

Nanostructures – density of states



Faculty of Physics UW
Jacek.Szczytko@fuw.edu.pl

Local density of states

Gęstość stanów (ogólnie) można zdefiniować jako:

$$N(E) = \sum_n \delta(E - \varepsilon_n)$$

Jak widać po scałkowaniu:

$$\int_{E_1}^{E_2} N(E) dE = \int_{E_1}^{E_2} \sum_n \delta(E - \varepsilon_n) dE = \sum_n \int_{E_1}^{E_2} \delta(E - \varepsilon_n) dE$$

Przykładowo:

$$N^{1D}(E) = \sum_k \delta(E - \varepsilon(k)) = \frac{1}{2\pi} \int \frac{1}{E'(k)} \delta(k - k') 2 dk = \frac{1}{\pi} \sqrt{\frac{2m}{E}}$$

$$N^{2D}(E) = \sum_k \delta(E - \varepsilon(k)) = \frac{1}{(2\pi)^2} \int \frac{1}{E'(k)} \delta(k - k') 2\pi k dk = \frac{m}{\pi \hbar^2}$$

$$N^{3D}(E) = \sum_k \delta(E - \varepsilon(k)) = \frac{1}{(2\pi)^3} \int \frac{1}{E'(k)} \delta(k - k') 4\pi k^2 dk = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}$$

Electrons statistics in crystals

The case of a semiconductor, in which both the electron gas and hole gas are far from the degeneracy:

the probability of filling of the electronic states:

$$f_e \approx e^{-\frac{E_G}{2k_B T} - \frac{E_e}{k_B T} + \frac{\xi}{k_B T}}$$

and of holes $f_h = 1 - f_e$

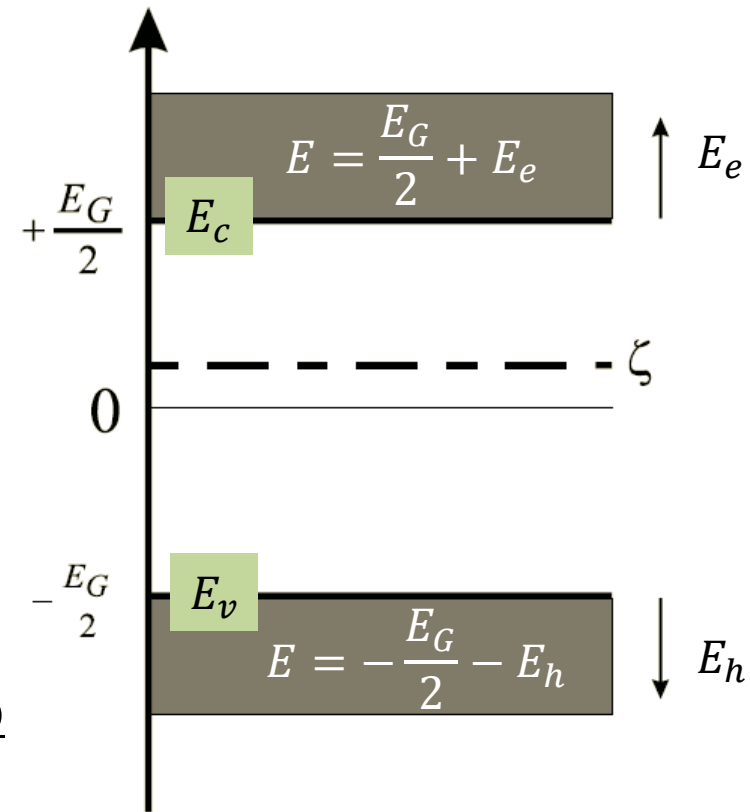
$$f_h \approx e^{-\frac{E_G}{2k_B T} - \frac{E_h}{k_B T} - \frac{\xi}{k_B T}}$$

$$\int_0^{\infty} \sqrt{x} e^{-x} dx = \frac{\sqrt{\pi}}{2}$$

Thus:

$$n(\xi) = 2 \left(\frac{m_e^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\frac{E_G}{2k_B T}} \cdot e^{\frac{\xi}{k_B T}} = N_c(T) e^{\frac{-(E_c - \xi)}{k_B T}}$$

$$p(\xi) = 2 \left(\frac{m_h^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\frac{E_G}{2k_B T}} \cdot e^{-\frac{\xi}{k_B T}} = N_v(T) e^{\frac{-(\xi - E_v)}{k_B T}}$$



Electrons statistics in crystals

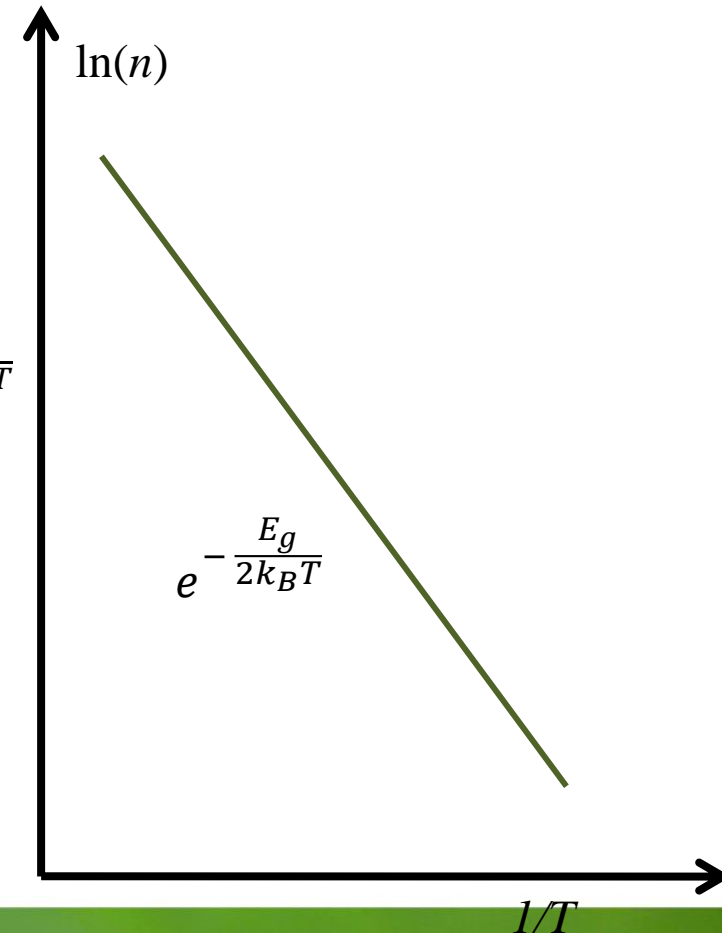
What is the concentration of carriers for $T > 0$?

In the thermodynamic equilibrium for an intrinsic semiconductors (*półprzewodniki samoistne*), the concentration of electrons in the conduction band is equal to the concentration of holes in the valence band (because they appear only as a result of excitation from the valence band).

$$n = p = n_i \text{ (an intrinsic case)}$$

$$n \cdot p = n_i^2 = 4 \left(\frac{k_B T}{2\pi \hbar^2} \right)^3 (m_e^* m_h^*)^{\frac{3}{2}} e^{-\frac{E_g}{k_B T}} = N_c N_v e^{-\frac{E_g}{k_B T}}$$

$$n = p = n_i = 2 \left(\frac{k_B T}{2\pi \hbar^2} \right)^{\frac{3}{2}} (m_e^* m_h^*)^{\frac{3}{4}} e^{-\frac{E_g}{2k_B T}} = \sqrt{N_c N_v} e^{-\frac{E_g}{2k_B T}}$$



Intrinsic carrier concentration

What is the concentration of carriers for $T > 0$?

In the thermodynamic equilibrium for an intrinsic semiconductors (*półprzewodniki samoistne*), the concentration of electrons in the conduction band is equal to the concentration of holes in the valence band (because they appear only as a result of excitation from the valence band).

$$n \cdot p = n_i^2 = 4 \left(\frac{k_B T}{2\pi \hbar^2} \right)^3 (m_e^* m_h^*)^{\frac{3}{2}} e^{-\frac{E_g}{k_B T}} = N_c N_v e^{-\frac{E_g}{k_B T}}$$

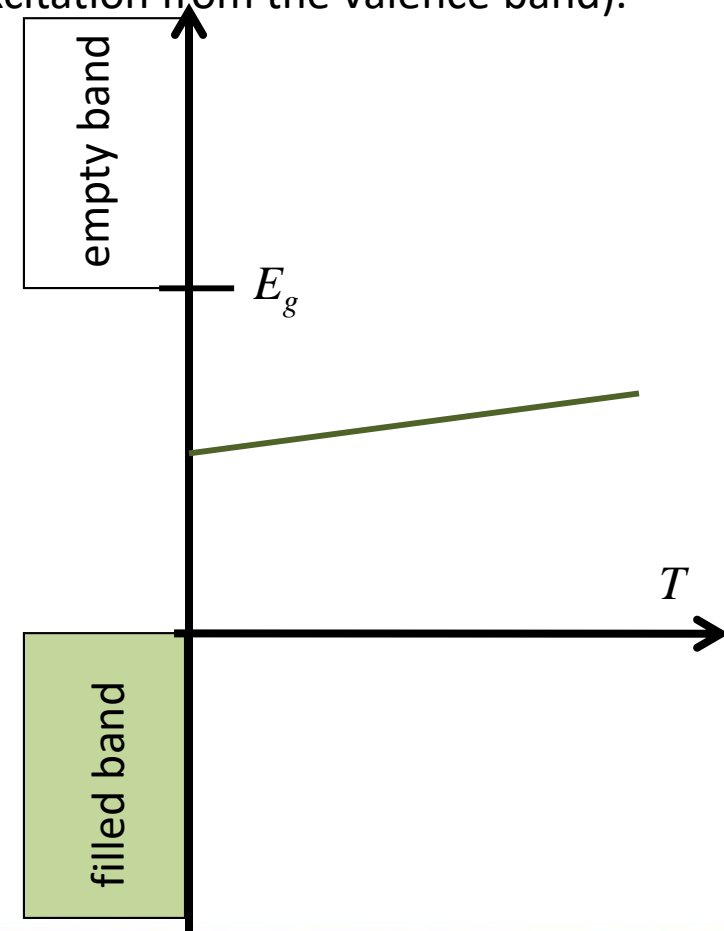
(general formula)

$$n = p = n_i \text{ (an intrinsic case)}$$

$$n = p = n_i = 2 \left(\frac{k_B T}{2\pi \hbar^2} \right)^{\frac{3}{2}} (m_e^* m_h^*)^{\frac{3}{4}} e^{-\frac{E_g}{2k_B T}} = \sqrt{N_c N_v} e^{-\frac{E_g}{2k_B T}}$$

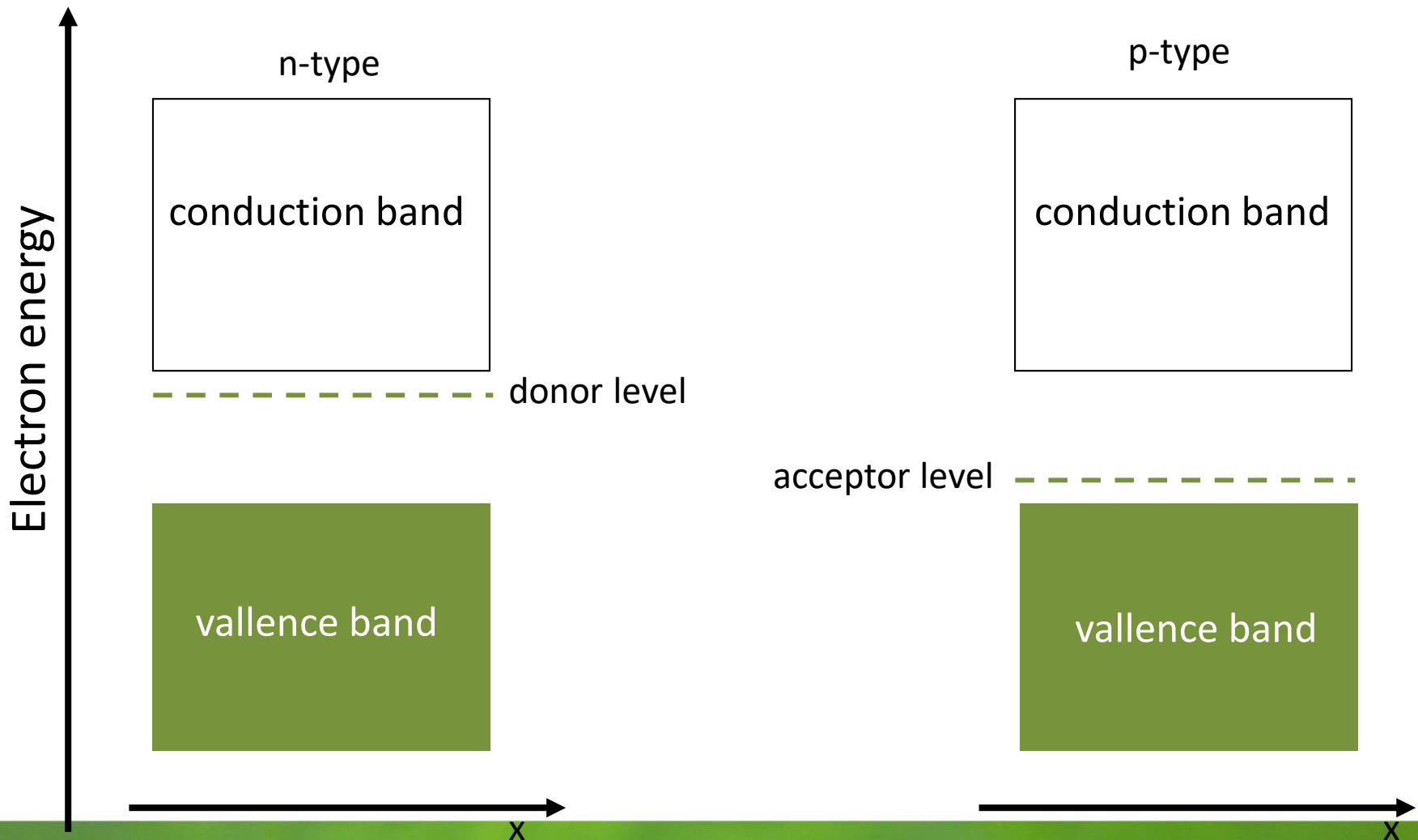
$$\frac{N_c}{N_v} = e^{\frac{2\xi - E_g}{k_B T}} \Rightarrow \xi = \frac{1}{2}(E_c + E_v) + \frac{3}{4}k_B T \ln \left(\frac{m_h^*}{m_e^*} \right)$$

in our notation the middle of the band is 0



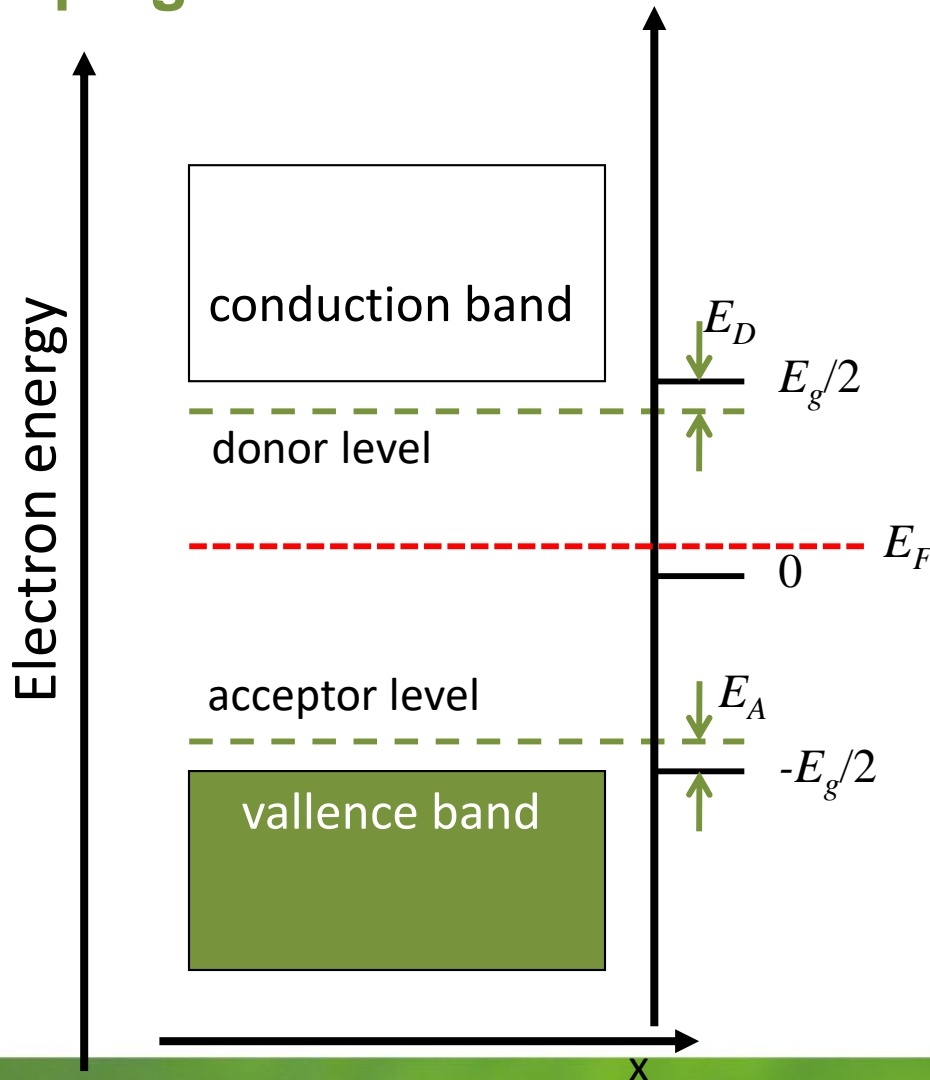
Dopants, impurities and defects

Hydrogen-like model – ionization of the dopant



Dopants, impurities and defects

Doping



The carrier concentration in extrinsic semiconductor (*niesamoistny*)

Consider a semiconductor, in which:

N_A – concentration of acceptors

N_D – concentration of donors

p_A – concentration of neutral acceptors

n_D – concentration of neutral donors

n_c – concentration of electrons in conduction band

p_v – concentration of holes in valence band

From the charge neutrality of the crystal:

$$n_c + (N_A - p_A) = p_v + (N_D - n_D)$$

$$n_c + n_D = (N_D - N_A) + p_v + p_A$$

The occupation of impurity levels

Occupation of impurity / defect levels in the thermodynamic equilibrium

„Occupation” of localized or band states means the exchange of particles (electrons) between the reservoir and considered subsystem (microstate).

The grand canonical ensemble (subsystem exchange particles and energy with the environment)

Thermodynamic probability (unnormalized) of finding subsystem in a state j , in which there are n_j particles (electrons) and which subsystem energy is E_j (the total energy of all n_j particles):

$$P_j = e^{-\beta(E_j - n_j \xi)}, \quad \beta = \frac{1}{k_B T}$$

ξ - chemical potential.

Statistical sum:

$$Z = \sum_j P_j = \sum_j e^{-\beta(E_j - n_j \xi)}$$

The occupation of impurity levels

Statistical sum :

$$Z = \sum_j P_j = \sum_j e^{-\beta(E_j - n_j \xi)}$$

Statistical means:

$$\langle A \rangle = \frac{\sum_j A_j \cdot e^{-\beta(E_j - n_j \xi)}}{\sum_j e^{-\beta(E_j - n_j \xi)}}$$

Examples:

free electron occupying (or not) the quantum state of the \vec{k} -vector and spin:
2 possible states of the subsystem (microstate):

$$n_0 = 0; E_0 = 0$$

$$n_1 = 1; E_1 = E \quad (\text{the occupation only for one spin state})$$

the average number of particles of the subsystem:

$$\langle n \rangle = \frac{0 \cdot e^0 + 1 \cdot e^{-\beta(E - \xi)}}{1 + e^{-\beta(E - \xi)}} = \frac{1}{e^{\beta(E - \xi)} + 1} = f(E, T)$$

(Fermi-Dirac distribution)

The occupation of impurity levels

Examples :

free electron occupying (or not) the quantum state of the \vec{k} -vector and ANY spin:
4 possible states of the subsystem (microstate):

$$n_0 = 0; E_0 = 0$$

$$n_1 = 1; E_1 = E \text{ (spin } \uparrow)$$

$$n_2 = 1; E_2 = E \text{ (spin } \downarrow)$$

$$n_3 = 2; E_3 = 2E \text{ (spin } \uparrow\downarrow)$$

the average number of particles of the subsystem:

$$\begin{aligned} \langle n \rangle &= \frac{0 \cdot e^0 + 1 \cdot e^{-\beta(E-\xi)} + 1 \cdot e^{-\beta(E-\xi)} + 2 \cdot e^{-\beta(2E-2\xi)}}{1 + e^{-\beta(E-\xi)} + e^{-\beta(E-\xi)} + e^{-\beta(2E-2\xi)}} = 2 \frac{e^{-\beta(E-\xi)} (1 + e^{-\beta(E-\xi)})}{(e^{-\beta(E-\xi)} + 1)^2} = \\ &= 2f(E, T) \end{aligned}$$

(Fermi-Dirac distribution x2)

The occupation of impurity levels

The ratio of the probability of finding dopant / defect of $n + 1$ electrons and of n electrons:

$$\frac{p_{n+1}}{p_n} = \frac{N_{n+1}/N_{total}}{N_n/N_{total}} = \frac{\sum_{j:n_j=n+1} e^{-\beta[E_j-(n+1)\xi]}}{\sum_{k;n_k=n} e^{-\beta[E_k-n\xi]}} = \frac{g_{n+1}}{g_n} \cdot e^{-\beta[(E_{n+1}-E_n)-\xi]}$$

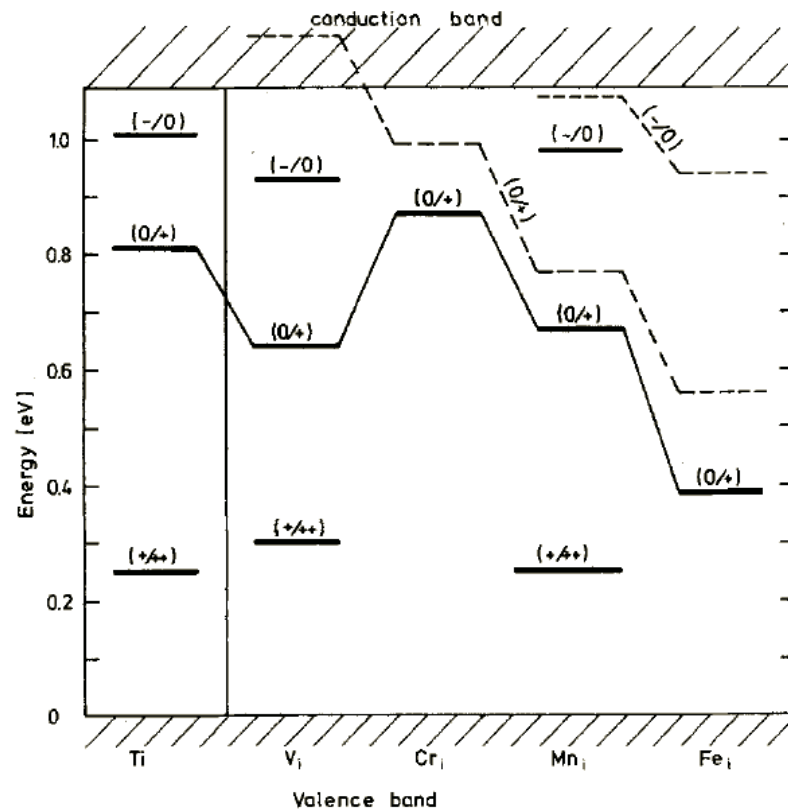


Fig. 15. Energy levels of interstitial 3d metals in silicon (full lines), see Table 3, compared with the results of X_α calculations of DeLeo et al. [15] (broken lines)

$\sum_n N_n = N$ – impurity (dopants) concentration

E_{n+1} i E_n – the lowest of all subsystem energies E_j with $n + 1$ and n electrons respectively

Successive impurity energy levels are filled with the increase of the Fermi level.

$E^{n+1/n}$ – so-called *energy level* of the impurity/defect „numbered” by charge states $n + 1$ and n

g_{n+1} , g_n – so-called degeneracy of states of subsystem of $n + 1$ and n electrons

The occupation of impurity levels

g_{n+1}, g_n – so-called degeneration of states of subsystem of $n + 1$ and n electrons.

The degeneracy g_{n+1} and g_n takes into account the possibility of the existence of different subsystem states corresponding to a same number of particles (including the excited states):

$$g_n = \alpha_{n,0} + \sum_{i=1,2,\dots} \alpha_{n,i} e^{-\beta \varepsilon_{n,i}}$$

$\alpha_{n,0}$ i $\alpha_{n,i}$ they are respectively: the degeneracies of the n -electronic ground state and its excited states of energies higher than the ground state by $\varepsilon_{n,i}$ (excitation energies)

Such defined degeneration g_n generally depends on temperature

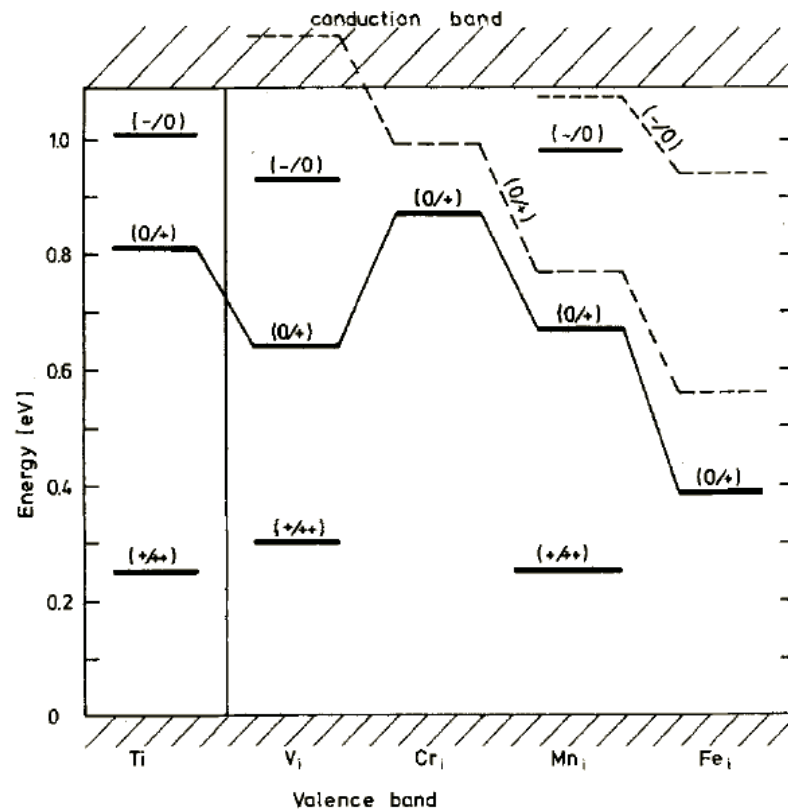


Fig. 15. Energy levels of interstitial 3d metals in silicon (full lines), see Table 3, compared with the results of X_α calculations of DeLeo et al. [15] (broken lines)

The occupation of impurity levels

Example – donor (we omit the excited states)

charge state (+) implemented in 1 way : $g_+ = 1$

charge state(0) implemented in 2 ways (spin \uparrow or \downarrow): $g_0 = 2$

the energy of the donor state $E^{0/+} = E_D$

Doping concentration of donors N_D

$$\frac{p_{n+1}}{p_n} = \frac{p_0}{p_+} = \frac{g_0}{g_+} \cdot e^{-\beta[E_D - \xi]}, \quad p_+ + p_0 = 1$$

The occupation probability of the donor state:

$$p_0 = \langle n \rangle = \frac{1}{1 + \frac{g_+}{g_0} \cdot e^{\beta[E_D - \xi]}} = \frac{1}{1 + \frac{1}{2} \cdot e^{\beta[E_D - \xi]}}$$

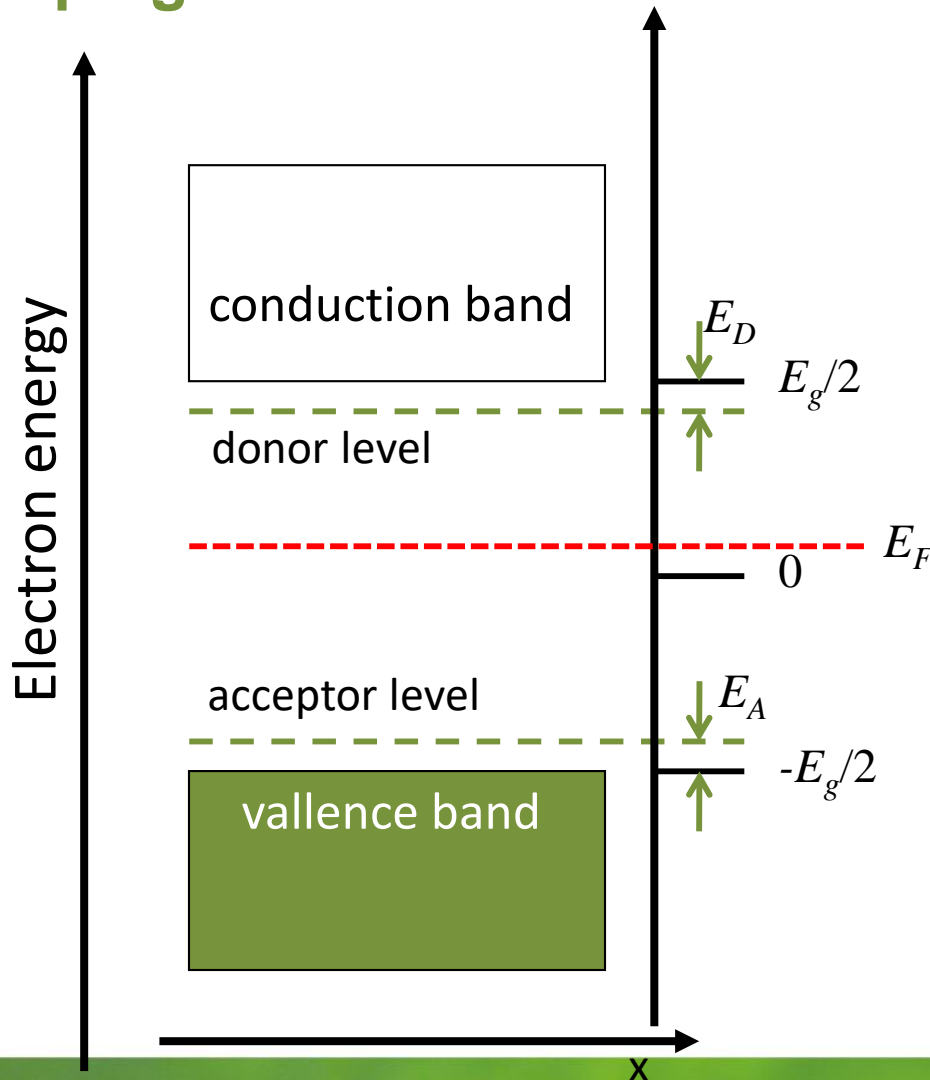
The concentration of occupied donor states (neutral donors are N_D^0)

$$N_D^0 = \frac{N_D}{1 + \frac{1}{2} \cdot e^{\beta[E_D - \xi]}}$$

TUTAJ 2017.04.10

Dopants, impurities and defects

Doping



The carrier concentration in extrinsic semiconductor (niesamoistny)

Consider a semiconductor, in which:

N_A – concentration of acceptors

N_D – concentration of donors

p_A – concentration of neutral acceptors

n_D – concentration of neutral donors

n_c – concentration of electrons in conduction band

p_v – concentration of holes in valence band

From the charge neutrality of the crystal:

$$n_c + (N_A - p_A) = p_v + (N_D - n_D)$$

$$n_c + n_D = (N_D - N_A) + p_v + p_A$$

The occupation of impurity levels

If both the donors and acceptors are shallow, and the electron and hole gas are not degenerated, then : $E_D - \xi \gg k_B T$, $\xi - E_A \gg k_B T$, $N_D^0 \ll N_D$, $N_A^0 \ll N_A$ (that is, virtually all impurities are ionized) .

$$\begin{cases} \Delta n = n - p \approx N_D - N_A \\ n \cdot p = n_i^2 \end{cases} \Rightarrow \begin{cases} n = \frac{1}{2} \left[\sqrt{(\Delta n)^2 + 4n_i^2} + \Delta n \right] \\ p = \frac{1}{2} \left[\sqrt{(\Delta n)^2 + 4n_i^2} - \Delta n \right] \end{cases}$$

If $\Delta n > 0$ (*n*-type semiconductor – for *p*-type is the same) and $\Delta n \gg n_i$, (at $T=300\text{K}$: $n_i(\text{Ge}) < 10^{13} \text{ cm}^{-3}$, $n_i(\text{Si}) < 10^{11} \text{ cm}^{-3}$, $n_i(\text{GaAs}) < 10^{10} \text{ cm}^{-3}$):

$$n \approx N_D - N_A$$

$$p \approx \frac{n_i^2}{N_D - N_A} = \frac{N_C(T) \cdot N_V(T)}{N_D - N_A} \cdot e^{-\frac{E_g}{k_B T}}$$

majority carrier concentration is determined by the effective concentration of impurities, the concentration of minority carriers may be very small (e.g. Si).

The occupation of impurity levels

Compensation

compensated semiconductors - containing both donors and acceptors

At appropriately high temperatures majority carrier concentration given by the effective concentration of dopants $|N_D - N_A|$

the concentration of scattering centers (charges): $N_D + N_A$

compensation ratio - the ratio of impurity concentration: minority to majority. It is a measure of the total number of ionized impurities :

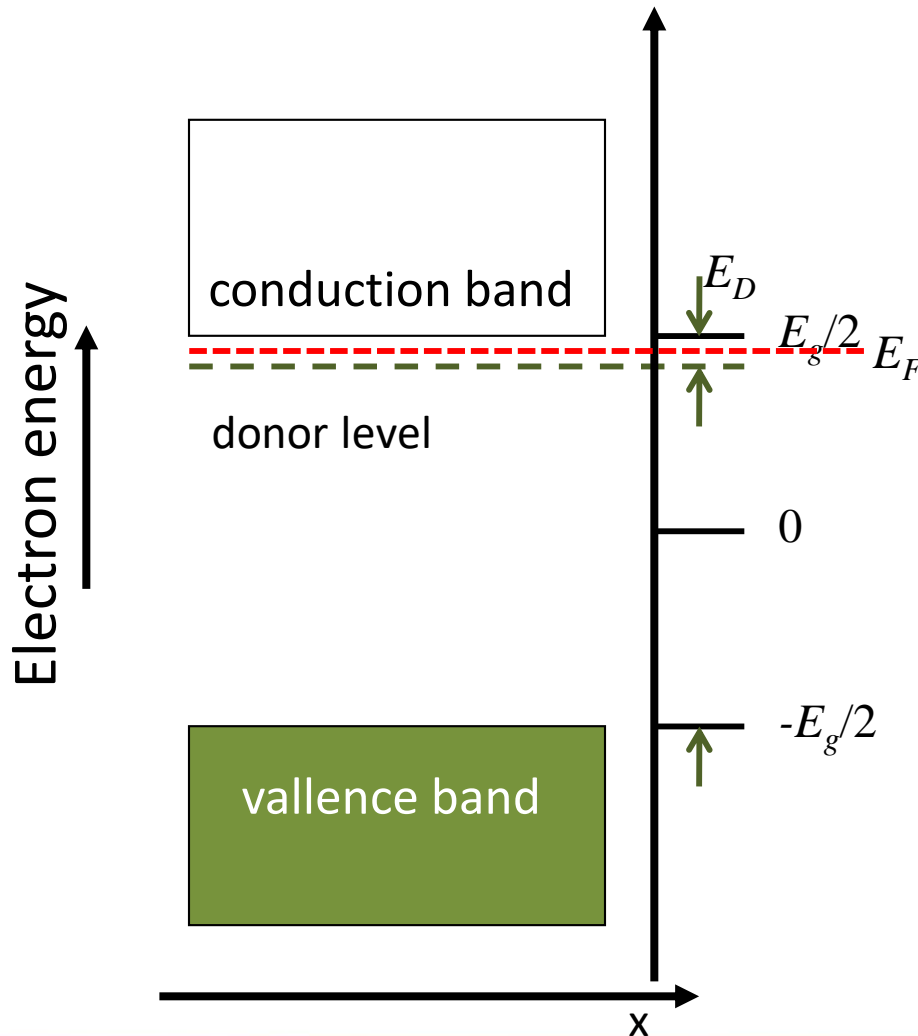
$$k = \frac{N_A}{N_D} - \text{for } n\text{-type}$$

$$k = \frac{N_D}{N_A} - \text{for } p\text{-type}$$

in highly compensated semiconductors ($k \approx 1$) strong electrostatic potential fluctuations are present – originating from the impurities, the disorder localization, the percolation effects etc.

The occupation of impurity levels

Equation of Charge Neutrality



low temperature,
thermal ionization of impurities

Consider a semiconductor, in which:

$N_A \approx 0$ – ~~concentration of acceptors~~

N_D – concentration of donors

p_A – concentration of neutral acceptors

n_D – concentration of neutral donors

n_c – concentration of electrons in conduction band

$p_v \approx 0$ – ~~concentration of holes in valence band~~

From the charge neutrality of the crystal:

$$n = N_D - N_D^0$$

The occupation of impurity levels

Now, a large part of donors will be neutral (the energies calculated from the bottom of the conduction band)

$$N_D - N_D^0 = N_D - \frac{N_D}{1 + \frac{1}{2} \cdot e^{\beta[E_D - \xi]}} = \dots = \frac{N_D}{2} \cdot e^{\beta[E_D - \xi]}$$

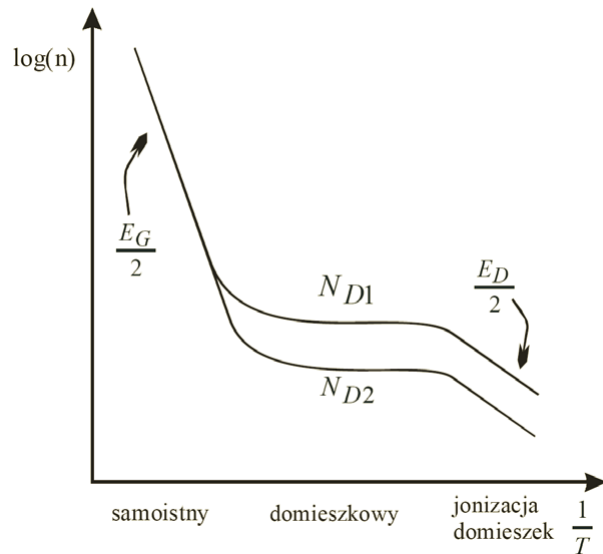
to calculate the occupation of the conduction band we use the Boltzmann distribution :

$$n = 2 \left(\frac{m_e^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{\frac{\xi - E_C}{k_B T}} = N_C(T) \cdot e^{\frac{\xi}{k_B T}}$$

Having $n = N_D - N_D^0$ we got:

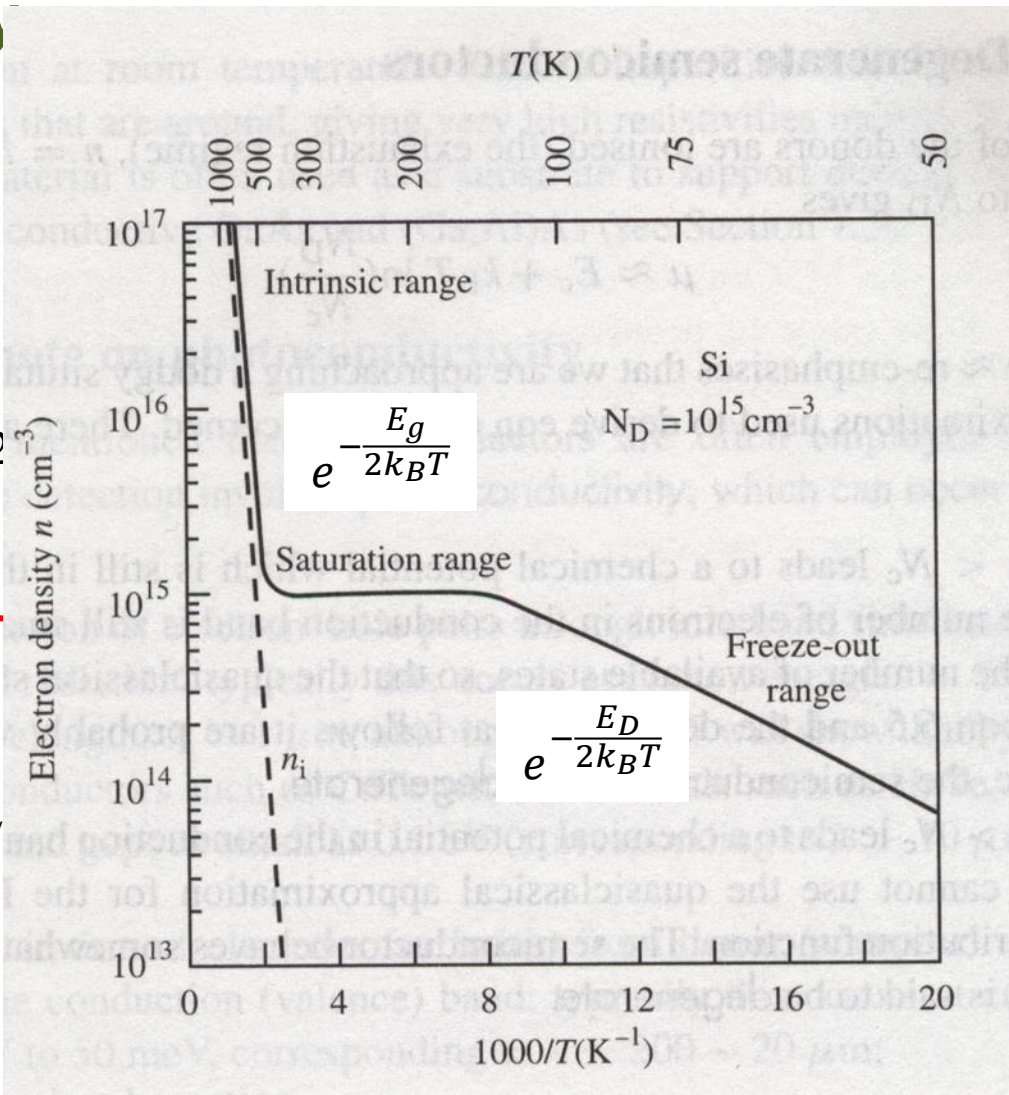
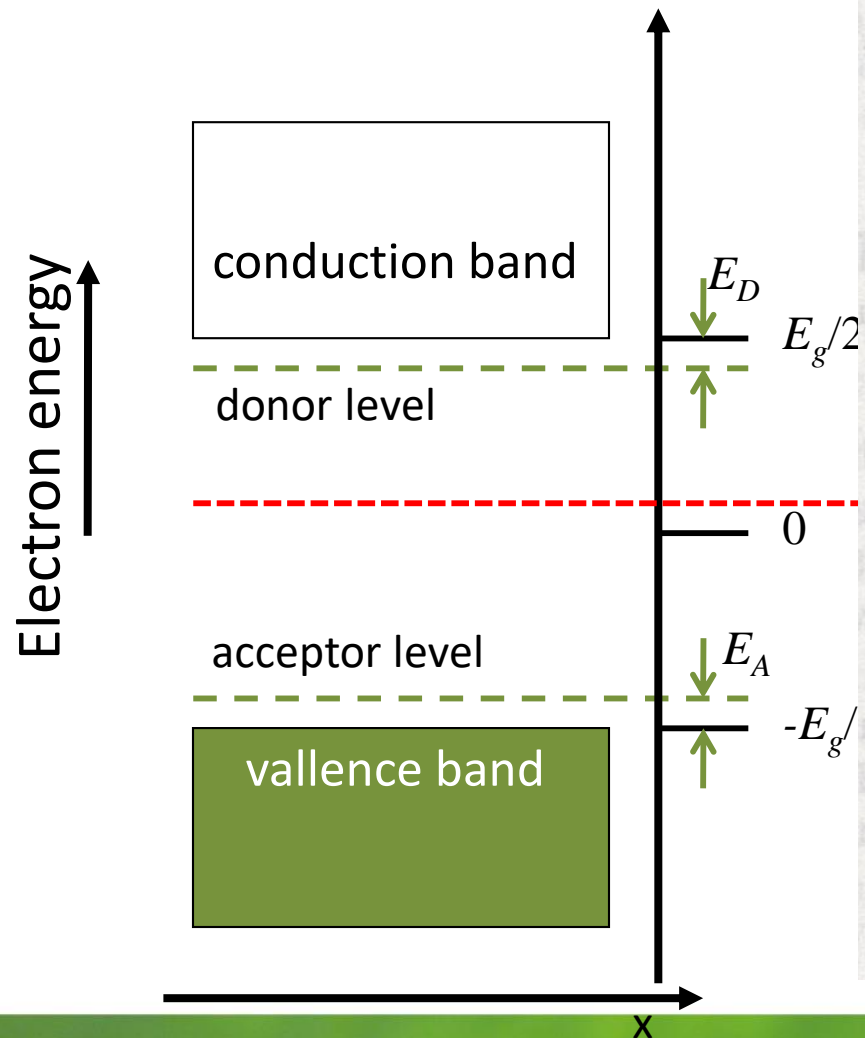
$$\xi = \frac{E_D}{2} + \frac{k_B T}{2} \ln \left(\frac{N_D}{2N_C(T)} \right)$$

$$n(T) = \sqrt{\frac{N_C(T) \cdot N_D}{2}} \cdot e^{\frac{E_D}{2k_B T}}$$



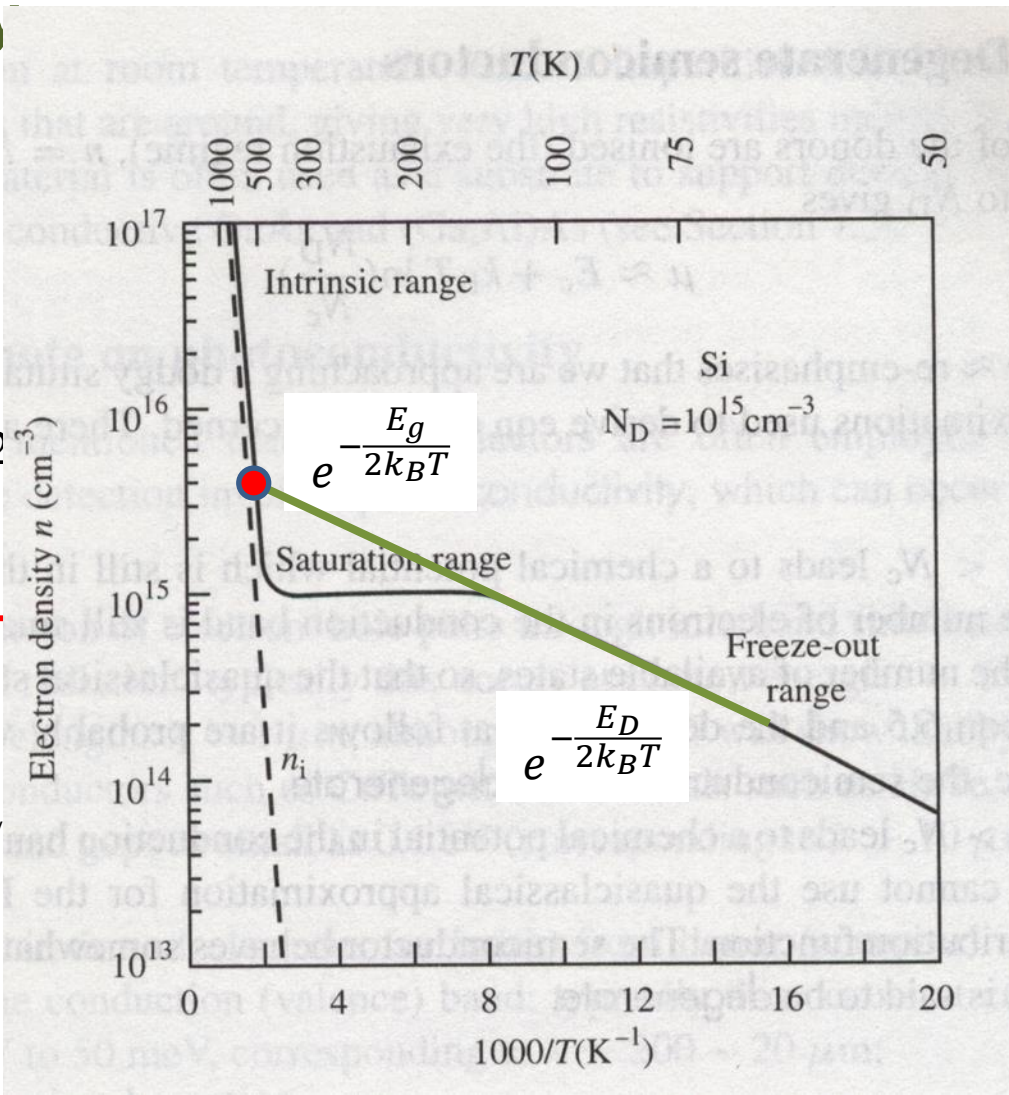
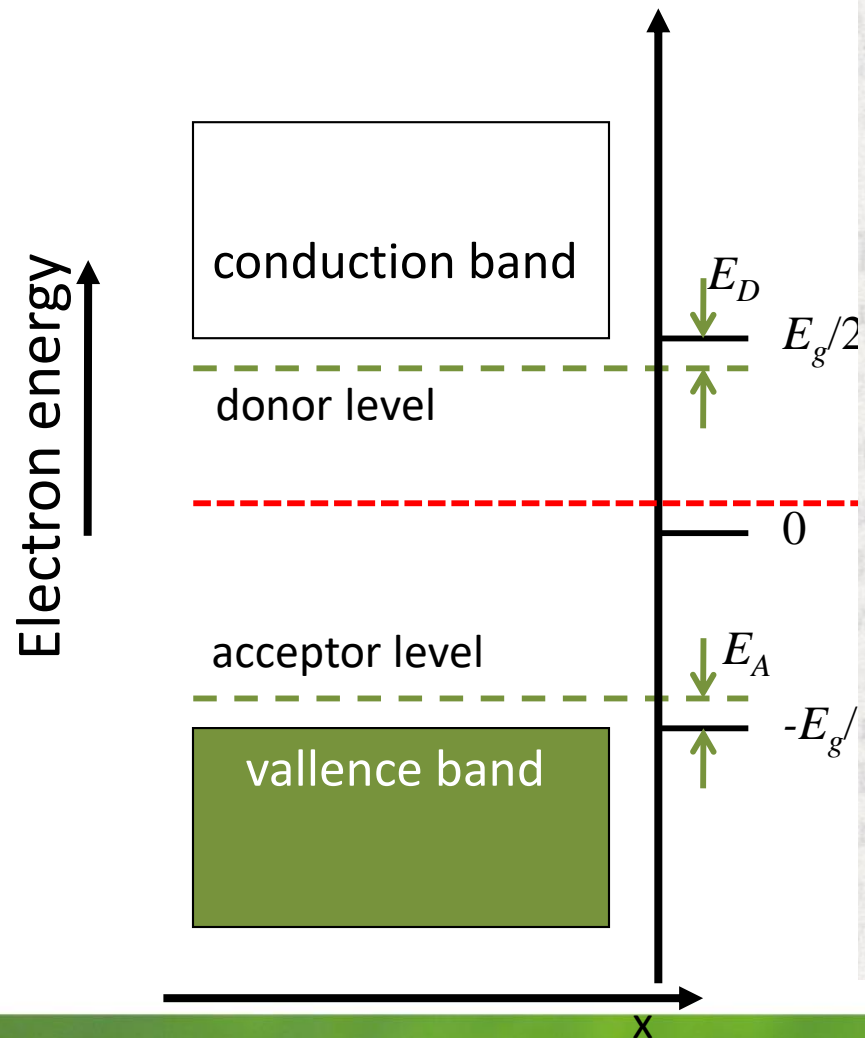
Dopants, impurities and defects

Equation of Charge Neutrality



Dopants, impurities and defects

Equation of Charge Neutrality



The occupation of impurity levels

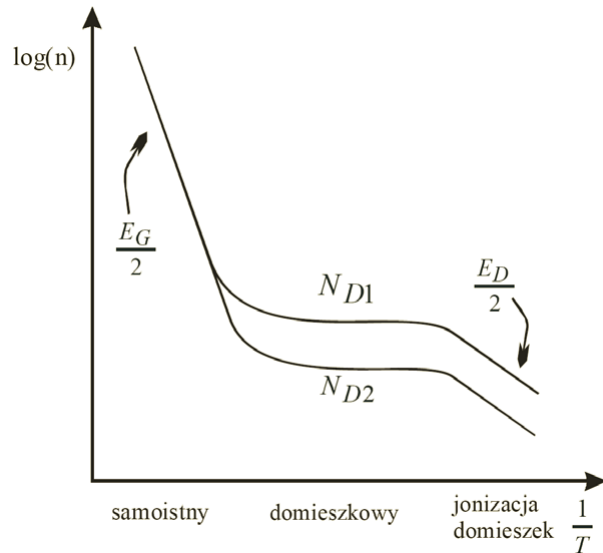
For compensated semiconductors the thermal activation energy at low temperature is E_D , not $\frac{E_D}{2}$

If there is a lot of impurities, also the wave functions of electrons bound to them overlap - ionization energies decrease, formed the **impurity band**.

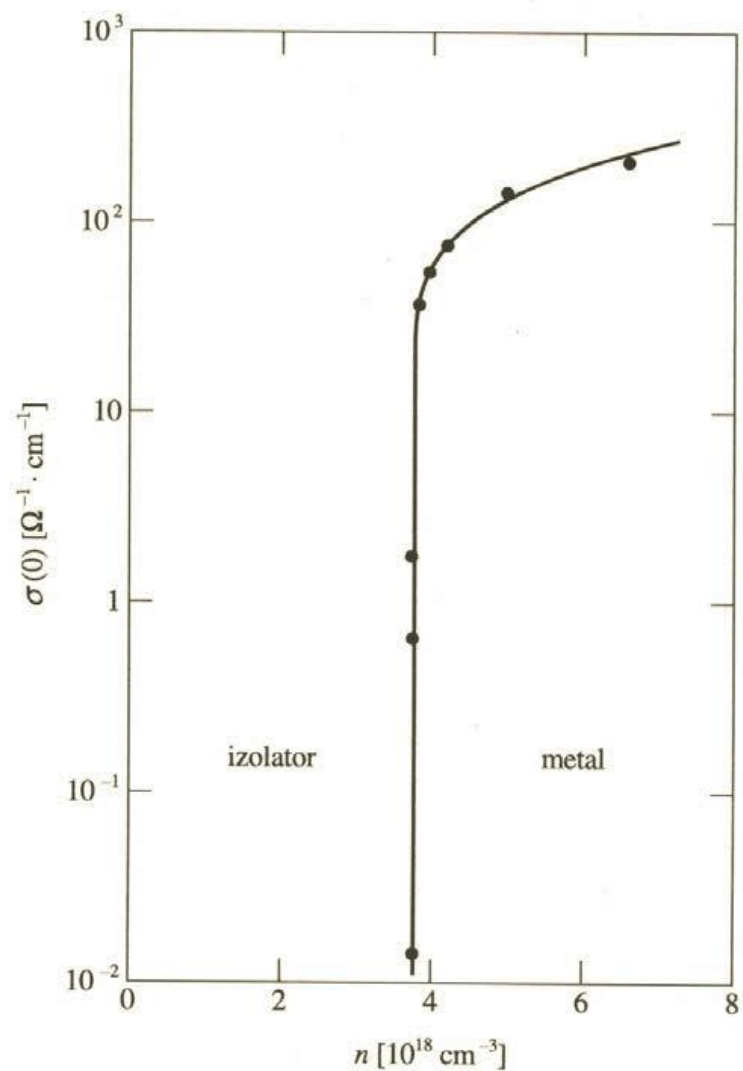
When impurity concentration is of the order of:

$$a_B^* \cdot (N_D)^{\frac{1}{3}} \approx 0.26$$

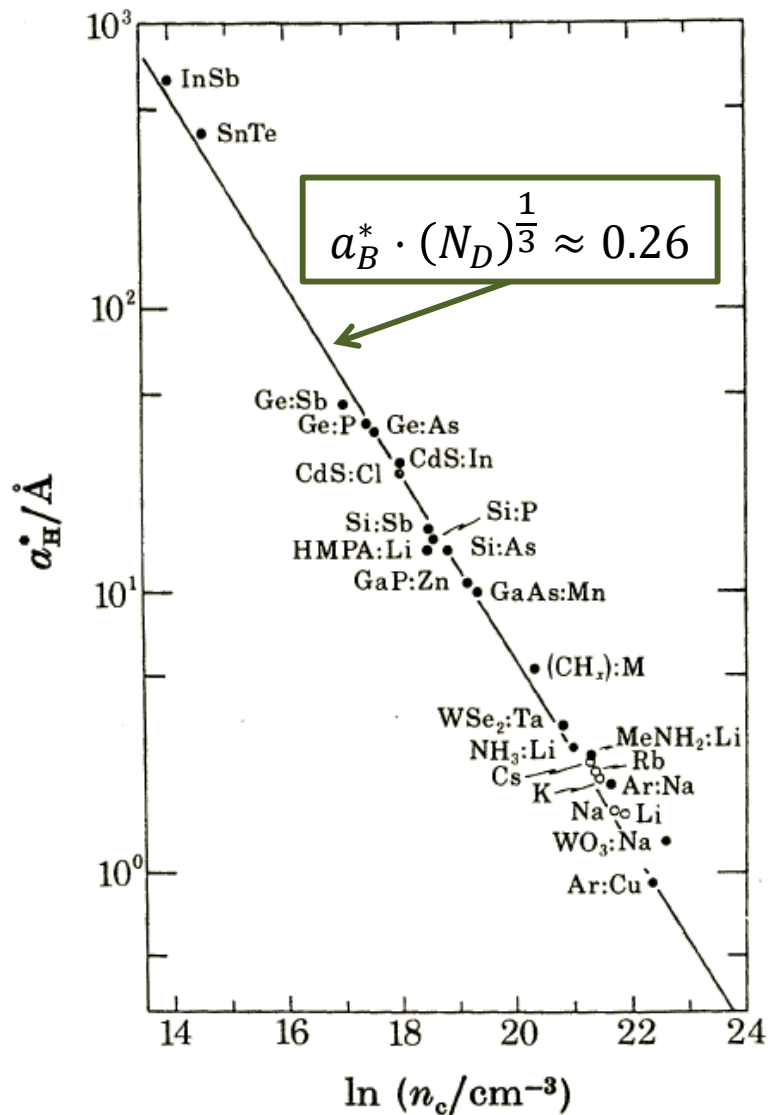
there is a nonmetal - metal phase transition (**Mott transition**)



The occupation of impurity levels

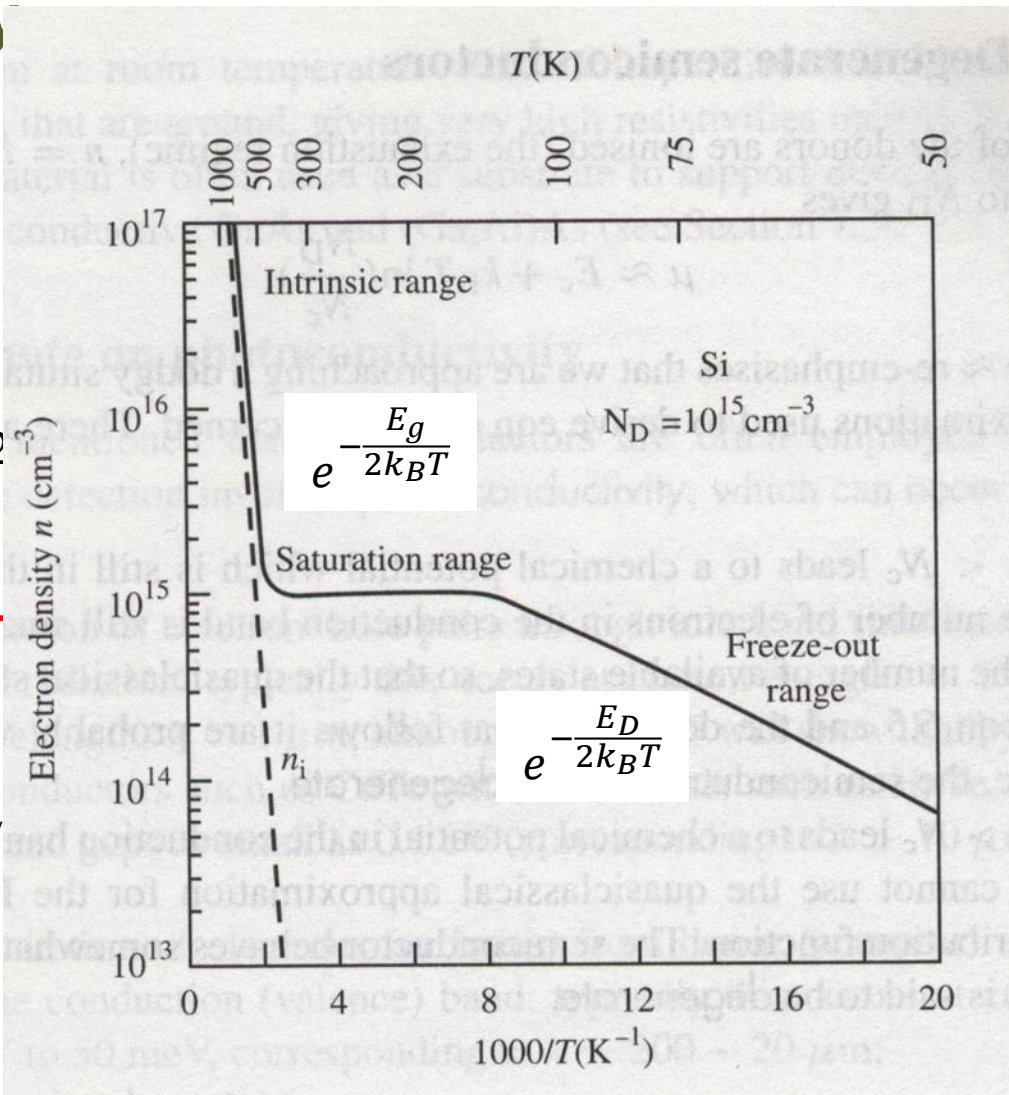
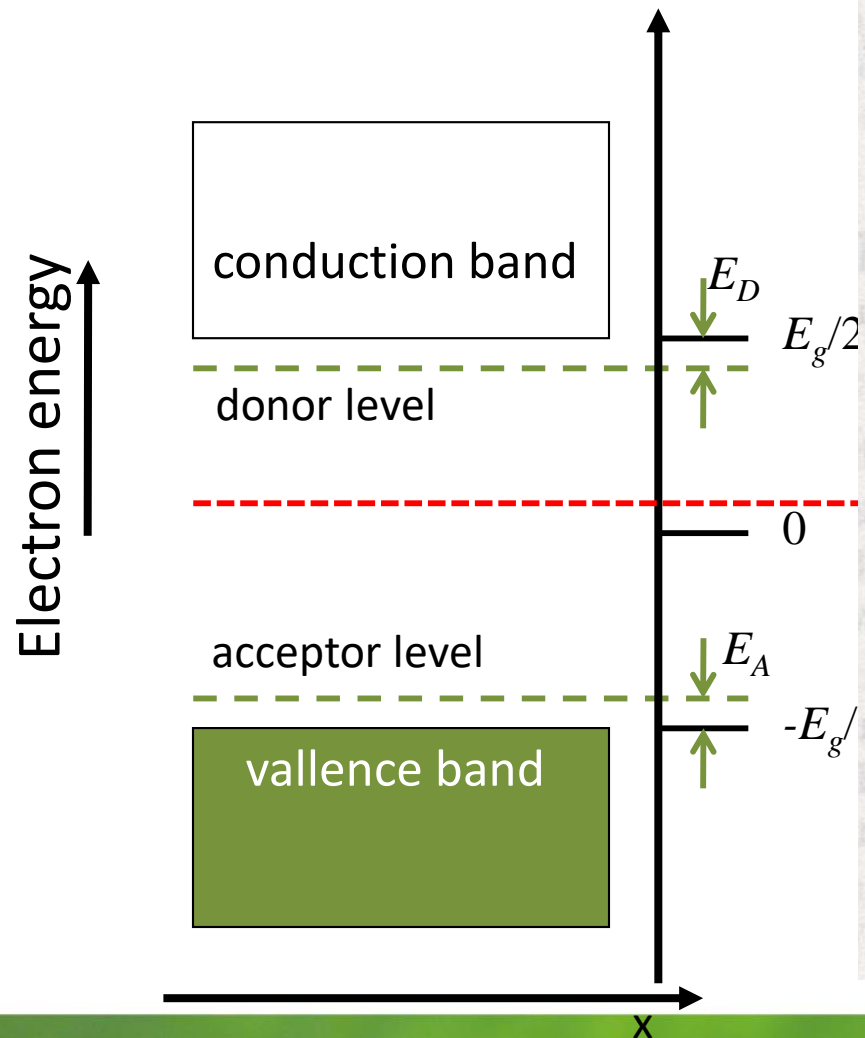


P.P. Edwards, M.J. Sienko, *J. Am. Chem. Soc.* **103**, 2967 (1981)



Dopants, impurities and defects

Equation of Charge Neutrality



Quasi-Fermi level (imref)

What happens if there is no equilibrium?

The problem is much more complicated, requires statistical analysis, but one can introduce a very useful concept of "quasi Fermi level" close to the equilibrium.

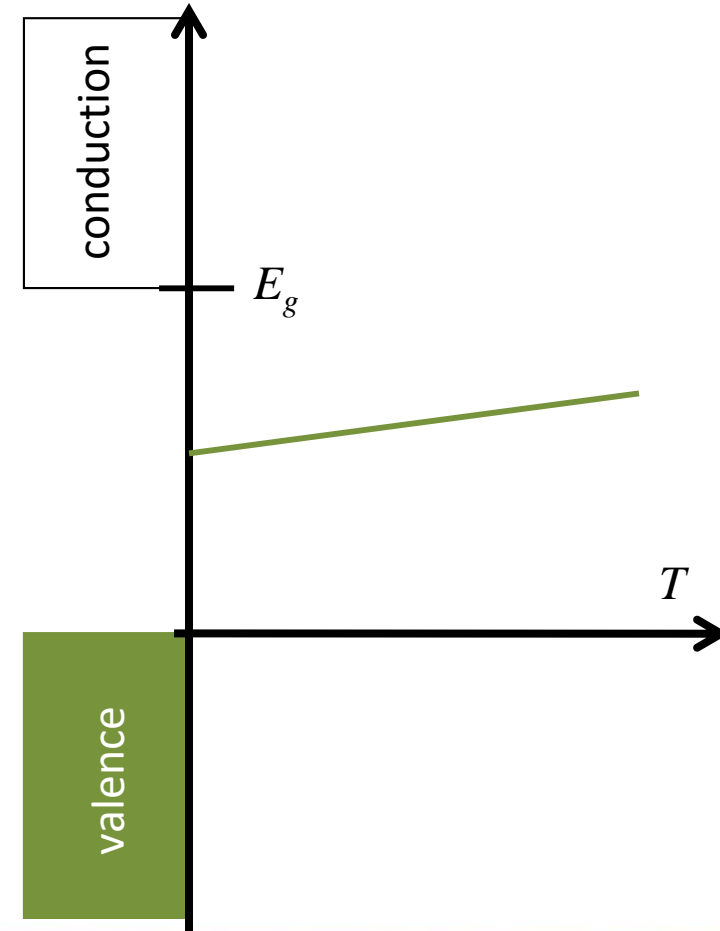
$$np > n_i^2$$

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

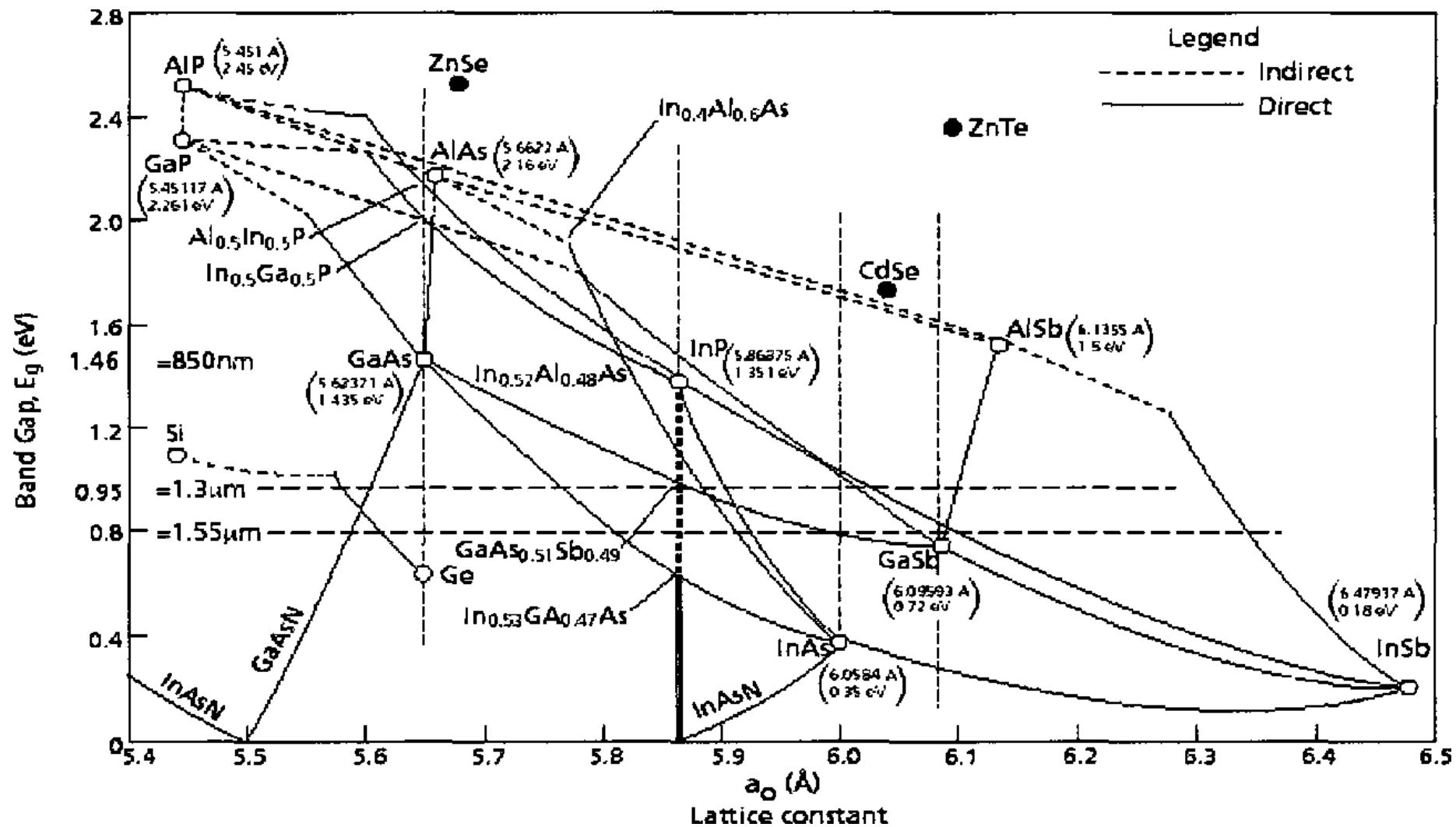
$$p = N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right)$$

$$E_F^n = E_c + k_B T \ln \frac{n}{N_c}$$

$$\frac{N_c}{N_v} = e^{\frac{2E_F - E_g}{k_B T}} \Rightarrow E_F = \frac{1}{2}(E_c + E_v) + \frac{3}{4}k_B T \ln\left(\frac{m_h^*}{m_e^*}\right)$$



Semiconductor heterostructures



Investigation of high antimony-content gallium arsenic nitride-gallium arsenic antimonide heterostructures for long wavelength application

Bandgap engineering

Valence band offset

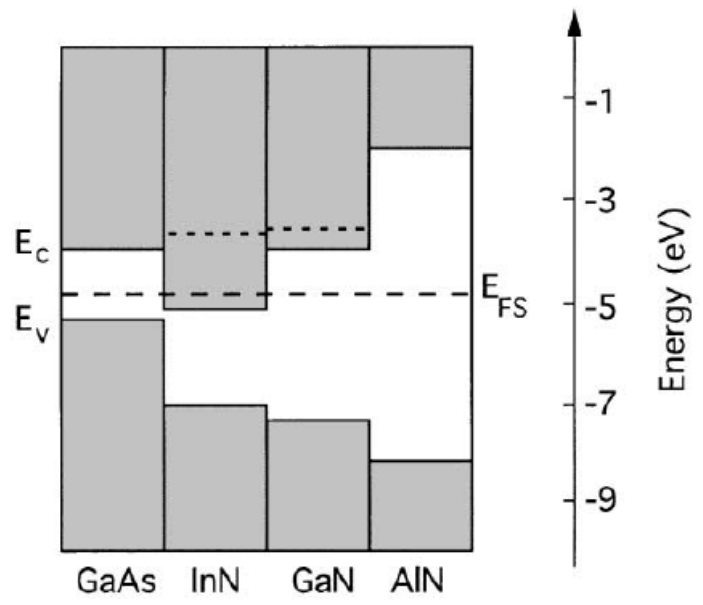


Fig. 4. Band offsets for group III-Nitrides. The dashed lines represent the Fermi energy for the maximum achievable free electron concentration in GaN and InN.

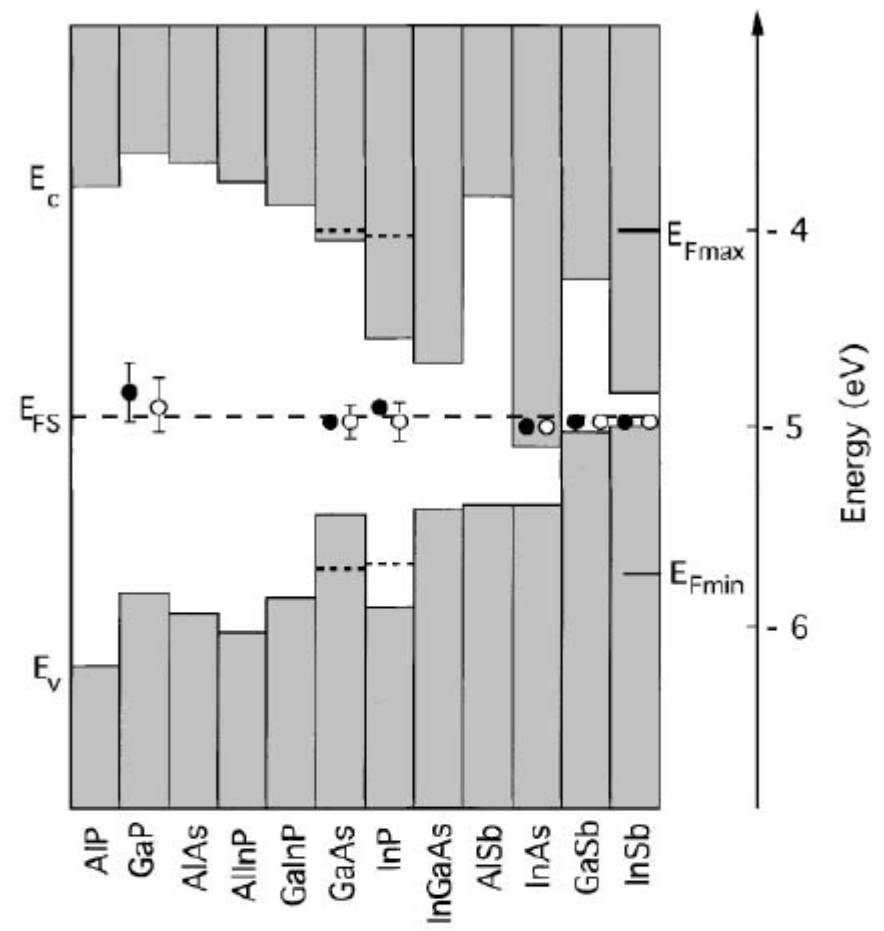
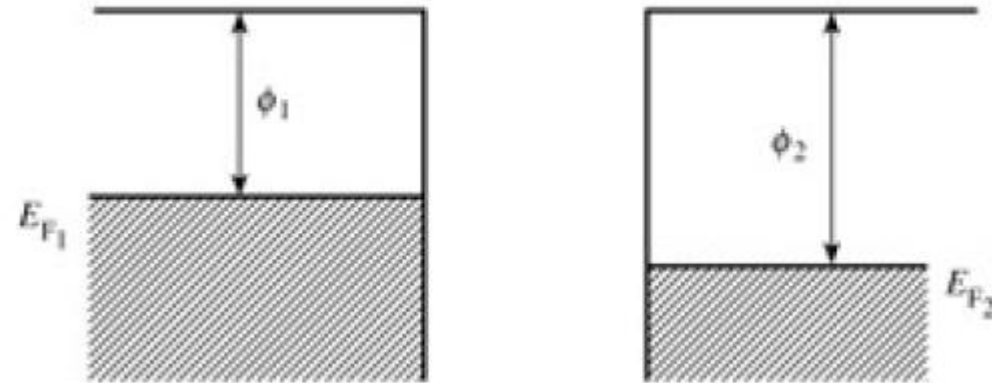


Fig. 1. Band offsets and the Fermi level stabilization energy (E_{FS}) in III-V compounds. The energy is measured relative to the vacuum level. The filled circles represent stabilized Fermi energies in heavily damaged materials, exposed to high energy radiation. The open circles correspond to the location of the Fermi energy on pinned semiconductor surfaces and at metal/semiconductor interfaces. The dashed lines show the location of the Fermi energy for a maximum equilibrium n- and p-type doping in GaAs and InP.

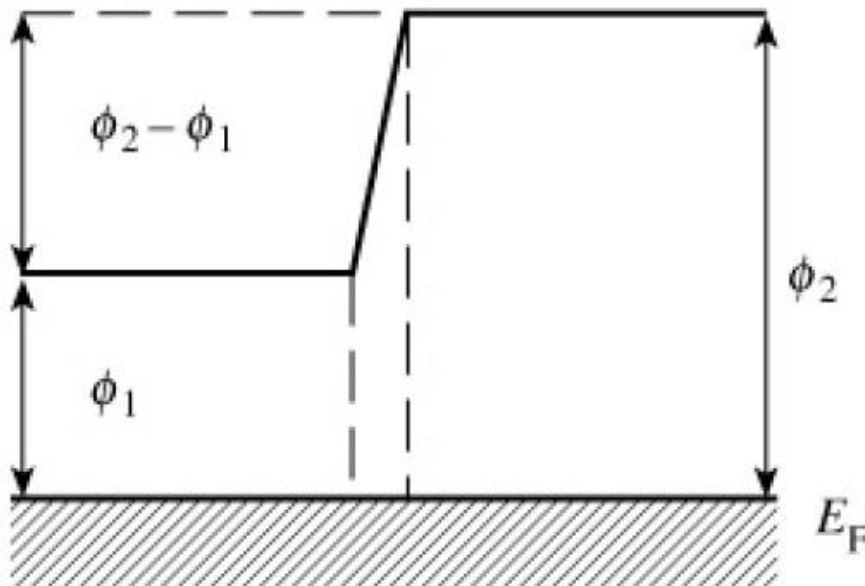
Walukiewicz Physica B 302-303 (2001) 123-134

The construction of energy band diagrams

Złącze metal-metal



Suppose, that $\phi_2 - \phi_1 \approx 1 \text{ eV}$
 Estimate the number of electrons that pass from one metal to another to create equilibrium potential difference. Assume that the distance between the metals is $5 \times 10^{-10} \text{ m}$.



Electric field: $E = \frac{\Delta\phi}{d} = 2 \times 10^9 \frac{\text{V}}{\text{m}}$

The surface charge: $\sigma = \epsilon_0 E$

The concentration: $n^{2D} = \frac{\sigma}{e} = 1.12 \times 10^{13} \text{ cm}^{-2}$

The concentration in metal

$$n^{3D} = 5 \times 10^{22} \text{ cm}^{-3}$$

$$n^{2D} = 1.5 \times 10^{15} \text{ cm}^{-2}$$

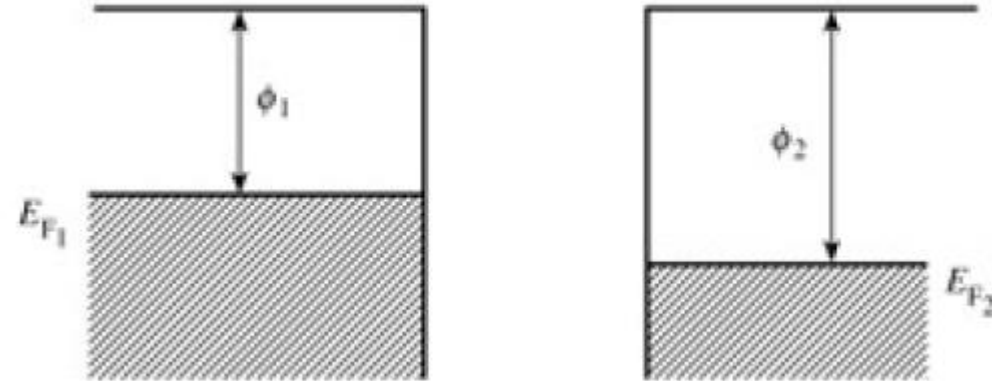
Within the width of 1 lattice parameter ~1% of charge

Electrical properties of materials Solymar, Walsh (6.11)

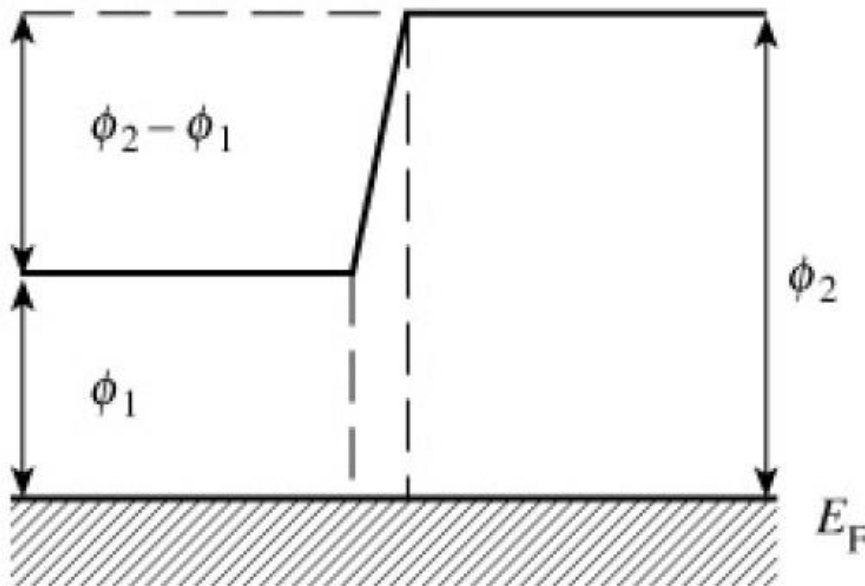
Pg. 143

The construction of energy band diagrams

Złącze metal-metal



Suppose, that $\phi_2 - \phi_1 \approx 1 \text{ eV}$
 Estimate the number of electrons that pass from one metal to another to create equilibrium potential difference. Assume that the distance between the metals is $5 \times 10^{-10} \text{ m}$.



Electric field: $E = \frac{\Delta\phi}{d} = 2 \times 10^9 \frac{\text{V}}{\text{m}}$

The surface charge: $\sigma = \epsilon_0 E$

The concentration: $n^{2D} = \frac{\sigma}{e} = 1.12 \times 10^{13} \text{ cm}^{-2}$

The concentration in metal

$n^{3D} = 5 \times 10^{22} \text{ cm}^{-3}$

$n^{2D} = 1.5 \times 10^{15} \text{ cm}^{-2}$

Within the width of 1 lattice parameter ~1% of charge

Electrical properties of materials Solymar, Walsh (6.11)

Pg. 143

The doping of semiconductors

From the Maxwell equations:

$$\nabla \vec{D} = \rho_s - \text{net charge density}$$

$$\vec{E} = -\nabla \phi = -\nabla U$$

$$\nabla \vec{D} = \epsilon_0 \epsilon \nabla \vec{E} = -\epsilon_0 \epsilon \nabla^2 \phi \stackrel{\text{def}}{=} -\epsilon \Delta U = \rho_s$$

Charge conservation

$$eN_A x_p = eN_D x_n = Q$$

Poisson equation:

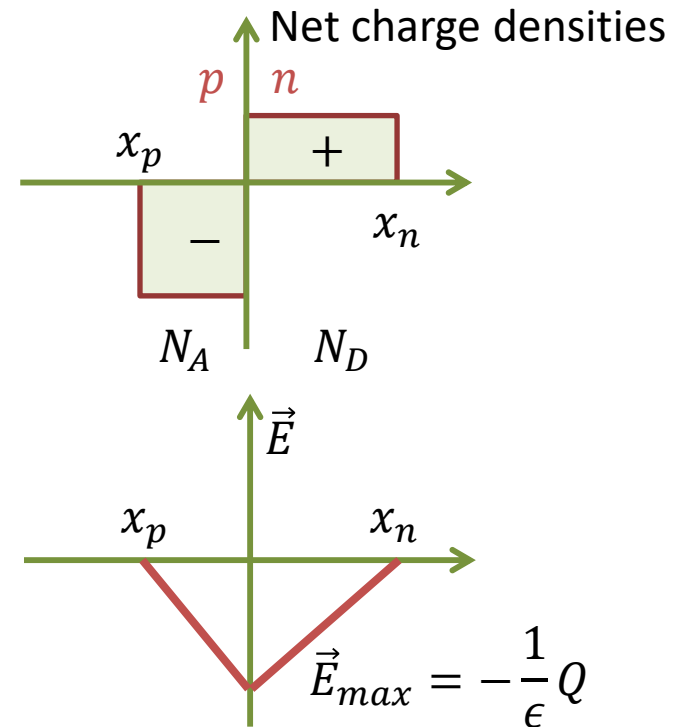
$$\frac{d^2 U}{dx^2} = -\frac{1}{\epsilon} \rho_s = \frac{1}{\epsilon} eN_A$$

Thus the electric field in the range $(x_p, 0)$:

$$\vec{E} = -\frac{dU}{dx} = \frac{1}{\epsilon} eN_A (x + C) = \frac{1}{\epsilon} eN_A (x - x_p)$$

Similarly for $(0, x_n)$:

$$\vec{E} = -\frac{dU}{dx} = \frac{1}{\epsilon} eN_D (x + C) = \frac{1}{\epsilon} eN_D (x - x_n)$$



The doping of semiconductors

Thus the electric field in the range $(x_p, 0)$:

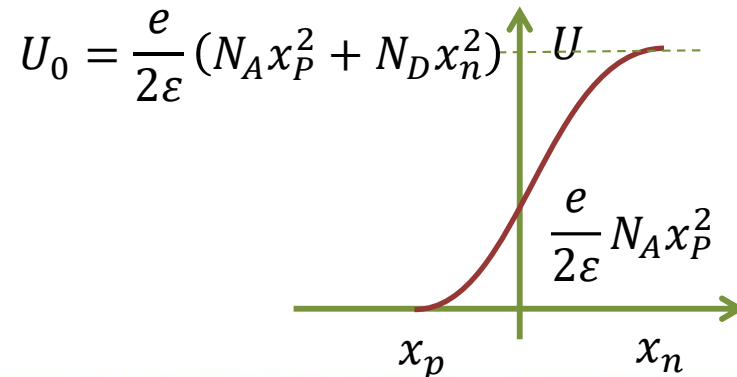
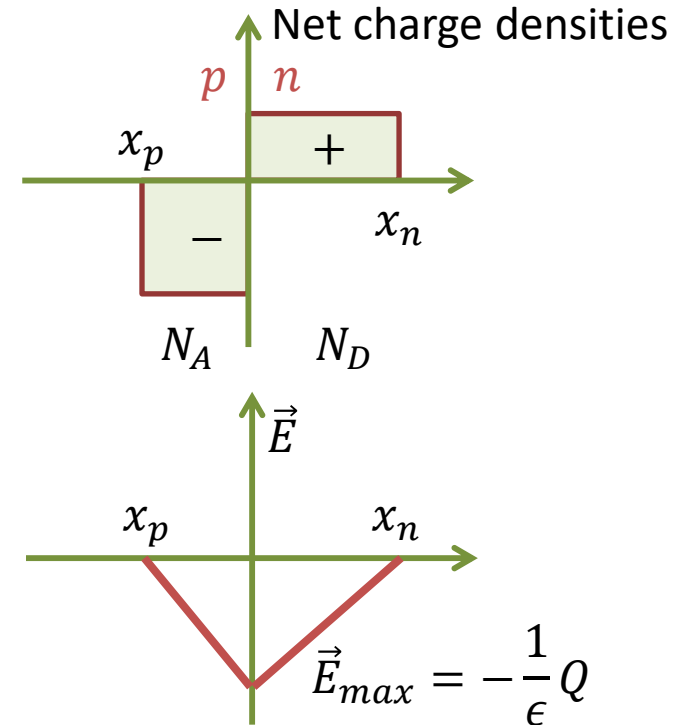
$$\vec{E}_A = -\frac{dU}{dx} = \frac{1}{\epsilon} e N_A (x + C) = \frac{1}{\epsilon} e N_A (x - x_p)$$

Similarly for $(0, x_n)$:

$$\vec{E}_D = -\frac{dU}{dx} = \frac{1}{\epsilon} e N_D (x + C) = \frac{1}{\epsilon} e N_D (x - x_n)$$

$$U = -\int_{x_p}^0 E_A dx \quad x < 0$$

$$U = -\int_0^{x_n} E_D dx \quad x > 0$$



The built-in voltage in the pn -junction

$$U_0 = U(x_n) - U(x_p) = \frac{e}{2\epsilon} (N_A x_p^2 + N_D x_n^2)$$

The doping of semiconductors

Charge conservation

$$eN_A x_p = eN_D x_n = Q$$

The total width of the depletion region w

$$w = x_n - x_p = \sqrt{\frac{2\epsilon U_0}{e(N_A + N_D)}} \left(\sqrt{\frac{N_A}{N_D}} + \sqrt{\frac{N_D}{N_A}} \right)$$

If, say, $N_A \gg N_D$ (p -type doping)

then:

$$w = \sqrt{\frac{2\epsilon U_0}{eN_D}} \quad \text{i} \quad |x_n| > |x_p|$$

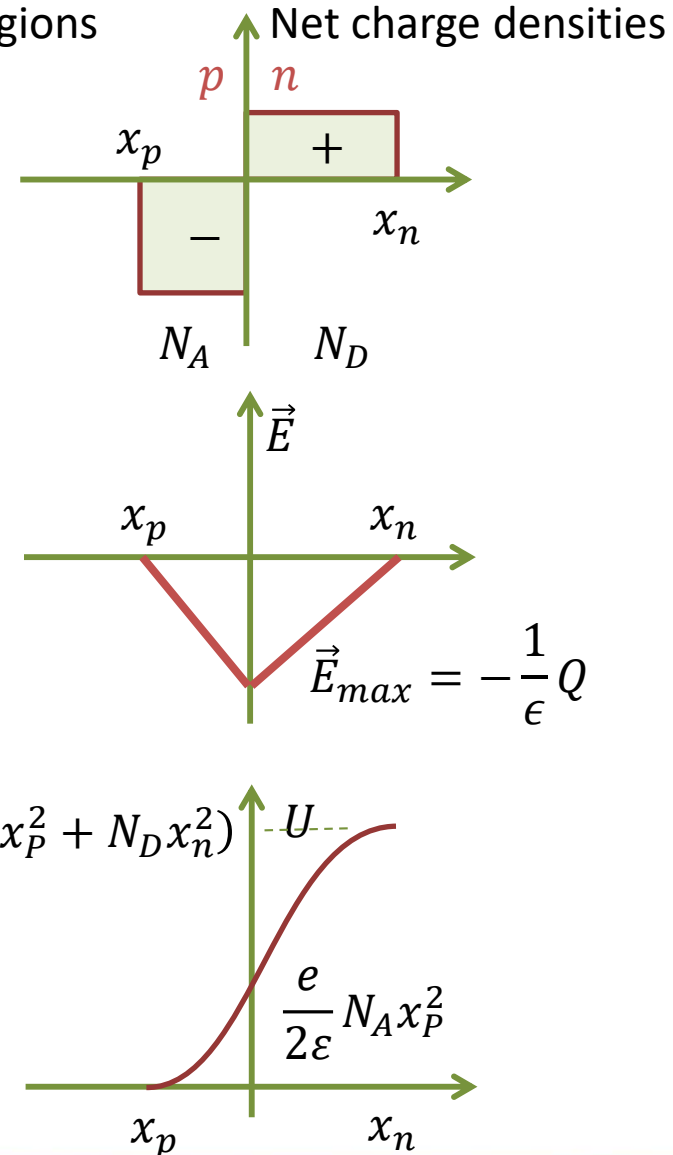
if the p -region is more highly doped, practically all of the potential drop is in the n -region. The less donors are the wider this region is.

(for $N_A \ll N_D$ is vice-versa!)

E.g. $N_D = 10^{15} \text{ cm}^{-3}$ for typical $U_0 = 0.3 \text{ V}$

We have $w \approx 180 \text{ nm}$. If the change from acceptor impurities to donor impurities is gradual, then $w \approx 1 \mu\text{m}$

Depletion regions



$$U_0 = \frac{e}{2\epsilon} (N_A x_p^2 + N_D x_n^2)$$

The doping of semiconductors

Charge conservation

$$eN_A x_p = eN_D x_n = Q$$

The total width of the depletion region w

$$w = x_n - x_p = \sqrt{\frac{2\epsilon U_0}{e(N_A + N_D)}} \left(\sqrt{\frac{N_A}{N_D}} + \sqrt{\frac{N_D}{N_A}} \right)$$

If, say, $N_A \gg N_D$ (p -type doping)

then:

$$w = \sqrt{\frac{2\epsilon U_0}{eN_D}} \quad \text{i} \quad |x_n| > |x_p|$$

if the p -region is more highly doped, practically all of the potential drop is in the n -region. The less donors are the wider this region is.

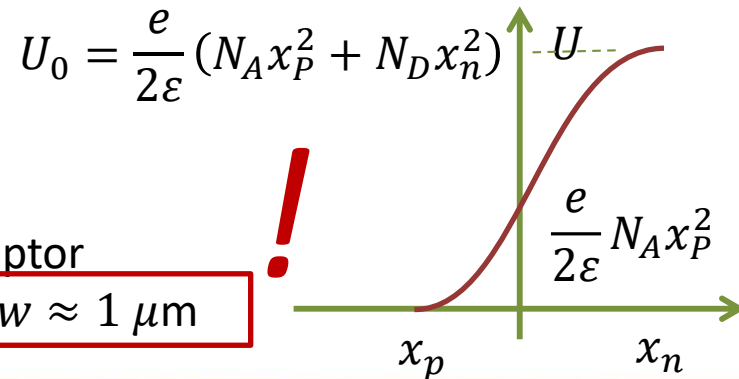
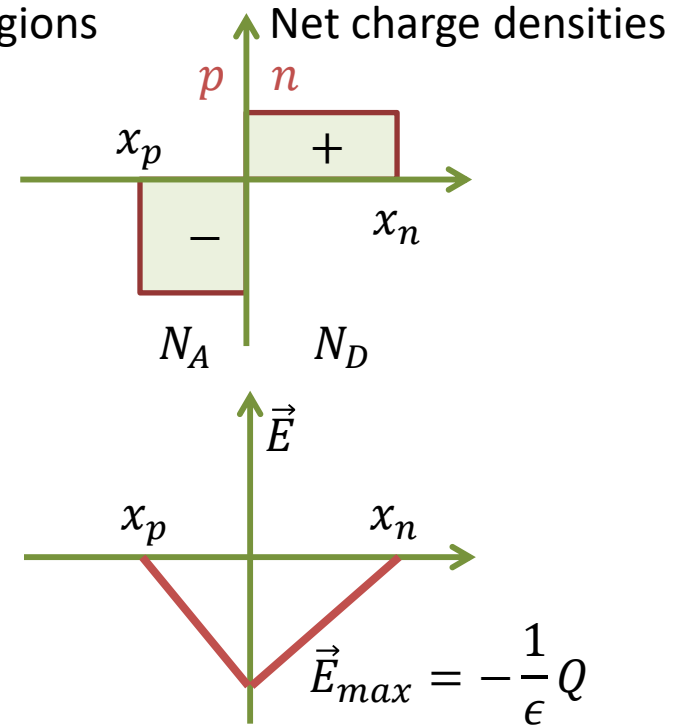
(for $N_A \ll N_D$ is vice-versa!)

E.g. $N_D = 10^{15} \text{ cm}^{-3}$ for typical $U_0 = 0.3 \text{ V}$

We have $w \approx 180 \text{ nm}$. If the change from acceptor

impurities to donor impurities is gradual, then $w \approx 1 \mu\text{m}$

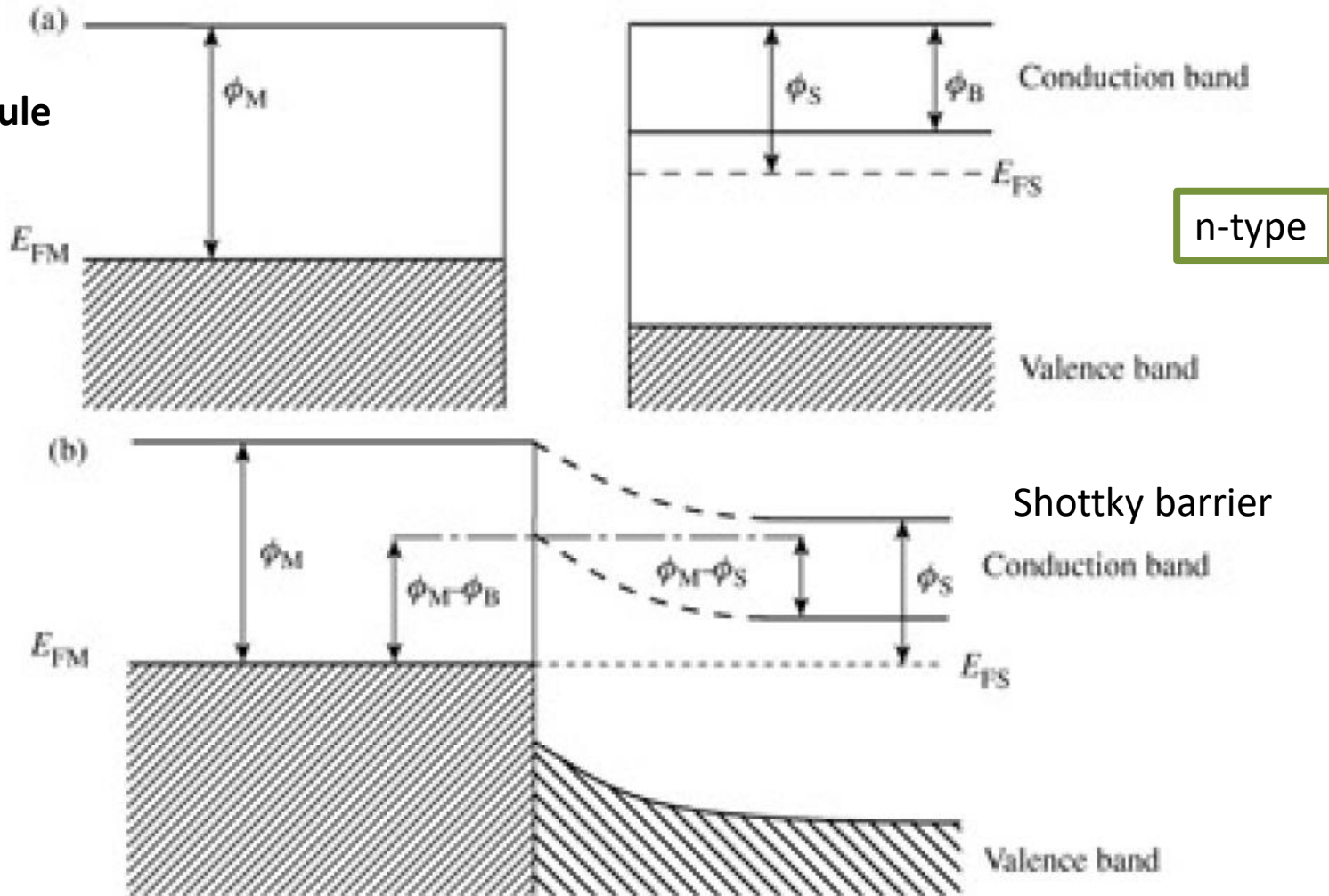
Depletion regions



The construction of energy band diagrams

The metal-semiconductor junction ($\phi_M > \phi_S$) Work function ϕ_S , electron affinity ϕ_B

Anderson's rule



n-type

Electrical properties of materials Solymar, Walsh (9.16)

Pg. 257

The construction of energy band diagrams

The metal-semiconductor junction ($\phi_M > \phi_S$)

Shottky barrier

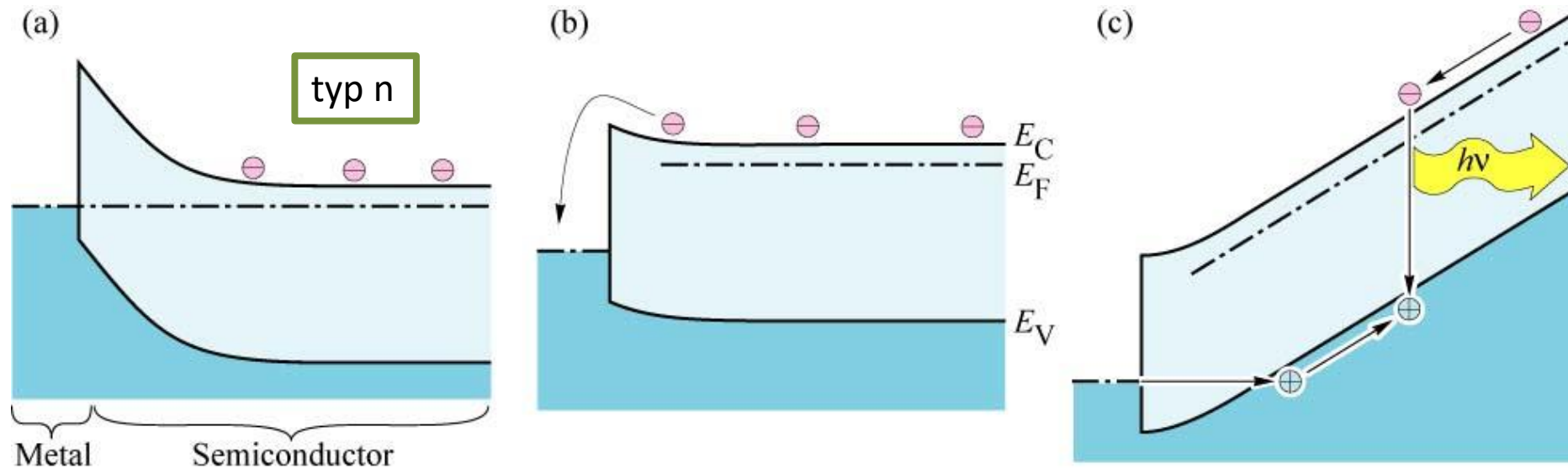
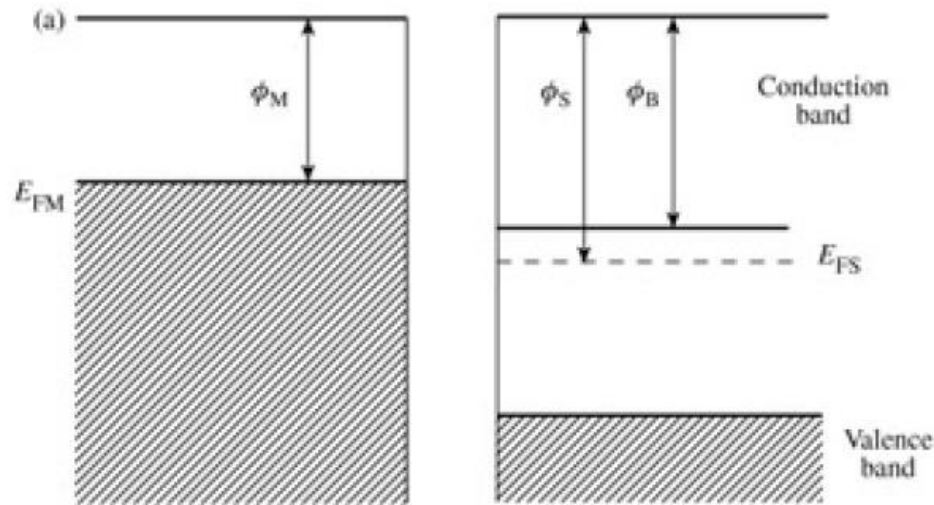


Fig. 1.2. Band diagram of a Schottky diode under (a) equilibrium conditions, (b) forward bias, and (c) strong forward bias. Under strong forward bias, minority carrier injection occurs making possible near-bandgap light emission.

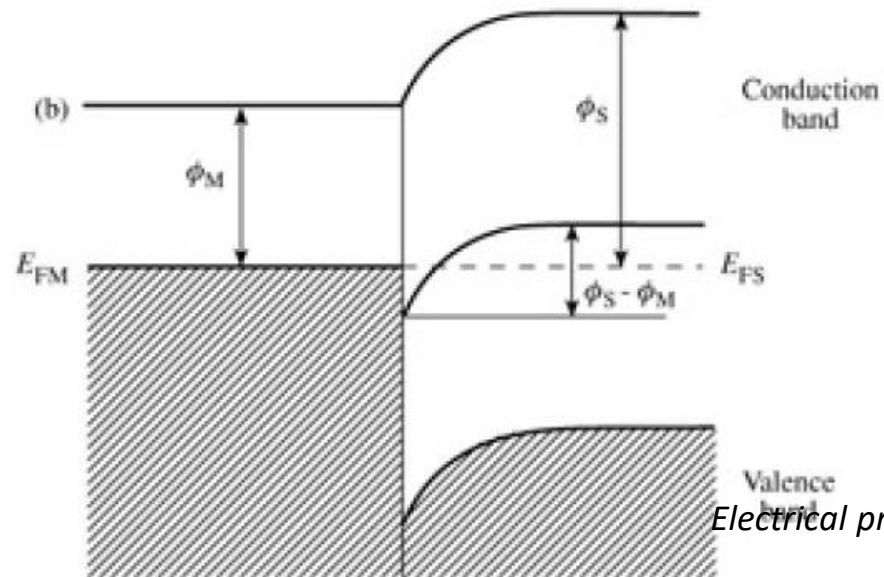
E. F. Schubert
Light-Emitting Diodes (Cambridge Univ. Press)
www.LightEmittingDiodes.org

The construction of energy band diagrams

The metal-semiconductor junction ($\phi_M > \phi_S$)



n-type



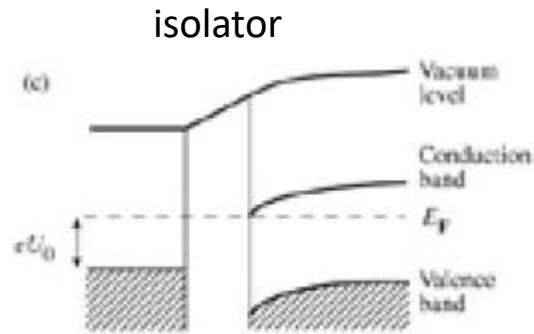
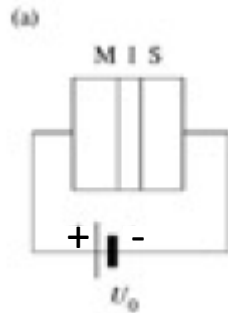
Theoretically there should be no Schottky barrier

Electrical properties of materials Solymar, Walsh

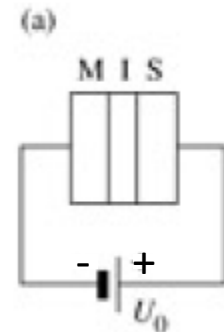
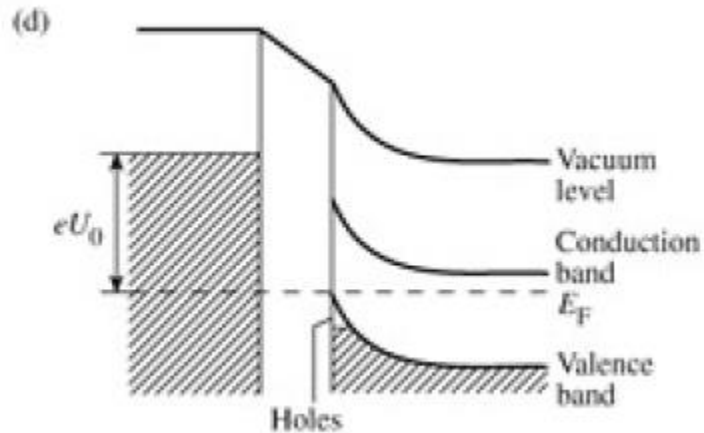
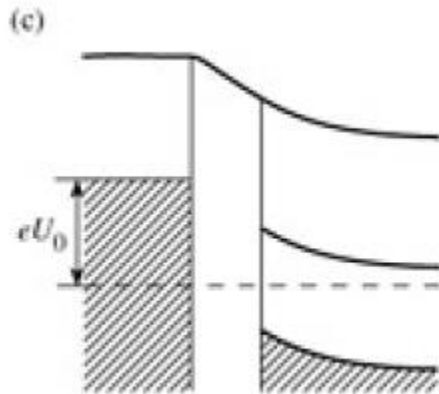
The construction of energy band diagrams

The metal-semiconductor junction ($\phi_M > \phi_S$)

n-type



forward bias
napięcie przewodzenia

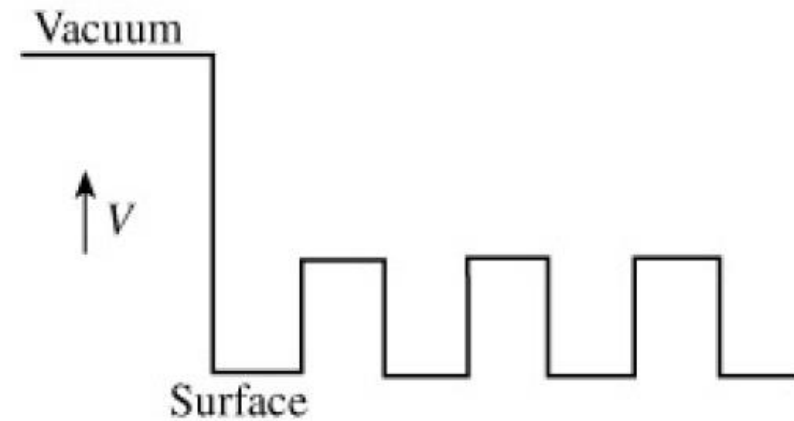
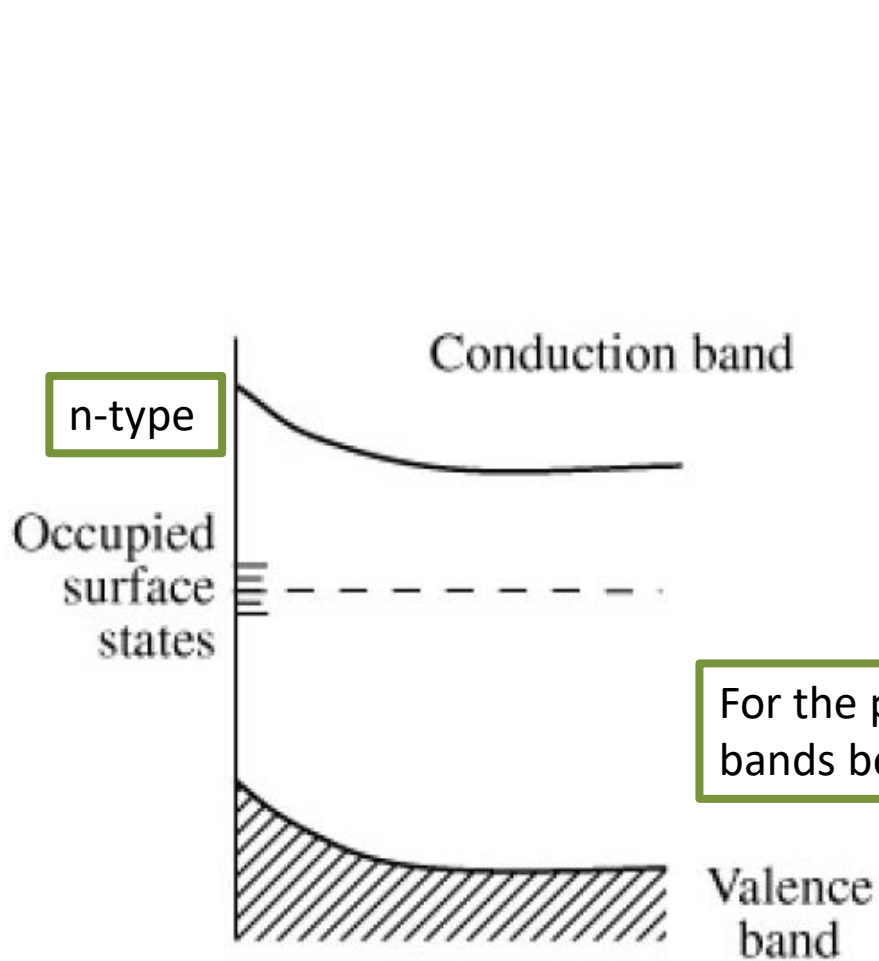


reverse bias
napięcie zaporowe

Electrical properties of materials Solymar, Walsh

The construction of energy band diagrams

The surface of the semiconductor is usually charged

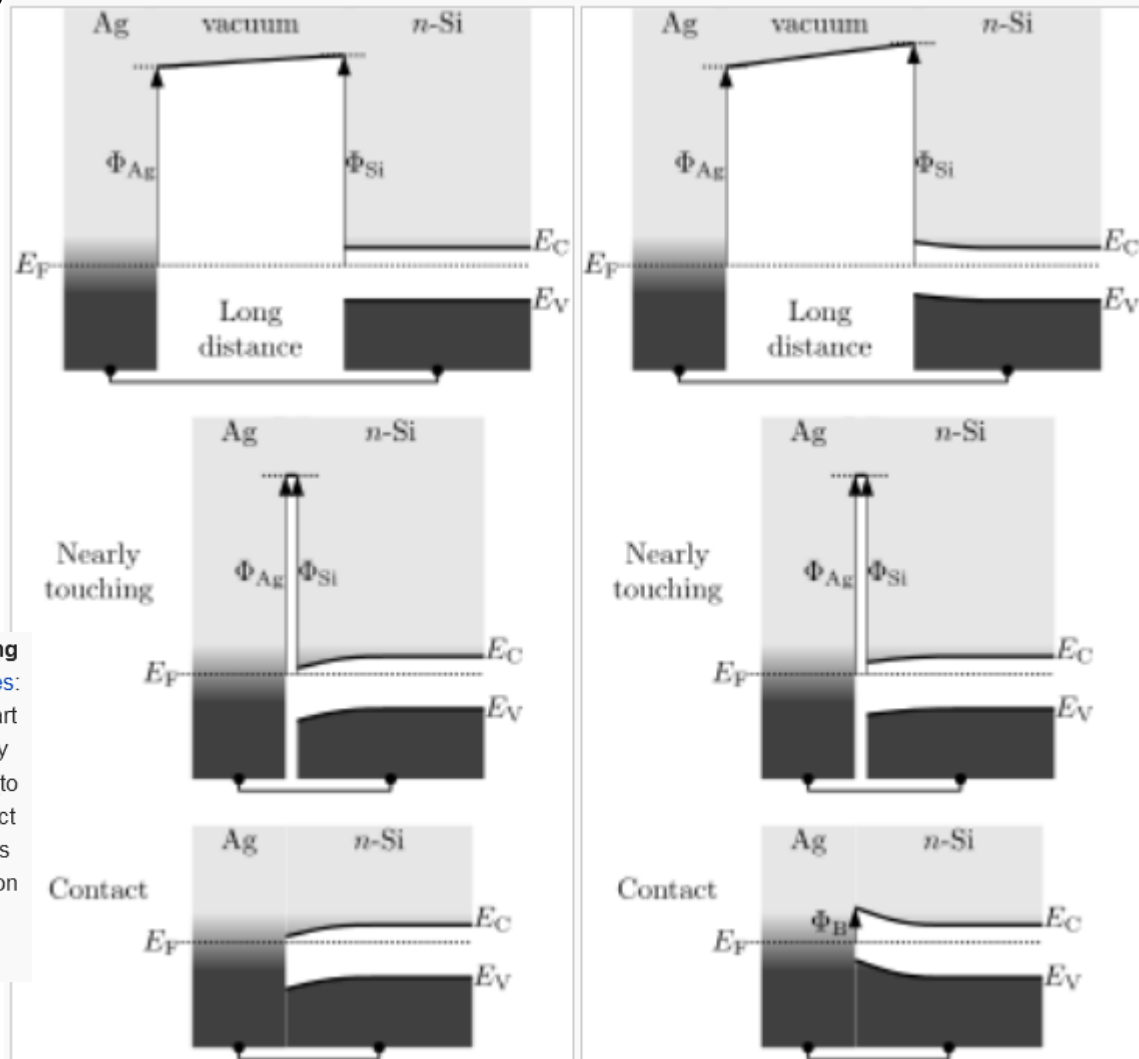


For the p-type the opposite is true - the bands bend downwardly the diagram!

The construction of energy band diagrams

The metal-semiconductor junction ($\phi_{Ag} > \phi_{Si}$)

n-type



Schottky-Mott rule: As the materials are brought together, the bands in the silicon bend such that the silicon's work function Φ matches the silver's. The bands retain their bending upon contact. This model predicts silver to have a very low Schottky barrier to n-doped silicon, making an excellent ohmic contact.

Picture showing **Fermi level pinning** effect from **metal-induced gap states**: The bands in the silicon already start out bent due to **surface states**. They are bent again just before contact (to match work functions). Upon contact however, the band bending changes completely, in a way that depends on the chemistry of the Ag-Si bonding.^[4]

https://en.wikipedia.org/wiki/Metal%20semiconductor_junction

WKB approximation

$$V(x) = V_b \left[1 - \left(\frac{x}{d} \right)^2 \right]$$

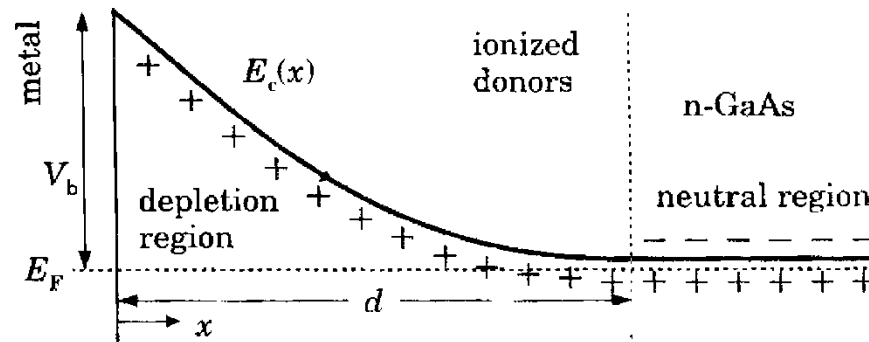


FIGURE 7.7. Schottky barrier in the conduction band $E_c(x)$ between a metal and n-GaAs. The potential is parabolic with height V_b and thickness d .

$$k_n(x) = \frac{1}{\hbar} \sqrt{2mV(x)} = \frac{1}{\hbar} \sqrt{2mV_b \left[1 - \left(\frac{x}{d} \right)^2 \right]}$$

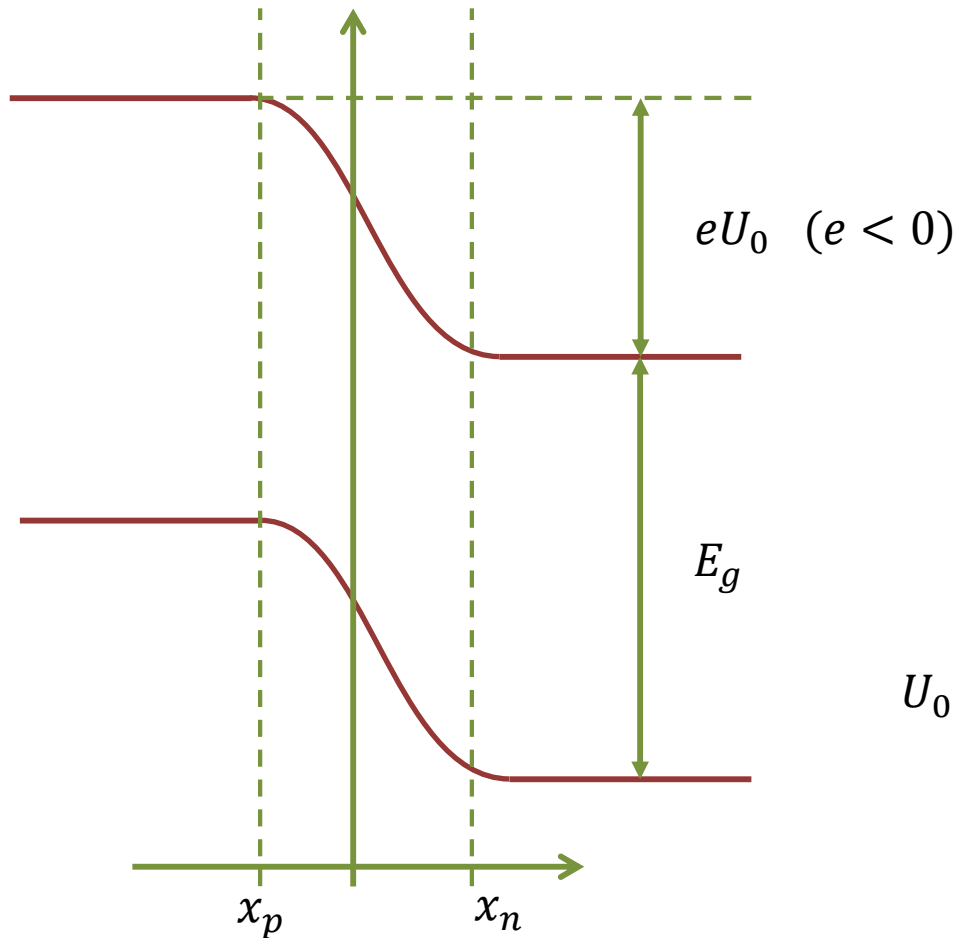
We will return discussing the transport

Heterojunction

Charge conservation

$$eN_A x_p = eN_D x_n = Q$$

TUTAJ 20151126



$$U_0 = \frac{e}{2\epsilon} (N_A x_p^2 + N_D x_n^2)$$

The graph shows the potential U versus position x . The potential is zero in the neutral regions and increases parabolically in the depletion regions. The depletion widths are marked as x_p and x_n on the x-axis. The potential values at the edges of the depletion regions are labeled $\frac{e}{2\epsilon} N_A x_p^2$ and U .

Heterojunction

Heterozłącze (heterojunction)

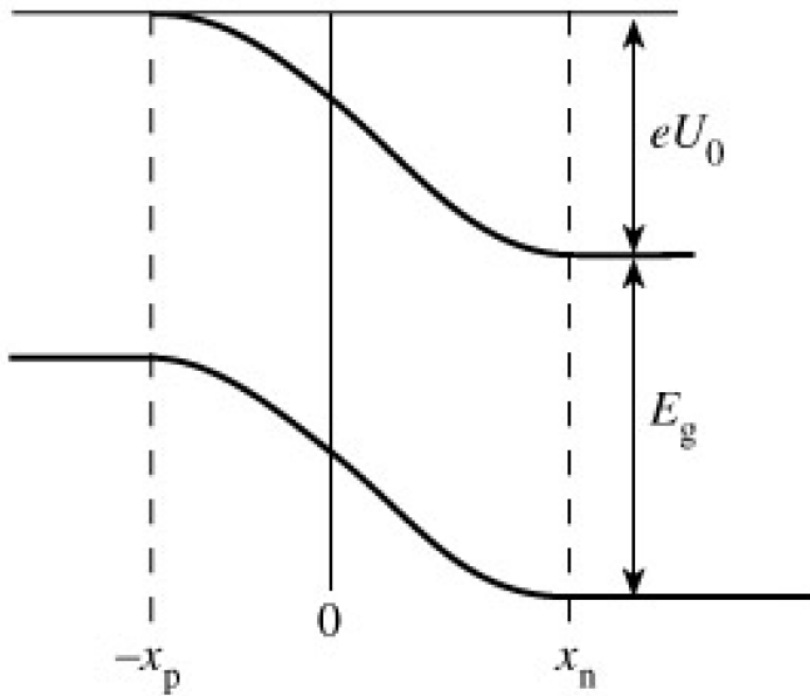


Figure 9.3: The energy diagram for the transition region of a p-n junction.

