# Part II Electrical Properties of Materials

Chap. 7 Electrical Conduction in Metals and Alloys

Chap. 8 Semiconductors

Chap. 9 Electrical Properties of Polymers, Ceramics, Dielectrics, and Amorphous Materials

# 8.1 band Structure

Material characterization by band structure

- **Metal:** partially filled valence bands with electrons

- **Insulator:** completely filled valence bands and a large energy gap up to unfilled conduction band

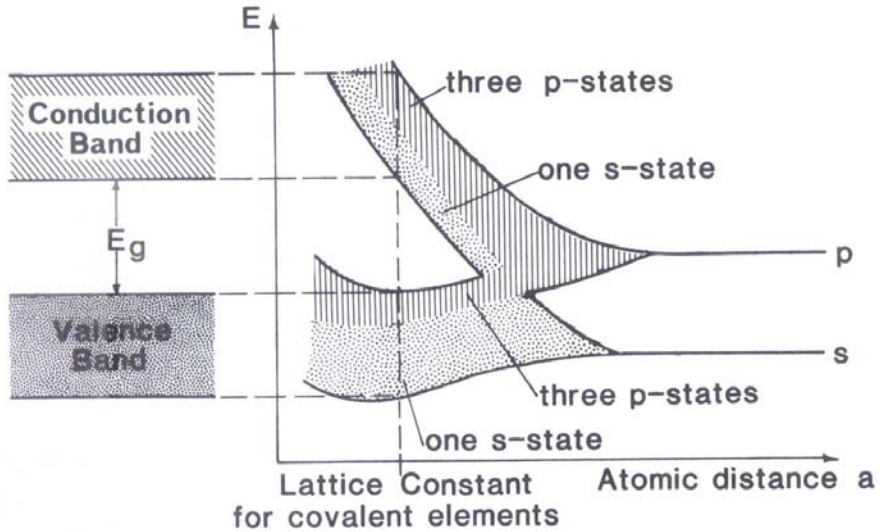



Figure 8.1. Sharp energy levels, widening into bands, and band overlapping with decreasing atomic distance for covalent elements. (Compare with Fig. 4.14.)

- **Semiconductor:** in low temperature, completely filled valence band and a narrow gap between this and the next higher, unfilled conduction band

Because of band overlapping, the valence band as well as the conduction band consist of *hybrid (mixed) s-* and *p-*state → the eight highest *s* + *p* states(2 *s-* and 6 *p-* states split into two separate (*s* + *p*) bands) (Fig. 8.1)

# 8.1 band Structure

**Fig. 8.2: calculated band structure of Si**

**The valence band can accommodate $4N_a$ electrons: one lowest *s*-state and three *p*-states (4 *sp*- hybrids) and empty conduction band of 4 *sp*-hybrids**

**Gap energy, $E_g$ for group IV elements (Table 8.1)**

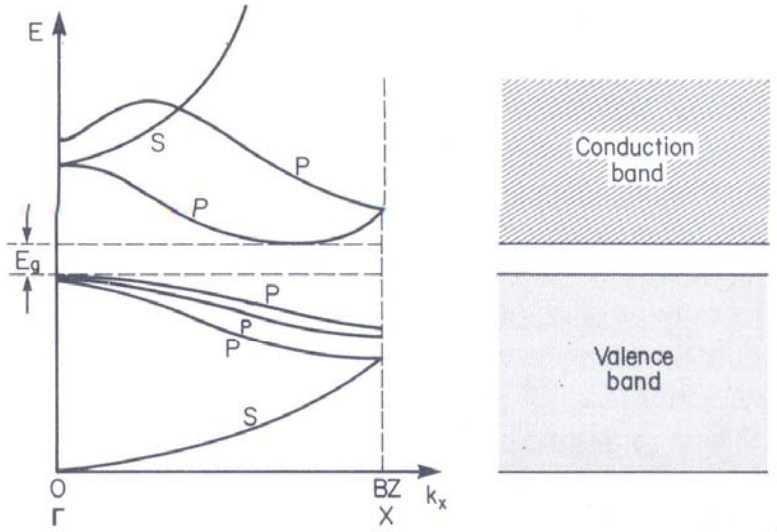



Figure 8.2. Schematic band structure of silicon in the $k_x$ (or $X$) direction (plotted in the reduced zone scheme). The separation of the two highest $p$-states in the valence band is strongly exaggerated. Compare with the complete band structure of Fig. 5.23.

**Temperature dependence of gap energy**

**(empirical equation)**

$$E_{gT} = E_{g0} - \frac{\xi T^2}{T + \theta_D}$$

**$E_{g0}$ is the band gap energy at $T$= 0 K,**

$\xi \approx 5 \times 10^{-4} eV/K$ $\theta_D$ : Debye temperature

Table 8.1. Gap Energies for Some Group IV Elements at 0 K (see also Appendix 4).

| Element | $E_g$ [eV] |
|---|---|
| C (diamond) | 5.48 |
| Si | 1.17 |
| Ge | 0.74 |
| Sn (gray) | 0.08 |

# 8.2 Intrinsic Semiconductors

**The conduction mechanism is predominated by the properties of the pure crystal**

**(i) Electron excitation from the valence band into conduction band, usually by thermal energy (interband transition)**

**(ii) Electron holes left behind in the valence band can also contribute to the conduction**

**- Fermi energy in semiconductor:**

**Energy for which the Fermi distribution function, $F(E) = 1/2$**

$$E_F = -E_g/2$$

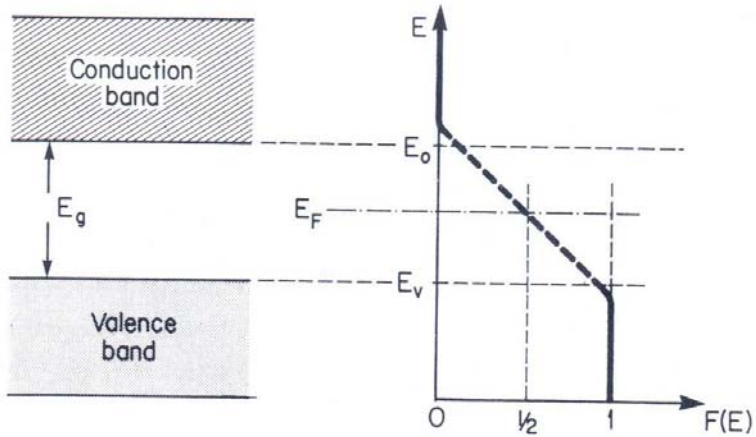



Figure 8.3. Schematic Fermi distribution function and Fermi energy for an intrinsic semiconductor for $T > 0$ K. The "smearing out" of the Fermi distribution function at $E_0$ and $E_V$ is exaggerated. For reasons of convenience, the zero point of the energy scale is placed at the bottom of the conduction band.

# 8.2 Intrinsic Semiconductors

## Number of electrons in the conduction band

$N^*$: number of electrons that have an energy equal to or smaller than a given energy $E_n$

For an energy interval between $E$ and $E + dE$,

$$dN^* = N(E)dE$$

Where the population density $N(E) = 2 \cdot Z(E) \cdot F(E)$

Density of state $Z(E)$ (see eqn. (6.5))

$$Z(E) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \qquad F(E) = \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1} \approx \exp\left[-\left(\frac{E - E_F}{k_B T}\right)\right]$$

Because $E - E_F$ is about 0.5eV and $k_B T$ at $R.T.$ is of the order of $10^{-2}$eV, the exponential factor is large compared to 1

# 8.2 Intrinsic Semiconductors

**Integration over all available electrons that have energies larger than the energy at the bottom of the conduction band (*E = 0*)**

$$N^* = \frac{V}{2\pi^2}\cdot\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty E^{1/2}\cdot\exp\left[-\left(\frac{E-E_F}{k_BT}\right)\right]dE$$

$$N^* = \frac{V}{2\pi^2}\cdot\left(\frac{2m}{\hbar^2}\right)^{3/2}\exp\left(\frac{E_F}{k_BT}\right)\int_0^\infty\cdot E^{1/2}\cdot\exp\left[-\left(\frac{E}{k_BT}\right)\right]dE$$

$$N^* = \frac{V}{2\pi^2}\cdot\left(\frac{2m}{\hbar^2}\right)^{3/2}\exp\left(\frac{E_F}{k_BT}\right)\frac{k_BT}{2}(\pi k_BT)^{1/2}$$

$$= \frac{V}{4}\left(\frac{2mk_BT}{\pi\hbar^2}\right)^{3/2}\exp\left(\frac{E_F}{k_BT}\right)$$

# 8.2 Intrinsic Semiconductors

Introducing $E_F = -E_g/2$ and effective mass ratio $m^*_e/m_0$

$N_e = N^*/V$: number of conduction band electrons per unit volume

$$N_e = \frac{1}{4}\left(\frac{2mk_B}{\pi\hbar^2}\right)^{3/2}\left(\frac{m_e^*}{m_0}\right)^{3/2} T^{3/2}\exp\left[-\left(\frac{E_g}{2k_BT}\right)\right]$$

where the constant factor $\frac{1}{4}\left(\frac{2mk_B}{\pi\hbar^2}\right)^{3/2}$ has the value $4.84\times10^{15}\,(cm^{-3}K^{-3/2})$

$$N_e = 4.84\times10^{15}\left(\frac{m_e^*}{m_0}\right)^{3/2} T^{3/2}\exp\left[-\left(\frac{E_g}{2k_BT}\right)\right]$$

- The number of electrons in the conduction band per $cm^3$ is a function of $E_g$ and $T$. A numerical evaluation of $N_e$ per $cm^3$ in Si at RT ~ $10^9$ : only one in $10^{13}$ atoms contributes an electron to the conduction

- "The number of electrons in the conduction band" = "the number of holes in the valence band". Thus equation for $N_e$ can be written for the holes by assuming $m^*_e = m^*_h$

# 8.2 Intrinsic Semiconductors

- Conductivity of an intrinsic semiconductor is determined by number of current carriers (electrons and holes) and also by their mobility

The mobility of the current carriers $\mu$:

$$\mu = \frac{\upsilon}{E}$$ drift velocity per unit *E*

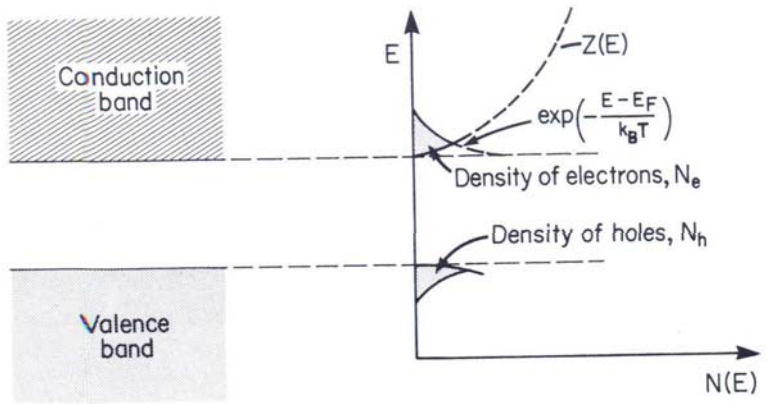



Figure 8.4. Density of electrons ($N_e$) and holes ($N_h$) for an intrinsic semiconductor

From $j = \sigma E$ & $j = N\upsilon e$

$$\sigma = N\frac{\upsilon}{E}e = N\mu e$$

$$\sigma = N_e e\mu_e + N_h e\mu_h,$$

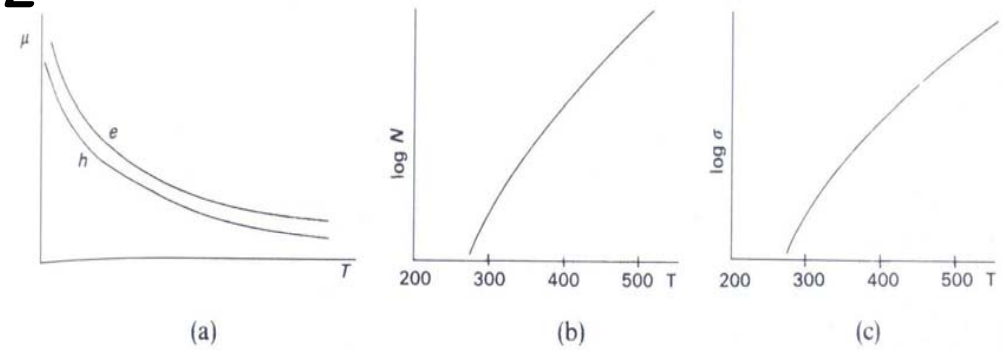



Figure 8.5. Schematic representation of the temperature dependence of (a) electron and hole mobilities, (b) number of carriers in an intrinsic semiconductor, and (c) conductivity for an intrinsic semiconductor. ($T$ is given in Kelvin.)

$$\sigma = 4.84\times10^{15}\left(\frac{m^*}{m_0}\right)^{3/2} T^{3/2} e(\mu_e + \mu_h)\exp\left[-\left(\frac{E_g}{2k_B T}\right)\right]$$

# 8.3 Extrinsic Semiconductors

## 8.3.1 Donors and Acceptors

**Extrinsic semicondutors: in most semiconductor devices, a considerably higher number of charge carriers are introduced by doping,i.e., by adding small amount of impurities (dopants) to the semiconductor materials**

**- n-type semiconductor: dopants (donor, element of group V : P,As,Sb)**

**→ major carrier :donor electrons (negative carrier)**

**- p-type semiconductor: dopants (acceptor, elements of group III : B,Al,Ga,In)**

**→ major carrier: holes (positive carriers)**

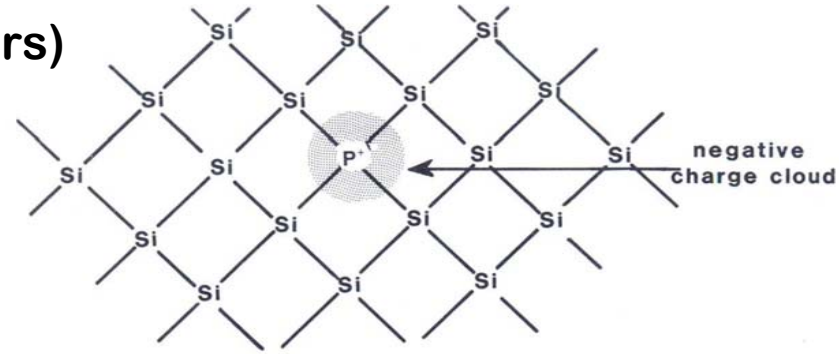



Figure 8.6. Two-dimensional representation of the silicon lattice. An impurity atom of group V of the periodic table ($P$) is shown to replace a silicon atom. The charge cloud around the phosphorus atom stems from the extra phosphorus electron. Each electron pair between two silicon atoms constitutes a covalent bond (electron sharing). The two electrons of such a pair are indistinguishable, but must have opposite spin to satisfy the Pauli principle.

# 8.3 Extrinsic Semiconductors

## 8.3.2 Band Structure

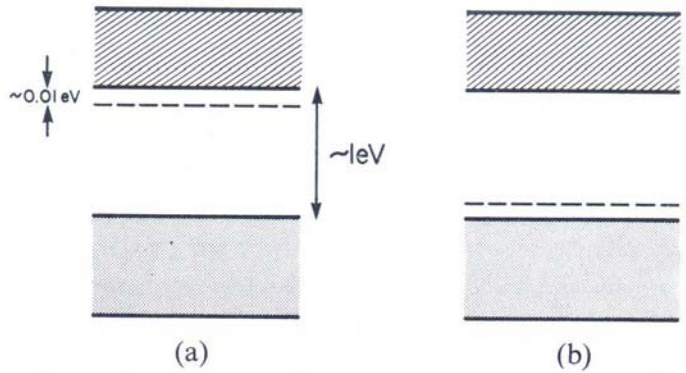



Figure 8.7. (a) Donor and (b) acceptor levels in extrinsic semiconductors.

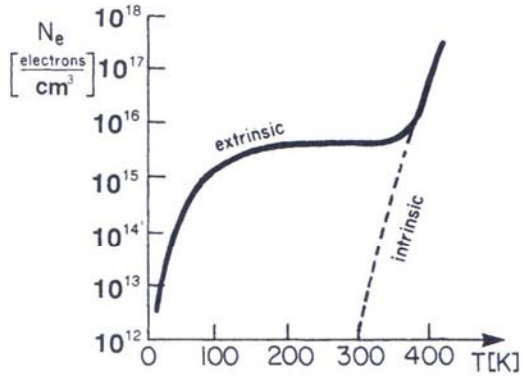



Figure 8.8. Schematic representation of the number of electrons per cubic centimeter in the conduction band versus temperature for an extrinsic semiconductor with low doping.

## 8.3.3 Temperature Dependence of the Number of Carriers

**With increasing temperature,**

**- n-type: the donor electrons overcome small potential barrier (Fig 8.7) : excite from the donor levels into the conduction band. → $N_e$ deviation from intrinsic way. Once all electron in donor levels have been excited into conduction band, further temperature increase does not create additional electron (Fig8.8)**

**- p-type : electrons excite from valence band into the acceptor levels, creating positive charge carriers (holes).**

# 8.3 Extrinsic Semiconductors

## 8.3.4 Conductivity

$$\sigma = N_{de} e \mu_e$$

where $N_{de}$: number of donor electrons

$\mu_e$ : mobility of the donor electrons

$N_{de}$, $\mu_e$ : two competing effects on conductivity of semiconductors

- For low doping and at low temperature, the conductivity decreases with increasing temperature : lattice vibration → decrease mobility

At higher temperature: conductivity increase : intrinsic effects → increase number of carriers

- For high doping : temperature dependence on conductivity is less pronounced due to the already higher number of carrier

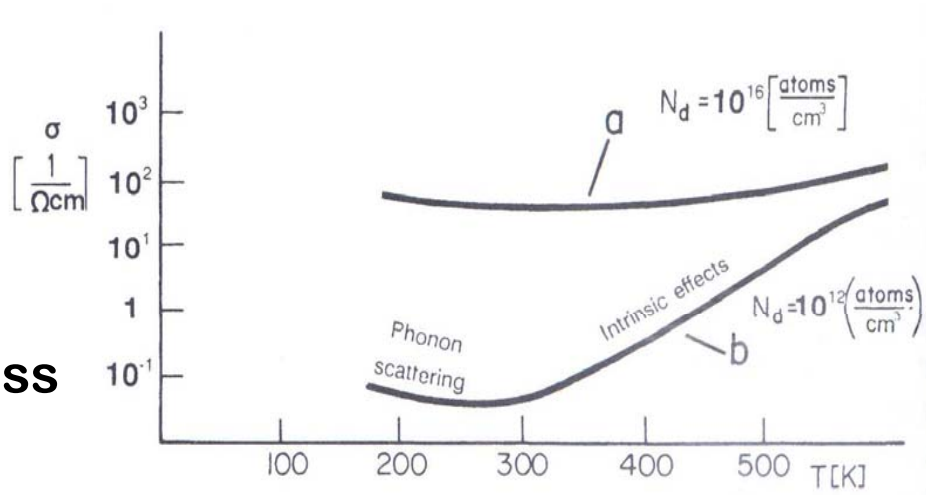



Figure 8.9. Conductivity of two extrinsic semiconductors, (a) high doping and (b) low doping. $N_d$ = number of donor atoms per cubic centimeter.

# 8.3 Extrinsic Semiconductors

## 8.3.5 Fermi Energy

$E_F$ level position

- n-type semiconductor

: between donor level and

conduction band

- p-type semiconductor

: between acceptor level

and valence band

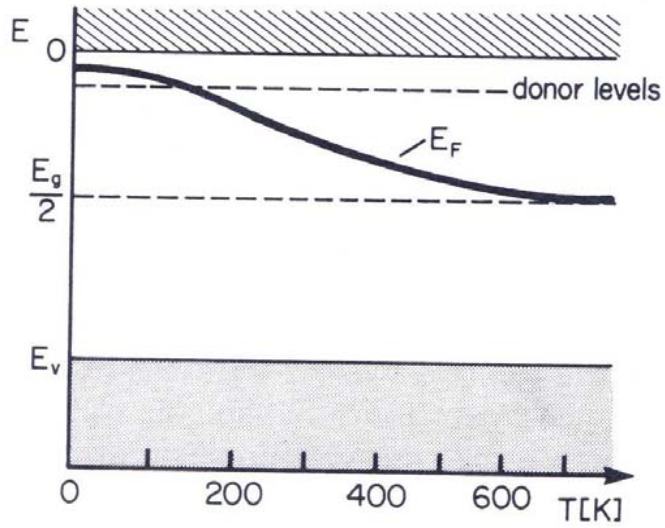



Figure 8.10. Fermi level of an *n*-type semiconductor as a function of temperature. $N_d \approx 10^{16}$ (atoms per cubic centimeter).

With increasing temperature, $E_F$ of both type semiconductors approach the value for intrinsic semiconductors, i.e., - $E_g/2$

# 8.4 Effective Mass, $m^*$

## *Evaluation of the effective mass of the charge carriers in semiconductors*

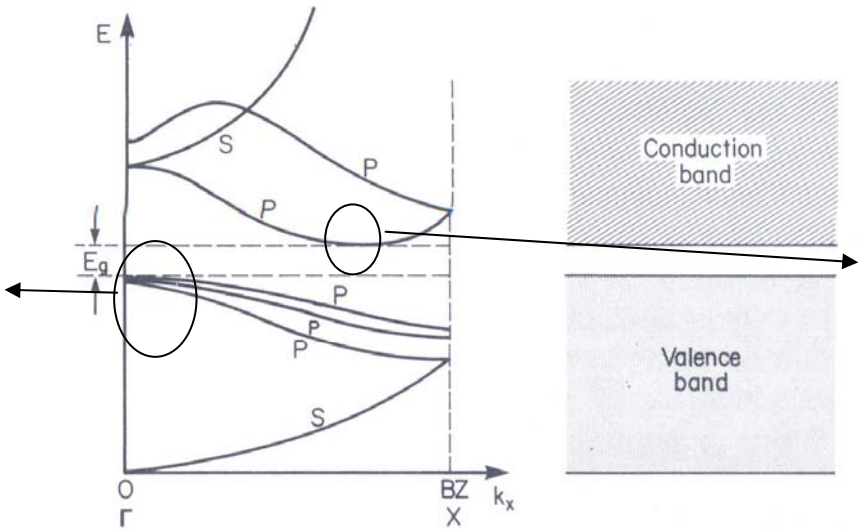
***m***is inversely proportional to the curvature of an electron band.*

**Consider the upper portion of the valence bands and the lower portion of the conduction bands for Si**

**Curvature: convex downward -> a negative effective mass, implying this band is populated by electron holes.**

**2 heavy holes : smaller curvature**

**1 light hole : larger curvature**




**Curvature : convex upward -> populated by electrons**

**In 3-d, a spheroid shape:**

**Longitudinal mass $m_l^*$**

**~~Transverse mass $m_t^*$~~**

Figure 8.2. Schematic band structure of silicon in the $k_x$ (or $X$) direction (plotted in the reduced zone scheme). The separation of the two highest $p$-states in the valence band is strongly exaggerated. Compare with the complete band structure of Fig. 5.23.

# 8.5 Hall Effect

"Number and type of charge carriers can be measured by making use of Hall effect"

## Consider n-type semiconductor

Suppose electric current density j flow in the positive *x* direction and magnetic field is applied *z* direction

Lorentz force, $F_L$ on electrons:

$$F_L = \upsilon_x B_z e$$

The electron accumulate on one side of the slap → cause Hall field $F_H$, thus Hall force

$$F_H = eE_y$$

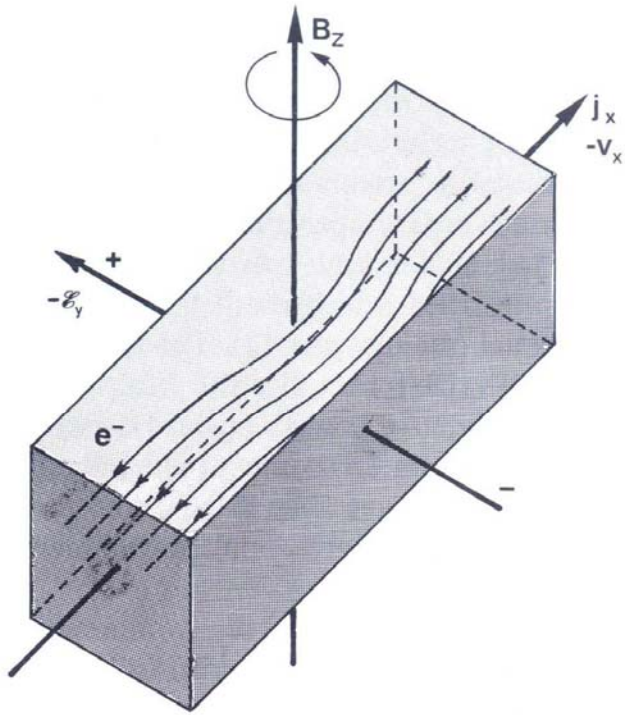



Figure 8.11. Schematic representation of the Hall effect in an *n*-type semiconductor (or a metal in which electrons are the predominant current carriers).

# 8.5 Hall Effect

(continued) In equilibrium $F_L + F_H = 0$ $\upsilon_x B_z e = eE_y$

$$E_y = \upsilon_x B_z$$

$$j_x = -N\upsilon_x e$$

Combining the two, yields for the number of conduction electrons per unit volume

$$N = -\frac{j_x B_z}{eE_y}$$

variables on the right side of this equation can be measured and thus $N$ can be obtained.

- **Hall constant** is defined as $R_H = -\frac{1}{Ne}$

which is inversely proportional to the density of charge carriers, $N$.

- negative (positive) $R_H$ : major charge carrier are electrons (holes)

# Additional Materials

**(Chap. 19 in Materials Science & Engineering, An Introduction, 4th Ed., W.D. Callister Jr.)**

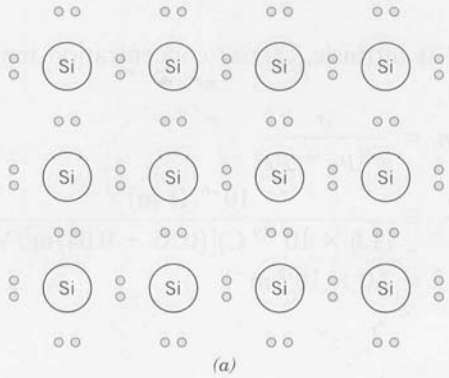



FIGURE 18.10 Electron bonding model of electrical conduction in intrinsic silicon: (*a*) before excitation, (*b*) and (*c*) after excitation (the subsequent free-electron and hole motions in response to an external electric field).

## Intrinsic Semiconductor

## Atomic bonding model

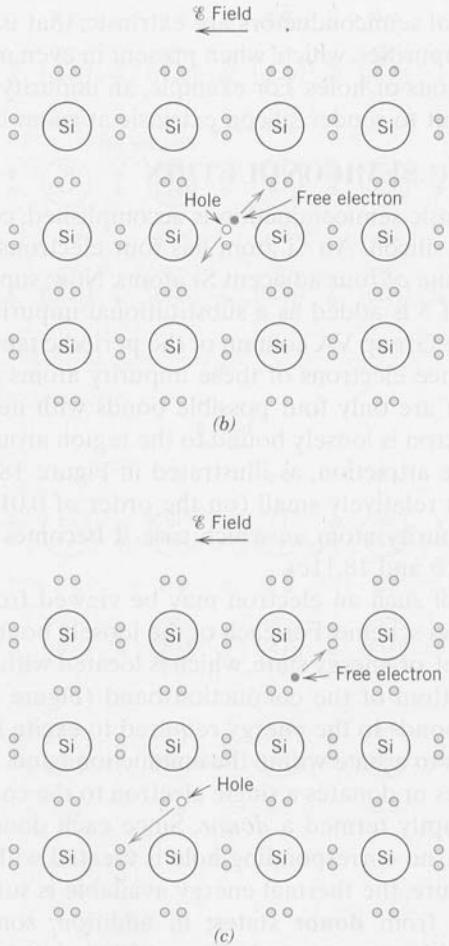
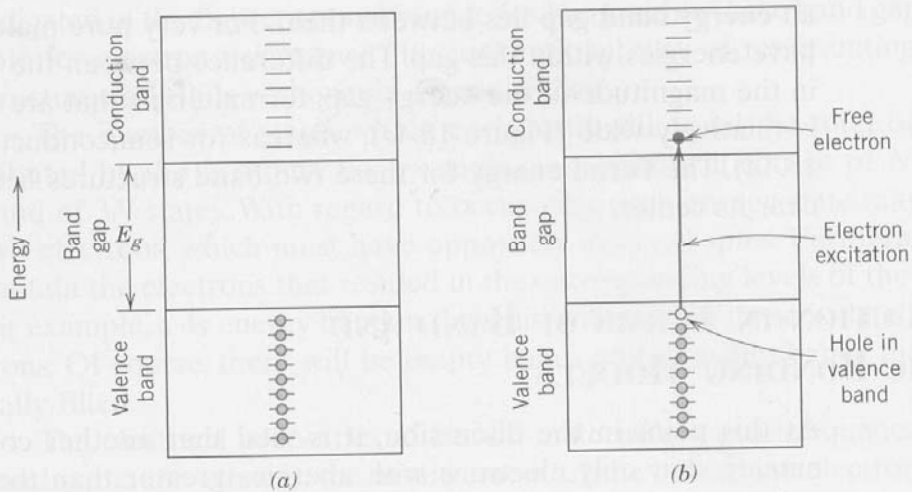



FIGURE 18.6 For an insulator or semiconductor, occupancy of electron states (*a*) before and (*b*) after an electron excitation from the valence band into the conduction band, in which both a free electron and a hole are generated.




## Band model

# n-type semiconduction

- Addition of 5 valence electrons to Si:
  P, As, Sb
  (group VA in periodic table)

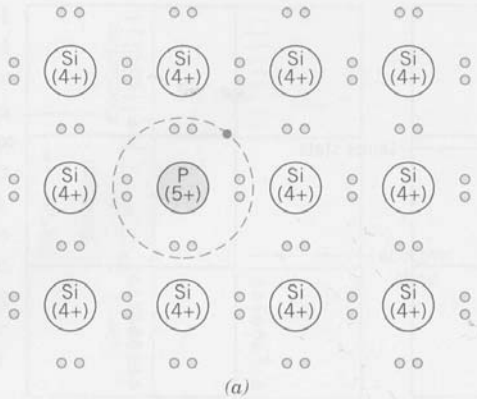



FIGURE 18.11 Extrinsic *n*-type semiconduction model (electron bonding). (*a*) An impurity atom such as phosphorus, having five valence electrons, may substitute for a silicon atom. This results in an extra bonding electron, which is bound to the impurity atom and orbits it. (*b*) Excitation to form a free electron. (*c*) The motion of this free electron in response to an electric field.

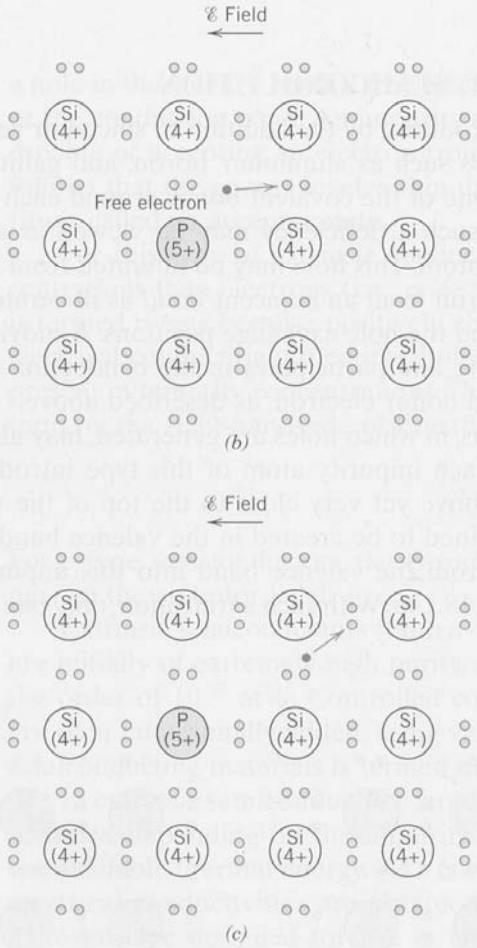
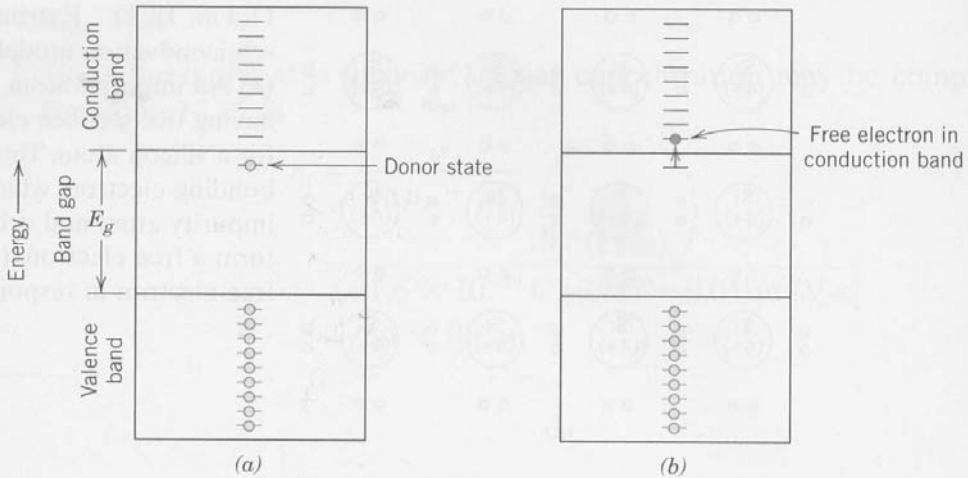



FIGURE 18.12 (*a*) Electron energy band scheme for a donor impurity level located within the band gap and just below the bottom of the conduction band. (*b*) Excitation from a donor state in which a free electron is generated in the conduction band.



## p-type semiconduction

-Addition of 3 valence electrons to Si, Ge: B, Al (group IIIA in periodic table)

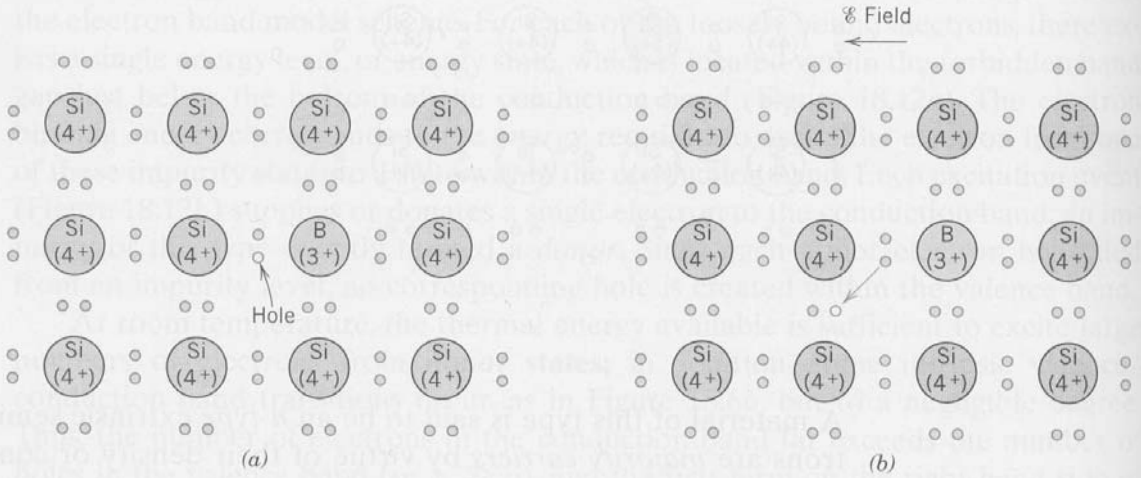



FIGURE 18.13 Extrinsic *p*-type semiconduction model (electron bonding). (*a*) An impurity atom such as boron, having three valence electrons, may substitute for a silicon atom. This results in a deficiency of one valence electron, or a hole associated with the impurity atom. (*b*) The motion of this hole in response to an electric field.

FIGURE 18.14 (*a*) Energy band scheme for an acceptor impurity level located within the band gap and just above the top of the valence band. (*b*) Excitation of an electron into the acceptor level, leaving behind a hole in the valence band.