

# Lecture 9

# 5 SEMICONDUCTOR IN EQUILIBRIUM

- Interested in determining the current-voltage characteristics of semiconductor devices.
- Current is due to net flow of charges, there is a need to determine the number of charge carriers available for generating the currents, i.e. the electron concentration in the conduction band and hole concentration in the valence band.
- Therefore, first of all, we will look at the electrons and hole concentrations in thermal equilibrium at temperature  $T$ 
  - Thermal equilibrium implies that no external forces, such as voltages, electric fields, magnetic fields or **temperature gradients** are acting on the semiconductor.

- However, if the presence of external forces do not create excess electrons in the conduction band and holes in the valence band, i.e. the electrons and holes are solely created by the thermal energy, then we can use the thermal equilibrium electron and hole concentrations to analyze the behavior of the semiconductor in the presence of the external forces.
- In thermal equilibrium, all properties of semiconductor will be independent of time

To determine the thermal equilibrium electron and hole concentrations at temperature  $T$ , essentially we need to know the following:

- The density of quantum states, that is the number of quantum states per unit volume of the crystal per unit energy, in the conduction and valence bands
- The probability of a quantum states at energy  $E$  is occupied by an electron at temperature  $T$

## 5.1 Fermi-Dirac Distribution Function

The probability that a quantum state is occupied by an electron at temperature  $T$  is given by the Fermi-Dirac distribution function.

The Fermi-Dirac probability function describes the distribution of electrons over a range of allowed energy levels at thermal equilibrium.

To develop this probability function, we must consider the following:

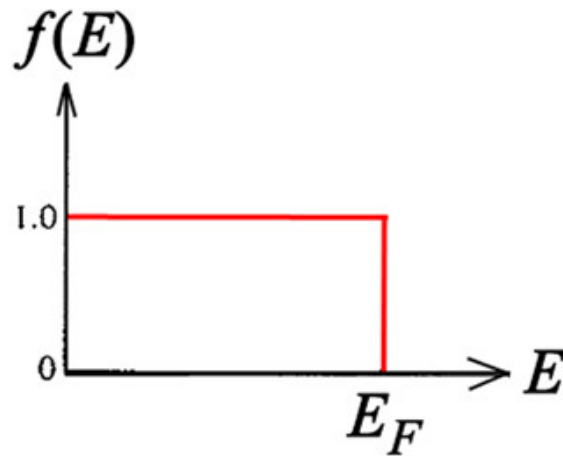
- The quantum nature of electrons
- Electrons are indistinguishable
- Only one particle is permitted in each quantum state (Pauli's exclusion principle)

- The Fermi-Dirac probability function is given by

$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]} \quad (5.1)$$

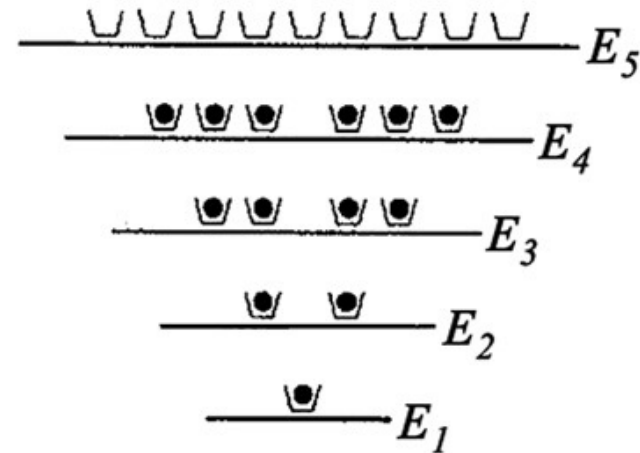
- it gives the probability that a quantum state at energy  $E$  will be occupied by an electron at temperature  $T$
- it is also the ratio of the filled states to the total quantum states at energy  $E$

$E_F$  is called the Fermi energy level. It determines the statistical distribution of electrons and does not have to correspond to an allowed energy state. The Fermi level is an important reference level.



**Fig. 5.1**

The Fermi probability function versus energy for  $T = 0^\circ\text{K}$



Discrete energy states and quantum states for a particular system at  $T = 0^\circ\text{K}$

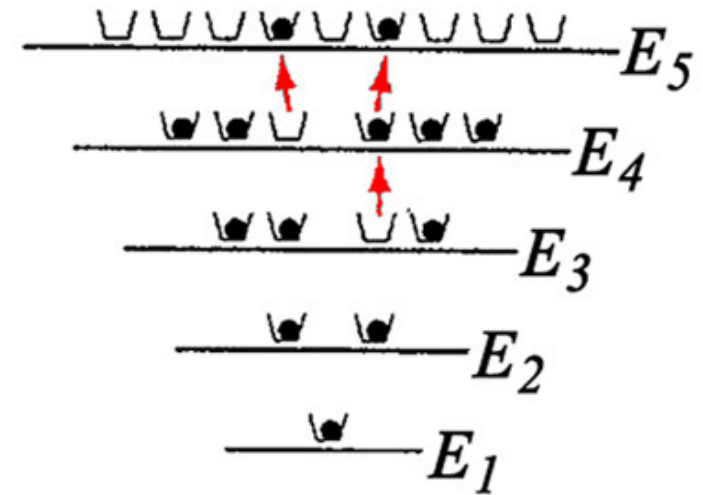
**At  $T = 0 \text{ K}$ ,**

$$f(E) = \begin{cases} 1 & \text{for } E < E_F \\ 0 & \text{for } E > E_F \end{cases} \quad (5.2)$$

- all electrons are in their lowest possible energy levels, up to the Fermi level
- probability of quantum states being occupied is unity for  $E < E_F$

At  $T > 0$  K,

- electrons gain a thermal energy so that some of them can jump to higher energy levels
  - change in distribution of electrons among available energy states



**Fig. 5.2** Discrete energy states and quantum states for the same system at  $T > 0^\circ\text{K}$

- At  $E > E_F$ , the Fermi-Dirac distribution in eqn. (5.1) is no longer zero. This means that some probabilities exists for a state above  $E_F$  is occupied by an electron.
- At  $E < E_F$ , the Fermi-Dirac distribution in eqn. (5.1) is no longer unity. This means that some probabilities exists for a state below  $E_F$  is empty.

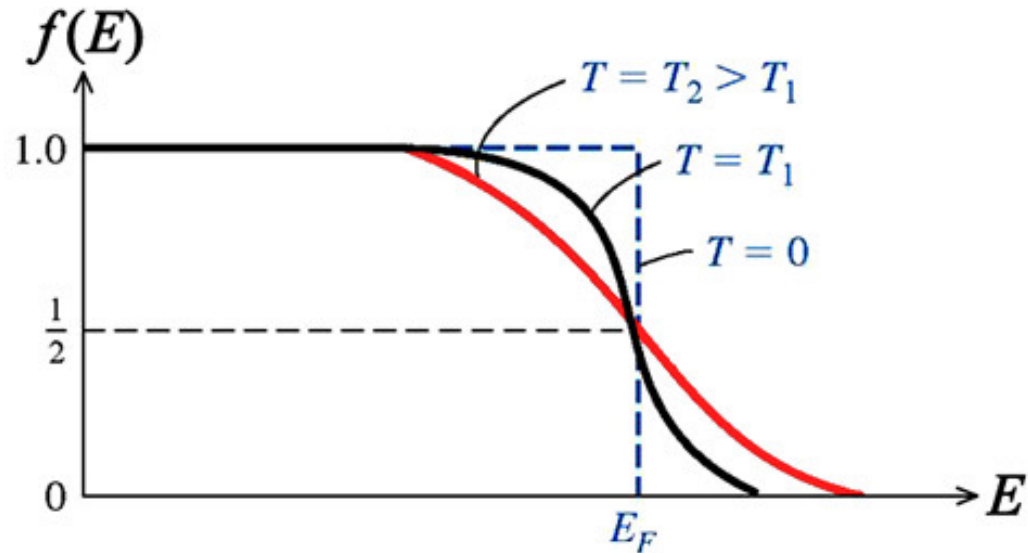
- At  $E = E_F$ , the Fermi-Dirac distribution is

$$f(E = E_F) = \frac{1}{1 + \exp(0)} = \frac{1}{2} \quad (5.3)$$

i.e. the probability of a state having energy  $E = E_F$  being occupied by an electron is  $\frac{1}{2}$

**Fig. 5.3**

The Fermi probability function vs energy for different temperatures



- Fig. 5.3 shows the Fermi-Dirac distribution function at various temperature  $T$ 
  - **symmetrical** about the Fermi energy  $E_F$  at all temperature.



- Consider the Fermi-Dirac function at temperature  $T_2$  in Fig. 5.3
  - The probability of a state having energy  $\Delta E$  above  $E_F$ , ( $E_F + \Delta E$ ), to be occupied by an electron is  $f(E_F + \Delta E)$
  - The probability of a state having energy  $\Delta E$  below  $E_F$ , ( $E_F - \Delta E$ ), to be empty is  $[1 - f(E_F - \Delta E)]$
  - Since the Fermi-Dirac function is symmetrical about the Fermi energy  $E_F$ , it follows that the probability of a state having energy  $\Delta E$  above  $E_F$  is occupied is the same as the probability of a state having energy  $\Delta E$  below  $E_F$  is empty.
  - mathematically, this means (and can be easily proved)

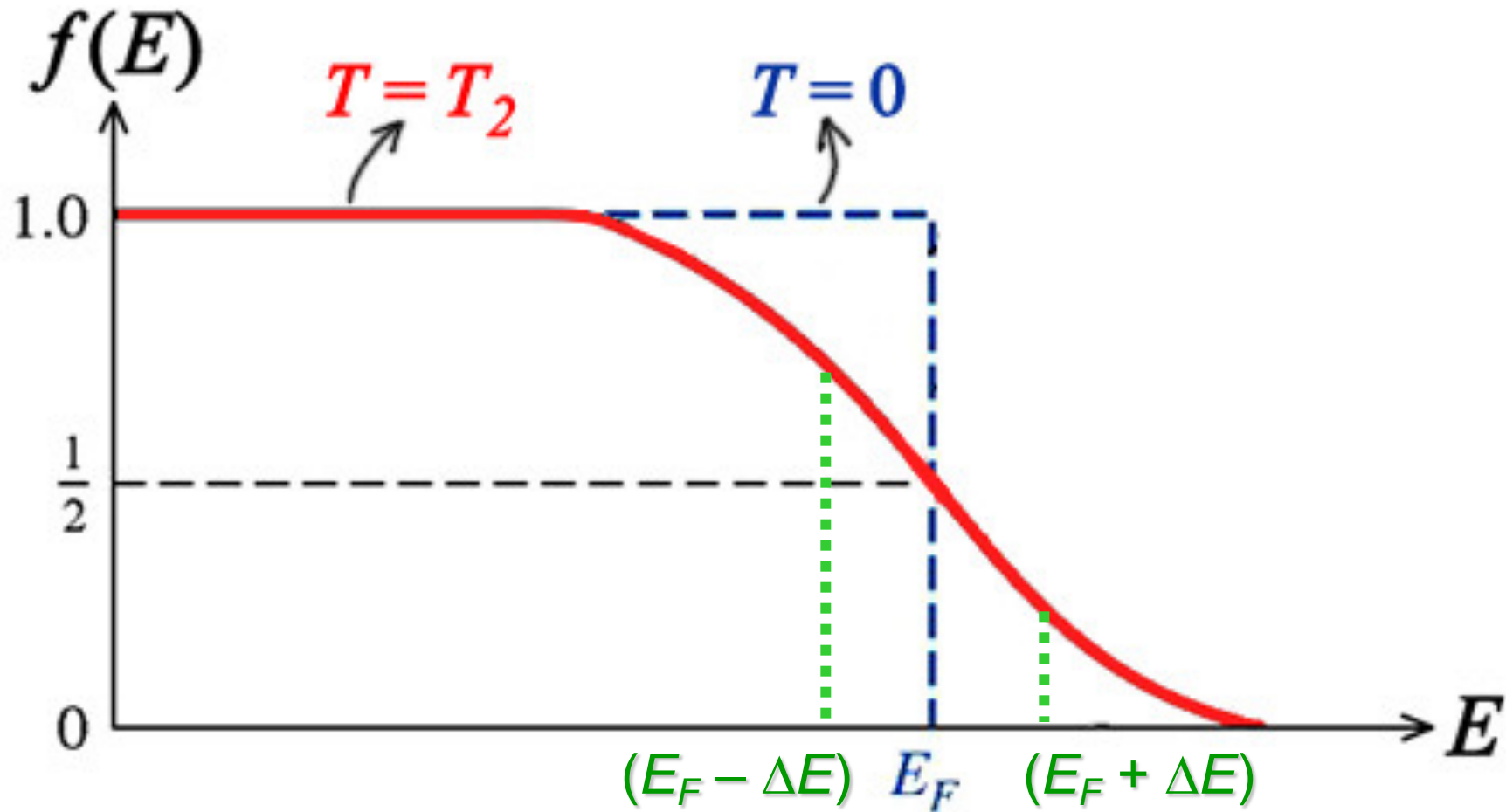
$$f(E_F + \Delta E) = 1 - f(E_F - \Delta E) \quad (5.4)$$

probability of a state  
having energy  $\Delta E$  above  
 $E_F$  is occupied

probability of a state  
having energy  $\Delta E$  below  
 $E_F$  is empty

Tutorial #3

- In terms of electrons and holes, we can say that probability of not finding an electron at energy  $E$ ,  $[1 - f(E)]$ , is the probability of finding a hole at energy  $E$ .



## Example 5.1

Calculate the probability that an energy state 0.56 eV above the Fermi energy is occupied by an electron for temperatures of 0 °C and 100 °C.

The probability of an energy state  $E = E_F + 0.56$  eV to be occupied by an electron is

$$f(E) = \frac{1}{1 + \exp \left[ \frac{E - E_F}{k_B T} \right]} = \frac{1}{1 + \exp \left[ \frac{0.56 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} T} \right]}$$

Hence, for  $T = 0$  °C = 273 K,  $f(E) = 4.69 \times 10^{-11}$ ,

and for  $T = 100$  °C = 373 K,  $f(E) = 2.76 \times 10^{-8}$

Note that as temperature increases by 100 °C, the probability increases by ~ 600 times. This shows the great sensitivity of this probability on temperature

## 5.2 Density of States

In addition to the Fermi-Dirac distribution function, we also need to consider the density of quantum states available for electrons to occupy.

### 5.2.1 Free electrons

To discuss the density of states of electrons in a crystal, let us start with the density of states of free electrons in 3-dimensions (3-D).

- Density of states is the number of quantum states per unit volume of the crystal per unit energy.
- The density of states  $g(E)$  for free electrons in 3-D is derived in Appendix B. It is given by

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3} \sqrt{E} \quad (5.5)$$

where the energy  $E$  is the free electron energy in 3-D [see Appendix B, eqn. (B.3)], that is

$$E = \frac{\hbar^2 k^2}{2m}$$

so, alternatively we can write eqn. 5.5 as

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3} \sqrt{\frac{\hbar^2 k^2}{2m}} \quad (5.6)$$

## 5.2.2 Electrons in crystals

The electrons in a crystal are not completely free, they interact with the periodic potential formed by the ions and electrons.

In section 3.4.4, we have seen that the effective mass takes into account the interaction of charge carriers with the lattice, which then allow us to regard the charge carriers as free carriers.

Consider now electrons in the conduction band

- Near the conduction band minima the  $E - k$  relation is approximately parabolic (see Fig. 5.4). The electrons behave like free electrons with effective mass  $m_n^*$ . Therefore we can express the energy  $E$  as

$$E - E_c = \frac{\hbar^2 k^2}{2m_n^*} \quad (5.7)$$

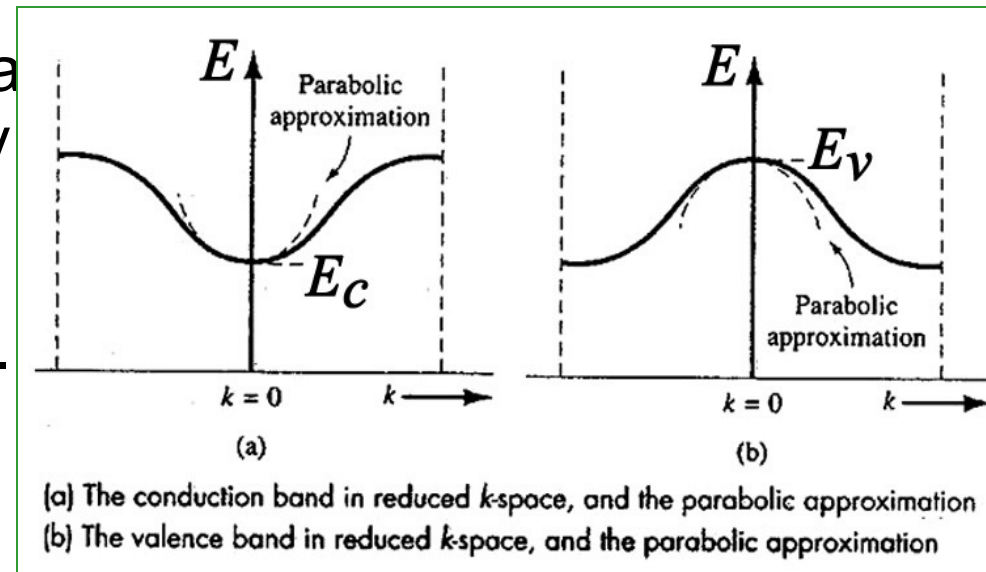


Fig.5.4

- Using eqn. (5.7) and the effective mass  $m_n^*$  in eqn. (5.6), we obtain the density of states in the conduction band  $g_c(E)$

$$g_c(E) = \frac{4\pi (2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c} \quad (5.8)$$

We can obtain the density of states in the valence band  $g_v(E)$  in the same way as we obtain the density of states in the conduction band

- Near the top of the valence band, the  $E - k$  relation is also approximately parabolic (see Fig. 5.4) with the effective mass  $m_p^*$ . The energy  $E$  is then

$$E_v - E = \frac{\hbar^2 k^2}{2m_p^*} \quad (5.9)$$

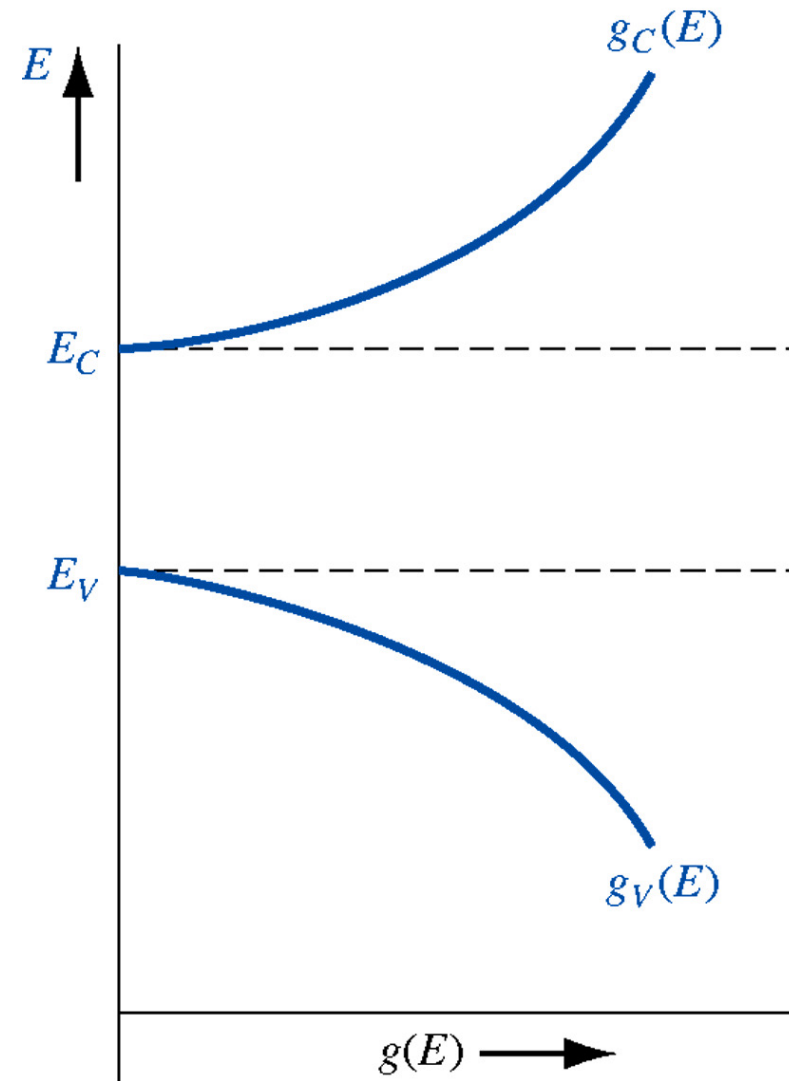
- Therefore, the density of states in the valence band is

$$g_v(E) = \frac{4\pi (2m_p^*)^{3/2}}{h^3} \sqrt{E_v - E} \quad (5.10)$$

Fig. 5.5 shows the density of states in the conduction and valence bands as function of energy  $E$

If quantum states do not exist within forbidden energy band, the density of states

$$g(E) = 0 \text{ for } E_v < E < E_c$$



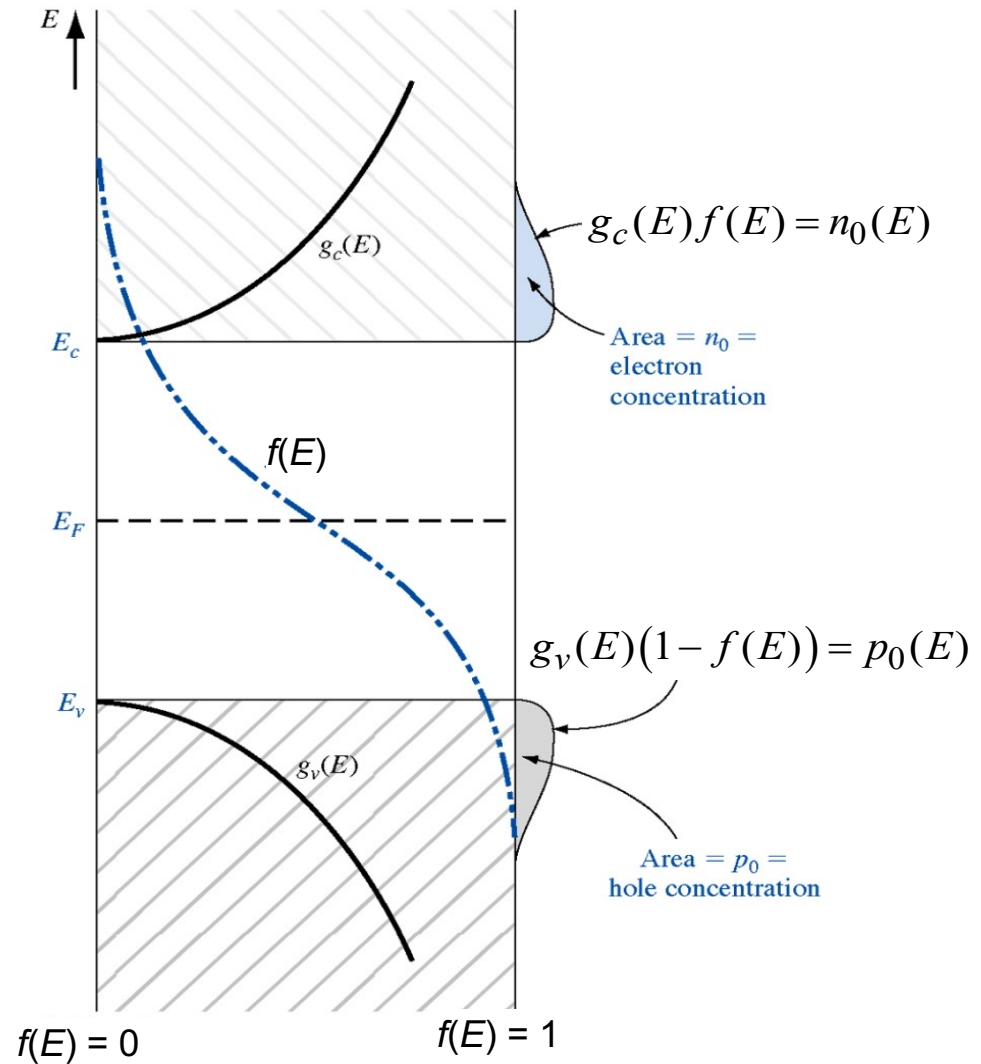
**Fig. 5.5**



## 5.3 Thermal equilibrium carrier concentrations

- At thermal equilibrium, the electron concentration at energy  $E$  in the conduction band, denoted by  $n_0(E)$ , is :

$$n_0(E) = g_c(E) f(E) \quad (5.11)$$



**Fig. 5.6**

Density of states function, Fermi-Dirac probability function, and areas representing electron and hole concentration for the case  $E_F$  is near the midgap

- The thermal equilibrium electron concentration in the conduction band  $n_0$  is then given by the integration over all the energies  $E$  in the entire conduction band, i.e. from the bottom of the conduction band  $E_c$  to  $\infty$

$$n_0 = \int_{E_c}^{\infty} n(E) dE = \int_{E_c}^{\infty} g_c(E) f(E) dE \quad (5.12)$$

- We will calculate the thermal equilibrium electron concentration  $n_0$  for the Fermi energy  $E_F$  within the bandgap below the conduction band edge  $E_c$ , such that

$$E_c - E_F \gg k_B T \quad (5.13)$$

To satisfy eqn. (5.13), it is sufficient to take  $E_c - E_F > 3k_B T$

- The energy of electrons in the conduction band  $E$  is above  $E_c$ , it follows

$$E - E_F \gg k_B T \quad (5.14)$$

The Fermi-Dirac distribution can then be reduced as follow

$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]} \approx \exp\left[-\frac{E - E_F}{k_B T}\right] \quad (5.15)$$

- Now, we evaluate the thermal equilibrium electron concentration  $n_0$  in eqn. (5.12) using the density of states  $g_c(E)$  in eqn. (5.8) and the reduced  $f(E)$  in eqn. (5.15). We obtain

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right] \quad (5.16)$$

where  $N_c$  is the effective density of states in the conduction band, given by

$$N_c = 2 \left( \frac{2\pi m_n^* k_B T}{h^2} \right)^{3/2} \quad (5.17)$$

# Problem

Q1: Determine the probability that a quantum state energy  $E = E_c + kT$  is occupied by an electron, and calculate the electron concentration in GaAs at  $T = 300\text{K}$  if the Fermi level is 0.25 eV below  $E_c$ . (Ex 4.1)



# Problem

Q1: Determine the probability that a quantum state energy  $E = E_c + kT$  is occupied by an electron, and calculate the electron concentration in GaAs at  $T = 300\text{K}$  if the Fermi level is 0.25 eV below  $E_c$ . (Ex 4.1)

$$\begin{aligned} f_F &\cong \exp\left[\frac{-(E - E_F)}{kT}\right] \\ &= \exp\left[\frac{-(E_c + kT - E_F)}{kT}\right] \\ &= \exp\left[\frac{-(0.25 + 0.0259)}{0.0259}\right] \end{aligned}$$

$$f_F = 2.36 \times 10^{-5}$$

$$\begin{aligned} n_o &= N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right] \\ &= (4.7 \times 10^{17}) \exp\left[\frac{-0.25}{0.0259}\right] \end{aligned}$$

$$n_o = 3.02 \times 10^{13} \text{ cm}^{-3}$$



## Key takeaways (Lecture #9)

- To determine the thermal equilibrium electron and hole concentrations at temperature  $T$ , we need:
  - The density of quantum states in the conduction and valence bands
  - The probability of a quantum states at energy  $E$  is occupied by an electron at temperature  $T$

- Fermi-Dirac Distribution Function: 
$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]}$$

- Equilibrium electron concentration  $n_0$  in CB:

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right] \quad N_c = 2 \left( \frac{2\pi m_n^* k_B T}{h^2} \right)^{3/2}$$

# Lecture 10

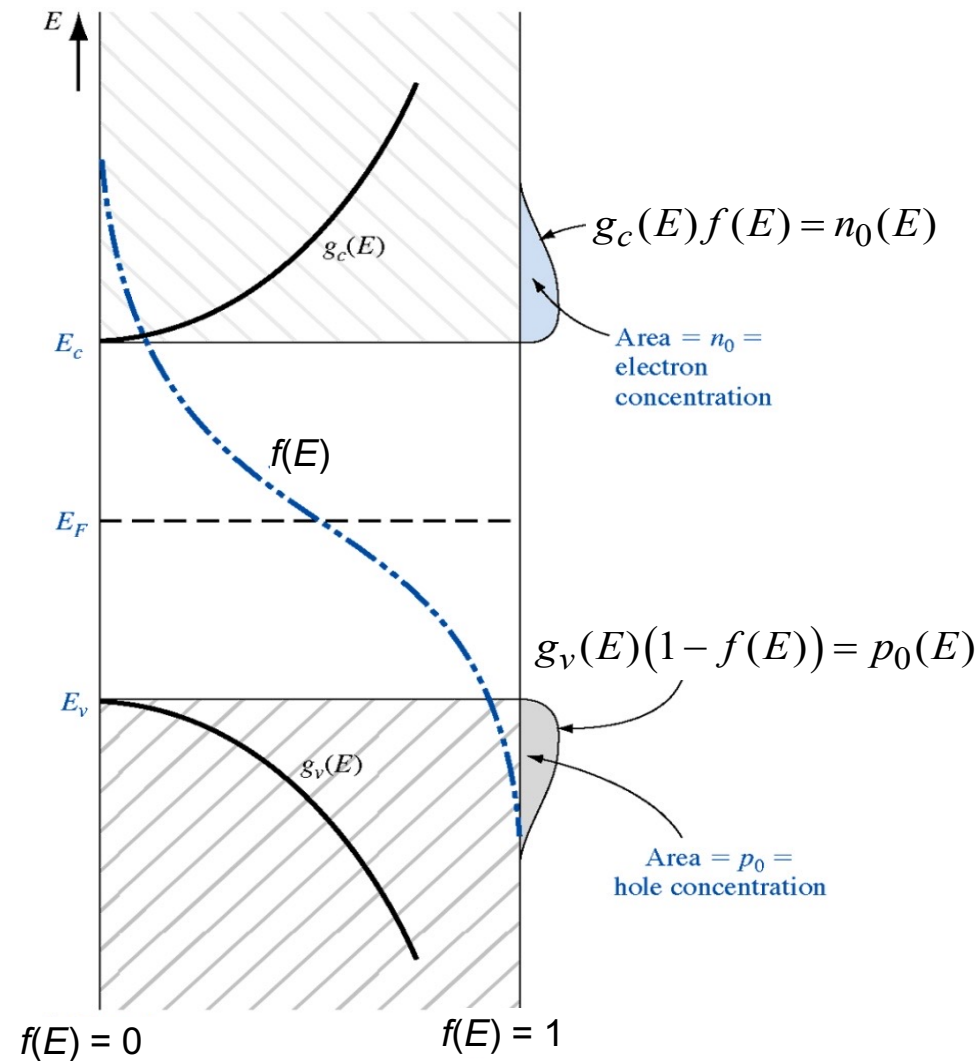


In a similar way, we can obtain the thermal equilibrium hole concentration in the valence band, denoted by  $p_0$ .

- The thermal equilibrium hole concentration at energy  $E$  in the valence band,  $p_0(E)$ , is

$$p_0(E) = g_v(E) \{1 - f(E)\} \quad (5.18)$$

the probability of a state at energy  $E$  is not occupied by an electron



Density of states function, Fermi-Dirac probability function, and areas representing electron and hole concentration for the case  $E_F$  is near the midgap

**Fig. 5.6**

- The thermal equilibrium holes concentration in the valence band is then given by

$$p_0 = \int_{-\infty}^{E_v} g_v(E) \{1 - f(E)\} dE \quad (5.19)$$

the integration is over all the energy  $E$  in the valence band, i.e. from  $-\infty$  to the top of valence band  $E_v$ .

- Now, we evaluate  $p_0$  for the Fermi energy  $E_F$  above the valence band edge  $E_v$ , such that

$$E_F - E_v \gg k_B T \quad (5.20)$$

Again,  $E_F - E_v > 3k_B T$  is sufficient to satisfy eqn. (5.20)

- Since the energy  $E$  in the valence band is below  $E_v$ , it follows

$$E_F - E \gg k_B T \quad (5.21)$$

Using eqn. (5.21), the term  $\{1 - f(E)\}$  in eqn. (5.19) can then be approximated as follow

$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \approx \exp\left(-\frac{E_F - E}{k_B T}\right) \quad (5.22)$$

- We can now evaluate the thermal equilibrium hole concentration  $p_0$  in eqn. (5.19) using the density of states  $g_v(E)$  in eqn. (5.10) and the reduced  $\{1 - f(E)\}$  in eqn. (5.22). We obtain

$$p_0 = N_v \exp \left[ - \frac{E_F - E_v}{k_B T} \right] \quad (5.23)$$

where  $N_v$  is the effective density of states in valence band and given by

$$N_v = 2 \left( \frac{2\pi m_p^* k_B T}{h^2} \right)^{3/2} \quad (5.24)$$

Semiconductors with electron and hole concentrations described by eqn. (5.16) and (5.23) respectively are called nondegenerate semiconductors. It is obvious, for nondegenerate semiconductors the position of the Fermi level  $E_F$  in the bandgap follows eqns. (5.13) and (5.20).

It is important to note the following

- The assumption used in deriving the thermal equilibrium electron and hole concentrations is that the Fermi energy  $E_F$  is not too close to the conduction and valence band edges,  $E_c$  and  $E_v$  respectively.
- So long as this assumption is valid, the expressions for the thermal equilibrium electron and hole concentrations,  $n_0$  and  $p_0$ , are valid for intrinsic and extrinsic semiconductors.
- $n_0$  and  $p_0$  are directly related to the effective density of states and to the Fermi energy level
  - temperature factor present in the effective density of states and the exponential term (representative of probability)
  - hence, thermal equilibrium concentrations will be very sensitive to the temperature

## 5.4 Intrinsic Material

For an intrinsic semiconductor,

- concentration of electrons in conduction band is equal to concentration of holes in valence band
- if we denote the electron and hole concentrations in an intrinsic semiconductor as  $n_i$  and  $p_i$  (subscript  $i$  refers to intrinsic), then

$$n_i = p_i \quad (5.25)$$

- the Fermi energy level of an intrinsic semiconductor is called the intrinsic Fermi energy,  $E_i$ . We understand that the expression of the thermal equilibrium electron and hole concentrations, eqns. (5.16) and (5.23) respectively, valid for both intrinsic and extrinsic semiconductors. If we apply eqns. (5.16) and (5.23) to an intrinsic semiconductor we obtain

$$n_i = N_c \exp\left[-\frac{E_c - E_i}{k_B T}\right] \quad (5.26)$$

and

$$p_i = N_v \exp\left[-\frac{E_i - E_v}{k_B T}\right] \quad (5.27)$$

- Now, multiply eqn. (5,26) with eqn. (5.27) and use the condition in eqn. (5.25) we obtain

$$n_i^2 = N_c N_v \exp\left[-\frac{E_c - E_v}{k_B T}\right] = N_c N_v \exp\left[-\frac{E_g}{k_B T}\right] \quad (5.28)$$

$$n_i = \sqrt{N_c N_v} \exp\left[-\frac{E_g}{2k_B T}\right] \quad (5.29)$$

It is very important to note here, that for a given semiconductor material at a constant temperature, the value of the intrinsic carrier concentration,  $n_i$ , is a constant and is independent of the Fermi energy.

This is true regardless whether the semiconductor is intrinsic (undoped) or extrinsic (doped).



- Recall eqns. (5.16) and (5.23), the thermal equilibrium electron and hole concentrations,  $n_0$  and  $p_0$ . The product of  $n_0$  and  $p_0$  is

$$n_0 p_0 = N_c N_v \exp\left[-\frac{E_c - E_v}{k_B T}\right] = N_c N_v \exp\left[-\frac{E_g}{k_B T}\right] \quad (5.30)$$

We see that the product of  $n_0$  and  $p_0$  is a constant for a particular material and temperature  $T$ . This is exactly the same as the expression for  $n_i^2$  in equation (5.28). We, therefore, obtain

$$n_0 p_0 = n_i^2 \quad (5.31)$$

This equation valid for intrinsic and extrinsic semiconductors.

- At a particular temperature  $T$ , the value of  $n_i$  is dependent on material parameters, like electron and hole effective masses,  $m_n^*$  and  $m_p^*$  respectively, and the bandgap energy  $E_g$ .

- For example, silicon at 300 K

$m_n^* = 1.08 m_0$  and  $m_p^* = 0.56 m_0$ , where  $m_0$  is the free electron rest mass.  $E_g = 1.12$  eV.

Using equations (5.17) and (5.24),

$$N_c = 2.8 \times 10^{19} / \text{cm}^3 \text{ and } N_v = 1.05 \times 10^{19} / \text{cm}^3$$

and then using equation (5.29)

$$n_i = 6.84 \times 10^9 / \text{cm}^3$$

- experimentally, the accepted value of  $n_i$  for silicon at 300 K is  $1.5 \times 10^{10} / \text{cm}^3$ . The discrepancy is due to the simple theoretical model adopted.

- Table 5.1 list the value of  $n_i$  for some semiconductors at 300 K. We see that  $n_i$  increases with decreasing energy gap  $E_g$ . This is expected since  $n_i$  is exponentially dependent on  $E_g$  (see eqn. 5.29)

**Table 5.1**

Materials	$n_i$ (/cm <sup>3</sup> )	$E_g$ (eV)
<b>GaAs</b>	$1.8 \times 10^6$	1.43
<b>Si</b>	$1.5 \times 10^{10}$	1.11
<b>Ge</b>	$2.4 \times 10^{13}$	0.67

- If we substitute the effective density of states  $N_c$  in eqn. (5.17) and  $N_v$  in eqn. (5.24) into the intrinsic carrier concentration  $n_i$  in eqn. (5.29), we obtain

$$n_i = 2 \underbrace{\left( \frac{2\pi k_B T}{h^2} \right)^{3/2}}_{\text{relatively constant over temperature range}} \left( m_n^* m_p^* \right)^{3/4} \exp \left[ \underbrace{-\frac{E_g}{2k_B T}}_{\text{dominant term}} \right] \quad (5.32)$$

- In eqn. (5.32), we note that, for a given material, all the parameters, except  $T$ , are constant
  - temperature  $T$  appears twice in eqn. (5.32):  $T^{3/2}$  and  $\exp(-1/T)$ .
  - the dominant term is the exponential term, the  $T^{3/2}$  term is relatively constant over a temperature range.

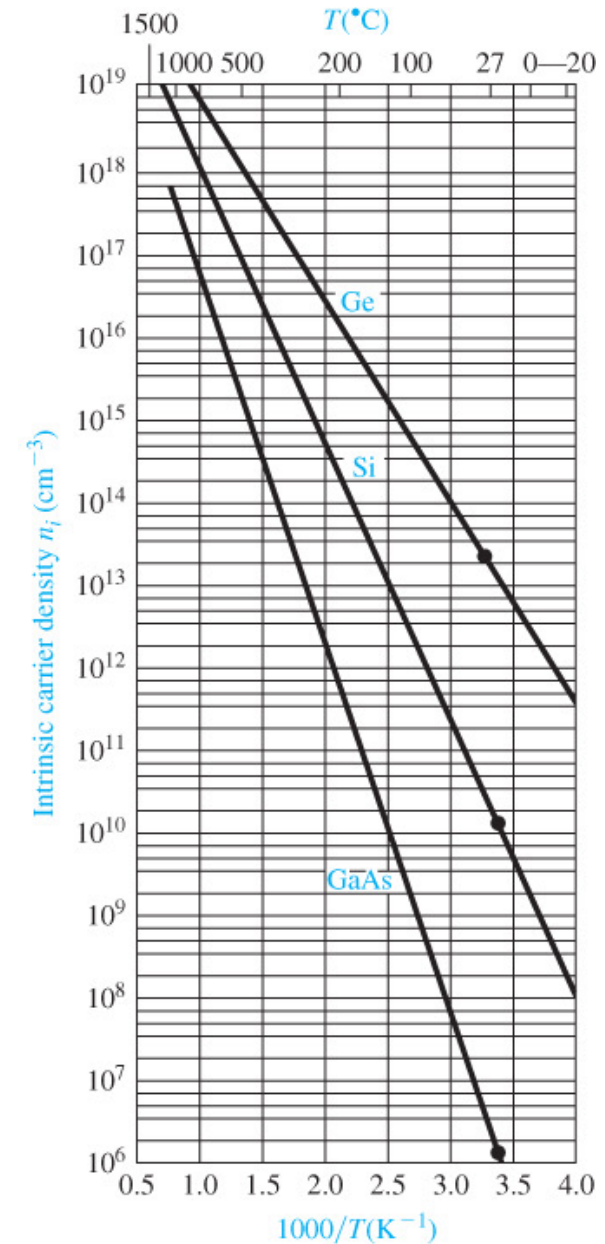
Hence, we could write

$$n_i \approx \text{constant} \times \exp\left[-\frac{E_g}{2k_B T}\right]$$

$$\ln n_i = \ln(\text{constant}) - \frac{E_g}{2k_B T} \quad (5.33)$$

this is a straight line equation, so if we plot  $\ln n_i$  versus  $1/T$ , we will get a straight line with the slope of  $-E_g/2k_B$

- The plot of eqn. (5.33) for some semiconductors is shown in Fig. 5.7.



**Figure 4.2** | The intrinsic carrier concentration of Ge, Si, and GaAs as a function of temperature.  
(From Sze [14].)

- To calculate the exact position of the intrinsic Fermi level  $E_i$ , we equate  $n_i$  in eqn. (5.26) and  $p_i$  in eqn. (5.27). We obtain

$$n_i = N_c \exp\left[-\frac{E_c - E_i}{k_B T}\right] \quad (5.26)$$

$$E_i = \frac{1}{2}(E_c + E_v) + \frac{1}{2}k_B T \ln\left(\frac{N_v}{N_c}\right) \quad (5.34)$$

Using the expressions of  $N_c$  and  $N_v$  in eqns. (5.17) and (5.24) respectively, we change the ratio of the effective density of states into the ratio of the effective masses

$$E_i = E_{mid} + \frac{3}{4}k_B T \ln\left(\frac{m_p^*}{m_n^*}\right) \quad (5.35)$$

$$\text{where } E_{mid} = \frac{1}{2}(E_c + E_v) \quad (5.36)$$

**Example:** Calculate the displacement of  $E_i$  from  $E_{mid}$  at 300 K, assuming the electron and hole effective masses are  $1.1 m_0$  and  $0.56 m_0$  respectively.

The displacement of the intrinsic Fermi energy from the center of the bandgap at 300 K is

$$E_i - E_{mid} = \frac{3k_B T}{4} \ln \left( \frac{m_p^*}{m_n^*} \right)$$
$$E_i - E_{mid} = \frac{3 \times 1.38 \times 10^{-23} \times 300}{4 \times 1.6 \times 10^{-19}} \ln \left( \frac{0.56}{1.1} \right)$$

$$E_i - E_{mid} = -0.013 \text{ eV}$$

At room temperature the displacement of the intrinsic Fermi level from the centre of the bandgap is very small.  $E_i$  is very close to the center of the bandgap.

- From eqn. (5.36), we see that the intrinsic Fermi level is exactly in the middle of the bandgap, i.e.  $E_i = E_{mid}$ , if
  - the temperature  $T = 0$  K or
  - $m_n^* = m_p^*$
- The deviation of  $E_i$  from  $E_{mid}$  is very small and in many cases the position  $E_i$  can be considered to be at the center of the bandgap.



- To express  $n_0$  and  $p_0$ , in terms of the intrinsic carrier concentration  $n_i$  and the intrinsic Fermi level  $E_i$ , we can easily do that by dividing eqn. (5.16) with eqn. (5.26) and eqn. (5.23) with eqn. (5.27). We obtain

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right] \quad (5.37)$$

$$p_0 = n_i \exp\left[\frac{E_i - E_F}{k_B T}\right] \quad (5.38)$$

Multiplying eqn. (5.37) with eqn. (5.38) will give us

$$n_0 p_0 = n_i^2$$

which is exactly the same result as we obtained in eqn. (5.31).

## Interpreting the relative position of Fermi level

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right]$$

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right]$$

$$p_0 = N_v \exp\left[-\frac{E_F - E_v}{k_B T}\right]$$

$$p_0 = n_i \exp\left[\frac{E_i - E_F}{k_B T}\right]$$

<http://www.acsu.buffalo.edu/~wie/applet/applet.old>

Three applets for the concept of Fermi Level:

# Key takeaways (Lecture #10)

- Equilibrium hole concentration  $p_0$  in VB :

$$p_0 = N_v \exp\left[-\frac{E_F - E_v}{k_B T}\right] \quad N_v = 2 \left( \frac{2\pi m_p^* k_B T}{h^2} \right)^{3/2}$$

- $n_i$  increases with decreasing energy gap  $E_g$  :

$$n_i = \sqrt{N_c N_v} \exp\left[-\frac{E_g}{2k_B T}\right]$$

- The product of  $n_0$  and  $p_0$  is a constant for a particular material and temperature  $T$ :

$$n_0 p_0 = n_i^2$$

# Lecture 11

## 5.5 Extrinsic materials

In this section we will calculate the thermal equilibrium electron and hole concentrations,  $n_0$  and  $p_0$ , as a function of the impurity concentration.

### 5.5.1 Donor impurity

Let us start with an n-type semiconductor where donor concentration is  $N_d$ . The majority carrier is electrons.

From section 4.2.:

- The thermal equilibrium majority electron concentration  $n_0$  is the sum of the electron concentration from the donor impurity and the electron concentration due to the excitation from the valence band to the conduction band creating the electron-hole pairs.

- At temperature  $T$  where all donor atoms are all ionized we have (recall eqn. 4.1)

$$n_0 = N_d + p_0 \quad (4.1)$$

negative charge concentration

positive charge concentration

- How can we now calculate  $n_0$  and  $p_0$  ?

We first calculate the majority carrier concentration  $n_0$  by simply using eqn. (5.31)

$$n_0 p_0 = n_i^2$$

to substitute  $p_0$  in eqn. (4.1) in terms of  $n_0$  and  $n_i$ .

We obtain

$$n_0 = N_d + \frac{n_i^2}{n_0} \quad (5.39)$$

Multiplying eqn. (5.39) throughout by  $n_0$  and rearranging the equation, we get

$$n_0^2 - N_d n_0 - n_i^2 = 0 \quad (5.40)$$

this is a quadratic equation in  $n_0$ . The solution of this equation is

$$n_0 = \frac{N_d \pm \sqrt{N_d^2 + 4n_i^2}}{2} \quad (5.41)$$

- We only take the positive solution in eqn. (5.41). The negative solution is omitted since it has no physical meaning.

- So, the thermal equilibrium majority electron concentration is

$$n_0 = \frac{N_d + \sqrt{N_d^2 + 4n_i^2}}{2} \quad (5.42)$$

- It is important to note the following in eqn. (5.42):
  - If the doping concentration is much larger than the intrinsic carrier concentration, that is

$$N_d \gg n_i \quad (5.43)$$

then the  $4n_i^2$  term in eqn. (5.42) can be ignored and  $n_0$  is approximately equal to  $N_d$ ,

$$n_0 \approx N_d \quad (5.44)$$



- If the doping concentration is not much larger than the intrinsic carrier concentration, then  $n_0$  cannot be approximated to  $N_d$ , and eqn. (5.42) needs to be used to calculate  $n_0$ .
- Once we obtain  $n_0$ , the thermal equilibrium minority hole concentration can be calculated using eqn. (5.31)

$$p_0 n_0 = n_i^2$$

- Using the value of  $n_0$ , the position of the Fermi level  $E_F$  in the bandgap can be determined using either eqn. (5.16) or eqn. (5.37), depending on the question, of course

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right] \quad (5.16)$$

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right] \quad (5.37)$$

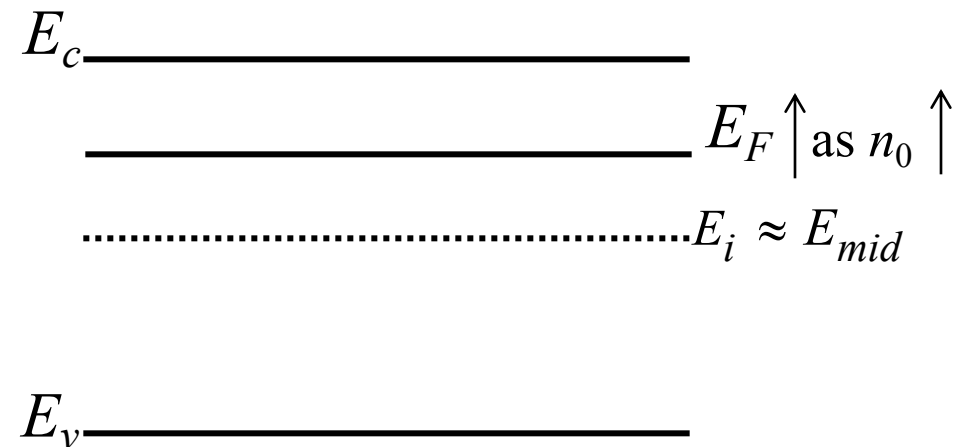
- At thermal equilibrium, the position of the Fermi level in the bandgap can also be determined using the value of  $p_0$ . In this case, we use either eqn. (5.23) or eqn. (5.38).

$$p_0 = N_v \exp \left[ -\frac{E_F - E_v}{k_B T} \right] \quad (5.23)$$

$$p_0 = n_i \exp \left[ \frac{E_i - E_F}{k_B T} \right] \quad (5.38)$$

At thermal equilibrium, the position of the Fermi level  $E_F$  is the same regardless we use  $n_0$  or  $p_0$  (see example 5.2)

- For n-type semiconductor ( $n_0 > p_0$ ),  $E_F$  is above the intrinsic Fermi level  $E_i$ . The Fermi level  $E_F$  moves up as  $n_0$  increases. This is clear from eqns. (5.16) and (5.37) and illustrated in Fig. 5.8.



**Fig. 5.8**

## Example 5.2

Consider a Si sample doped with  $10^{16}$  P atoms/cm<sup>3</sup> at 300 K. The intrinsic carrier concentration is  $1.5 \times 10^{10}$  /cm<sup>3</sup>. Calculate

- i) the thermal equilibrium minority concentration
- ii) and the position of the Fermi level relative to the intrinsic Fermi level

The impurity P atom is from Group V in the periodic table. So, in the Si sample, the P atom acts as donor and hence the majority carrier is electrons.

Using eqn. (5.42) we obtain the majority carrier concentration

$$n_0 = \frac{10^{16} + \sqrt{(10^{16})^2 + 4(1.5 \times 10^{10})^2}}{2} = 10^{16} \text{ / cm}^3$$

From the above calculation we show that for  $N_d \gg n_i$ ,  $n_0 = N_d$

From eqn. (5.31), the thermal equilibrium minority hole concentration is

$$n_0 p_0 = n_i^2$$

$$p_0 = \frac{(1.5 \times 10^4)^2}{10^{16}} = 2.25 \times 10^4 \text{ /cm}^3$$

The position the Fermi level can be obtained using either the value of  $n_0$  (eqn. 5.37) or  $p_0$  eqn. (eqn. 5.38)

Using the value of  $n_0$

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right] \quad (5.37)$$

$$E_F - E_i = k_B T \ln\left(\frac{n_0}{n_i}\right) = 1.38 \times 10^{-23} \times 300 \times \ln\left(\frac{10^{16}}{1.5 \times 10^{10}}\right) = 5.55 \times 10^{-20} \text{ J}$$

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}, \quad \therefore E_F - E_i = 0.347 \text{ eV}$$

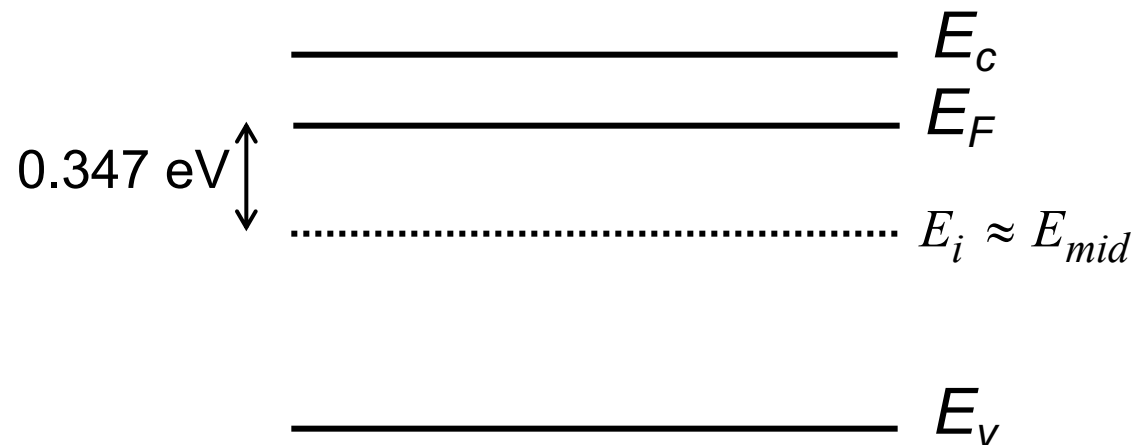
Using the value of  $p_0$

$$p_0 = n_i \exp\left[\frac{E_i - E_F}{k_B T}\right] \quad (5.38)$$

$$E_i - E_F = k_B T \ln\left(\frac{p_0}{n_i}\right) = 1.38 \times 10^{-23} \times 300 \times \ln\left(\frac{2.25 \times 10^4}{1.5 \times 10^{10}}\right) = -5.55 \times 10^{-20} \text{ J}$$

$$E_i - E_F = -0.347 \text{ eV} \quad \text{or} \quad E_F - E_i = 0.347 \text{ eV}$$

This is exactly the same result as obtained previously using eqn. (5.37)



### Example 5.3

Consider a germanium sample at 330 K in which  $N_d = 5 \times 10^{13} \text{ /cm}^3$ . Assume  $n_i = 2.4 \times 10^{13} \text{ /cm}^3$ , calculate the thermal equilibrium majority and minority concentration.



### Example 5.3

Consider a germanium sample at 330 K in which  $N_d = 5 \times 10^{13} \text{ /cm}^3$ . Assume  $n_i = 2.4 \times 10^{13} \text{ /cm}^3$ , calculate the thermal equilibrium majority and minority concentration.

At 330 K, the donor impurity is fully ionized. From eqn. (5.42), the majority carrier concentration is

$$n_0 = \frac{5 \times 10^{13} + \sqrt{(5 \times 10^{13})^2 + 4(2.4 \times 10^{13})^2}}{2} = 5.97 \times 10^{13} \text{ /cm}^3$$

Notice that, since  $N_d$  is not much larger than  $n_i$ ,  $n_0 \neq N_d$

From eqn. (5.31), the minority carrier concentration is

$$p_0 = \frac{n_i^2}{n_0} = \frac{(2.4 \times 10^{13})^2}{5.97 \times 10^{13}} = 9.65 \times 10^{12} \text{ /cm}^3$$

## 5.5.2 Acceptor impurity

Let us now consider a p-type semiconductor with acceptor concentration  $N_a$ . Here, the majority carrier is holes.

From section 4.3:

- The thermal equilibrium majority hole concentration  $p_0$  is the sum of the holes created due to the excitation of electrons from the valence band to the acceptor level and the excitation of electron from the valence band to the conduction band.
- At  $T$  where all acceptor atoms are fully ionized we have (see eqn. 4.6)

$$p_0 = N_a + n_0 \quad (4.6)$$

positive charge concentration

negative charge concentration



- We can obtain the majority carrier concentration  $p_0$  and the minority carrier concentration  $n_0$  by using the same procedure as we did in section 5.5.1.
- Firstly, we calculate the majority carrier concentration  $p_0$  by substituting the minority carrier concentration  $n_0$  in eqn. (4.6) in terms of  $p_0$  and  $n_i$ . Of course, we use eqn. (5.31). We obtain

$$p_0 = N_a + \frac{n_i^2}{p_0} \quad (5.45)$$

from eqn. (5.45), the majority carrier concentration is

$$p_0 = \frac{N_a + \sqrt{N_a^2 + 4n_i^2}}{2} \quad (5.46)$$

- Again, using eqn. (5.31), the minority carrier concentration is

$$n_0 = \frac{n_i^2}{p_0}$$

- For  $N_a \gg n_i$ ,  $p_0 \approx N_a$  (5.47)
- Having obtained  $p_0$  and  $n_0$ , the position of the Fermi level can be easily determined as discussed in section 5.5.1.
  - Using the value of  $p_0$  we use

$$\text{either } p_0 = N_v \exp \left[ -\frac{E_F - E_v}{k_B T} \right] \quad (5.23)$$

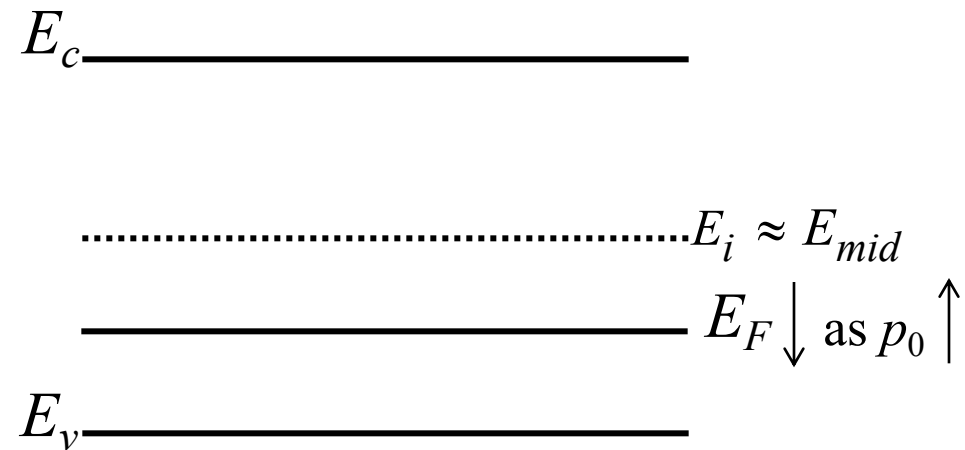
$$\text{or } p_0 = n_i \exp \left[ \frac{E_i - E_F}{k_B T} \right] \quad (5.38)$$

- Using the value of  $n_0$  we use

either  $n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right]$  **(5.16)**

or  $n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right]$  **(5.37)**

- For p-type semiconductor ( $p_0 > n_0$ ),  $E_F$  is below  $E_i$ . The Fermi level  $E_F$  moves down with increasing  $p_0$ . This is clear from eqns. (5.23) and (5.38) and illustrated in Fig. 5.9.



**Fig. 5.9**

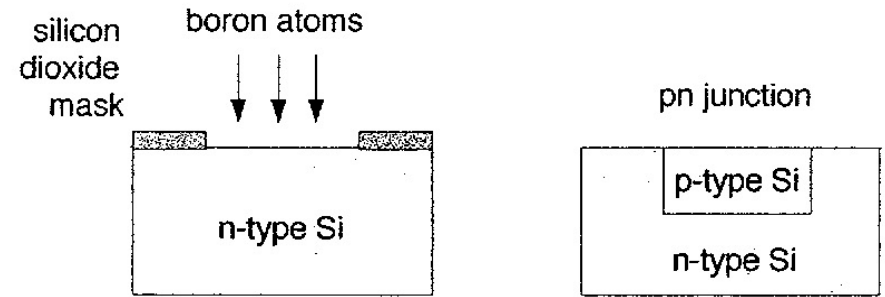
### 5.5.3 Compensated semiconductor

A compensated semiconductor is a semiconductor that contains both donor and acceptor impurity atoms in the same region.

- It can be formed by diffusing acceptor impurities into n-type material or donor impurities into a p-type material
- Considering all impurities are fully ionized
  - n-type is created when  $N_d > N_a$
  - p-type is created when  $N_a > N_d$
  - Intrinsic is created when  $N_d = N_a$

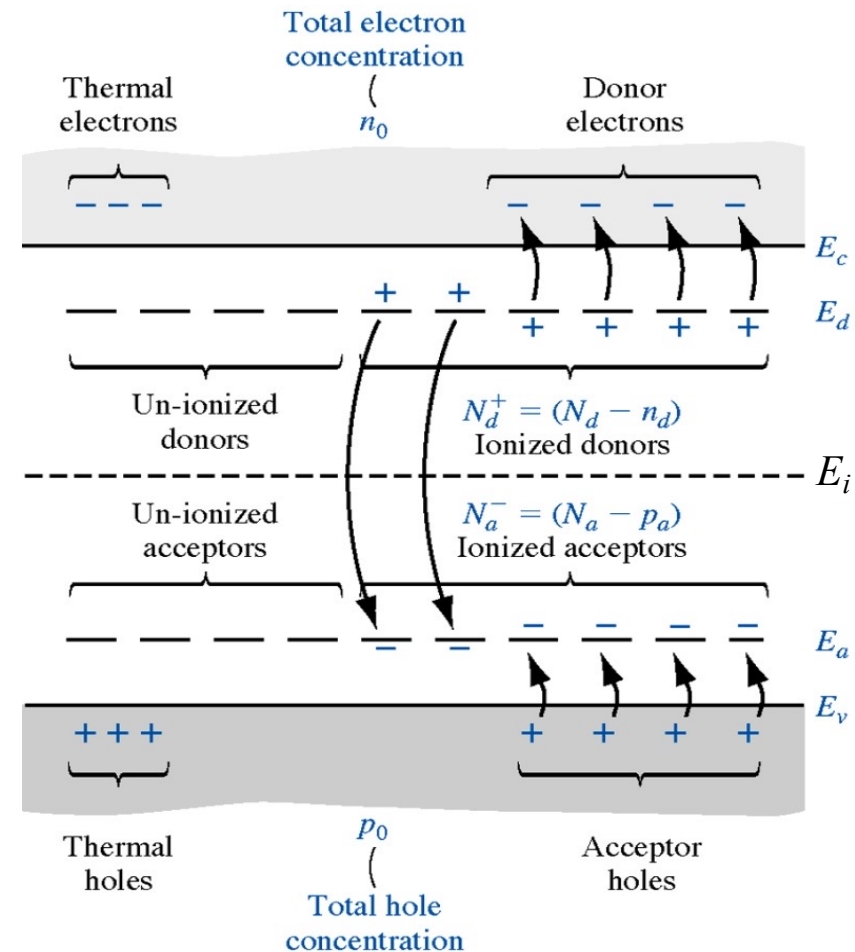
- Compensated semiconductors are created naturally during device fabrication.

Fig. 5.10 shows the formation a p-type semiconductor by diffusing acceptor boron impurities into an n-type Si sample thereby forming a p-n junction.



**Fig. 5.10**

- We will now calculate the thermal equilibrium carrier concentration,  $n_0$  and  $p_0$ , where both donor and acceptor impurities are present.
- At thermal equilibrium the semiconductor is electrically neutral. As we did in previous sections (sections 5.5.1 and 5.5.2) we will use the charge neutrality condition to obtain the thermal equilibrium carrier concentrations.



Energy-band diagram of a compensated semiconductor showing ionized and un-ionized donors and acceptors

**Fig. 5.11**

- The charge neutrality (often referred to as the space charge neutrality):

The sum of positive charges = the sum of negative charges

- The general form of the charge neutrality condition is

$$\underbrace{p_0 + N_d^+}_{\text{sum of positive charges}} = \underbrace{n_0 + N_a^-}_{\text{sum of negative charges}} \quad (5.48)$$

Here, for generality, we have considered a relatively low temperature where the impurities are not fully ionized. So, we have in eqn. (5.48)

- $N_d^+$  : ionized donor concentration
- $N_a^-$  : ionized acceptor concentration

- At temperature  $T$  where all impurities are ionized eqn. (5.48) becomes

$$\boxed{p_0 + N_d = n_0 + N_a} \quad (5.49)$$

Note that, when only donor impurity is present, i.e.  $N_a = 0$ , eqn. (5.49) reduces to eqn. (4.1)

$$p_0 + N_d = n_0$$

and when only acceptor impurity is present, i.e.  $N_d = 0$ , eqn. (5.49) reduces to eqn. (4.6)

$$p_0 = n_0 + N_a$$



- Let us calculate the thermal equilibrium carrier concentration where both donor and acceptor impurities are present and consider only the case where the temperature is high enough so that all impurities are ionized.

We start with eqn. (5.49):  $p_0 + N_d = n_0 + N_a$

- Consider first a case where  $N_d > N_a$ , i.e. n-type semiconductor. As before, we express  $p_0$  in eqn. (5.49) in terms of  $n_0$  and  $n_i$  using eqn. (5.31), we obtain

$$n_0^2 - (N_d - N_a)n_0 - n_i^2 = 0 \quad (5.50)$$

The solution this quadratic equation is

$$n_0 = \frac{(N_d - N_a) + \sqrt{(N_d - N_a)^2 + 4n_i^2}}{2} \quad (5.51)$$

as usual we obtain the minority carrier concentration  $p_0$  from eqn. (5.31)

- For  $N_a > N_d$ , i.e. p-type semiconductor, we express  $n_0$  in terms of  $p_0$  and  $n_i$ . We can then write eqn. (5.49) as follow

$$p_0^2 - (N_a - N_d)p_0 - n_i^2 = 0 \quad (5.51)$$

The solution is

$$p_0 = \frac{(N_a - N_d) + \sqrt{(N_a - N_d)^2 + 4n_i^2}}{2} \quad (5.52)$$

the minority carrier concentration  $n_0$  is then obtained from eqn. (5.31)

- It is important to note here that the charge neutrality equation is always true and can be used to determine the carrier concentrations in a semiconductor sample regardless
  - whether there is only one type of impurity or two types of impurities present
  - and whether the concentrations of the impurities are much larger or in the order of  $n_i$
- From eqns. (5.42), (5.46), (5.51) or (5.52), we see that the majority carrier concentration is not a simple sum of dopant concentration and intrinsic carrier concentration.

### Example 5.4

A piece of germanium crystal is doped with donor impurities to a concentration of  $5.8 \times 10^{14} \text{ /cm}^3$ , as well as acceptor impurities to a concentration of  $5.4 \times 10^{14} \text{ /cm}^3$ . Taking the intrinsic concentration at 300 K to be  $2.4 \times 10^{13} \text{ /cm}^3$ , calculate the thermal equilibrium electron and hole concentrations.

Material has 2 types of impurities  $N_d = 5.8 \times 10^{14} \text{ /cm}^3$

$$N_a = 5.4 \times 10^{14} \text{ /cm}^3$$

Since  $N_d > N_a$ , the material is an n-type compensated material.

From eqn. (5.51), the majority carrier concentration is

$$n_0 = \frac{(N_d - N_a) + \sqrt{(N_d - N_a)^2 + 4n_i^2}}{2}$$

$$n_0 = \frac{(5.8 \times 10^{14} - 5.4 \times 10^{14}) + \sqrt{(5.8 \times 10^{14} - 5.4 \times 10^{14})^2 + 4(2.4 \times 10^{13})^2}}{2}$$

$$n_0 = 5.12 \times 10^{13} \text{ /cm}^3$$

From eqn. (5.31), the minority carrier concentration is

$$p_0 = \frac{(2.4 \times 10^{13})^2}{5.12 \times 10^{13}} = 1.125 \times 10^{13} \text{ /cm}^3$$

## Problem

**Q1:** Consider a compensated GaAs semiconductor at  $T = 300\text{K}$  doped at  $N_d = 5 \times 10^{15} \text{ cm}^{-3}$  and  $N_a = 2 \times 10^{16} \text{ cm}^{-3}$ . Calculate the thermal equilibrium electron and hole concentration. (TYU 4.11)

$$\begin{aligned} p_o &= N_a - N_d = 2 \times 10^{16} - 5 \times 10^{15} \\ &= 1.5 \times 10^{16} \text{ cm}^{-3} \end{aligned}$$

Then

$$\begin{aligned} n_o &= \frac{n_i^2}{p_o} = \frac{(1.8 \times 10^6)^2}{1.5 \times 10^{16}} \\ &= 2.16 \times 10^{-4} \text{ cm}^{-3} \end{aligned}$$



**Q2:** For a particular semiconductor,  $E_g = 1.50$  eV,  $m_p^* = 10m_n^*$ ,  $T = 300$  K, and  $n_i = 1 \times 10^5$  cm<sup>-3</sup>. (a) Determine the position of the intrinsic Fermi energy level with respect to the center of the bandgap. (b) Impurity atoms are added so that the Fermi energy level is 0.45 eV below the center of the bandgap: (i) Are acceptor or donor atoms added? (ii) What is the concentration of impurity atoms added? (4.53)

$$\begin{aligned} \text{(a)} \quad E_{Fi} - E_{midgap} &= \frac{3}{4} kT \ln \left( \frac{m_p^*}{m_n^*} \right) \\ &= \frac{3}{4} (0.0259) \ln(10) \end{aligned}$$

or

$$E_{Fi} - E_{midgap} = +0.0447 \text{ eV}$$

(b) Impurity atoms to be added so

$$E_{midgap} - E_F = 0.45 \text{ eV}$$

(i) p-type, so add acceptor atoms

$$\text{(ii)} \quad E_{Fi} - E_F = 0.0447 + 0.45 = 0.4947 \text{ eV}$$

Then

$$\begin{aligned} p_o &= n_i \exp \left( \frac{E_{Fi} - E_F}{kT} \right) \\ &= (10^5) \exp \left( \frac{0.4947}{0.0259} \right) \end{aligned}$$

or

$$p_o = N_a = 1.97 \times 10^{13} \text{ cm}^{-3}$$



# Key takeaways (Lecture #11)

- The general form of the charge neutrality condition in compensated (counter-doped) semiconductor (assuming full ionization):

$$p_0 + N_d = n_0 + N_a$$

- when only donor impurity is present, i.e.  $N_a = 0$  ( $n$ -type)

$$p_0 + N_d = n_0$$

- when only acceptor impurity is present, i.e.  $N_d = 0$  ( $p$ -type)

$$p_0 = n_0 + N_a$$