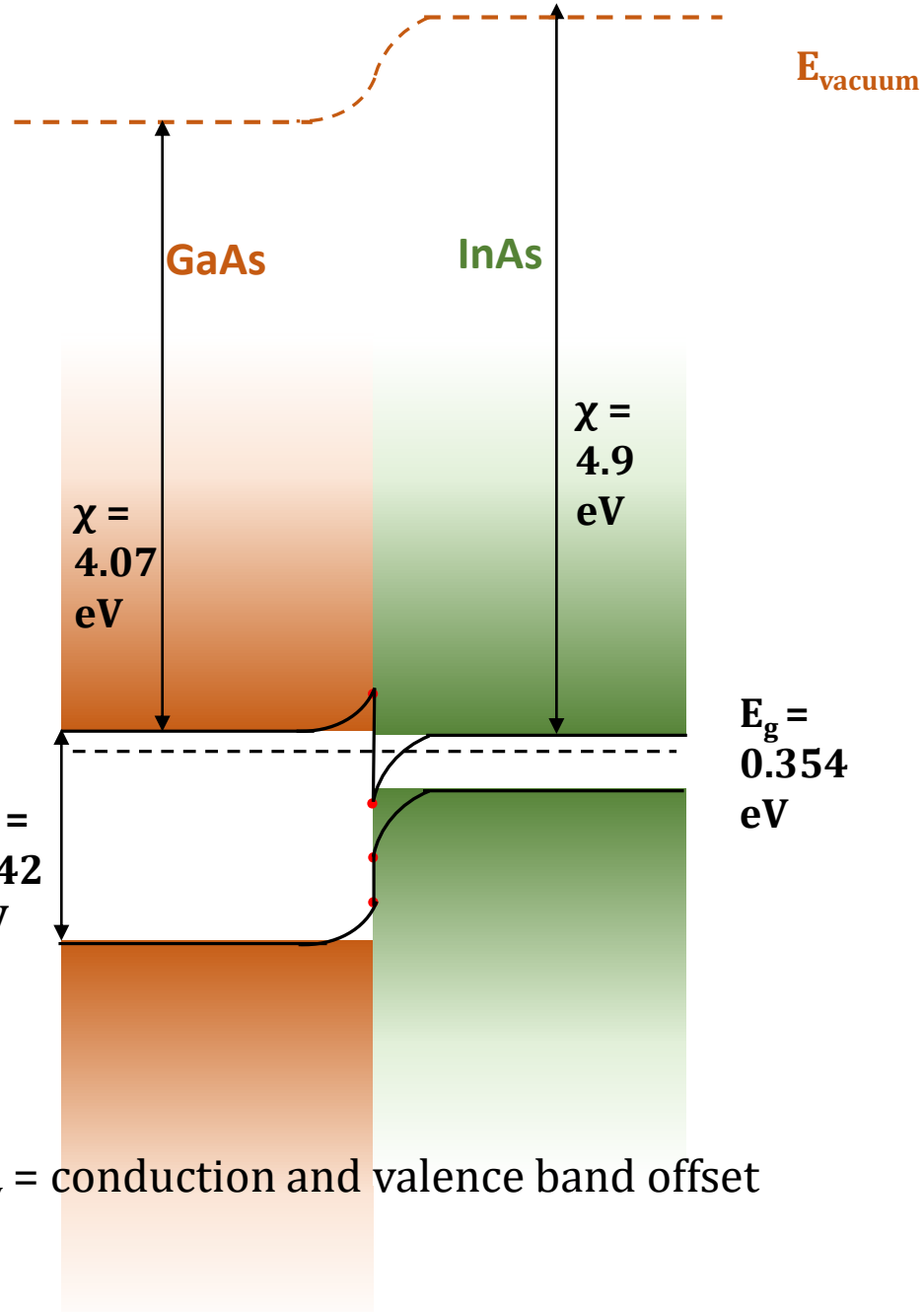
Anderson's rule for doped semiconductors



Anderson's rule:

- Align the vacuum energy at the interface
- Align the Fermi energy far from the interface

EXAMPLE	n-GaAs	n-InAs
E_g	1.42 eV	0.354 eV
χ	4.07 eV	4.9 eV
E_C-E_F	0.3 eV	0.1 eV



Φ_c, Φ_v = conduction and valence band offset

Functional heterostructures

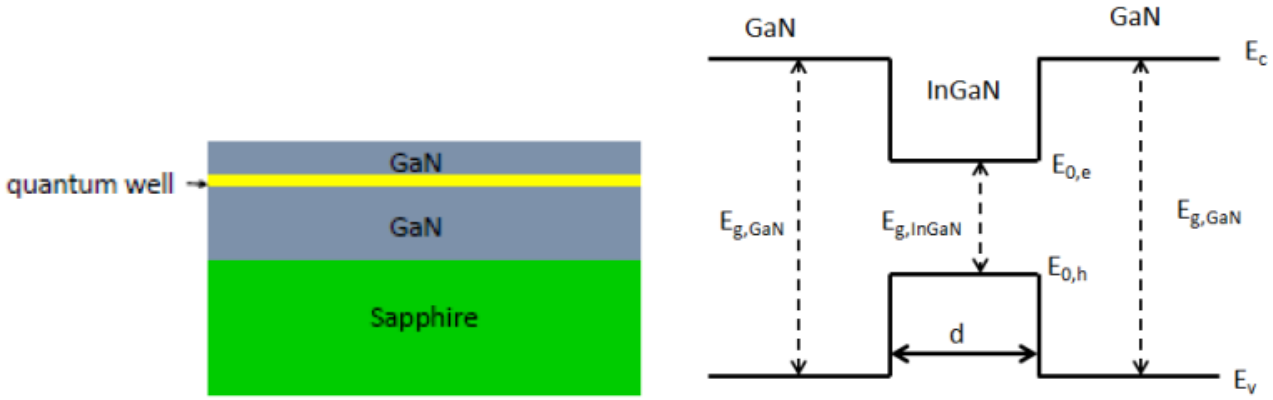
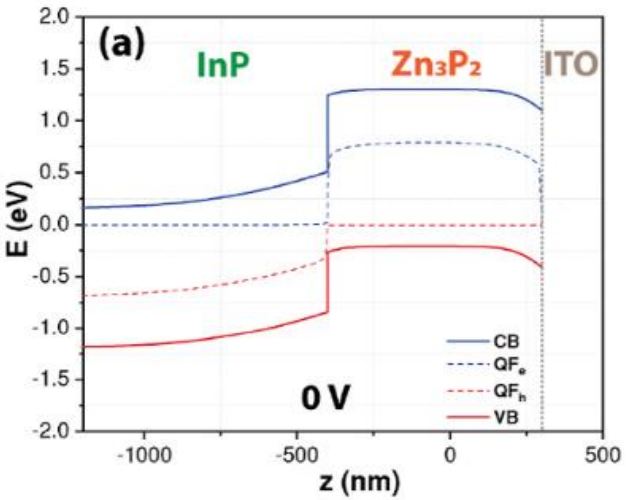
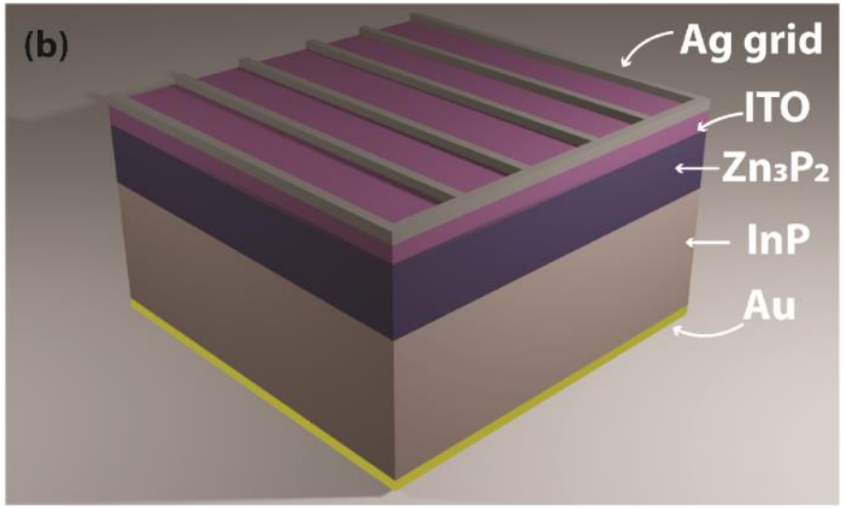


Figure 3.4: GaN/InGaN heterostructure. Cross section for a grown sample (left) and band edges of the heterostructure (right).

Accumulation of e^- and h^+ in the quantum well (LEDs)

Separation of e^- and h^+ at the hetero-interface (PV)





Lattice mismatch and strain

1D

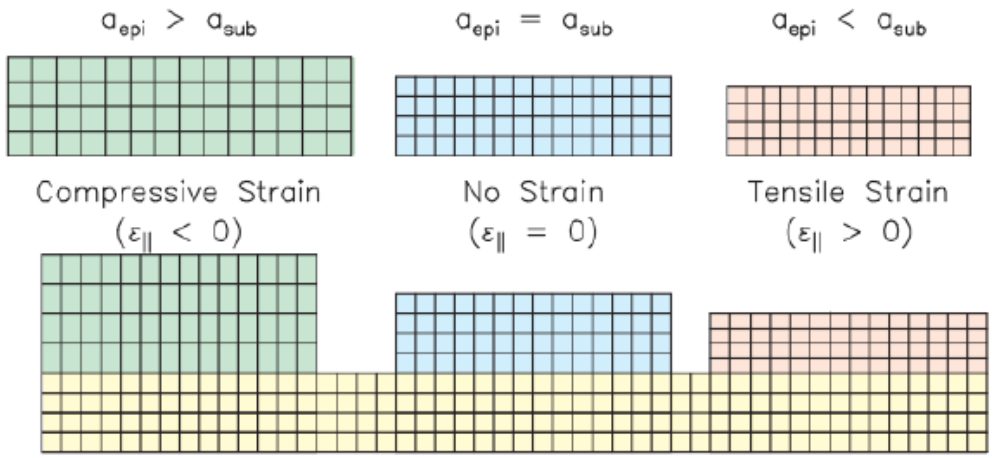
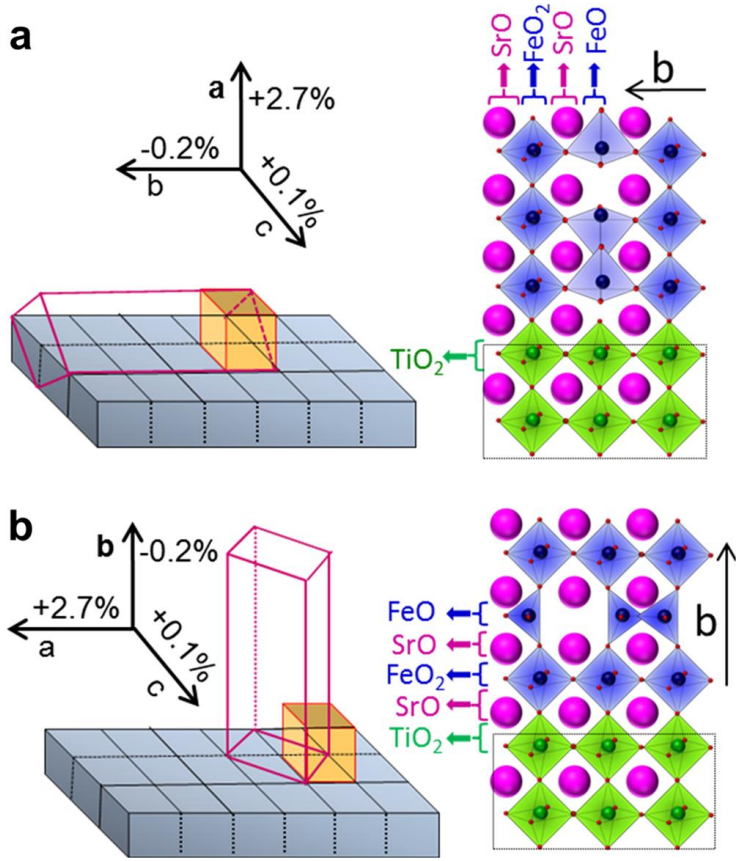


Figure 3.5: Schematic of a pseudomorphically strained lattice mismatched layer [7].

3D



Defect density

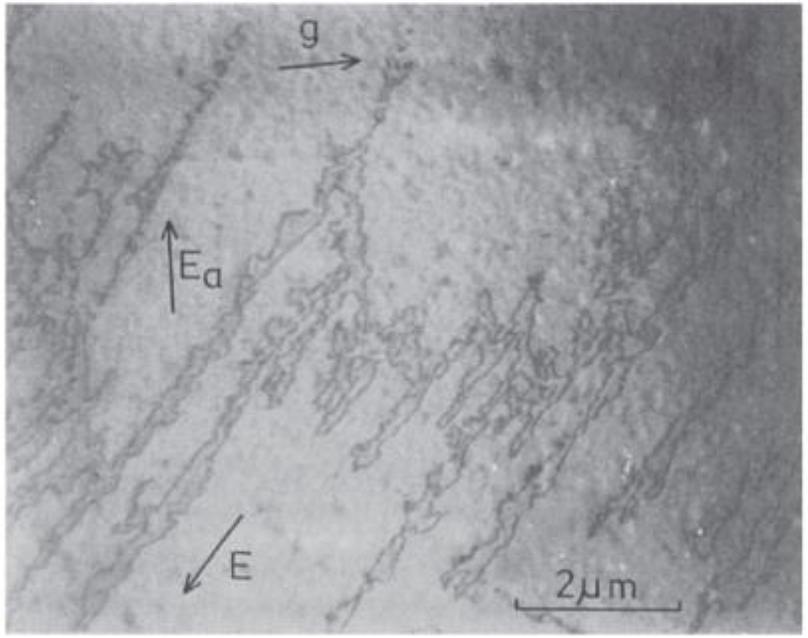


Figure 2. TEM image of a ⟨100⟩ DLD dislocation network in a plane parallel to the (001) growth surface of a GaAs laser. E indicates the [100] and Ea the [-1-10] crystal direction. Reprinted from [36] with the permission of Taylor and Francis Ltd (www.tandfonline.com).

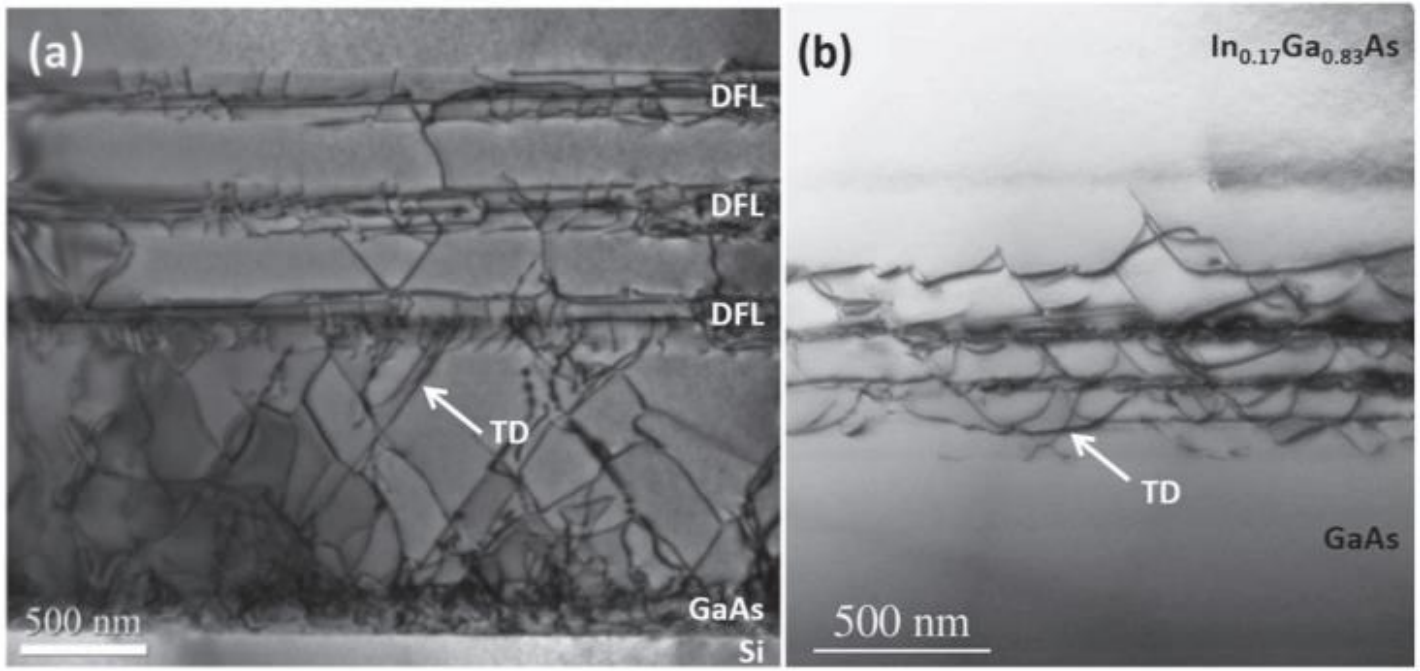
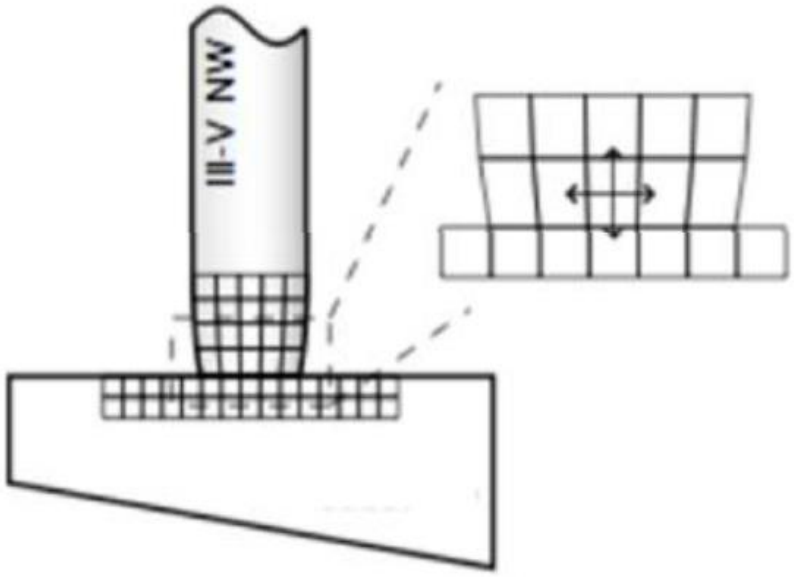


Figure 5. (a) is a bright field TEM image of GaAs deposited on a (001) Si substrate with 4° offcut containing three DFLs of InGaAs/GaAs SLSs © 2016 IEEE. Reprinted, with permission from [91]. (b) is a (002) two beam bright field TEM of an InGaAs graded buffer grown on a (001) Ge substrate with 6° offcut from [99].

DOI: 10.1088/1361-6641/aad655

Low dimensional materials



Low dimensional materials can have a different mechanical response due to their dimensionality or aspect ratio (i.e. Nanowires)

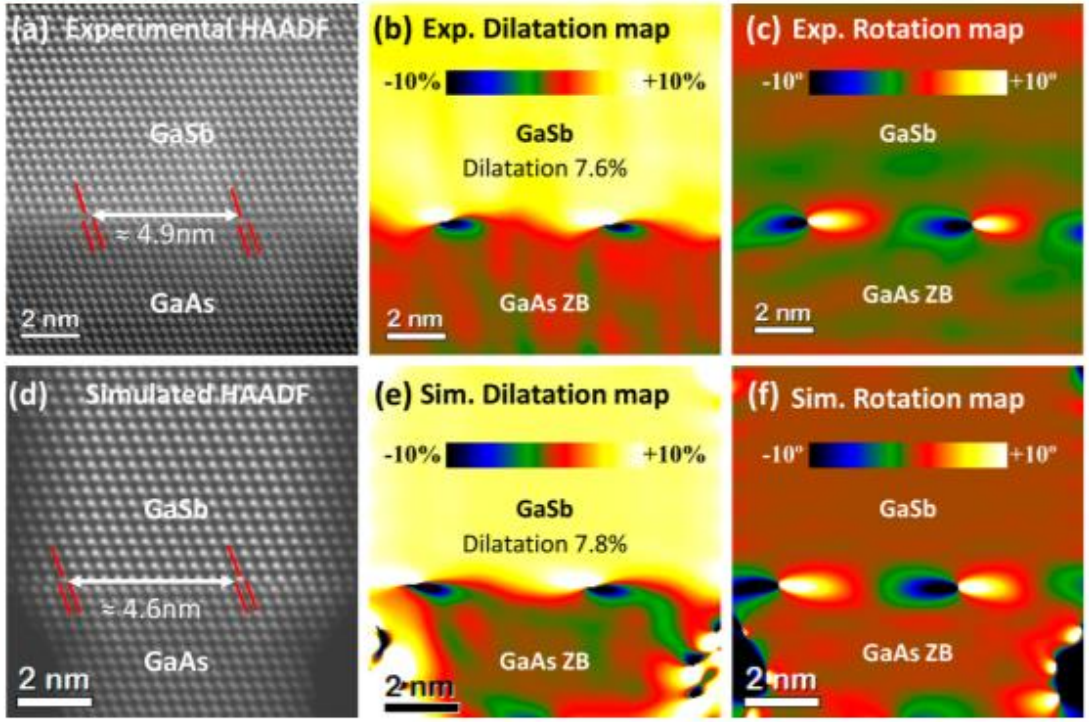


Figure 4. (a–c) Experimental data obtained at the GaAs/GaSb heterointerface. (a) HAADF image showing two misfit dislocations 4.9 nm apart. (b,c) Dilatation and rotation maps, respectively, obtained by performing GPA on the image in (a). (d–f) Simulated data on the GaAs/GaSb interface. (d) HAADF simulated image. (e,f) Simulated dilatation and rotation map, respectively, obtained by performing GPA on the image in (d).

dx.doi.org/10.1021/nl503273j | *Nano Lett.* 2014, 14, 6614–6620