# **Chapter 4: Semiconductor Physics**

Crystal structures of solids Energy band structures of solids Charge carriers in semiconductors Carrier transport

# **Equilibrium Distribution of Electrons and Holes**

The densities of electrons and holes are related to the density-of-states function and the Fermi distribution function.

$$n(E) = g_c(E) f_F(E)$$

$$p(E) = g_v(E) [1 - f_F(E)]$$

The total electron/hole concentration per unit volume is found by integrating the corresponding function over the entire conduction/valence band energy.

We need to determine the Fermi energy in order to find the thermalequilibrium electron and hole concentrations.

We first consider an **intrinsic semiconductor**. An ideal intrinsic semiconductor is pure semiconductor without impurities or lattice defects. At T = 0 K, all the energy states in the valence band are filled with electrons and all the energy states in the conduction band are empty. The Fermi energy must be somewhere between  $E_c$  and  $E_v$ . At T > 0 K, the number of electrons in the conduction band is equal to that of holes in the valence band.



#### **Equilibrium Distribution of Electrons and Holes**

# The $n_0$ and $p_0$ Equations

$$n_0 = \int g_c(E) f_F(E) dE$$

Because the Fermi distribution rapidly approaches zero with increasing energy, therefore  $\int_{-\infty}^{\infty} f(r) f(r) dr$ 

$$n_0 = \int_{E_c}^{\infty} g_c(E) f_F(E) dE$$

If  $(E_c - E_F) >> kT$ , then  $(E - E_F) >> kT$ , so that

$$f_F(E) = \frac{1}{1 + \exp\left(\frac{(E - E_F)}{kT}\right)} \cong \exp\left(\frac{\left[-(E - E_F)\right]}{kT}\right)$$

$$n_{0} = \int_{E_{c}}^{\infty} \frac{4\pi \left(2m_{n}^{*}\right)^{3/2}}{h^{3}} \sqrt{E - E_{c}} \exp\left[\frac{-\left(E - E_{F}\right)}{kT}\right] dE$$

If we let

$$\eta = \frac{E - E_c}{kT}$$

Then  

$$n_0 = \frac{4\pi \left(2m_n^* kT\right)^{3/2}}{h^3} \exp\left[\frac{-\left(E_c - E_F\right)}{kT}\right] \int_0^\infty \eta^{1/2} \exp(-\eta) d\eta$$

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The integral is a gamma function.

$$\int_0^\infty \eta^{1/2} \exp(-\eta) d\eta = \frac{1}{2} \sqrt{\pi}$$
  
So 
$$n_0 = 2 \left( \frac{2\pi m_n^* kT}{h^2} \right)^{3/2} \exp\left[ \frac{-(E_c - E_F)}{kT} \right]$$

We define a parameter  $N_c$  as

$$N_c = 2 \left( \frac{2\pi m_n^* kT}{h^2} \right)^3$$

 $\binom{3}{2}^{3/2}$   $N_c$  is called the effective density-of-states function in the conduction band.

Then

$$n_0 = N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right]$$

<u>*N<sub>c</sub>* is called the effective density-of-states function in the conduction</u> <u>band.</u> If we were to assume that  $m_n^* = m_0$ , then at T = 300 K,

$$N_{c} = 2 \left[ \frac{2\pi \left(9.109 \times 10^{-31} \right) \left(1.381 \times 10^{-23} \right) \left(300\right)}{\left(6.626 \times 10^{-34} \right)^{2}} \right]^{3/2} = 2.5 \times 10^{19} \,\mathrm{cm}^{-3}$$

For holes: 
$$p_0 = \int g_v(E) [1 - f_F(E)] dE$$
$$1 - f_F(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)} = \frac{\exp\left(\frac{E - E_F}{kT}\right)}{1 + \exp\left(\frac{E - E_F}{kT}\right)} = \frac{1}{1 + \exp\left(\frac{E_F - E_F}{kT}\right)}$$

If  $(E_F - E_v) >> kT$ , then  $(E_F - E) >> kT$ .  $1 - f_F(E) \approx \exp\left[\frac{-(E_F - E)}{kT}\right]$ 

$$p_{0} = \int_{-\infty}^{E_{v}} \frac{4\pi \left(2m_{p}^{*}\right)^{3/2}}{h^{3}} \sqrt{E_{v} - E} \exp\left[\frac{-\left(E_{F} - E\right)}{kT}\right] dE$$
  
If we let  
$$\eta' = \frac{E_{v} - E}{kT}$$
  
Then  
$$p_{0} = \frac{-4\pi \left(2m_{p}^{*}kT\right)^{3/2}}{h^{3}} \exp\left[\frac{-\left(E_{F} - E_{v}\right)}{kT}\right] \int_{+\infty}^{0} (\eta')^{1/2} \exp(-\eta') d\eta$$
  
$$\left(2\pi m_{v}^{*}kT\right)^{3/2} \left[-\left(E_{v} - E\right)\right]$$

$$p_0 = 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{n/2} \exp\left[\frac{-\left(E_F - E_v\right)}{kT}\right]$$

If we let  $N_{v} = 2 \left( \frac{2\pi m_{p}^{*} kT}{h^{2}} \right)^{3/2} \quad \text{then} \quad p_{0} = N_{v} \exp \left[ \frac{-\left(E_{F} - E_{v}\right)}{kT} \right]$ 

 $N_{\nu}$  is called the effective density-of-states function in the valence band. PHY4320 Chapter Four (II) 7

# **The Intrinsic Carrier Concentration**

We use  $n_i$  and  $p_i$  to denote electron and hole concentrations in an **intrinsic semiconductor**. Since  $n_i = p_i$ , we usually use  $n_i$  to denote either the intrinsic electron or hole concentration. The Fermi level for an intrinsic semiconductor is called the **intrinsic Fermi energy**,  $E_{Fi}$ .

$$n_{0} = n_{i} = N_{c} \exp\left[\frac{-(E_{c} - E_{Fi})}{kT}\right]$$
$$p_{0} = p_{i} = n_{i} = N_{v} \exp\left[\frac{-(E_{Fi} - E_{v})}{kT}\right]$$
$$n_{i}^{2} = N_{c}N_{v} \exp\left[\frac{-(E_{c} - E_{Fi})}{kT}\right] \exp\left[\frac{-(E_{Fi} - E_{v})}{kT}\right]$$
$$n_{i}^{2} = N_{c}N_{v} \exp\left[\frac{-(E_{c} - E_{v})}{kT}\right] = N_{c}N_{v} \exp\left[\frac{-E_{g}}{kT}\right]$$

# At T = 300 K

	$N_c(\mathrm{cm}^{-3})$	$N_{\nu}(\mathrm{cm}^{-3})$	$m_n^*/m_0$	$m_p^*/m_0$
Silicon	$2.8 \times 10^{19}$	$1.04 \times 10^{19}$	1.08	0.56
Gallium arsenide	$4.7 \times 10^{17}$	$7.0 \times 10^{18}$	0.067	0.48
Germanium	$1.04 \times 10^{19}$	$6.0 \times 10^{18}$	0.55	0.37

Silicon	$n_i = 1.5 \times 10^{10} \text{ cm}^{-3}$
Gallium arsenide	$n_i = 1.8 \times 10^6 \text{ cm}^{-3}$
Germanium	$n_i = 2.4 \times 10^{13} \text{ cm}^{-3}$

 $N_c, N_v$ , and  $n_i$  are constant for a given semiconductor material at a fixed temperature.



# **The Intrinsic Fermi Level Position**

We can calculate the Fermi level position since the electron and hole concentrations are equal for an intrinsic semiconductor:

$$n_0 = N_c \exp\left[\frac{-\left(E_c - E_{Fi}\right)}{kT}\right] = p_0 = N_v \exp\left[\frac{-\left(E_{Fi} - E_{Fi}\right)}{kT}\right]$$
$$-E_c + E_{Fi} + E_{Fi} - E_v = kT \ln\left(\frac{N_v}{N_c}\right)$$
$$If m_n^* = m_n^*, the$$

$$E_{Fi} = \frac{1}{2} \left( E_c + E_v \right) + \frac{1}{2} kT \ln \left( \frac{N_v}{N_c} \right)$$
$$E_{Fi} = E_{\text{midgap}} + \frac{3}{4} kT \ln \left( \frac{m_p^*}{m_n^*} \right)$$
$$E_{Fi} - E_{\text{midgap}} = \frac{3}{4} kT \ln \left( \frac{m_p^*}{m_n^*} \right)$$

If  $m_p^* = m_n^*$ , the intrinsic Fermi level will be in the center of the bandgap. If  $m_p^* > m_n^*$ , the intrinsic Fermi level will be slightly above the center. If  $m_p^*$  $< m_n^*$ , the intrinsic Fermi level will be slightly below the center of the bandgap.

# **Donor Atoms and Energy Levels**

Real power of semiconductors is realized by adding controlled amounts of specific dopant, or impurity atoms. The doped semiconductor is called an **extrinsic** material. Doping is the primary reason that we can fabricate various semiconductor devices.



Add **a group V element**, such as phosphorus, to silicon as a substitutional impurity. The group V element has five valence electrons. Four of these will contribute to the covalent bonding with the silicon atoms, leaving the fifth more loosely bound to the phosphorus atom.

# **Donor Atoms and Energy Levels**



At very low temperatures, the extra electron is bound to the phosphorus atom. However, it should be clear that the energy required to elevate the extra electron into the conduction band is considerably smaller than that for the electrons involved in the covalent bonding.

The electron elevated into the conduction band can move through the crystal to generate a current, while the positively charged phosphorous atoms are fixed in the crystal. This type of atom is called **a donor impurity atom**. The donor atoms add electrons to the conduction band without creating holes in the valence band. The resulting material is referred to as **an n-type semiconductor**.

### **Acceptor Atoms and Energy Levels**



Consider adding **a group III** element, such as boron, which has three valence electrons. One covalent bonding position is empty. If an electron were to occupy this "empty" position, its energy would have to be greater than that of the valence electrons, since the net charge of the B atom would become negative. However, the electron occupying this "empty" position does not have sufficient energy to be in the conduction band, so its energy is far smaller than the conduction band energy. The "empty" position associated with the B atom can be occupied and other valence electron positions become vacated. These other vacated electron positions can be thought of as **holes**.

# **Acceptor Atoms and Energy Levels**



The hole can move through the crystal to generate a current, while the negatively charged boron atoms are fixed in the crystal. The group III atom accepts an electron from the valence band and so is referred to as **an acceptor impurity atom**. The acceptor atom can generate holes in the valence band without generating electrons in the conduction band. This type of semiconductor material is referred to as **a p-type semiconductor**.

**An extrinsic semiconductor** will have either a preponderance of electrons (n-type) or a preponderance of holes (p-type).

# **Ionization Energy**

We can calculate the approximate distance of the donor electron from the donor impurity ion, and also the approximate energy required to elevate the donor electron into the conduction band. This energy is referred to as **the ionization energy**. We will use **the Bohr model of the atom** for these calculations.

The permittivity of the semiconductor material instead of the permittivity of free space will be used, and the effective mass of the electron will be used.

From the Coulomb force of attraction being equal to the centripetal force of the orbiting electron:

$$\frac{e^2}{4\pi\varepsilon r_n^2} = \frac{m^* v^2}{r_n}$$

Assume that the angular momentum is quantized,

$$m^* r_n v = n\hbar$$

$$v = \frac{n\hbar}{m^* r_n} \qquad n = 1, 2, 3, \dots$$
$$r_n = \frac{n^2 \hbar^2 4\pi \varepsilon}{m^* e^2}$$
$$a_0 = \frac{4\pi \varepsilon_0 \hbar^2}{m_0 e^2} = 0.053 \text{nm}$$
$$\frac{r_n}{a_0} = n^2 \varepsilon_r \left(\frac{m_0}{m^*}\right)$$

The Bohr radius is

Then

If we consider n = 1 state, and if we consider silicon, for which  $\varepsilon_r = 11.7$ ,  $m^*/m_0 = 0.26$ , then we have

$$r_1 = 45$$
  $r_1 = 2.39$  For silicon,  $a = 0.543$  nm.  
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$$v = \frac{e^2}{4\pi\epsilon n\hbar}$$
  
The kinetic energy is  $T = \frac{1}{2}m^*v^2 = \frac{m^*e^4}{2(n\hbar)^2(4\pi\epsilon)^2}$   
The potential energy is  $V = \frac{-e^2}{4\pi\epsilon r_n} = \frac{-m^*e^4}{(n\hbar)^2(4\pi\epsilon)^2}$   
The total energy is  $E = T + V = \frac{-m^*e^4}{2(n\hbar)^2(4\pi\epsilon)^2}$ 

The lowest energy state of the hydrogen atom is E = -13.6 eV. For silicon, the lowest energy is E = -25.8 meV ( $E_g = 1.12$  eV at T = 300 K).

Ge	
0.012 eV	
0.0127	
0.0104	
0.0102	

# **Group III-V Semiconductors**

The donor and acceptor impurities in III-V compound semiconductors is more complicated than that in Si. <u>When we talk about donors or acceptors in</u> <u>III-V semiconductors, we need to know for which atoms (III or V) impurity</u> <u>atoms are substituted.</u> For example, for Si atoms in gallium arsenide semiconductor, if Si atoms replace gallium atoms, Si impurities will act as donors. But if Si atoms replace arsenic atoms, they will act as acceptors.

#### For gallium arsenide

Donor impurity	Ionization energy (eV) 0.0059	
Selenium		
Tellurium	0.0058	
Silicon	0.0058	
Germanium	0.0061	
Acceptor impurity		
Beryllium	0.028	
Zinc	0.0307	
Cadmium	0.0347	
Silicon	0.0345	
Germanium	0.0404	

#### Equilibrium Distribution of Electrons and Holes in Extrinsic Semiconductors



Adding donor or acceptor impurity atoms to a semiconductor will change the distribution of electrons and holes in the material. Since the Fermi energy is related to the distribution function, <u>the</u> <u>Fermi energy will change as dopant</u> <u>atoms are added</u>.

In general, when  $E_F > E_{\text{midgap}}$ , the density of electrons is larger than that of holes, and the semiconductor is **n-type**.

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# Equilibrium Distribution of Electrons and Holes in the Extrinsic Semiconductor



In general, when  $E_F < E_{\text{midgap}}$ , the density of electrons is smaller than that of holes, and the semiconductor is **p-type**.

$$n_0 = N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right]$$
$$p_0 = N_v \exp\left[\frac{-(E_F - E_v)}{kT}\right]$$

The above are general equations for  $n_0$ and  $p_0$  in terms of the Fermi energy. The values of  $n_0$  and  $p_0$  will change with the Fermi energy,  $E_F$ .

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**Example**: consider silicon at T = 300 K so that  $N_c = 2.8 \times 10^{19}$  cm<sup>-3</sup> and  $N_v = 1.04 \times 10^{19}$  cm<sup>-3</sup>. If we assume the Fermi energy is 0.25 eV below the conduction band, calculate the thermal equilibrium concentrations of electrons and holes. The bandgap energy of silicon is 1.12 eV.

**Solution**:  $E_c - E_F = 0.25 \text{eV}$   $E_F - E_v = 0.87 \text{eV}$ 

$$n_{0} = (2.8 \times 10^{19}) \exp\left[\frac{-(0.25)(1.602 \times 10^{-19})}{(1.381 \times 10^{-23})(300)}\right] = 1.8 \times 10^{15} \,\mathrm{cm^{-3}}$$
$$p_{0} = (1.04 \times 10^{19}) \exp\left[\frac{-(0.87)(1.602 \times 10^{-19})}{(1.381 \times 10^{-23})(300)}\right] = 2.6 \times 10^{4} \,\mathrm{cm^{-3}}$$

**Comment**: electron and hole concentrations change by orders of magnitude from the intrinsic carrier concentrations (at 300 K,  $n_i = 1.5 \times 10^{10}$  cm<sup>-3</sup>) as the Fermi energy changes by a few tenths of an eV.

In an n-type semiconductor,  $n_0 > p_0$ , electrons are referred to as **majority** carriers and holes as **minority carriers**. In an p-type semiconductor,  $p_0 > n_0$ , holes are referred to as **majority carriers** and electrons as **minority** carriers.

We can derive another form of the equations for the thermalequilibrium concentrations of electrons and holes:

$$n_0 = N_c \exp\left[\frac{-\left(E_c - E_F\right)}{kT}\right] = N_c \exp\left[\frac{-\left(E_c - E_{Fi}\right) + \left(E_F - E_{Fi}\right)}{kT}\right]$$
$$n_0 = n_i \exp\left(\frac{E_F - E_{Fi}}{kT}\right)$$

$$p_0 = N_v \exp\left[\frac{-\left(E_F - E_v\right)}{kT}\right] = N_v \exp\left[\frac{-\left(E_{Fi} - E_v\right) + \left(E_{Fi} - E_F\right)}{kT}\right]$$

$$p_0 = n_i \exp\left[\frac{E_{Fi} - E_F}{kT}\right] = n_i \exp\left[\frac{-(E_F - E_{Fi})}{kT}\right]$$

# The $n_0 p_0$ Product

$$n_0 p_0 = N_c N_v \exp\left[\frac{-(E_c - E_F)}{kT}\right] \exp\left[\frac{-(E_F - E_v)}{kT}\right]$$

$$n_0 p_0 = N_c N_v \exp\left[\frac{-E_g}{kT}\right] = n_i^2$$

The product of  $n_0$  and  $p_0$  is always a constant for a given semiconductor material at a given temperature. It is one of the fundamental principles of semiconductors in thermal equilibrium.

It is important to keep in mind that <u>the above equation is derived using the</u> <u>Boltzmann approximation</u>.

We may think of the intrinsic concentration  $n_i$  simply as a parameter of the semiconductor material.

#### **The Fermi-Dirac Integral**

$$n_{0} = \int_{E_{c}}^{\infty} g_{c}(E) f_{F}(E) dE$$

$$n_{0} = \frac{4\pi}{h^{3}} (2m_{n}^{*})^{3/2} \int_{E_{c}}^{\infty} \frac{\sqrt{E - E_{c}} dE}{1 + \exp\left(\frac{E - E_{F}}{kT}\right)}$$
If we define
$$\eta = \frac{E - E_{c}}{kT} \quad \text{and} \quad \eta_{F} = \frac{E_{F} - E_{c}}{kT}$$

$$n_{0} = 4\pi \left(\frac{2m_{n}^{*}kT}{h^{2}}\right)^{3/2} \int_{0}^{\infty} \frac{\eta^{1/2} d\eta}{1 + \exp(\eta - \eta_{F})}$$

$$F_{1/2}(\eta_{F}) = \int_{0}^{\infty} \frac{\eta^{1/2} d\eta}{1 + \exp(\eta - \eta_{F})} \quad \leftarrow \quad \text{Fermi-Dirac integral}$$



We need to use the Fermi-Dirac integral when  $E_F$  is above  $E_c$  or below  $E_v$ .

$$p_0 = 4\pi \left(\frac{2m_p^* kT}{h^2}\right)^{3/2} \int_0^\infty \frac{(\eta')^{1/2} d\eta'}{1 + \exp(\eta' - \eta'_F)}$$

### **Degenerate and Nondegenerate Semiconductors**

When discussing donors and acceptors, the concentration of dopant atoms is assumed to be small compared to the density of host atoms. The impurities introduce <u>discrete</u>, <u>non-interacting donor and acceptor energy states</u> in the n-type and p-type semiconductor, respectively. These types of semiconductors are referred to as **nondegenerate semiconductors**.

As the impurity concentration increases, the distance between the impurity atoms decreases and the electrons from the impurity atoms will begin to interact. When this occurs, the discrete donor or acceptor energy level will split into a band of energies. As the impurity concentration further increases, the band of donor or acceptor states widens and overlaps with the bottom of the conduction band or the top of the valence band. When the concentration of electrons in the conduction band exceeds the density of states  $N_c$ , the Fermi energy lies within the conduction band. This type of semiconductors is called **degenerate n-type semiconductors**. When the concentration of holes exceeds the density of states  $N_v$ , the Fermi energy lies in the valence band. This type of semiconductors is called **degenerate p-type semiconductors**.

#### **Degenerate and Nondegenerate Semiconductors**



# Statistics of Donors and Acceptors

The probability of the donor energy level being occupied is



Each donor level could be empty, contain one electron of either spin, or two electrons of opposite spins. However, the  $\frac{1}{1 + \frac{1}{2} \exp\left(\frac{E_d - E_F}{kT}\right)} \quad \begin{array}{c} \text{Coulomb repulsion of two localized electrons raises the} \\ \text{energy of the doubly occupied level so high that double} \\ \text{for the reason for the reaso$ occupation is essentially prohibited. This is the reason for the factor of  $\frac{1}{2}$  appearing in the probability function.

$$n_d = \frac{N_d}{1 + \frac{1}{2} \exp\left(\frac{E_d - E_F}{kT}\right)}$$
$$n_d = N_d - N_d^+$$

 $n_d$  is the density of electrons occupying the donor level.

 $N_d$  is the concentration of donor atoms.  $N_d^+$  is the concentration of ionized donors.



 $p_a = \frac{Iv_a}{1 + \frac{1}{g} \exp\left(\frac{E_F - E_a}{kT}\right)}$ g is a degeneracy factor. The ground state g in normally taken as 4 for the acceptor level in Signature. g is a degeneracy factor. The ground state g is normally taken as 4 for the acceptor level in Si and

#### **Complete Ionization and Freeze-Out**

If  $(E_d - E_F) >> kT$ , we then have  $n_d = \frac{N_d}{1 + \frac{1}{2} \exp\left(\frac{E_d - E_F}{kT}\right)} \approx 2N_d \exp\left[\frac{-(E_d - E_F)}{kT}\right]$  $n_0 = N_c \exp\left|\frac{-(E_c - E_F)}{kT}\right|$ 

Because

We can determine the percentage of electrons in the donor state compared with the total number of electrons:

$$\frac{n_d}{n_d + n_0} = \frac{2N_d \exp\left[\frac{-\left(E_d - E_F\right)}{kT}\right]}{2N_d \exp\left[\frac{-\left(E_d - E_F\right)}{kT}\right] + N_c \exp\left[\frac{-\left(E_c - E_F\right)}{kT}\right]}$$

$$\frac{n_d}{n_d + n_0} = \frac{1}{1 + \frac{N_c}{2N_d} \exp\left[\frac{-\left(E_c - E_d\right)}{kT}\right]}$$

For phosphorus-doped silicon at T = 300 K,  $N_c = 2.8 \times 10^{19}$  cm<sup>-3</sup>,  $N_d = 10^{16}$  cm<sup>-3</sup>, and the ionization energy is 0.045 eV:

$$\frac{n_d}{n_d + n_0} = \frac{1}{1 + \frac{2.8 \times 10^{19}}{2(10^{16})}} \exp\left(\frac{-0.045}{0.0259}\right) = 0.004 = 0.4\%$$

At room temperature, the donor states are almost completely ionized, which is also true for the acceptor states at room temperature.



At T = 0 K, all electrons are in their lowest energy state. For an n-type semiconductor, each donor state must contain an electron, therefore,  $n_d = N_d$ .

$$\begin{cases} \exp[(E_d - E_F)/kT] = 0 \\ T = 0 \end{cases} \Rightarrow E_F > E_d$$

The Fermi level is above the donor level for an n-type semiconductor at T = 0 K. Similarly, the Fermi level will be below the acceptor level for a p-type semiconductor at T = 0 K.

