

# IV Energy Bands in Crystals

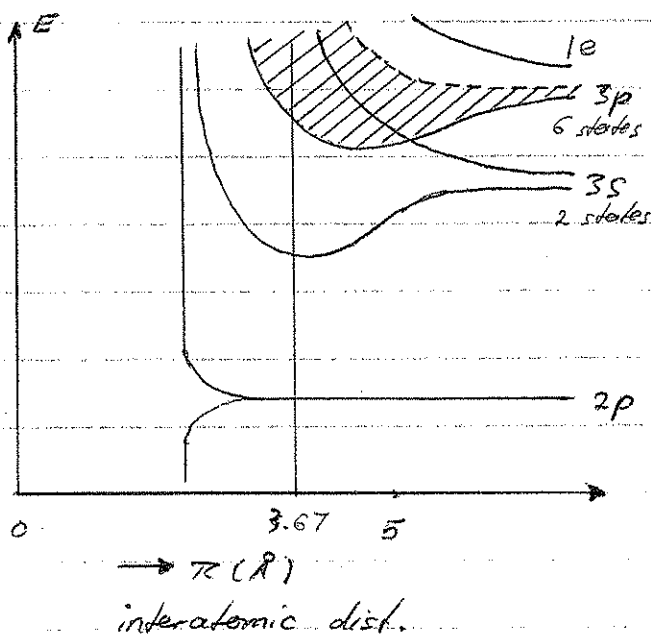
## 4.1 Energy-Band structures of Insulators, Semiconductors and Conductors

We know from the previous chapter that confined electrons exhibit discrete energy levels.

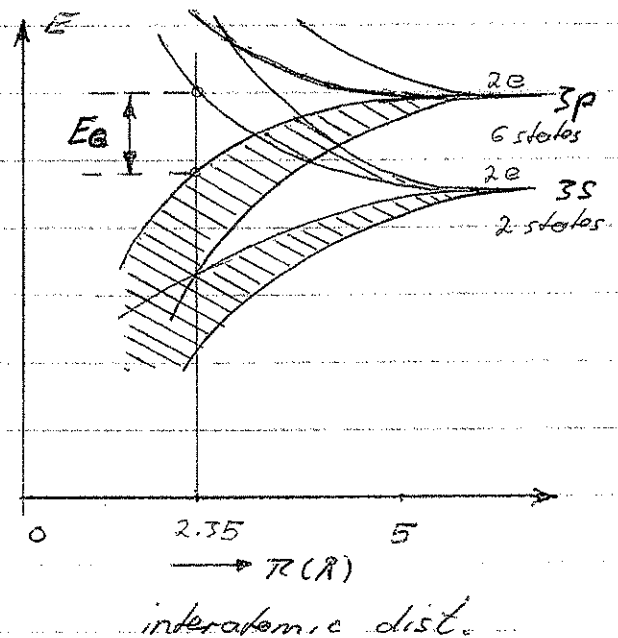
If two atoms with identical energy states are brought close together, the interacting electrons must slightly change their states, since the Pauli exclusion principle does not allow single-state pairs. Hence, the discrete energy levels associated with certain electrons split into closely packed energy bands.

### Example

Sodium



Silicon

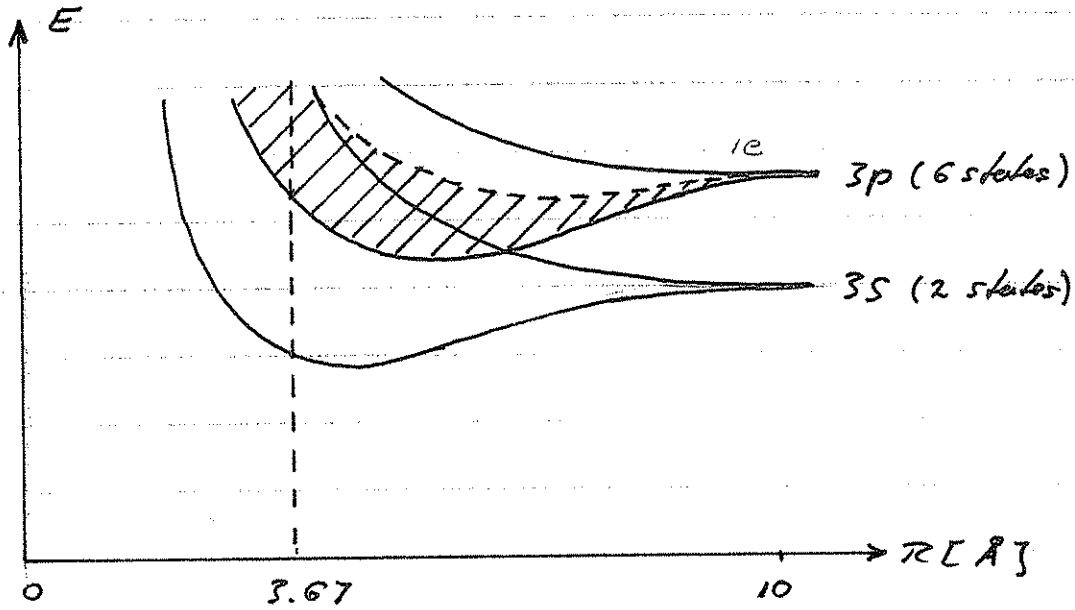


full

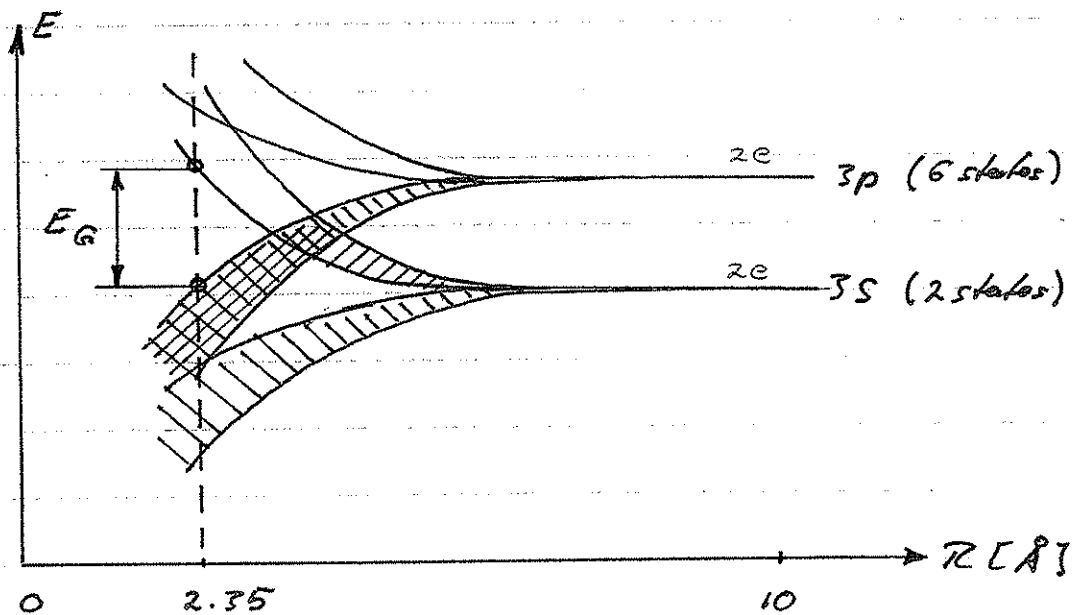
# Energy-Band Structures in Crystals

## Example

a) Sodium → Conductor



b) Silicon → Semiconductor

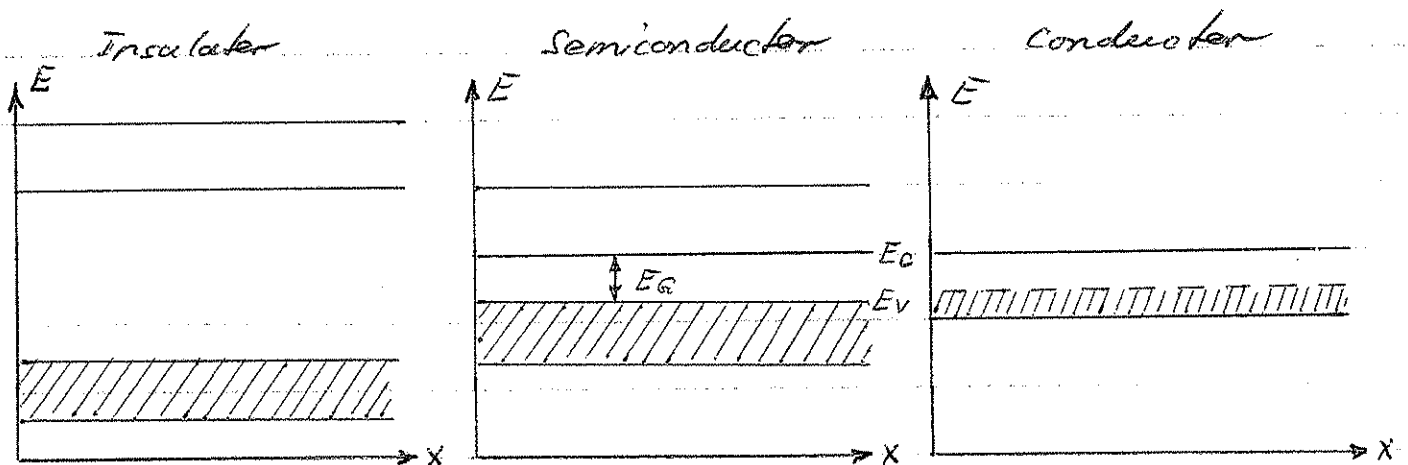


At the interatomic distance  $\pi_0 = 3.67 \text{ \AA}$ , Sodium exhibits an empty 3s band, which overlaps with a partially filled 3p band. Hence, Sodium provides free electrons and is a conductor.

At  $\pi_0 = 2.35 \text{ \AA}$ , Silicon exhibits a full lower 3s band, a full lower 3p band and two empty upper 3s and 3p bands, respectively. Since there is no overlap between a full and an empty band, Silicon provides no free electrons. Since the energy gap between the highest full band and the lowest empty band is relatively small ( $E_g = 1.12 \text{ eV}$ ), we call this type of material a semiconductor.

An insulator finally exhibits a band structure similar to that of silicon except for a larger band gap (e.g.  $5 \text{ eV} < E_g < 10 \text{ eV}$ ).

A convenient way to represent the three types of materials is by means of Energy-band diagrams



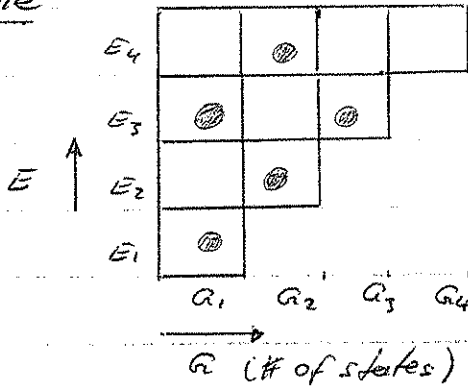
Note: This broad classification of materials into three categories is a sensitive function of the interatomic distance in the crystal.

## 4.2 The Fermi-Dirac Distribution

Quantum particles with half-odd-integral spin are also called Fermions (e.g. electron, proton, neutron,  $^3\text{He}$  nuclei). These Fermions are characterized by:

1. Particles are indistinguishable
2. They obey the Pauli exclusion principle
3. Particles are statistically independent

Example



Constraints:

$$N_i \leq g_i$$

$$\# \text{ of part. } N = \sum_i N_i$$

$$\text{Total Energ. } E = \sum_i N_i E_i$$

$g$  (# of states)

Thermodynamic probability (# of possible distributions)

$$W_{FD} = \prod_{i=1}^M \frac{g_i!}{N_i! (g_i - N_i)!} \quad M: \# \text{ of energy levels}$$

In the above example, we have:

$$N_1 = 1 \quad g_1 = 1$$

$$N_2 = 1 \quad g_2 = 2$$

$$N_3 = 2 \quad g_3 = 3$$

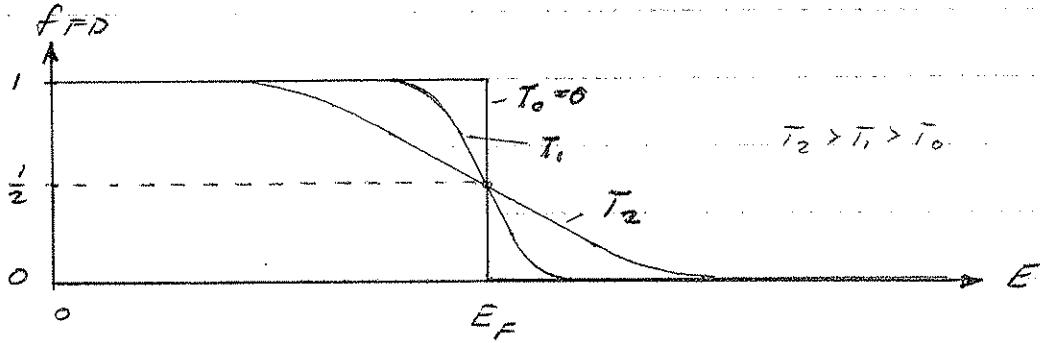
$$N_4 = 1 \quad g_4 = 4$$

$$\Rightarrow W_{FD} = 1 \cdot 2 \cdot 3 \cdot 4 = \underline{\underline{24}}$$

The energy distribution (or occupation index) for fermions is:

$$f_{FD} = \frac{1}{1 + \exp[(E - E_F) / kT]}$$

$E_F$ : Fermi energy



At  $T = 0$ , all available states below the Fermi energy  $E_F$  are occupied while all states above  $E_F$  are empty. The following table indicates some occupation indices for different temperatures.

$T$	$f_{FD}(E = E_F - 1eV)$	$f_{FD}(E = E_F)$	$f_{FD}(E = E_F + 1eV)$
$0^\circ K$	100%	50%	0%
$300^\circ K$	97.9%	50%	2.1%
$600^\circ K$	87.2%	50%	12.8%

Recall: at  $T = 300^\circ K$  Thermal energy  $kT \approx 0.026 eV$

Problem #2 Calculate  $f_{FD} = \frac{1}{1 + \exp[(E - E_F)/kT]}$  for  
 $E - E_F = 0, \pm kT, \pm 2kT, \pm 3kT, \pm 4kT, \pm 5kT$  and  $\pm 6kT$   
 if a)  $T = 100^\circ K$   
 b)  $T = 300^\circ K$   
 c)  $T = 600^\circ K$

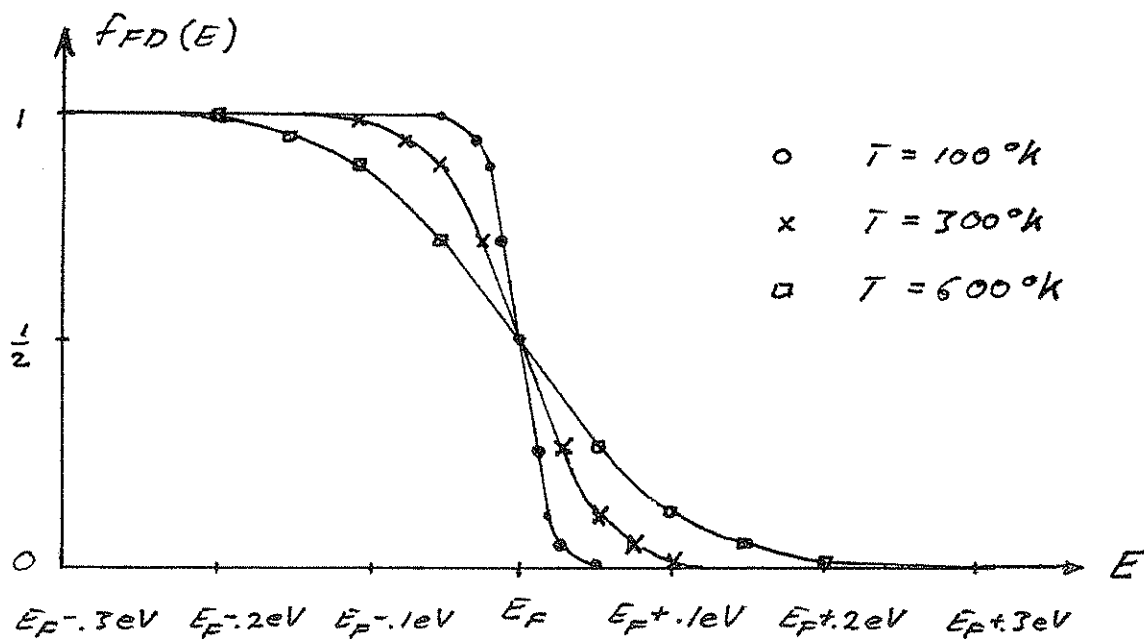
Solution

$(E - E_F)/kT$	$f_{FD}$
-6	0.9975
-5	0.9933
-4	0.9820
-3	0.9526
-2	0.8808
-1	0.7311
0	0.5
1	0.2689
2	0.1192
3	0.0474
4	0.0180
5	0.0067
6	0.0025

a)  $kT = 0.009 \text{ eV}$

b)  $kT = 0.026 \text{ eV}$

c)  $kT = 0.052 \text{ eV}$



### 4.3 Density of States

In order to determine the electron (hole) density in a semiconductor, it is necessary to know both the occupation index  $f_{FD}(E)$  and the density of available states  $g(E)$ . The particle density is then given by

$$|n(E) = g(E) \cdot f_{FD}(E)|$$

Electrons moving back and forth along the  $x$ -direction in a semiconductor can be described by standing waves. The wavelength  $\lambda$  of a standing wave is related to the length of the semiconductor  $L$  by

$$\frac{L}{\lambda} = n_x \quad n_x: \text{integer}$$

de Broglie  $\lambda = \frac{h}{\bar{p}_x} \quad \bar{p}_x = m^* v_x \text{ (crystal mom.)}$   
 $= \hbar k_x$

Thus  $n_x = \frac{L}{h} \bar{p}_x$

The incremental momentum required for a unity increase in  $n_x$  is

$$dn_x = 1 = \frac{L}{h} d\bar{p}_x$$

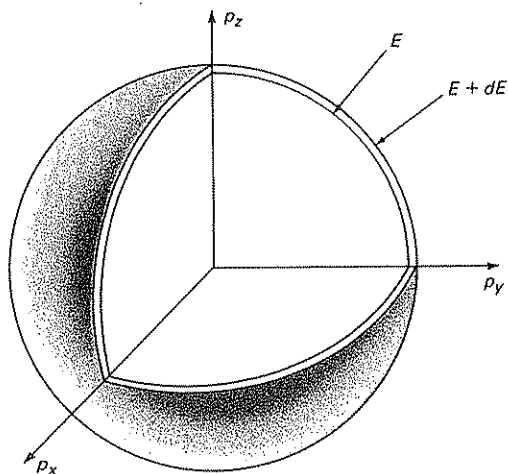
$$\Rightarrow \underline{d\bar{p}_x = \frac{h}{L}} \quad (\text{or } dk_x = \frac{2\pi}{L})$$

For a cube of side  $L$ , we have correspondingly

$$d\bar{p}_x d\bar{p}_y d\bar{p}_z = \left(\frac{h}{L}\right)^3 \quad (\text{or } dk_x dk_y dk_z = \left[\frac{2\pi}{L}\right]^3)$$

The above expression denotes the incremental momentum volume for a unity increase in the number of states in volume  $L^3$ .

if we describe the incremental momentum volume  $d\bar{p}_x d\bar{p}_y d\bar{p}_z$  by spherical coordinates in momentum space, we obtain



Note: Surface of sphere is proportional to Energy since  $4\pi\bar{p}^2 = 4\pi 2m^2 E$ .

$$d\bar{p}^3 = 4\pi\bar{p}^2 d\bar{p}$$

or

$$dk^3 = 4\pi k^2 dk$$

The number of energy states contained in this incremental spherical volume is then equal to

$$g(E) dE = 2 \cdot \frac{4\pi\bar{p}^2 d\bar{p}}{h^3} \quad (\text{or } 2 \frac{4\pi k^2 dk}{(2\pi)^3})$$

↑
↑

2 el. per state with spin ↑ and ↓
Volume for unity increase in # of states per unit volume



Since

$$E = \frac{\bar{p}^2}{2m^*} \quad (\text{or } E = \frac{(\hbar k)^2}{2m^*})$$

we can replace  $\bar{p}^2$  and  $d\bar{p}$  by

$$\frac{\bar{p}^2 = 2Em^* \text{ and } d\bar{p} = \frac{m^*}{\bar{p}} dE = \sqrt{\frac{m^*}{2E}} dE}{(k^2 = 2Em^*\hbar^{-2}) \quad dk = \hbar^{-2} \frac{m^*}{k} dE = \hbar^{-1} \sqrt{\frac{m^*}{2E}} dE}$$

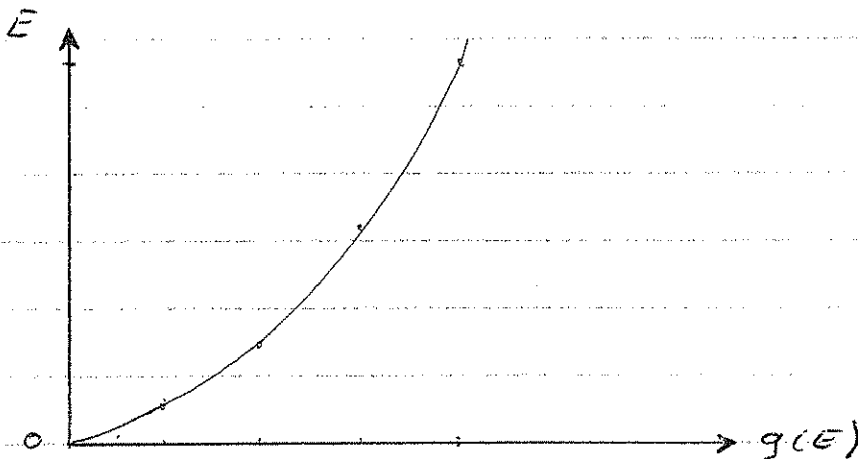
respectively. We finally obtain

$$g(E) dE = \frac{8\pi}{h^3} 2Em^* \sqrt{\frac{m^*}{2E}} dE$$

$$(g(E) dE = \frac{1}{\pi^2 \hbar^3} 2Em^* \sqrt{\frac{m^*}{2E}} dE)$$

Thus

$$\left| g(E) = \frac{8\pi}{h^3} \sqrt{2Em^*{}^3} \right| \quad \left[ \frac{\text{States}}{\text{Energy} \times \text{Vol}} \right]$$

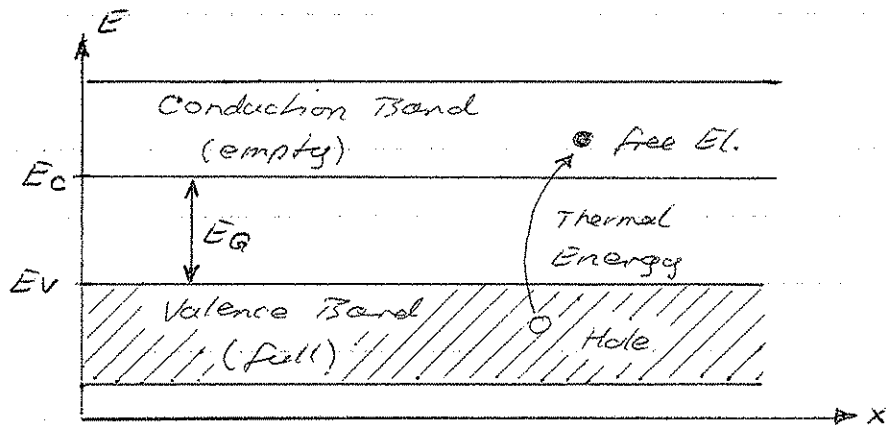


$$\underline{g(E) = 4\pi \left( \frac{2m^*}{h^2} \right)^{3/2} E^{1/2}}$$

## 4.4 Intrinsic Carrier Densities

### 4.4.1 Electrons and Holes

Recall: Energy-Band Structure in Semiconductors.



Each el. that is thermally excited to the conduction band leaves a hole in the valence band. Note that this vacancy can also contribute to the conduction of current by sequentially filling it up with adjacent electrons. Using the concept of the effective mass, we can even assign a mass to this "missing valence electron". Hence, we can view a hole in the valence band as a free particle carrying a positive unity charge.

Note: Since holes are created by thermally excited electrons, their number must be equal to the number of electrons in the conduction band.

$$\underline{n_{i0} = p_{i0}}$$

4.2 Electron and Hole Concentrations

For the conduction band, we assume zero energy at  $E = E_c$  (bottom of band). Thus

$$g_c(E) = 4\pi \left( \frac{2m_n^*}{h^2} \right)^{3/2} (E - E_c)^{1/2} \quad E \geq E_c$$

states/ev. x Vol

Similarly, we assume zero energy at  $E = E_v$  in the valence band (i.e. at the top of the band). So

$$g_v(E) = 4\pi \left( \frac{2m_p^*}{h^2} \right)^{3/2} (E_v - E)^{1/2} \quad E \leq E_v$$

The density of conduction electrons in an intrinsic semiconductor at thermal equilibrium is then given by:

$$n_{i0} = \int_{E_c}^{E_c} 4\pi \left( \frac{2m_n^*}{h^2} \right)^{3/2} \frac{(E - E_c)^{1/2}}{1 + \exp[(E - E_F)/kT]} dE$$

$E_c$  upper edge of conds B.  
Fermi level in intrinsic semic.

and the density of holes follows from:

$$p_{i0} = \int_{E_v}^{E_v} 4\pi \left( \frac{2m_p^*}{h^2} \right)^{3/2} \frac{(E_v - E)^{1/2}}{1 + \exp[(E_F - E)/kT]} dE$$

$E_v$  lower edge of valence B.

Unfortunately, there exists no closed form solution for these integrals.

Simplification: since  $E - E_{Fi} \gg kT$  conduction band  
 $E_{Fi} - E \gg kT$  valence band.

$$\Rightarrow \frac{1}{1 + \exp[(E - E_{Fi})/kT]} \cong \exp[-(E - E_{Fi})/kT] \quad \text{conduction b.}$$

$$\frac{1}{1 + \exp[(E_{Fi} - E)/kT]} \cong \exp[-(E_{Fi} - E)/kT] \quad \text{valence b.}$$

Furthermore:  $\exp[-(E_c - E_{Fi})/kT] \gg \exp[-(E_c' - E_{Fi})/kT]$   
 $\exp[-(E_{Fi} - E_v)/kT] \gg \exp[-(E_{Fi} - E_v')/kT]$

using these simplification yields:

$n_{i0} = N_c \exp\left[-\frac{(E_c - E_{Fi})}{kT}\right]$	intrinsic carrier
$p_{i0} = N_v \exp\left[-\frac{(E_{Fi} - E_v)}{kT}\right]$	concentrations
$N_c = 2 \left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}$	effective dens. of states in conduction b.
$N_v = 2 \left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2}$	eff. dens. of states in valence b.

Since  $n_{i0} = p_{i0}$

i.e.  $N_c \exp\left[-\frac{(E_c - E_{Fi})}{kT}\right] = N_v \exp\left[-\frac{(E_{Fi} - E_v)}{kT}\right]$

$$\Rightarrow \left| E_{Fi} = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln\left[\frac{N_v}{N_c}\right] \right|$$

$$\frac{3}{4} kT \ln\left[\frac{m_p^*}{m_n^*}\right]$$

we can also write

$$E_c - E_{Fi} = \underbrace{\frac{E_c - E_v}{2}}_{\frac{1}{2} E_G} - \underbrace{\frac{kT}{2} \ln \left[ \frac{N_v}{N_c} \right]}_{\frac{3}{4} kT \ln \left[ \frac{m_p^*}{m_n^*} \right]}$$

Example

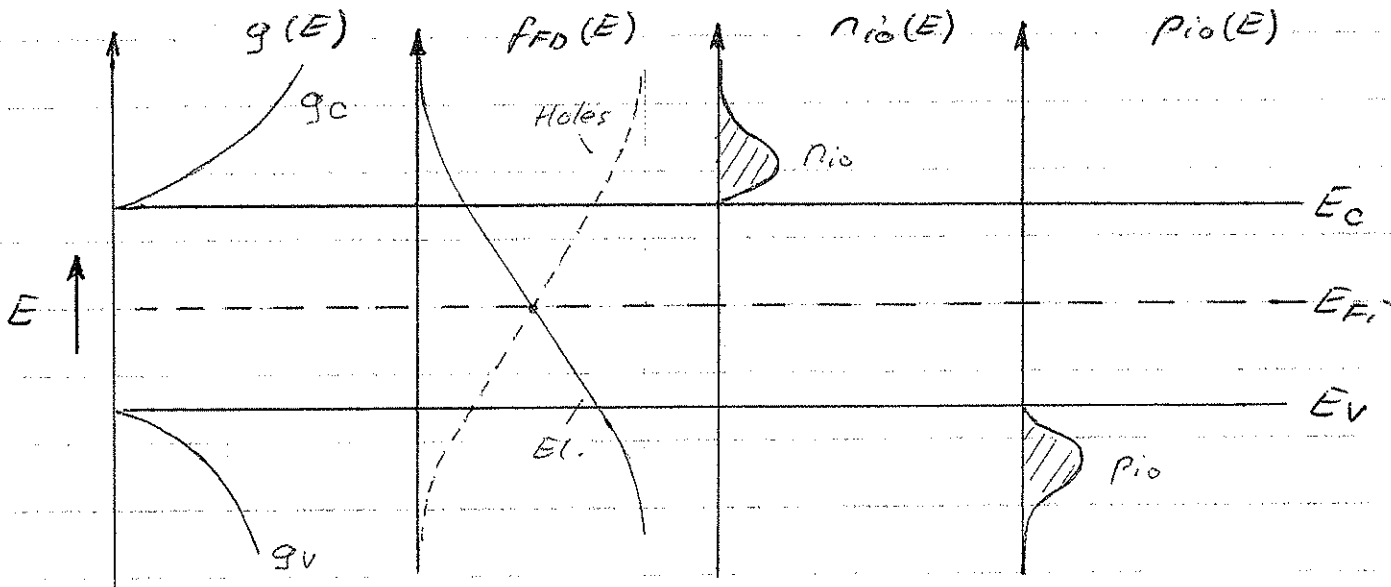
T = 300°K

Material	$m_n^*/m_0$	$m_p^*/m_0$	$\frac{3}{4} kT \ln \left[ \frac{m_p^*}{m_n^*} \right]$
Si	1.08	0.81	-0.006 eV
Ge	0.55	0.29	-0.012 eV
GaAs	0.068	0.82	+0.049 eV

intrinsic

At thermal equilibrium, the Fermi Energy  $E_{Fi}$  is very close to the center of the energy gap.

Carrier Concentration vs. Energy



4.4.3 Temp. dependence of the intrinsic carrier conc.

The product of el. and hole density is:

$$n_{i0} p_{i0} = n_{i0}^2 = p_{i0}^2 = N_c N_v \exp\left[-\frac{E_c - E_v}{kT}\right]$$

$$= 4 \left(\frac{2\pi kT}{h^2}\right)^3 (m_n^\alpha m_p^\alpha)^{3/2} e^{-\frac{E_g}{kT}}$$

Law of  
Mass action  
(indep. of  $E_F$ )  
⇒ holds for intr. +  
extr. semic.

Thus

$$n_{i0} = p_{i0} = 2 \left(\frac{2\pi kT}{h^2}\right)^{3/2} (m_n^\alpha m_p^\alpha)^{3/4} e^{-\frac{E_g}{2kT}}$$

$$= n_{i0}(T_0) \cdot \left[\frac{T}{T_0}\right]^{3/2} e^{-\frac{E_g}{2kT_0} \left(\frac{T_0}{T} - 1\right)}$$

Example

$T$	$n_{i0} = p_{i0}$		
	Ge	Si	GaAs
200°K	$2.3 \times 10^{16} \text{ m}^{-3}$	$1.7 \times 10^{11} \text{ m}^{-3}$	$1.2 \times 10^6 \text{ m}^{-3}$
300°K	$2.4 \times 10^{19} \text{ m}^{-3}$	$1.5 \times 10^{16} \text{ m}^{-3}$	$1.8 \times 10^{12} \text{ m}^{-3}$
400°K	$8.8 \times 10^{20} \text{ m}^{-3}$	$5.0 \times 10^{18} \text{ m}^{-3}$	$2.6 \times 10^{15} \text{ m}^{-3}$

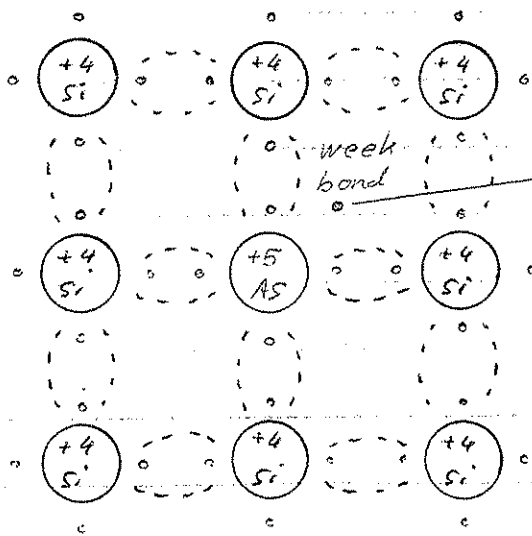
Recall: The concentration of free carriers in a metal is on the order of  $10^{28} \text{ m}^{-3}$  at  $T=300\text{K}$ , i.e. several orders of magnitudes higher than the free carrier concentration in semiconductors.

Note: Since  $E_g$  slightly changes with  $T$ , the actual carrier dens. at  $T=400\text{K}$  and  $T=200\text{K}$  are a little bit different from the values in the above table.

## 4.5 Extrinsic Semiconductors (doped semicond.)

When a semiconductor is doped with impurities, it becomes extrinsic.

2-Dim. Model of doped crystal Si doped with As



conduction electron

Each As atom donates 1 e.l. to the conduction band.

Si doped with B

→ Each B atom donates a hole to the valence band

### Ionization Energy

To obtain a rough estimate of the energy required to free the excess electron (hole) of the impurity atom, we can consider the core of this atom as a neg. (pos.) charged nucleus surrounded by a single electron (hole). Hence, we obtain a model similar to Bohr's model of the H-atom. The ionization energy can then be written as  $(E_H = -\frac{1}{2} \frac{meq^4}{(2\epsilon_0 h)^2 n^2})$

$$E_{ion} = -E_H \frac{\epsilon_0^2}{\epsilon_s^2} \approx 0.1 eV$$

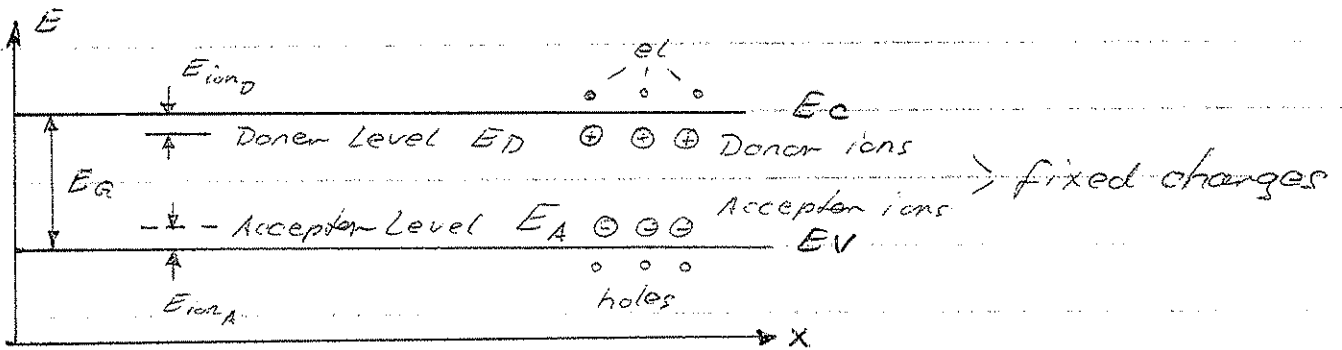
8  
12 · ε<sub>0</sub>

Measured ionization Energies:

Semic.	$E_{ion} \text{ (Donor) [eV]}$			$E_{ion} \text{ (Acceptor) [eV]}$		
	Sb	P	As	B	Al	Ga
Si	0.039	0.045	0.054	0.045	0.067	0.072
GaAs	S	Se	Sn	Te	Mg	Zn
	0.006	0.006	0.006	0.028	0.028	0.051

Recall: Thermal Energy at  $T = 300^\circ K$ :  $\frac{3}{2} kT = 0.039 eV$

Energy - Band diagram



The probability that an impurity atom is ionized is

for Donors:

$$P_D(E_D) = \frac{1}{1 + 2 \frac{1}{4} \exp[(E_D - E_F)/kT]} = \frac{1}{1 + 2 \exp[(E_F - E_D)/kT]}$$

probab. that el. is occupying donor site  
 ↑  
 for spin  $\pm \frac{1}{2} \rightarrow 2$  states

for Acceptors:

$$P_A(E_A) = \frac{1}{1 + \frac{1}{4} \exp[(E_A - E_F)/kT]}$$



### 4.5.1 Extrinsic Carrier Concentrations

As long as  $(E_c - E_F) \gg kT^*$  and  $(E_F - E_V) \gg kT^*$ , we can apply the same eq. to calculate the carrier concentr. as in case of intrinsic semiconductors.

i.e.

$$\left| \begin{array}{l} n_0 = N_c \exp \left[ -\frac{E_c - E_F}{kT} \right] \\ p_0 = N_v \exp \left[ -\frac{E_F - E_V}{kT} \right] \end{array} \right| \quad \begin{array}{l} N_c = 2 \left( 2\pi \frac{m_n^* kT}{h^2} \right)^{3/2} \\ N_v = 2 \left( 2\pi \frac{m_p^* kT}{h^2} \right)^{3/2} \end{array}$$

Note: If  $(E_c - E_F)$  and  $(E_F - E_V)$  are in the range of  $kT$ , the above equations cannot be applied any more.

The semiconductor is then called degenerate.

This will be the case if the semiconductor is highly doped (e.g.  $N_D > 10^{24} \text{ m}^{-3}$  in Si).

If the semiconductor is not degenerate, we can write:

$$\left| \begin{array}{l} E_c - E_F = kT \ln \left[ \frac{N_0}{n_0} \right] \\ E_F - E_V = kT \ln \left[ \frac{N_v}{p_0} \right] \\ n_0 p_0 = N_c N_v \exp \left[ -\frac{E_c - E_V}{kT} \right] = n_i^2 \end{array} \right| \quad \text{law of mass action}$$

Note: If  $n_0$  increases by a factor  $k$ ,  $p_0$  decreases by the same factor and vice versa.

\* This inequality is approx. satisfied if  $(E_c - E_F) > 3.0 kT$  since  $e^{3.0} \approx 20 \gg 1$   
 $(E_F - E_V)$

If we denote the impurity concentration in a semiconductor with  $N_D$  (donors) or  $N_A$  (accepters), respectively and assume that all impurity atoms are ionized, we can write

$$\left| \begin{array}{l} n_0^- = N_D^+ + p_0^+ \\ p_0^+ = N_A^- + n_0^- \end{array} \right| \quad \text{charge neutrality eq.}$$

From law of mass action, we obtain

$$p_0 = \frac{n_{i0}^2}{n_0} \quad \therefore p_0^2 = N_A p_0 + n_{i0}^2$$

$$n_0 = \frac{n_{i0}^2}{p_0} \quad \therefore n_0^2 = N_D n_0 + n_{i0}^2$$

Thus

$$n\text{-doped S.} \quad \left| n_0 = N_D \frac{1}{2} \left[ 1 + \sqrt{1 + 4 \frac{n_{i0}^2}{N_D^2}} \right] \cong N_D \right| \quad (N_D \gg n_{i0})$$

$$p\text{-doped S.} \quad \left| p_0 = N_A \frac{1}{2} \left[ 1 + \sqrt{1 + 4 \frac{n_{i0}^2}{N_A^2}} \right] \cong N_A \right| \quad (N_A \gg n_{i0})$$

⇓

$$n\text{-doped S.} \quad \left| N_D \cong N_C \exp \left[ -\frac{E_C - E_F}{kT} \right] \right| \quad E_C - E_F = kT \ln \left[ \frac{N_C}{N_D} \right]$$

$$p\text{-doped S.} \quad \left| N_A \cong N_V \exp \left[ -\frac{E_F - E_V}{kT} \right] \right| \quad E_F - E_V = kT \ln \left[ \frac{N_V}{N_A} \right]$$

Carrier Concentrations

Intrinsic and extrinsic semicond. at equilibrium

$$\left. \begin{aligned} n_0 &= N_C \exp\left[-\frac{E_C - E_F}{kT}\right] \\ p_0 &= N_V \exp\left[-\frac{E_F - E_V}{kT}\right] \\ n_0 p_0 &= N_C N_V \exp\left[-\frac{E_C - E_V}{kT}\right] = n_{i0}^2 \end{aligned} \right\}$$

Restriction for above eqs.

$$\left. \begin{aligned} \exp\left[\frac{E_C - E_F}{kT}\right] &\gg 1 \\ \exp\left[\frac{E_F - E_V}{kT}\right] &\gg 1 \end{aligned} \right\}$$

Charge neutrality eqs.

(100% ionization assumed)

$$\left. \begin{aligned} n_0 &= N_D \frac{1}{2} \left[ 1 + \sqrt{1 + 4 \frac{n_{i0}^2}{N_D}} \right] \cong N_D & (n\text{-doped}) \\ p_0 &= N_A \frac{1}{2} \left[ 1 + \sqrt{1 + 4 \frac{n_{i0}^2}{N_A}} \right] \cong N_A & (p\text{-doped}) \end{aligned} \right\}$$

↓

$$\left. \begin{aligned} N_D &\cong N_C \exp\left[-\frac{E_C - E_F}{kT}\right] \\ N_A &\cong N_V \exp\left[-\frac{E_F - E_V}{kT}\right] \end{aligned} \right\}$$

Fermi energy vs. dopant concentration

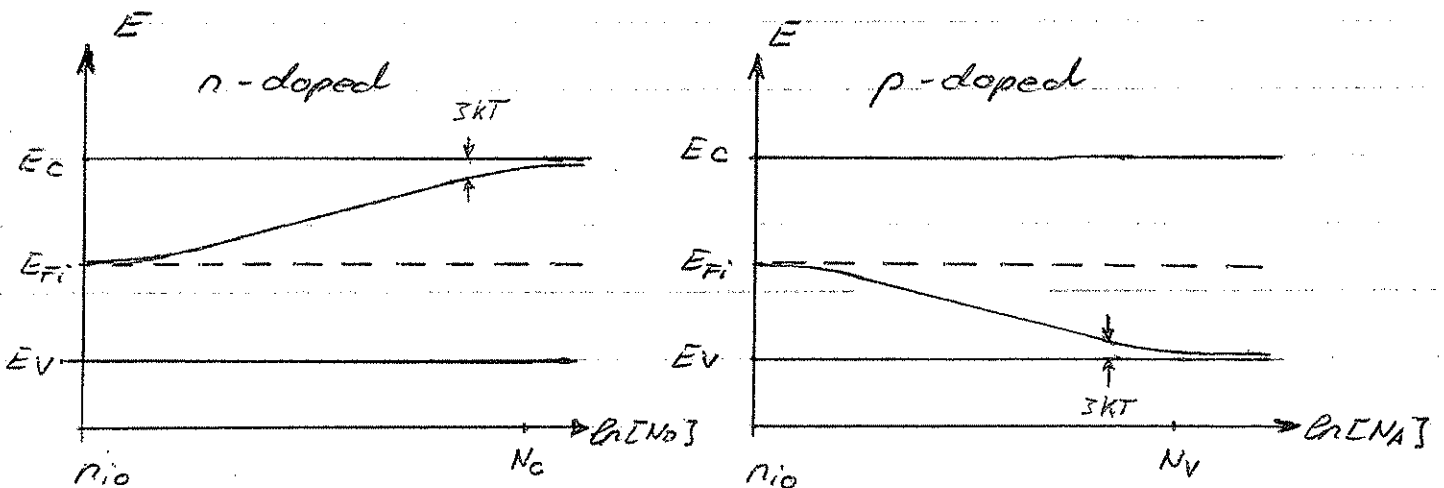
Under the assumption of 100% ionization, we have

$$\left| \begin{array}{l} E_C - E_F = kT \ln \left[ \frac{N_C}{N_D} \right] \\ E_F - E_V = kT \ln \left[ \frac{N_V}{N_A} \right] \end{array} \right| \quad \begin{array}{l} n\text{-doped} \\ p\text{-doped} \end{array}$$

with  $E_{Fi} = E_C - kT \ln \left[ \frac{N_C}{n_{i0}} \right] = E_V + kT \ln \left[ \frac{N_V}{n_{i0}} \right]$  we can rewrite the above eq. as

$$\left| \begin{array}{l} E_F = E_{Fi} + kT \ln \left[ \frac{N_D}{n_{i0}} \right] \\ E_F = E_{Fi} - kT \ln \left[ \frac{N_A}{n_{i0}} \right] \end{array} \right| \quad \begin{array}{l} n\text{-doped } (n_{i0} < N_D < N_C) \\ p\text{-doped } (n_{i0} < N_A < N_V) \end{array}$$

Note: The above eq. hold only as long as  $e^{\frac{(E_C - E_F)}{kT}} \gg 1$  or  $e^{\frac{(E_F - E_V)}{kT}} \gg 1$  (e.g.  $(E_C - E_F) = 3kT \rightarrow e^3 = 20 \gg 1$ )



Recall: probability that impurity atom is ionized

$$p_D(E_D) = \frac{1}{1 + 2 \exp[(E_F - E_D)/kT]} \quad \text{donor}$$

$$p_A(E_A) = \frac{1}{1 + \frac{1}{4} \exp[(E_A - E_F)/kT]} \quad \text{acceptor}$$

with  $E_C - E_F = kT \ln \left[ \frac{N_C}{N_D p_D} \right]$  and  $E_F - E_V = kT \ln \left[ \frac{N_V}{N_A p_A} \right]$   
we obtain

$$\left| \begin{array}{l} p_D(E_D) = \frac{1}{1 + 2 \exp[(E_C - E_D)/kT] \frac{N_D p_D}{N_C}} \quad \text{for donors} \\ p_A(E_A) = \frac{1}{1 + \frac{1}{4} \exp[(E_A - E_V)/kT] \frac{N_A p_A}{N_V}} \quad \text{for acceptors} \end{array} \right|$$

If we solve the above eqs. for the temp.  $T_{px}$  where  $p_D$  % or  $p_A$  %, respectively, of all impurity atoms are ionized, we obtain

Note:

$$\left| \begin{array}{l} T_{pD} = \frac{(E_C - E_D)}{k \ln \left[ \frac{N_C}{2N_D p_D} \left( \frac{1}{p_D} - 1 \right) \right]} \quad \text{for donors} \quad N_C = N_{C0} \left( \frac{T}{T_0} \right)^{3/2} \\ T_{pA} = \frac{(E_A - E_V)}{k \ln \left[ \frac{4N_V}{N_A p_A} \left( \frac{1}{p_A} - 1 \right) \right]} \quad \text{for acceptors} \quad N_V = N_{V0} \left( \frac{T}{T_0} \right)^{3/2} \end{array} \right|$$

e.g.

$$T_{D90\%} = \frac{(E_C - E_D)}{k \left( \ln \left[ \frac{N_{C0}}{N_D} \right] - \frac{3}{2} \ln \left[ \frac{T_0}{T} \right] - 2.785 \right)} \quad \text{Iterative Process}$$

$$T_{A90\%} = \frac{(E_A - E_V)}{k \left( \ln \left[ \frac{N_{V0}}{N_A} \right] - \frac{3}{2} \ln \left[ \frac{T_0}{T} \right] - 0.706 \right)} \quad \text{to find exact solution!}$$

Example Si is doped with P  $\rightarrow$  donor with  $E_C - E_D = 0.045 \text{ eV}$  (ionization energy)

Find  $T_{90\%}$  for

a) impurity conc.  $N_D = 10^{21} \text{ m}^{-3}$

b) " "  $N_D = 10^{23} \text{ m}^{-3}$

Solution: 
$$T_{90\%} = \frac{(E_C - E_D)}{k \left( \ln \left[ \frac{N_{Co}}{N_D} \right] - \frac{3}{2} \ln \left[ \frac{T_0}{T} \right] - 2.79 \right)}$$

$N_{Co}(T_0 = 300\text{K}) = \underline{2.85 \times 10^{25} \text{ m}^{-3}}$

a)  $T_{190\%} = \frac{522\text{K}}{\ln[2.85 \times 10^4] - 2.79} = 69.9\text{K}$

$T_{290\%} = \frac{522\text{K}}{\ln[2.85 \times 10^4] - 4.98} = 98.8\text{K}$

$\vdots$   $90.0\text{K}$

$\vdots$   $92.2\text{K}$

$T_{590\%}$  = 91.6K

b)  $T_{190\%} = \frac{522\text{K}}{\ln[2.85 \times 10^2] - 2.79} = 182.4\text{K}$

$T_{290\%} = \frac{522\text{K}}{\ln[2.85 \times 10^2] - 3.54} = 246.7\text{K}$

$\vdots$   $203.2\text{K}$

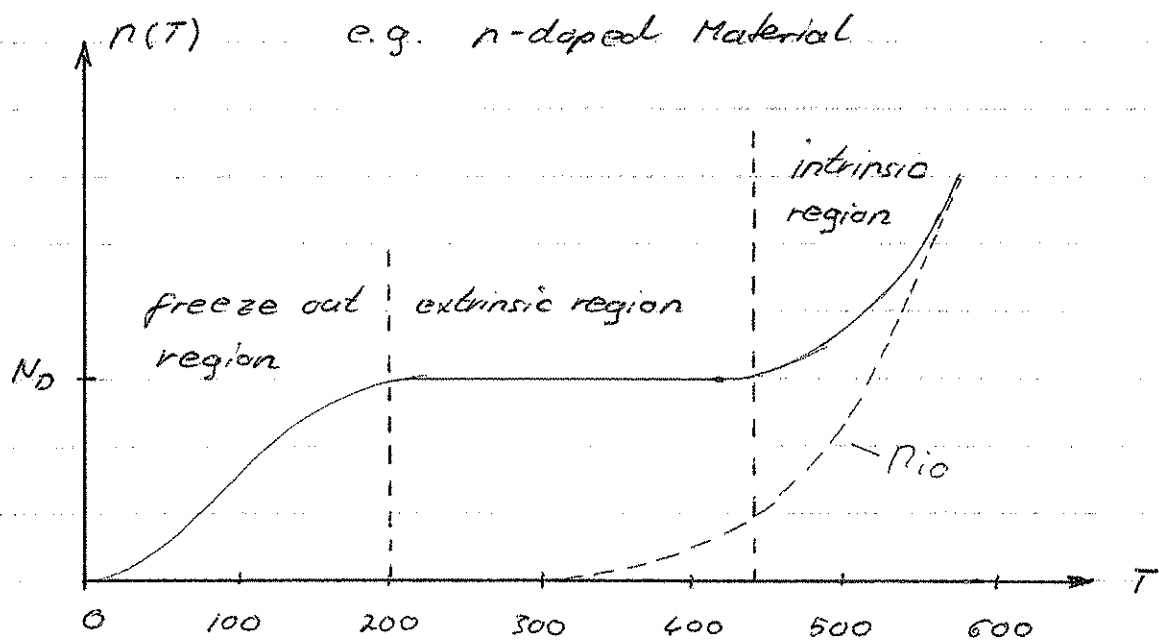
$\vdots$

$\vdots$

$\vdots$   $217.6\text{K}$

$T_{1090\%}$  = 218.2K

## Carrier Concentration vs. Temperature



### freeze out region

Thermal energy is not high enough to ionize all donor states

### extrinsic region

Carrier concentration is essentially equal to the impurity (donor) concentration. Note: This is the most important region for semiconductor device fabric.

### intrinsic region

Due to the high temp. the intrinsic carrier conc. ( $n_{i0}$ ) exceeds the donor concentration and the semiconductor becomes intrinsic.

Problem: Calculate the upper edge of the extrinsic region (assume  $n_{i0}(T) = \frac{1}{10} N_D$ ) for

a) Si doped with  $N_D = 10^{21} \text{ m}^{-3}$  donors

b) Ge " " "  $N_D = 10^{21} \text{ m}^{-3}$  donors

Solution

$$n_{i0}(T) = n_{i0}(T_0) \left[ \frac{T}{T_0} \right]^{3/2} e^{-\frac{E_G}{2kT_0} \left( 1 - \frac{T_0}{T} \right)}$$

if  $n_{i0}(T) = \frac{1}{10} N_D$

$$\Rightarrow \left| \frac{T_{10\%}}{T_0} = \frac{1}{1 - \frac{2kT_0}{E_G} \left( \ln \left[ \frac{N_D}{10 \times n_{i0}(T_0)} \right] - \frac{3}{2} \ln \left[ \frac{T}{T_0} \right] \right)} \right|$$

iterative solution:

a) Si at 300°K  $n_{i0}(300\text{K}) = 1.5 \times 10^{16} \text{ m}^{-3}$

$E_G = 1.12 \text{ eV}$

$kT_0 = 0.026 \text{ eV}$

$T_{110\%} = 507^\circ \text{K}$

$T_{210\%} = 478^\circ \text{K}$

$T_{310\%} = 481^\circ \text{K}$

b) Ge at 300°K  $n_{i0}(300\text{K}) = 2.4 \times 10^{19} \text{ m}^{-3}$

$E_G = 0.66 \text{ eV}$

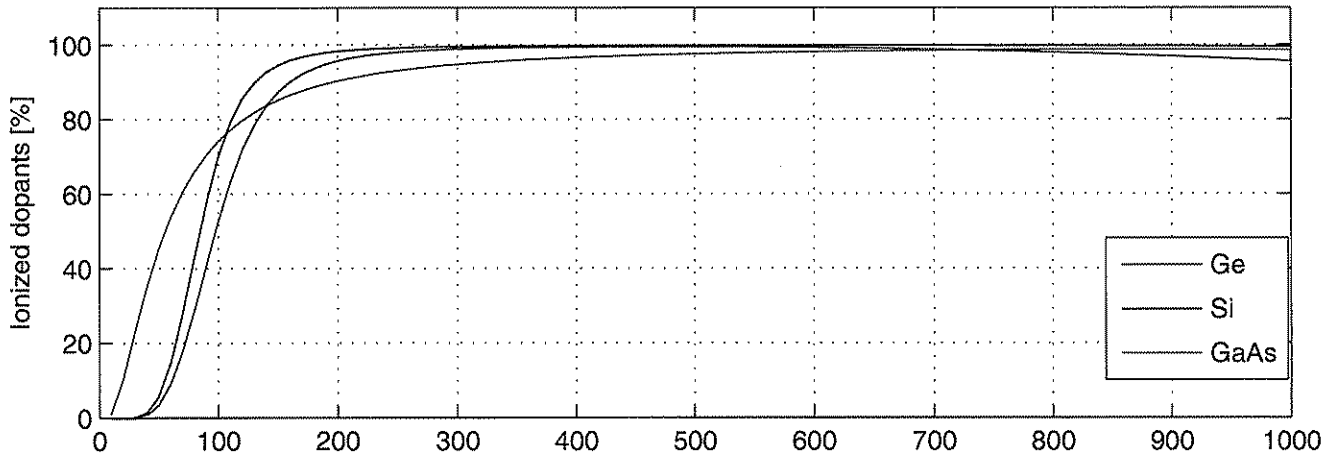
$T_{110\%} = 338^\circ \text{K}$

$T_{210\%} = 333^\circ \text{K}$

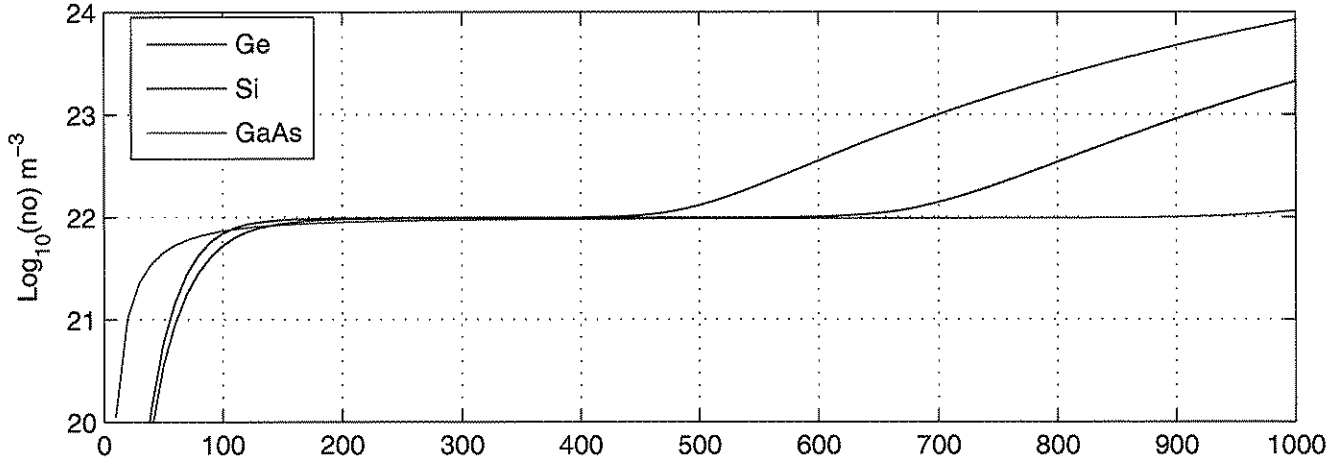
$T_{310\%} = 333^\circ \text{K}$



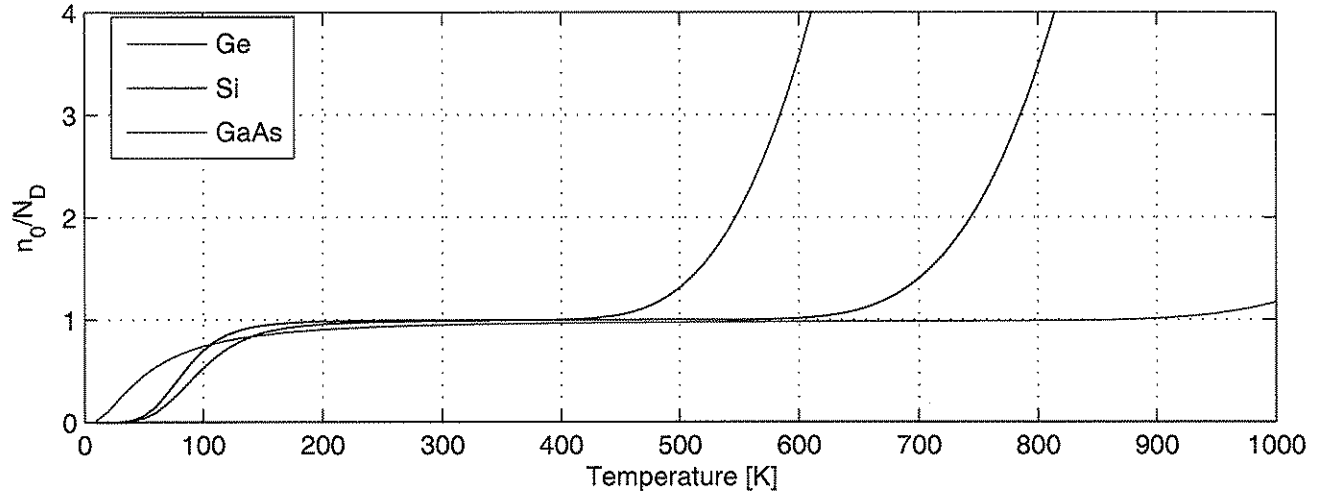
Percentage of ionized Impurities in Ge, Si and GaAs for  $N_D = 10^{22} \text{ m}^{-3}$



Absolute Carrier Concentration ( $N_D = 10^{22} \text{ m}^{-3}$ )



Relative Carrier Concentration  $n_0/N_D$  ( $N_D = 10^{22} \text{ m}^{-3}$ )



Carrier Concentration vs. Temperature

Silicon is doped with Phosphorus ( $N_D = 10^{22} \text{ m}^{-3}$ ).

Find  $n_0(T)$  for  $300 \text{ K} < T < 1000 \text{ K}$  if we know that the energy level  $E_D$  of Phosphorus lies 44 meV below the conduction band energy  $E_C$ .

Solution

Probability that Phosphorus is ionized

$$p_D = \frac{1}{1 + 2 e^{\frac{E_F - E_D}{kT}}} \quad (1)$$

Furthermore

$$n_0 = p_D \cdot N_D = N_C e^{-\frac{E_C - E_F}{kT}} \quad *$$

Solving for  $E_F$  in (2) yields

$$E_F = E_C + kT \ln\left(\frac{p_D N_D}{N_C}\right) \quad (3)$$

Insert (3) into (1)

$$\therefore p_D = \frac{1}{1 + 2 \frac{N_D}{N_C} p_D e^{\frac{E_C - E_D}{kT}}} \quad (4)$$

Solving for  $p_D$  yields

$$p_D = -\frac{1}{2} b_0 \pm \frac{1}{2} b_0 \sqrt{1 + \frac{4}{b_0}} \quad (5)$$

where  $b_0 = \frac{1}{2} \frac{N_C}{N_D} e^{-\frac{E_C - E_D}{kT}}$

charge neutrality equation

$$|n_0 = p_0 + p_D \cdot N_D| \quad (6)$$

law of mass action

$$|n_0 \cdot p_0 = n_{i0}^2| \quad (7)$$

Insert (7) into (6)

$$|n_0 = \frac{n_{i0}^2}{n_0} + p_D N_D| \quad (8)$$

solving for  $n_0$  yields

$$|n_0 = \frac{1}{2} p_D N_D \left[ 1 + \sqrt{1 + 4 \frac{n_{i0}^2}{(p_D N_D)^2}} \right]| \quad (9)$$

Note: if  $n_{i0} \ll p_D N_D$

$$\therefore |n_0 \cong p_D N_D| \quad \text{low to moderate temperature}$$

if  $n_{i0} \gg p_D N_D$

$$\therefore |n_0 \cong n_{i0}| \quad \text{high temperature}$$

\* The assumption that  $n_0 = p_D N_D$  does not hold for high temperatures as eq. (9) testifies. However, the resulting errors are replicably small since the decrease in  $p_D N_D$  is inconsequential in view of the exponential increase of  $n_0$  due to  $n_{i0}$ .

IV-25

