Energy Bands and Charge Carriers
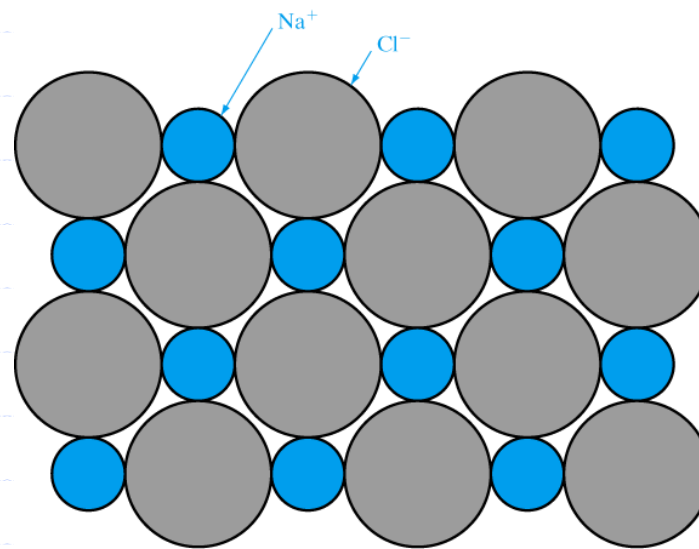
ELEC 424

John Peeples
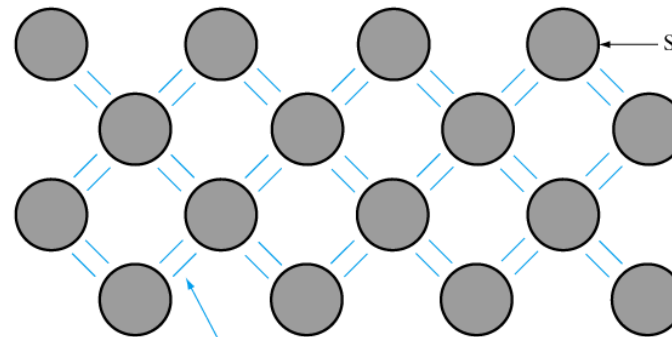
Ungraded "Homework" for Test Preparation
Chapter 2

- ## 2.5, 2.6, and 2.11 in text, p57

Na$^+$

Cl$^-$

(a)

Si

Two electrons per bond
(b)

Figure 3—1
Different types of chemical bonding in solids (a) an example of ionic bonding in NaCl; (b) covalent bonding in the Si crystal, veiwed along a <100> direction (see also Figs. 1–8 and 1–9).
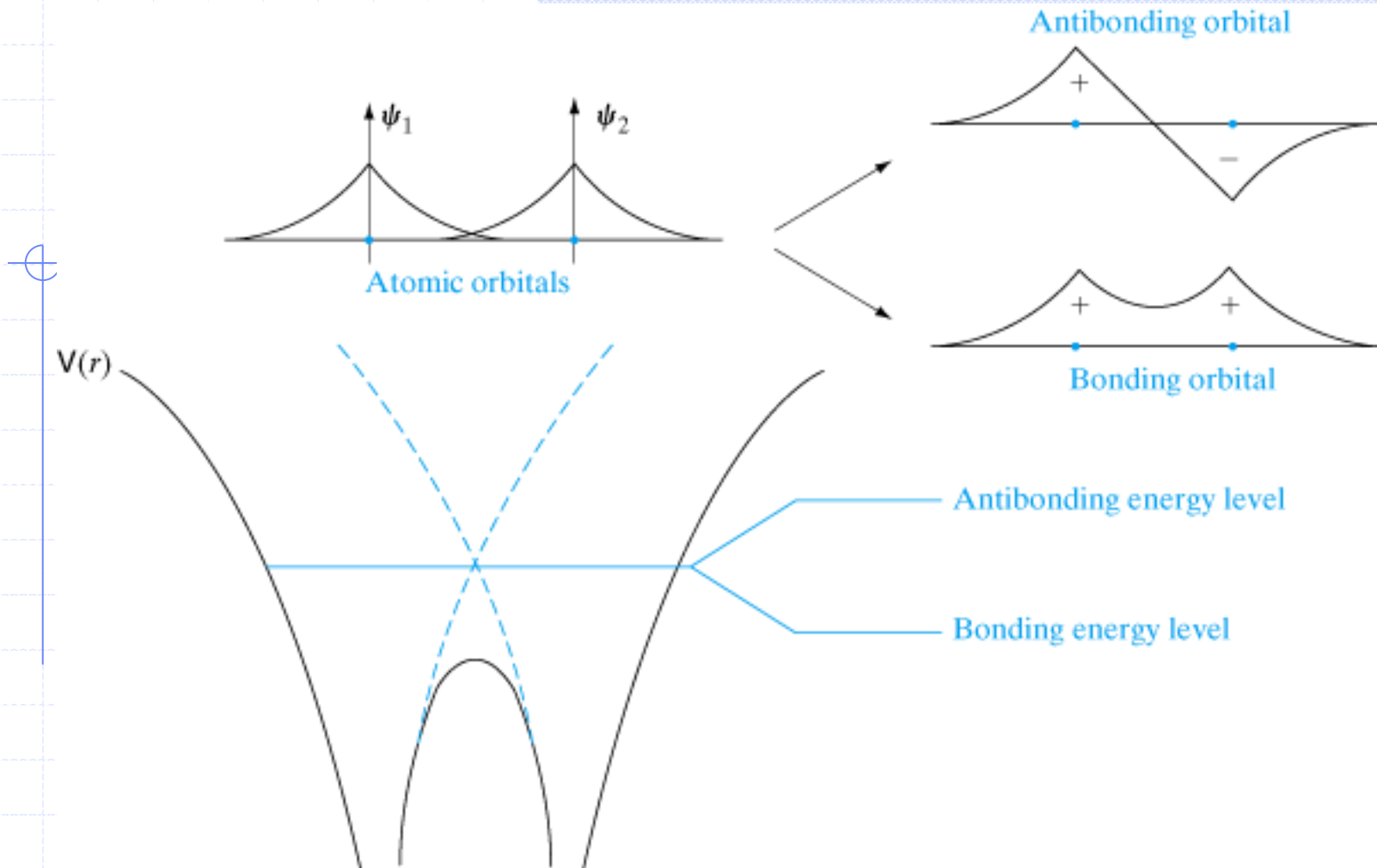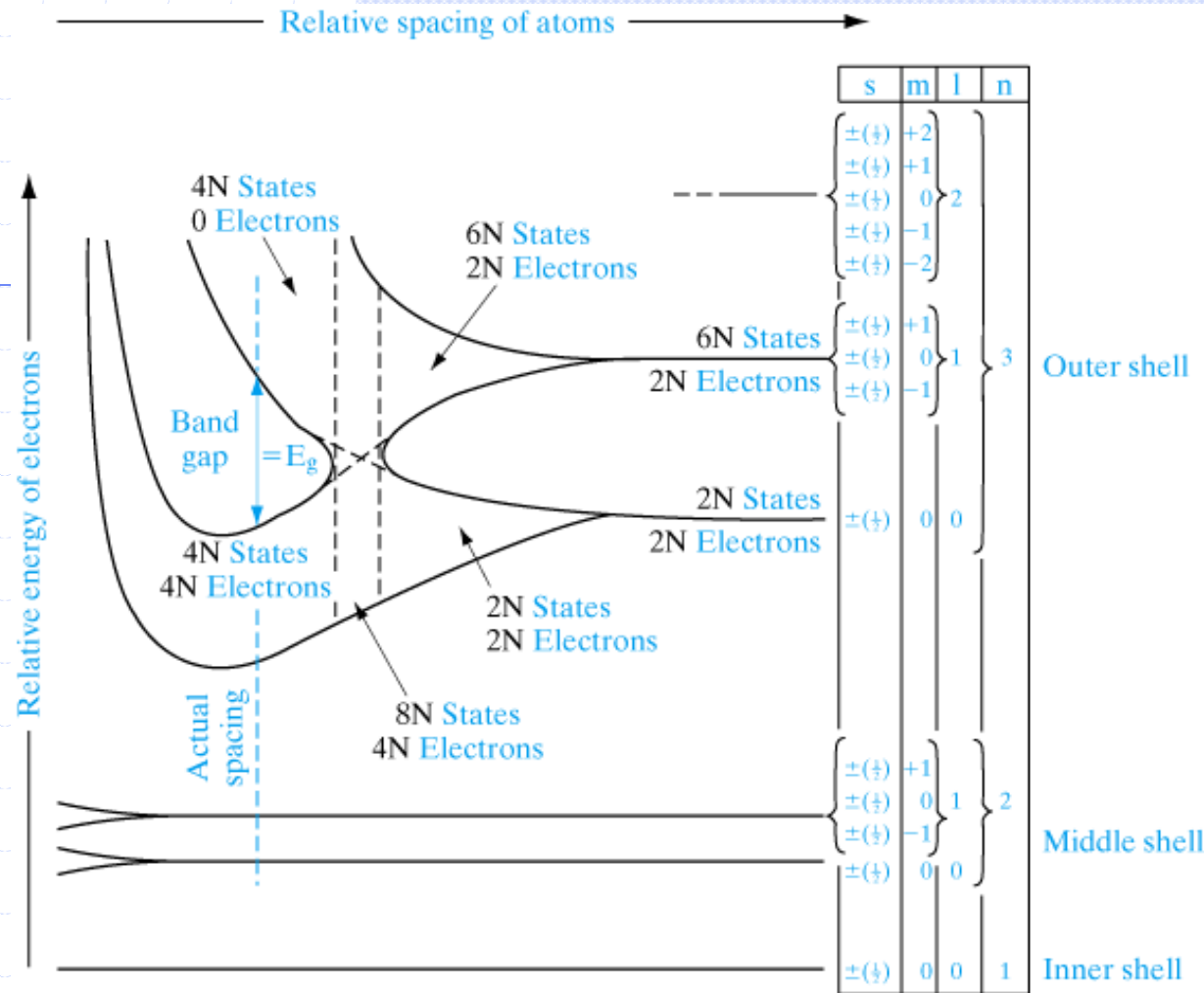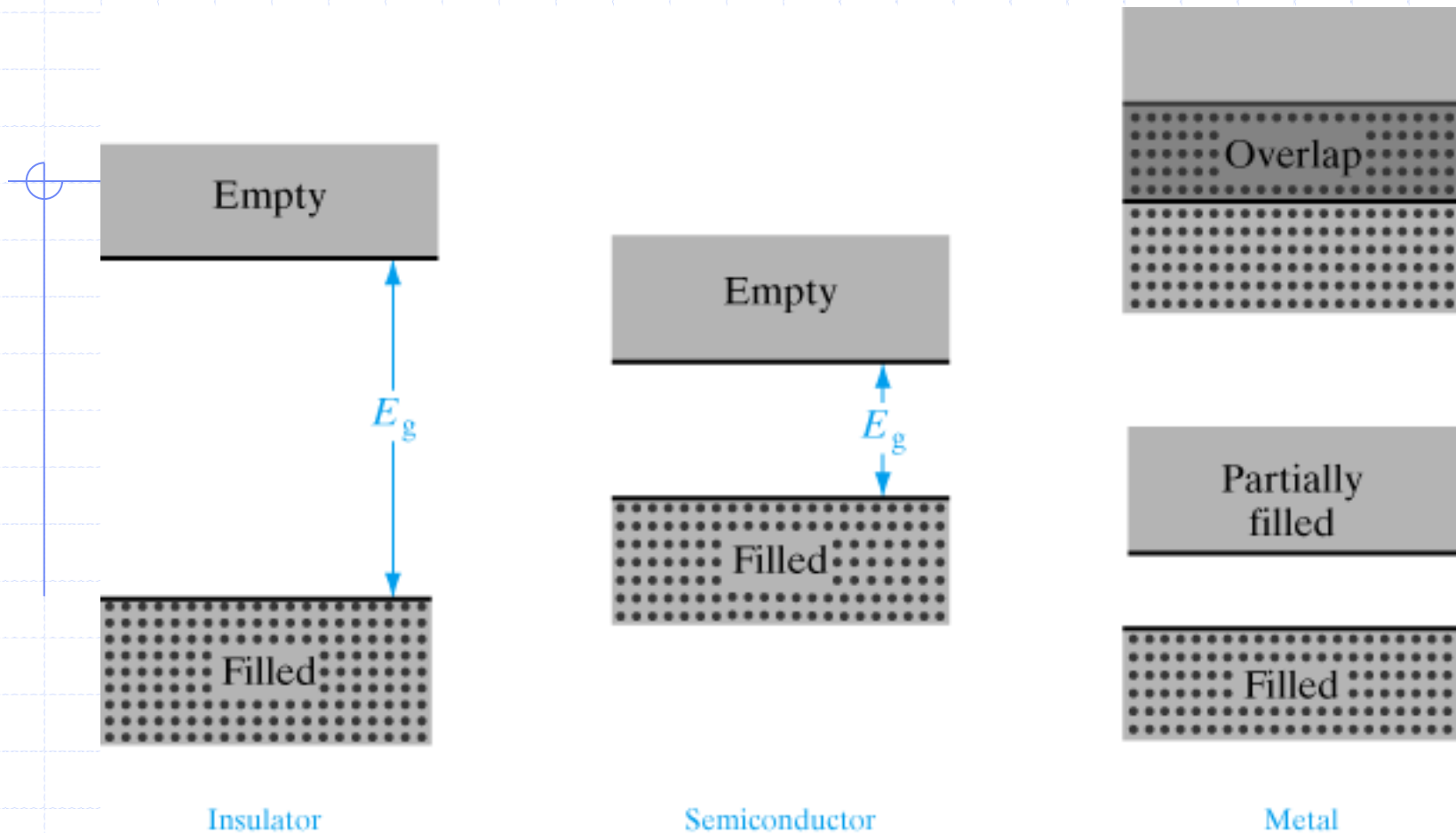
Figure 3—2
Linear combinations of atomic orbitals (LCAO): The LCAO when 2 atoms are brought together leads to 2 distinct "normal" modes—a higher energy anti-bonding orbital, and a lower energy bonding orbital. Note that the electron probability density is high in the region between the ion cores (covalent "bond"), leading to lowering of the bonding energy level and the cohesion of the crystal. If instead of 2 atoms, one brings together N atoms, there will be N distinct LCAO, and N closely-spaced energy levels in a band.
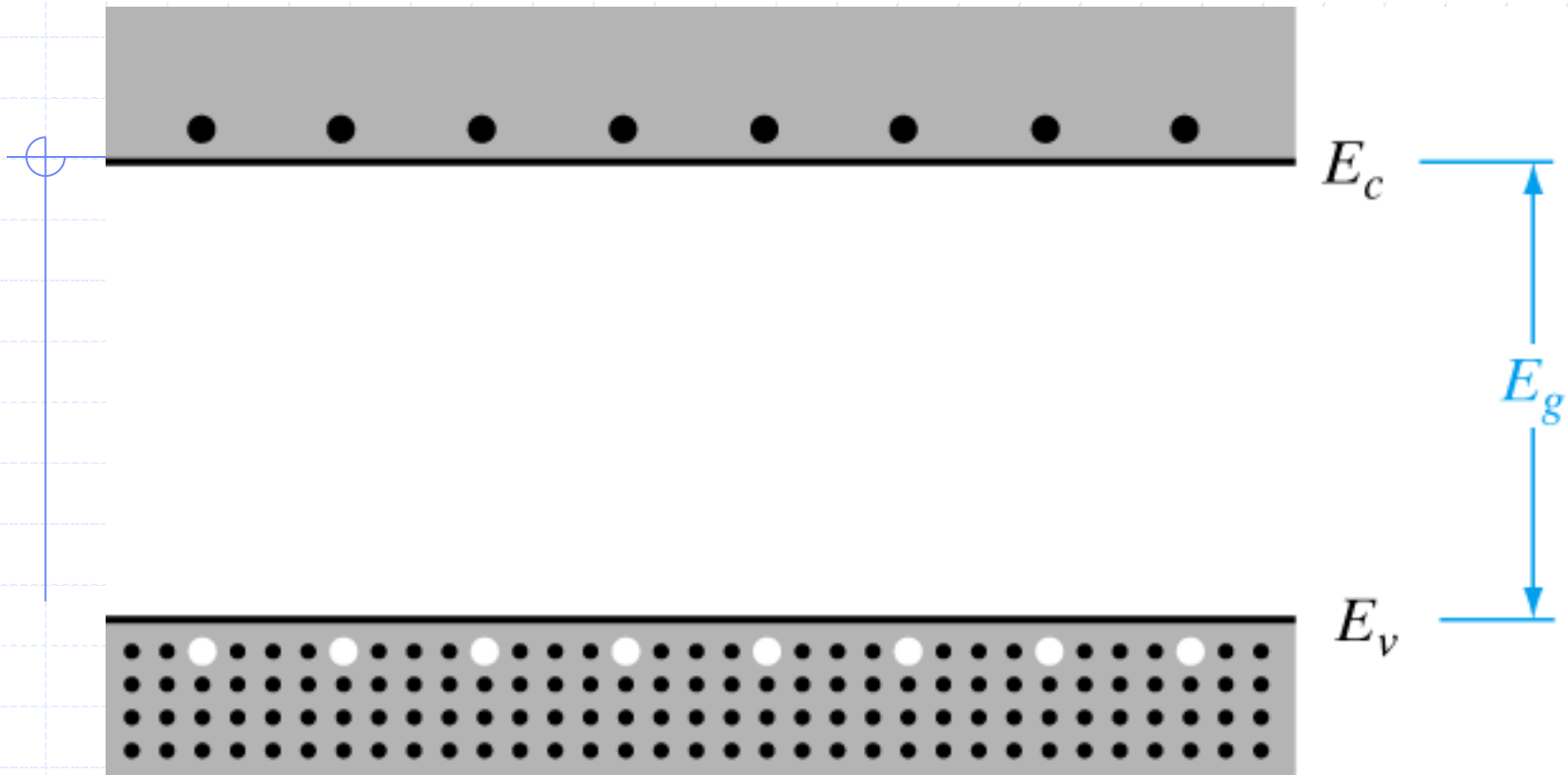
Relative spacing of atoms →

Relative energy of electrons →

4N States
0 Electrons

6N States
2N Electrons

6N States
2N Electrons

Band gap $= E_g$

4N States
4N Electrons

2N States
2N Electrons

2N States
2N Electrons

8N States
4N Electrons

Actual spacing

s	m	l	n	
$\pm(\frac{1}{2})$	+2			
$\pm(\frac{1}{2})$	+1			
$\pm(\frac{1}{2})$	0	2		
$\pm(\frac{1}{2})$	−1			
$\pm(\frac{1}{2})$	−2			
$\pm(\frac{1}{2})$	+1			
$\pm(\frac{1}{2})$	0	1	3	Outer shell
$\pm(\frac{1}{2})$	−1			
$\pm(\frac{1}{2})$	0	0		
$\pm(\frac{1}{2})$	+1			
$\pm(\frac{1}{2})$	0	1	2	
$\pm(\frac{1}{2})$	−1			Middle shell
$\pm(\frac{1}{2})$	0	0		
$\pm(\frac{1}{2})$	0	0	1	Inner shell

Things to remember
- **Inner and middle shell are unaffected (do not interact)**
- **The total number of valence states (2+6=8) is preserved, but due to Pauli's principle, banding occurs with a band of 4N lower energy states separated by a forbidden gap from a band of 4N higher energy states.**
- **At equilibrium the valence electrons will occupy the low energy states.**

Empty

E_g

Filled

Insulator

Empty

E_g

Filled

Semiconductor

Overlap

Partially filled

Filled

Metal

A look at material character as related to energy bands

E_c

E_g

E_v
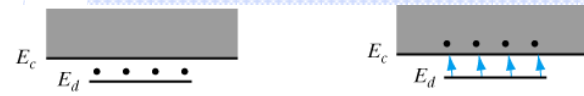
Things to remember
• Electron-hole pairs (EHPs) generation applies to INTRINSIC materials.
• Energies on the order of $1/10^{th}$ to $1/20^{th}$ the band gap are required to ionize donors or acceptors.
• Electrons in the conduction band have more freedom than do the holes in the valence band. This is our first hint of "effective mass".
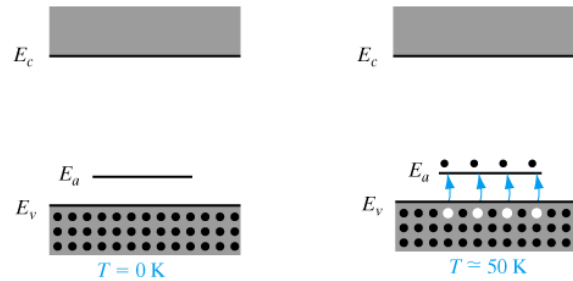
$$n = p = n_i$$

Si

e^-

e^-

h^+

h^+

e^- : Electron

h^+ : Hole
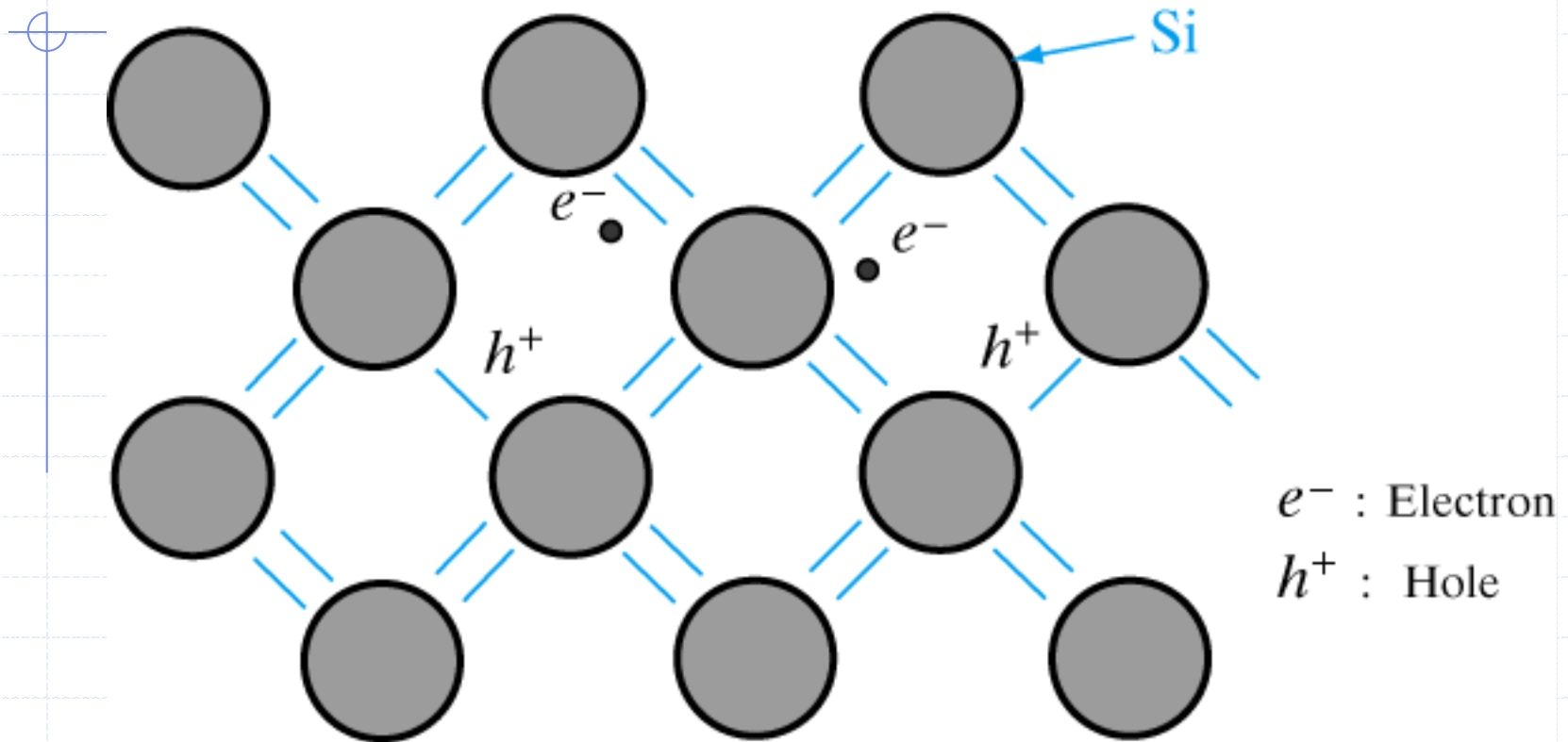
EHPs in Intrinsic Materials…about 1 pair per 10,000 billion electrons at 300K

E_c
E_d

E_c
E_d

(a)

E_v

E_v

$T = 0\,K$

$T \simeq 50\,K$

E_c

E_c

(b)

E_a
E_v

E_a
E_v

$T = 0\,K$

$T \simeq 50\,K$

Si

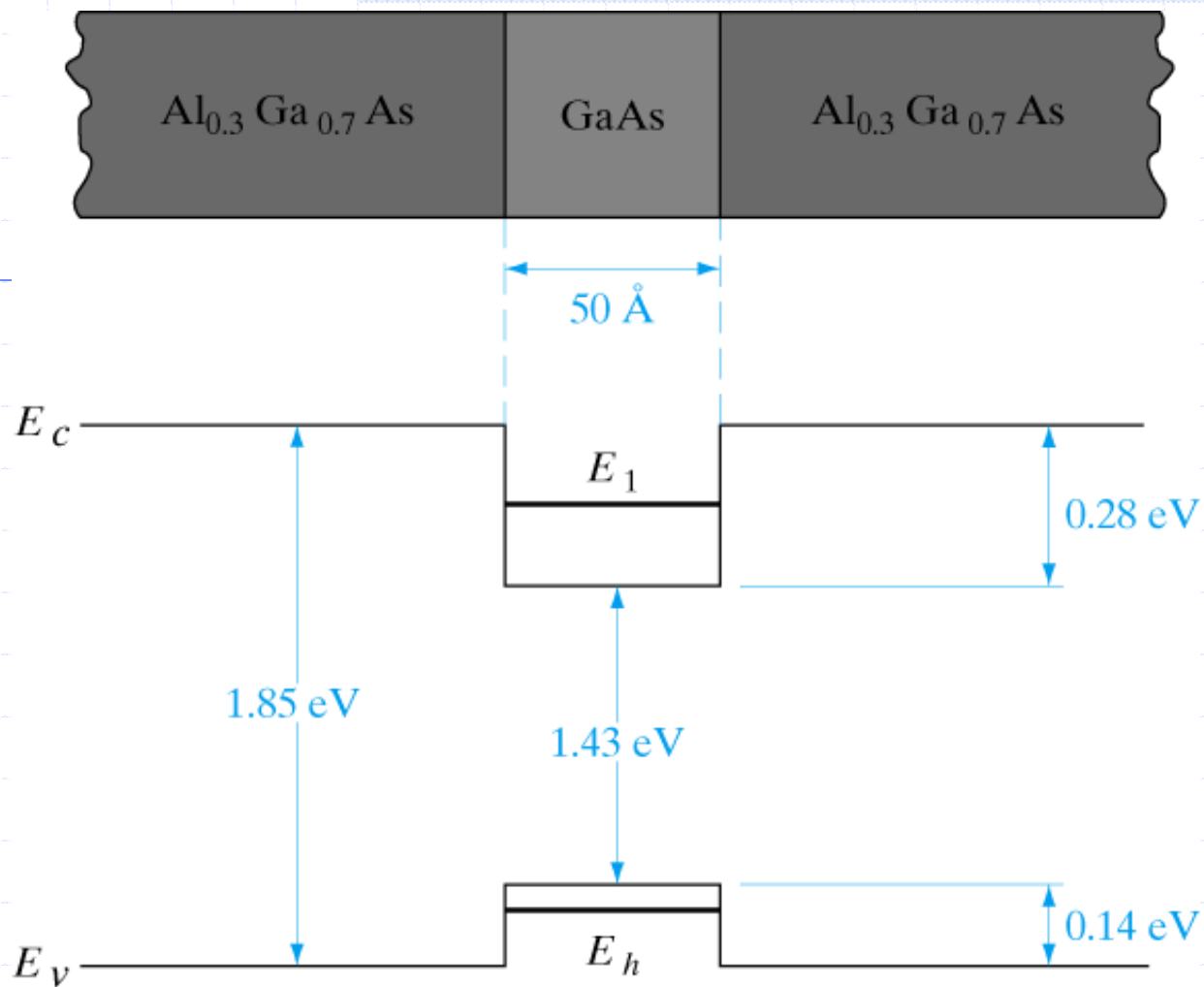As

$\bullet\, e^-$

h^+

B

(c)
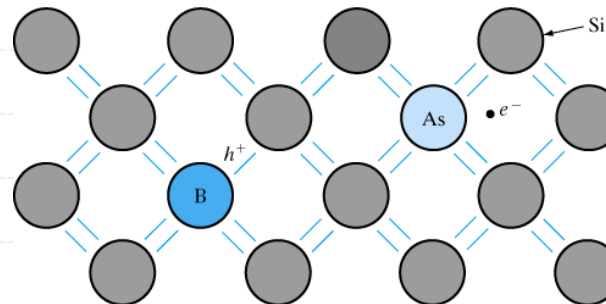
Dopants in the crystal lattice
- **Replace a Silicon atom with a group 3 or a group 5 atom**
- **Results in too few or too many electrons for pure covalent bonding**
- **Ionization energy (needed to break the extra electron off or to occupy the empty bond is much less than E_g**
- **The model is enhanced to show the new energy levels**

Al$_{0.3}$Ga$_{0.7}$As   GaAs   Al$_{0.3}$Ga$_{0.7}$As

50 Å

E_c

E_1

0.28 eV

1.85 eV

1.43 eV

0.14 eV

E_h

E_v

This is an aside
- Epitaxial methods can be used to grow very thin crystal sandwiches
- This will effectively create donor and acceptor levels that are in the middle materials conduction and valence bands.
- Ends up behaving like a particle in a box.

Chapter 3 Continued

Carrier concentration

Energy bands

Conduction

Fermi Level

◈ Fermi Dirac Distribution Function

- The probability that an available energy state is occupied by an electron at temperature T (absolute)

$$f(E) = \frac{1}{1 + e^{(E - E_f)/kT}}$$

$$k = Boltzmann's Consant$$

$$E_f = FermiLevel$$

If $E=E_f$
$$f(E) = \frac{1}{1 + e^{(E_f - E_f)/kT}} = \frac{1}{1 + e^0} = 1/2$$

So…the Fermi Level is the level of 50% probability of occupancy.
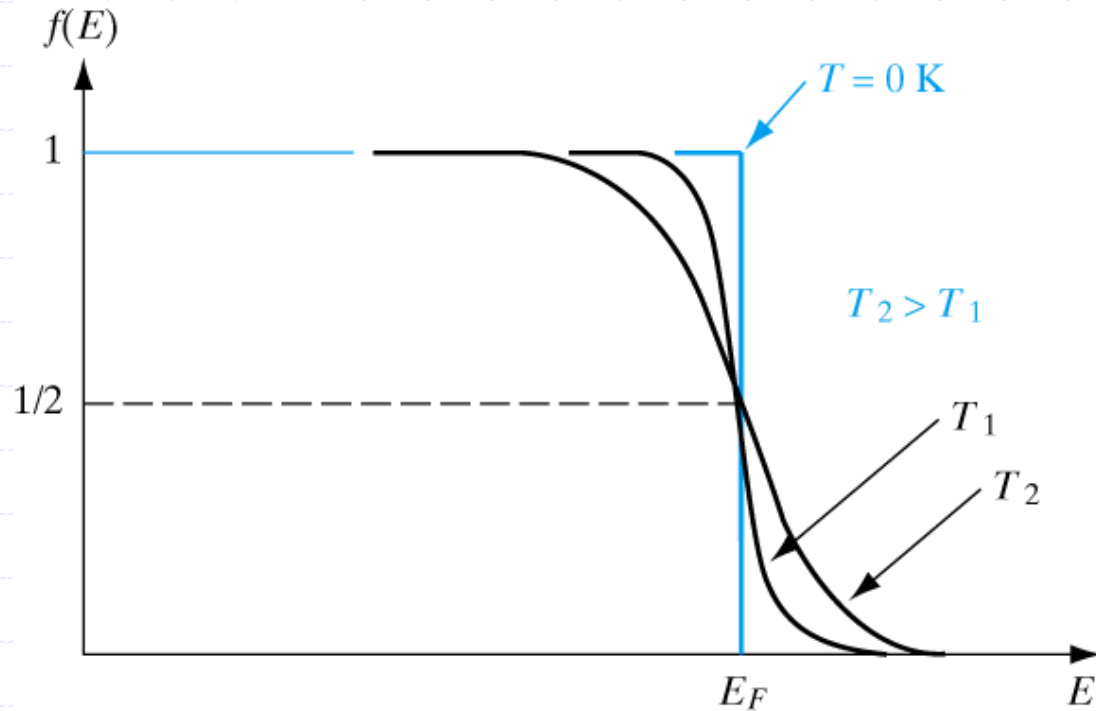
Fermi Level at *T=0K*

1 if $\quad E - E_f < 1$

$$f(E) = \cfrac{1}{1 + e^{E-E_f/0}}$$

0 if $\quad E - E_f > 1$

Figure 3—14
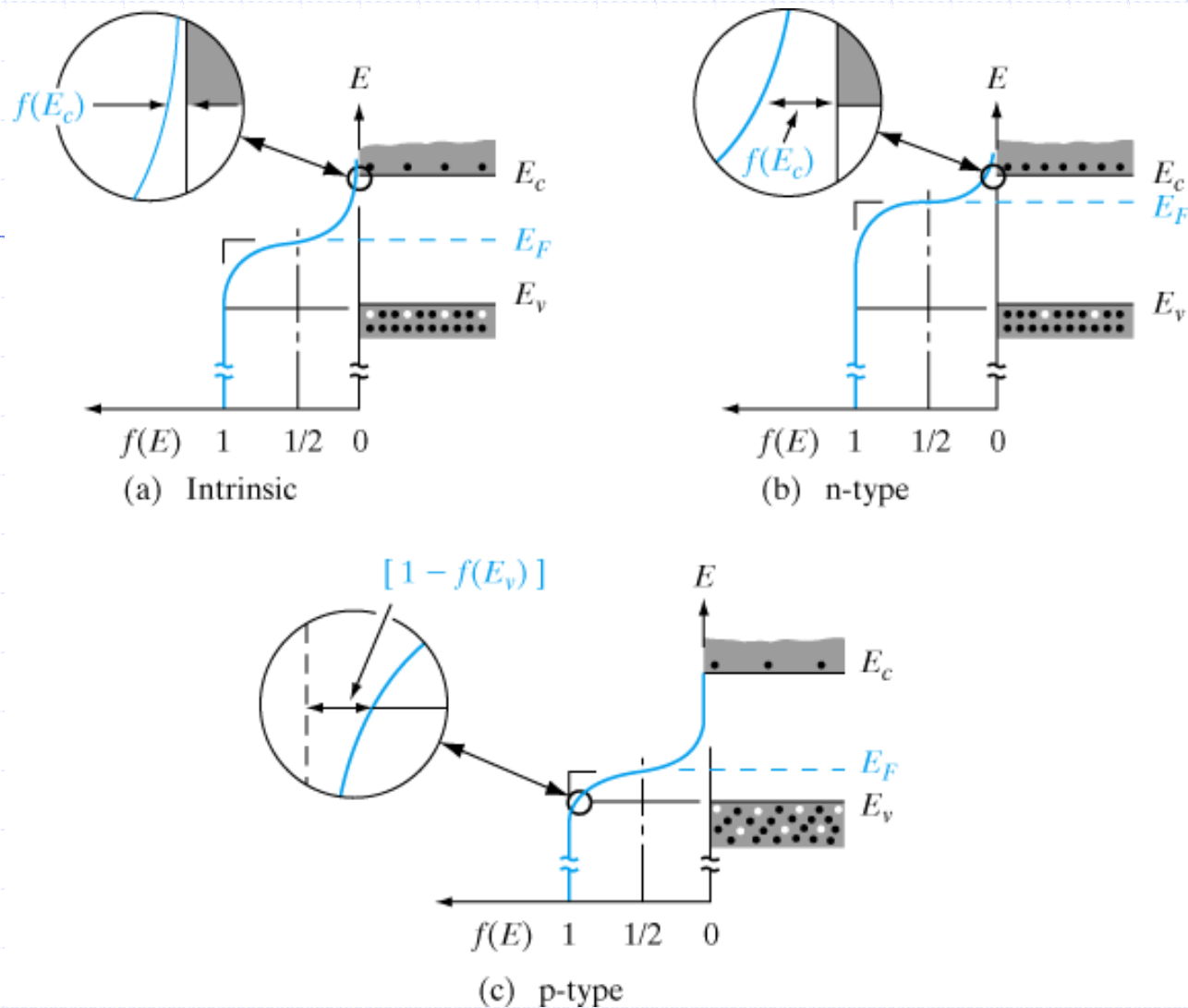The Fermi-Dirac distribution function.

Figure 3—15
The Fermi distribution function applied to semiconductors:
(a) intrinsic material; (b) n-type material; (c) p-type material.

Electron and Hole Concentrations

◆ Fermi Dirac Distribution Function gives a probability of occupancy, IF we know how many available states exist within the energy range of interest.

◆ *N(E)* = the Density of States

$$n_o = \int_{E_c}^{\infty} f(E)N(E)de$$

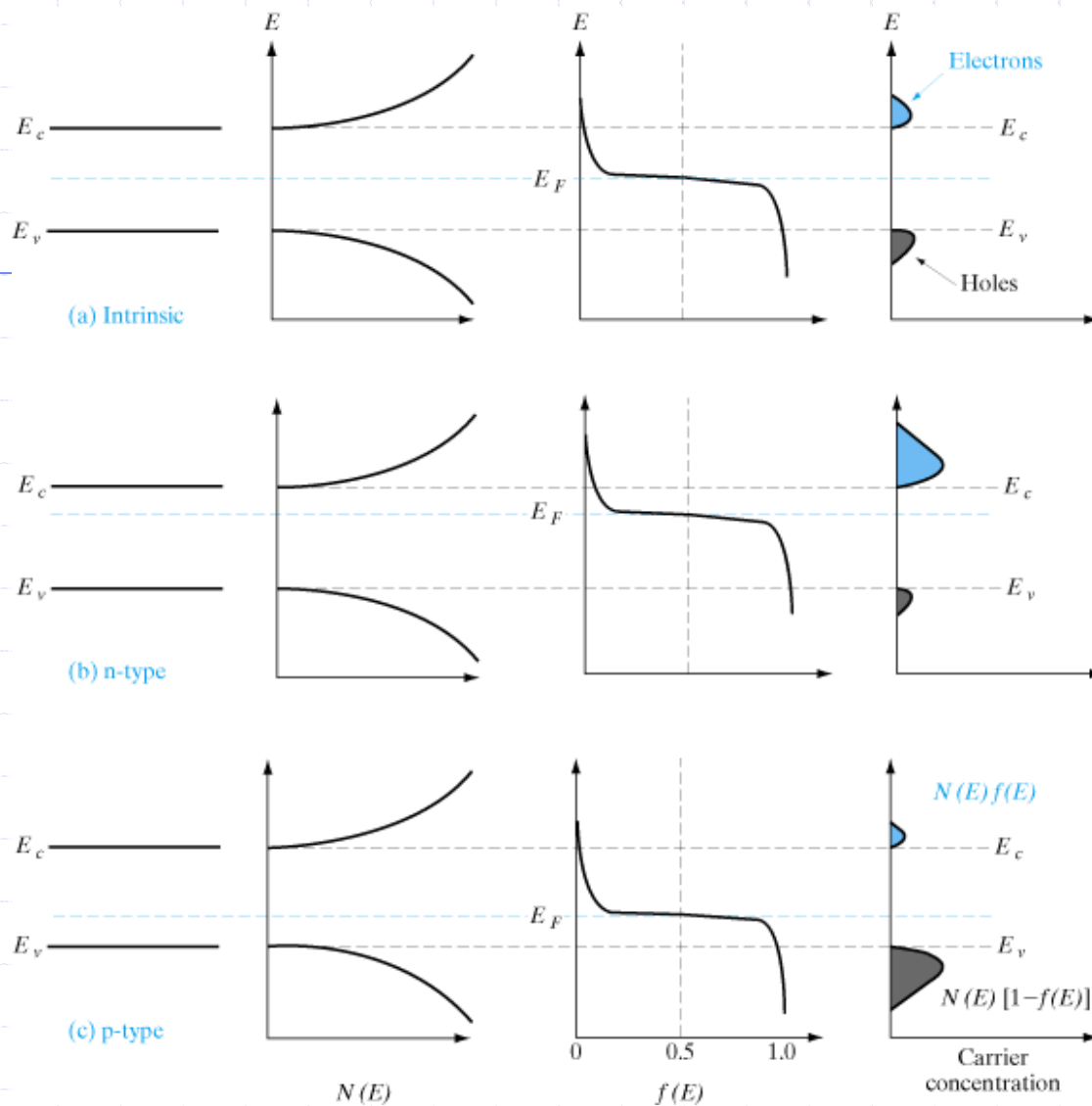$$N(E) \propto E^{\frac{1}{2}}$$

Which brings us to Figure 3-16.

Figure 3—16
Schematic band diagram, density of states, Fermi–Dirac distribution, and the carrier concentrations for (a) intrinsic, (b) n-type, and (c) p-type semiconductors at thermal equilibrium.

Electron and Hole Concentrations

Moving on

$$n_o = N_c f(E_c) = N_c e^{-(E_c - E_f)/kT}$$

and

$$p_o = N_v f(E_v) = N_v e^{-(E_f - E_v)/kT}$$

And

$$n_i = N_c e^{-(E_c - E_i)/kT}$$

and

$$p_i = N_v e^{-(E_i - E_v)/kT}$$

Equilibrium Electron and Hole Product

$$n_o p_o = n_i^2$$

- Because the product of hole and electron concentration is constant at a particular temperature in a particular material, regardless of doping,

$$n_o p_o = N_c N_v e^{-e_g / kT}$$

- and because the concentration of intrinsic holes is always equal to that of intrinsic electrons.

$$n_i = p_i \rightarrow n_i p_i = N_c N_v e^{-e_g / kT}$$

Electron and Hole Concentrations

$$n_o p_o = n_i^2$$

$$n_o = n_i e^{(E_F - E_i)/kT}$$

$$p_o = n_i e^{(E_i - E_F)/kT}$$

Example 3-5

A Si sample is doped with 10^{17} donor atoms/cm^3. At room temperature what is the hole concentration and where is the Fermi level relative to E_i?

Since $N_d >> n_i$, n_o is $\sim N_d$

$$n_o p_o = n_i^2 \Rightarrow p_o = \frac{n_i^2}{n_o} = \frac{2.25 \times 10^{20}}{10^{17}} = 2.25 \times 10^3 / cm^3$$

Example 3-5 (continued)

From
$$n_o = n_i e^{(E_F - E_i)/kT} \Rightarrow e^{(E_F - E_i)/kT} = \frac{n_o}{n_i}$$

$$\ln e^{(E_F - E_i)/kT} = \ln \frac{n_o}{n_i}$$

$$(E_F - E_i) = kT(\ln \frac{n_0}{n_i}) = 0.0259 x \ln \left[\frac{10^{17}}{1.5 x 10^{10}} \right] = 0.407 eV$$
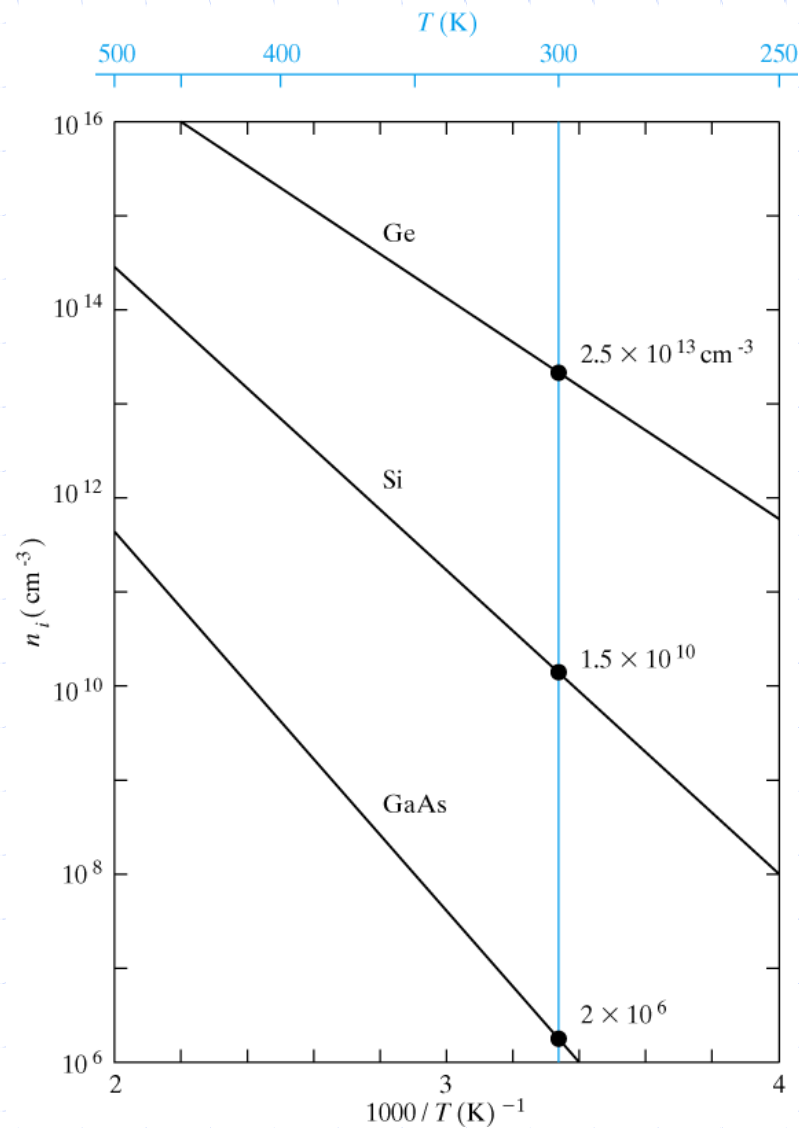
Figure 3—17
Intrinsic carrier concentration for Ge, Si, and GaAs as a function of inverse temperature. The room temperature values are marked for reference.

Compensation and Space Charge Neutrality

Space charge neutrality requires that − offset +

$$n_o + N_a^- = p_o + N_d^+$$

$$n_o = p_o + (N_d^+ - N_a^-)$$

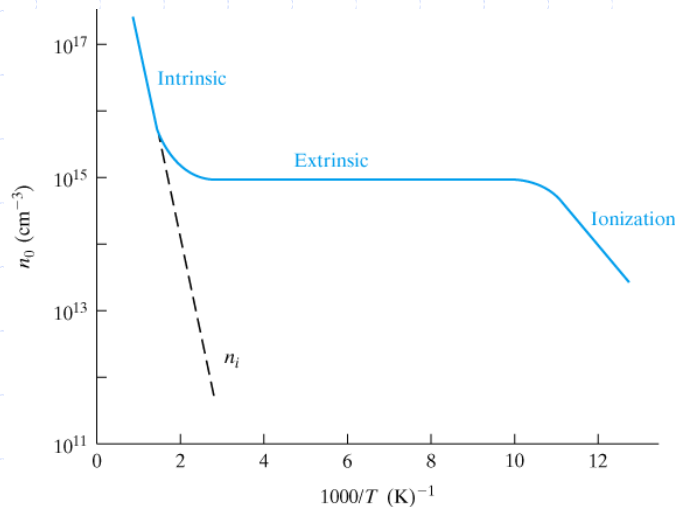Thus if $n_o >> p_o$ and all the dopants are ionized

$$n_o \cong N_d - N_a$$

E_c

E_d

E_F

E_i

E_a

E_v

Figure 3—19
Compensation in an *n-type* semiconductor (N d > N a).

Figure 3—18
Carrier concentration vs. inverse temperature for Si doped with 10^{15} donors/cm^3.

Intrinsic

Extrinsic

Ionization

n_i

n_0 (cm^{-3})

10^{17}

10^{15}

10^{13}

10^{11}

0   2   4   6   8   10   12

$1000/T$ (K)$^{-1}$

Charge Motion Carriers in Silicon
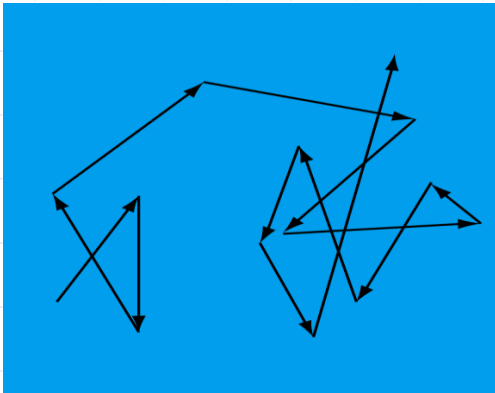
Free carrier motion due to thermal energy

$$\frac{1}{2} m_n^* v_{th}^2 = \frac{3}{2} kT$$

m_n^* is the effective mass of the carrier

v_{th} is the thermal velocity of the carrier

k is Boltzmann's constant

T is temperature in kelvin

Thermal Motion

Drift

Motion due to E-field

Diffusion

Motion due to carrier concentration gradient

Thermal Motion in Silicon

$$\frac{1}{2} m_n^* v_{th}^2 = \frac{3}{2} kT$$

$$v_{th} = \sqrt{\frac{3(1.38x10^{-23})300}{0.26 m_o}} = \sqrt{\frac{1.242x10^{-20}}{0.26(9.11*10^{-31})}}$$

$$v_{th} = 2.3*10^5 \, m/s = 2.3*10^7 \, cm/s$$

Or about 1/1300th of the speed of light

Terminology

μ is mobility

$\bar{t}$ is time between scattering events, lifetime

$\bar{l}$ is mean free length

$$\langle v_x \rangle = \frac{\langle p_x \rangle}{m_n^*} = -\frac{q\bar{t}}{m_n^*}\xi_x \qquad J_x = \sigma\xi_x \quad \text{where} \quad \sigma \equiv \frac{nq^2\bar{t}}{m_n^*}$$

$$J_x = -qn\langle v_x \rangle = \frac{nq^2\bar{t}}{m_n^*}\xi_x \qquad \sigma = qn\mu_n \quad \text{where} \quad \mu_n \equiv \frac{q\bar{t}}{m_n^*}$$

$$\mu = -\frac{\langle v_x \rangle}{\xi_x} \rightarrow \frac{cm/\text{sec}}{V/cm} = cm^2/V\cdot\text{sec}$$

Current Density

$$J_x = q(n\mu_n + p\mu_p)\xi_x = \sigma\xi_x$$

Conductivity is a function of mobility

Mobility depends on effective mass and mean free path (scattering)
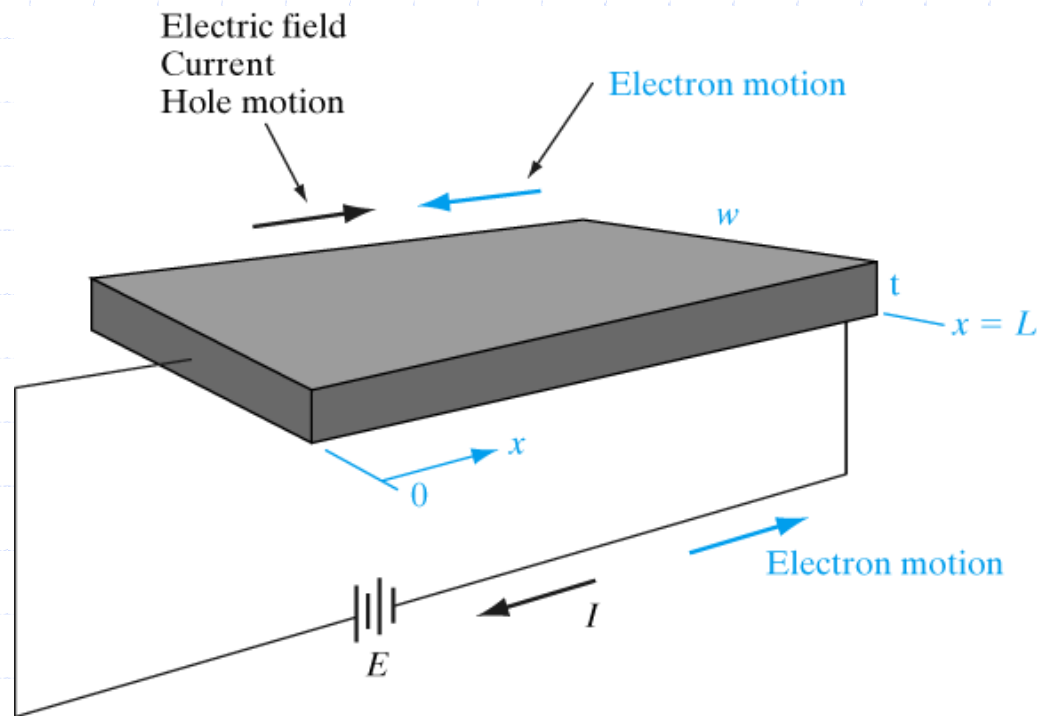
Drift and Resistance

Figure 3—21 Drift of electrons and holes in a semiconductor bar.

Carrier Drift in Homogenously Doped Silicon

$$I = \frac{V}{R} = \frac{V}{\rho \dfrac{l}{A}}$$

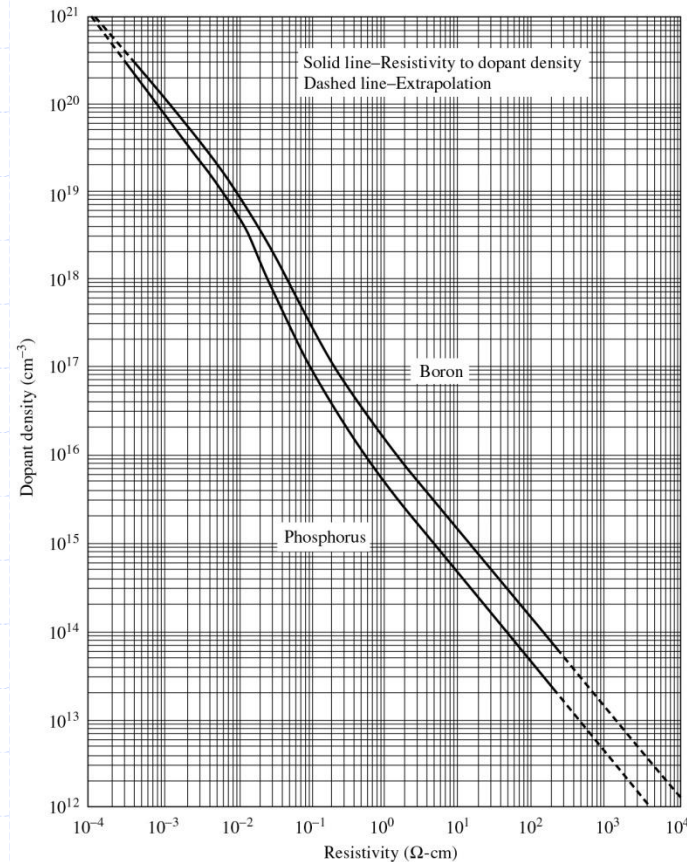…but…ρ depends on temperature, doping species, doping density and mobility


Figure 1.15 (p. 29 of *Device Electronics for Integrated Circuits*, Muller, et al, Third Edition)
Dopant density versus resistivity at 23°C (296 K) for silicon doped with phosphorus and with boron. The curves can be used with little error to represent conditions at 300 K. [W. R. Thurber, R. L. Mattis, and Y. M. Liu, National Bureau of Standards Special Publication 400–64, 42 (May 1981).]

Modeling Carrier Drift
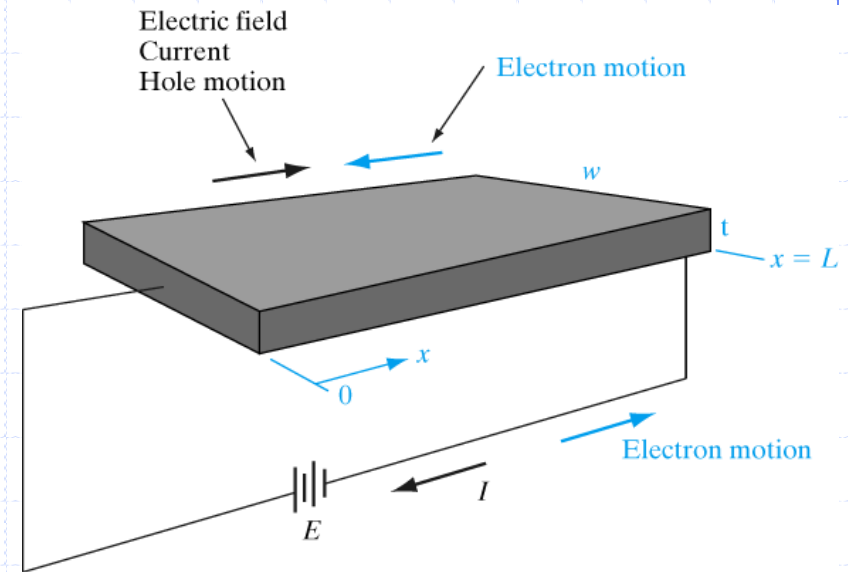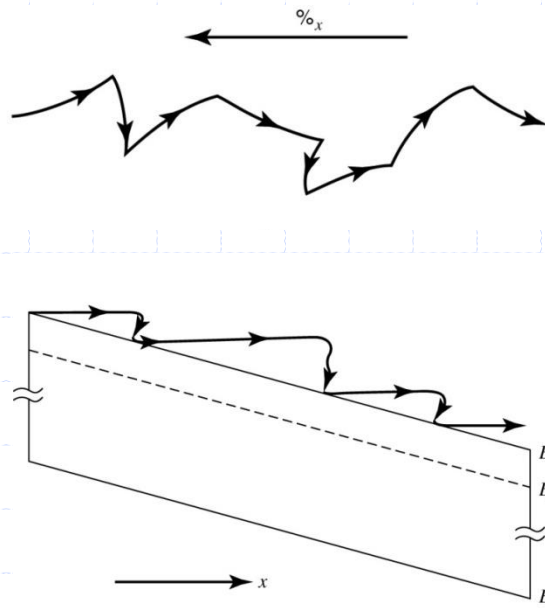
$$R = \frac{\rho L}{wt} = \frac{L}{wt}\frac{1}{\sigma}$$

Figure 1.14 (p. 27, Muller, et al)
(*a*) The motion of an electron in a solid under the influence of an applied field.
(*b*) Energy-band representation of the motion, indicating the loss of energy when the electron undergoes a collision.

Example 3-7

Si bar, 0.1 *cm* by 100 *um²*, 10^{17} Phosphorous, what is the current at 10V at 300*K*?

E-field is low enough for ohmic conduction. Figure 3-23 gives the conductivity vs. doping. The rest is accounting for the dimensions of the bar and using Ohm's Law.
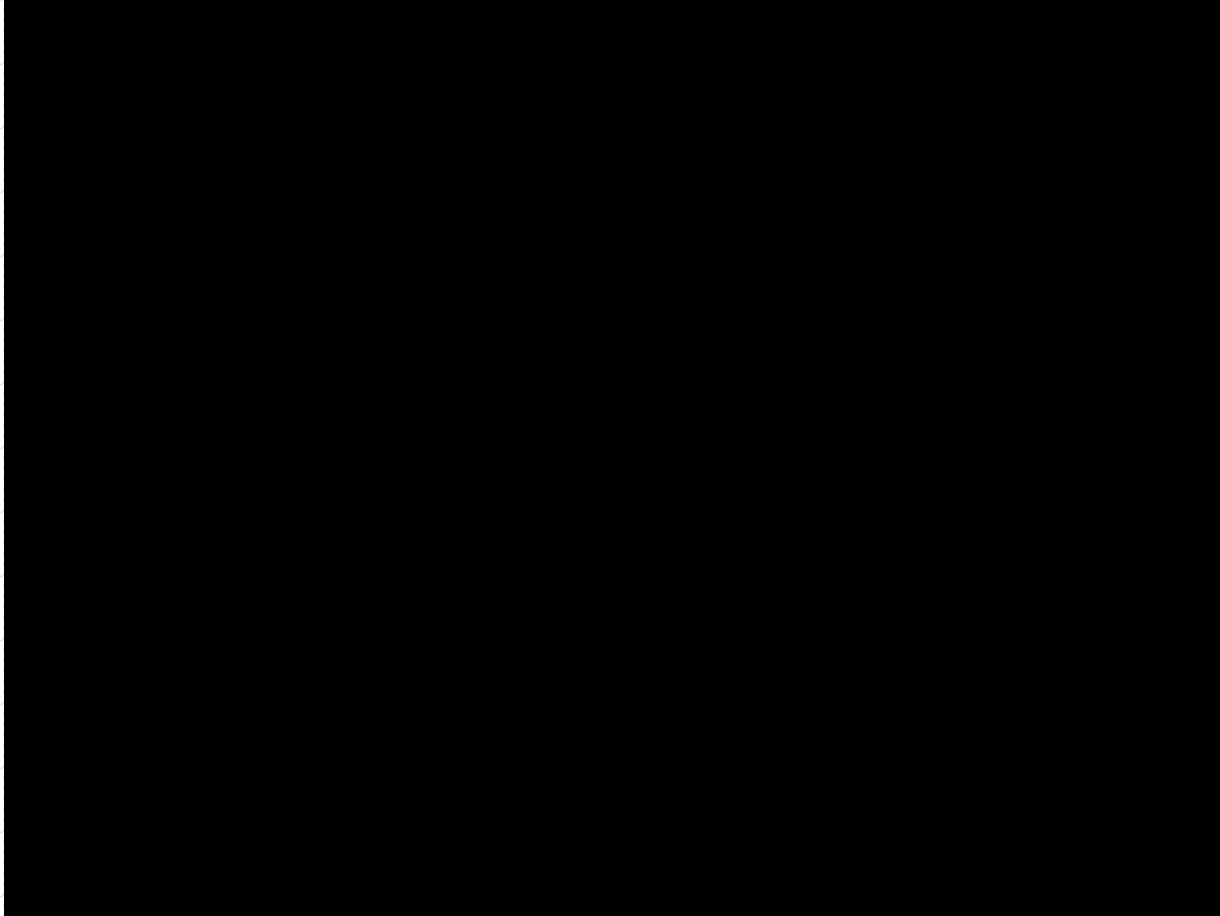
From Fig. 3-23, μ_n=700 *cm²/V-s*,

$$\sigma = qn\mu_n = 1.9*10^{-19}*700*10^{17} = 11.2 = \frac{1}{\rho}$$

$$R = \rho\frac{L}{A} = \left(\frac{1}{11.2}\right)\left(\frac{.1}{10^{-6}}\right) = 8930\Omega$$

$$I = 10V/8930\Omega = 1.12ma$$

Where did the 10^{-6} come from?

Thermal Impact on Mobility

Thermal and Doping Impact on Mobility

$T^{3/2}$ $T^{-3/2}$

Impurity scattering   Lattice scattering

μ (cm²/V-s) (log scale)
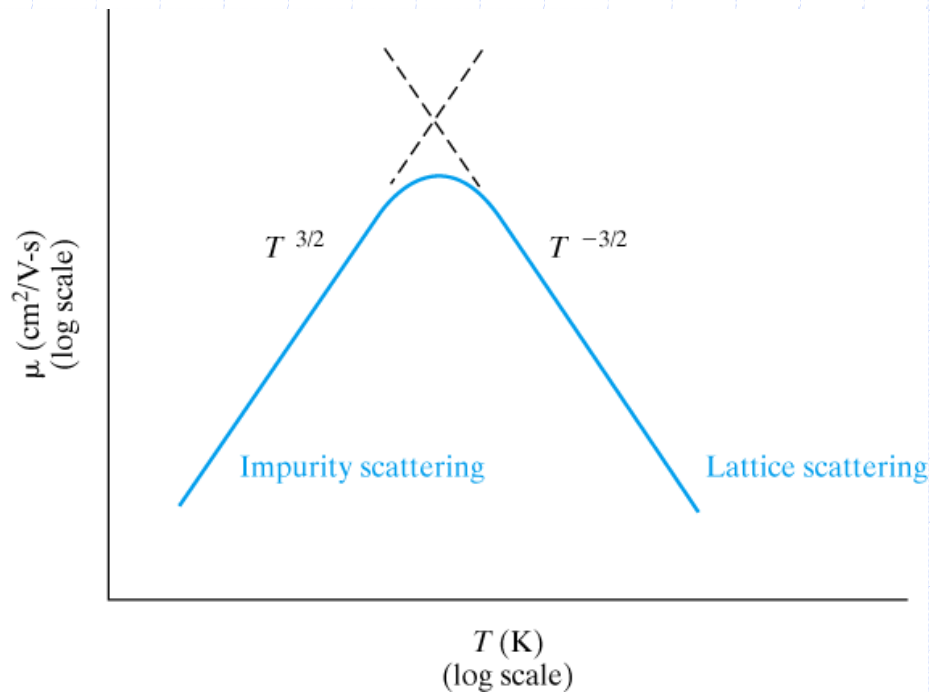
T (K) (log scale)

Figure 3—21
Approximate temperature dependence of mobility with both lattice and impurity scattering.

Streetman, p103

Mobility decreases with temperature due to lattice scattering

Impurity scattering (often ionic) events decrease mobility as temperature decreases, BUT increase with the concentration of impurities

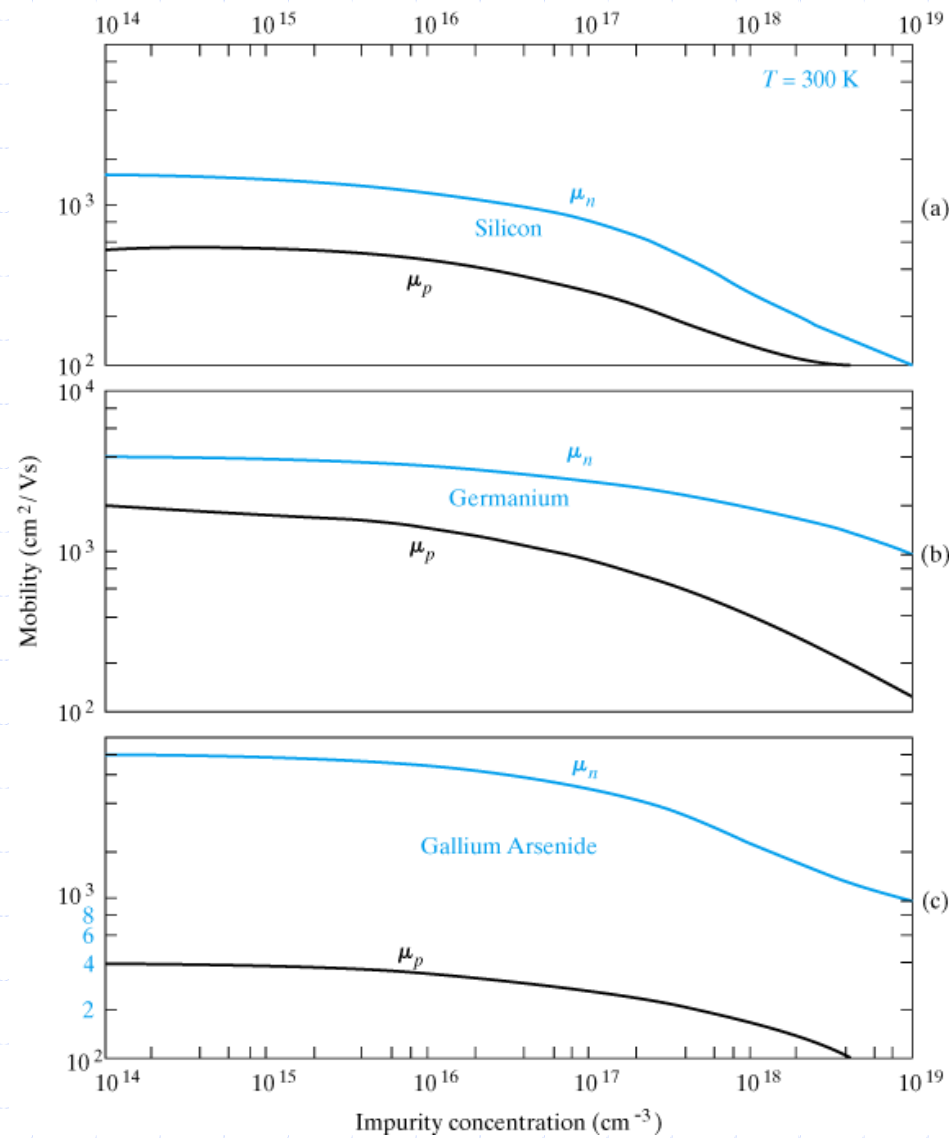Mobilities due to multiple mechanisms add like parallel resistors.

Figure 3—23

Variation of mobility with total doping impurity concentration $(N_a + N_d)$ for Ge, Si, and GaAs at 300 K.

Ohm's Law

~~Ohm's Law~~ due to critical electric field ($>10^3$ V/cm) driving carriers to a scattering limited velocity of $\sim 10^7$ cm/s.
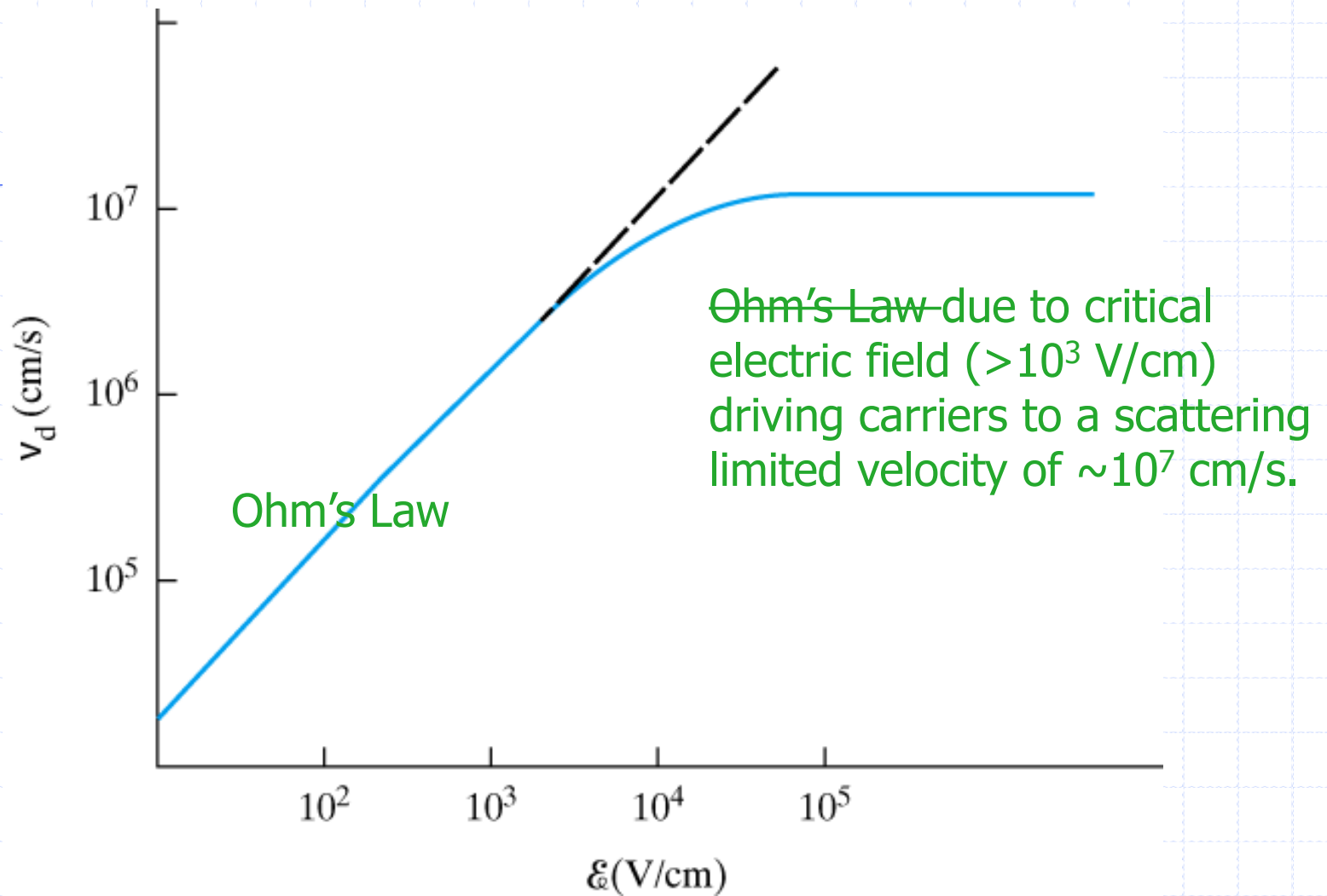
Figure 3—24
Saturation of electron drift velocity at high electric fields for Si.

Chapter 3 Homework
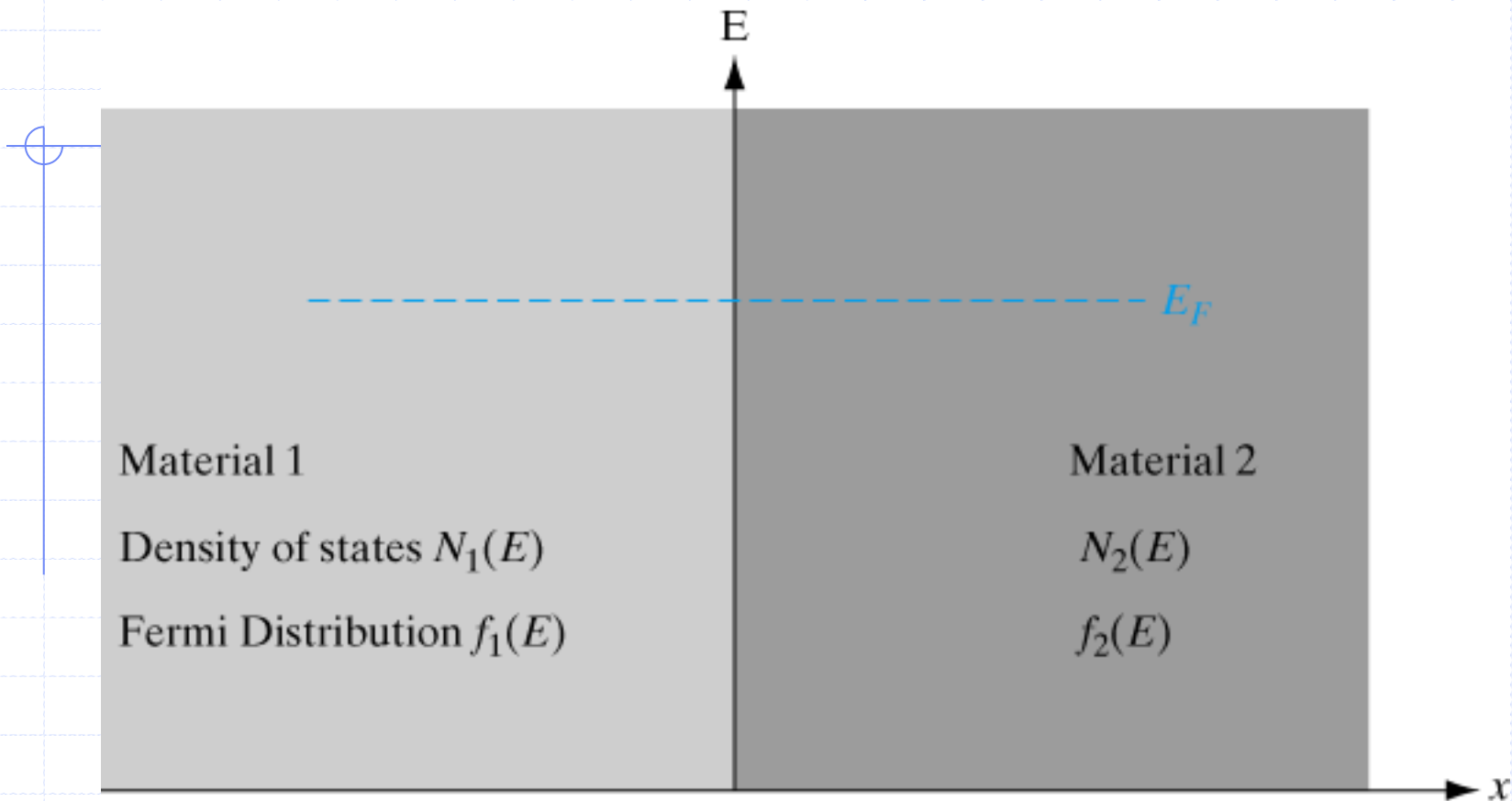
- 3.2
- 3.6
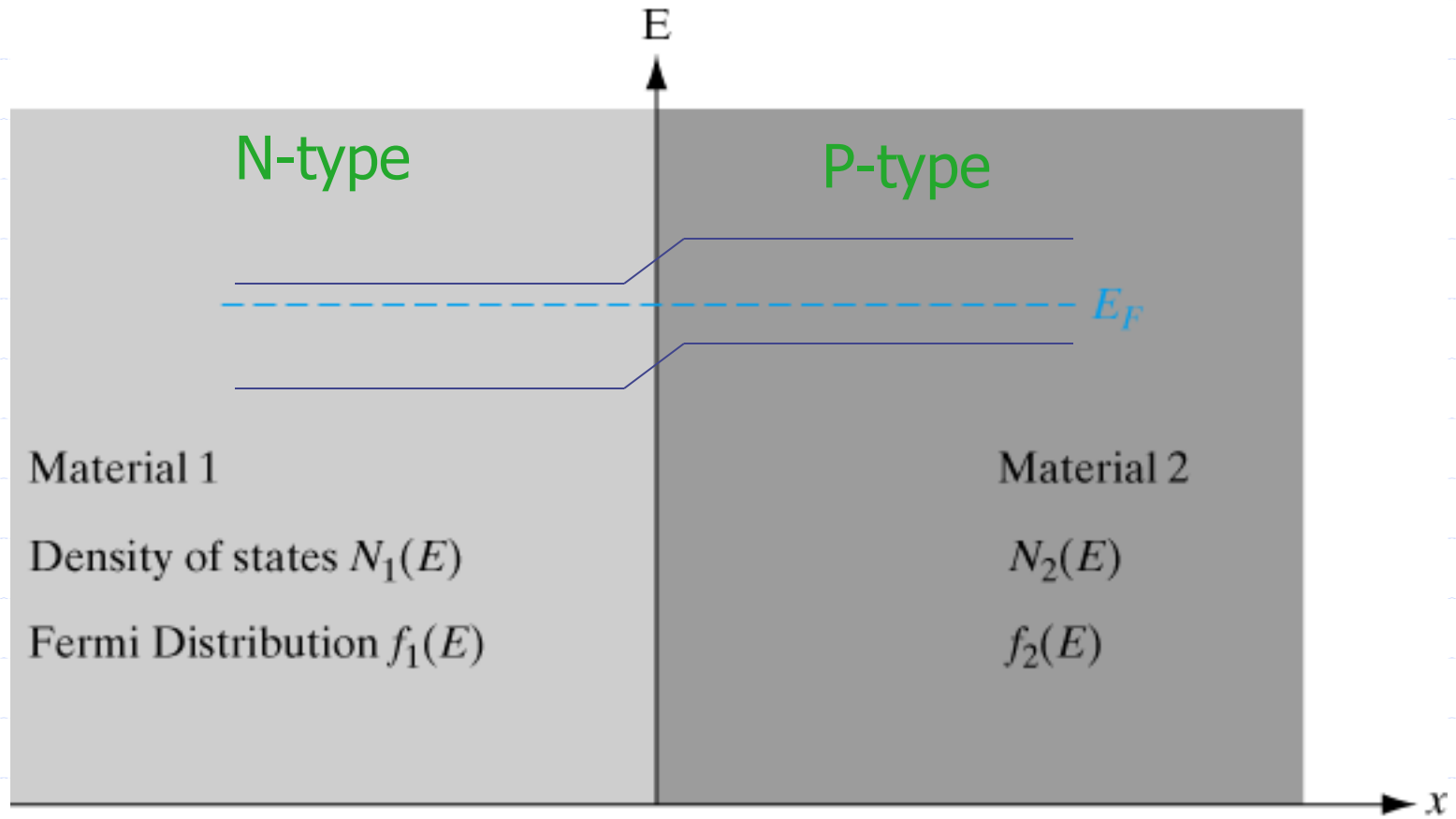- 3.10
- 3.13

◆ Due on June 8, 2015

Figure 3—26
Two materials in intimate contact at equilibrium. Since the net motion of electrons is zero, the equilibrium Fermi level must be constant throughout.
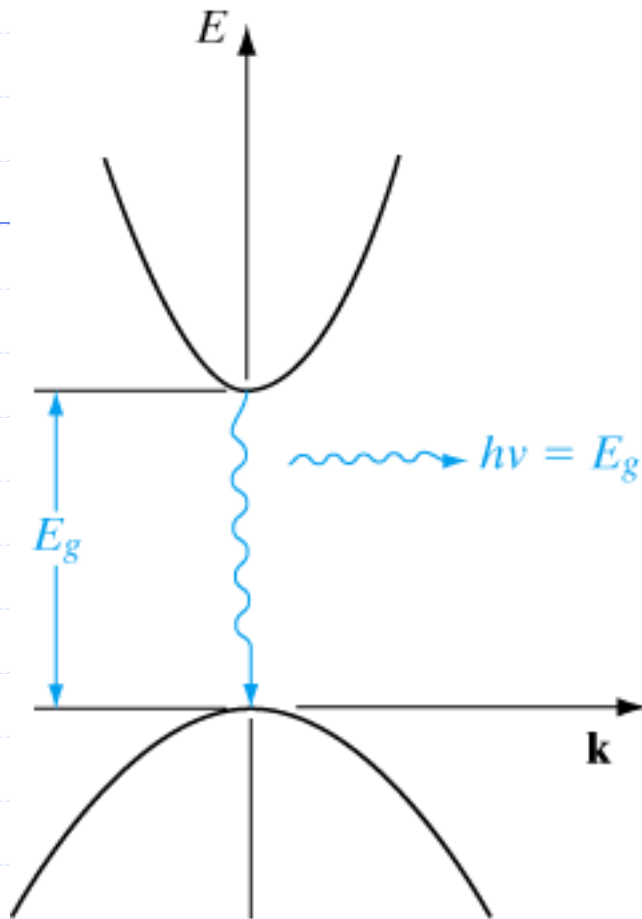
What If?

P-N junction

E

N-type

P-type

E_F

Material 1

Density of states $N_1(E)$

Fermi Distribution $f_1(E)$

Material 2

$N_2(E)$

$f_2(E)$

x

Hyperphysics

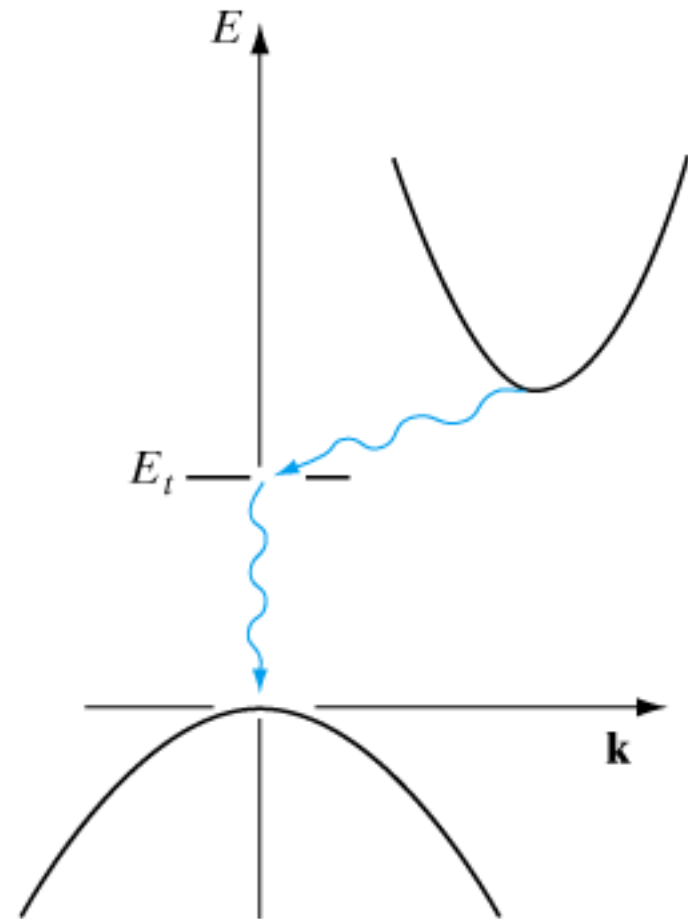http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html

Extra Slides if Needed

(a) Direct

(b) Indirect

WHOA!!! What is this _k_ value? Its called propagation constant
Direct and indirect electron transitions in semiconductors: (a) direct transition with
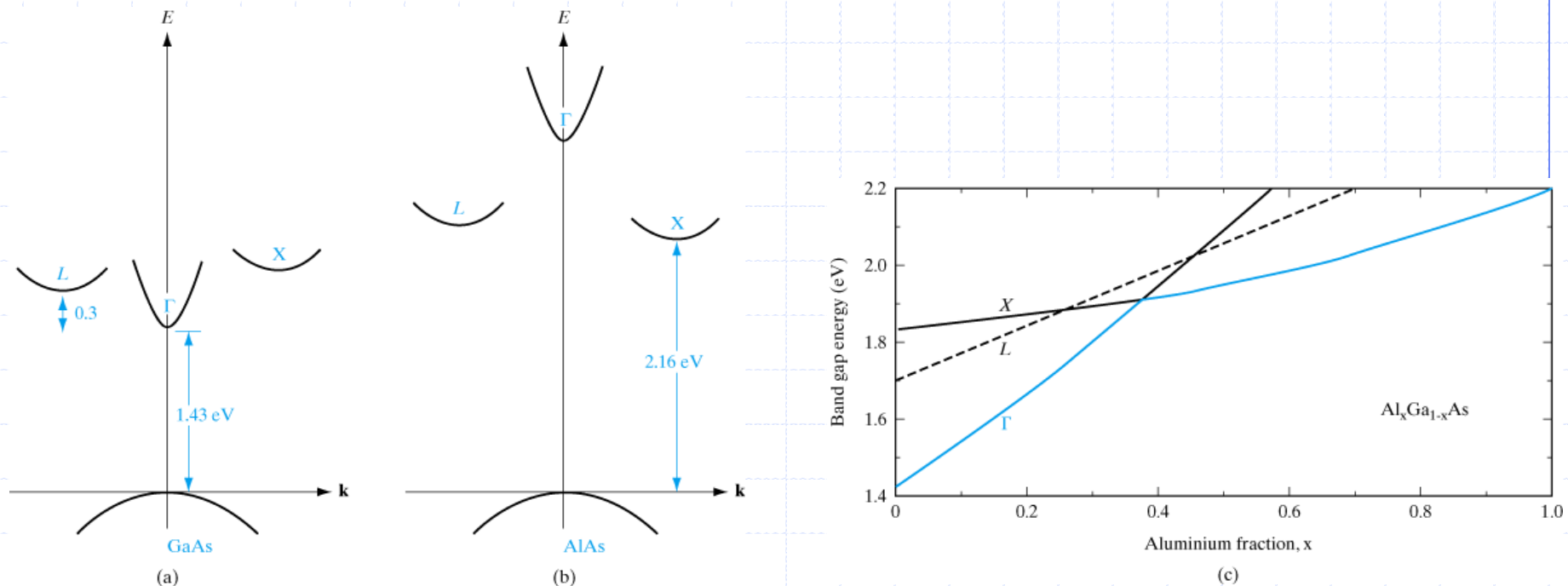accompanying photon emission; (b) indirect transition via a defect level.

Figure 3—6
Variation of direct and indirect conduction bands in AlGaAs as a function of composition: (a) the (E,k) diagram for GaAs, showing three minima in the conduction band; (b) AlAs band diagram; (c) positions of the three conduction band minima in Al x Ga 1- x As as x varies over the range of compositions from GaAs (x = 0) to AlAs (x = 1). The smallest band gap, E g (shown in color), follows the direct band to x = 0.38, and then follows the indirect X band.
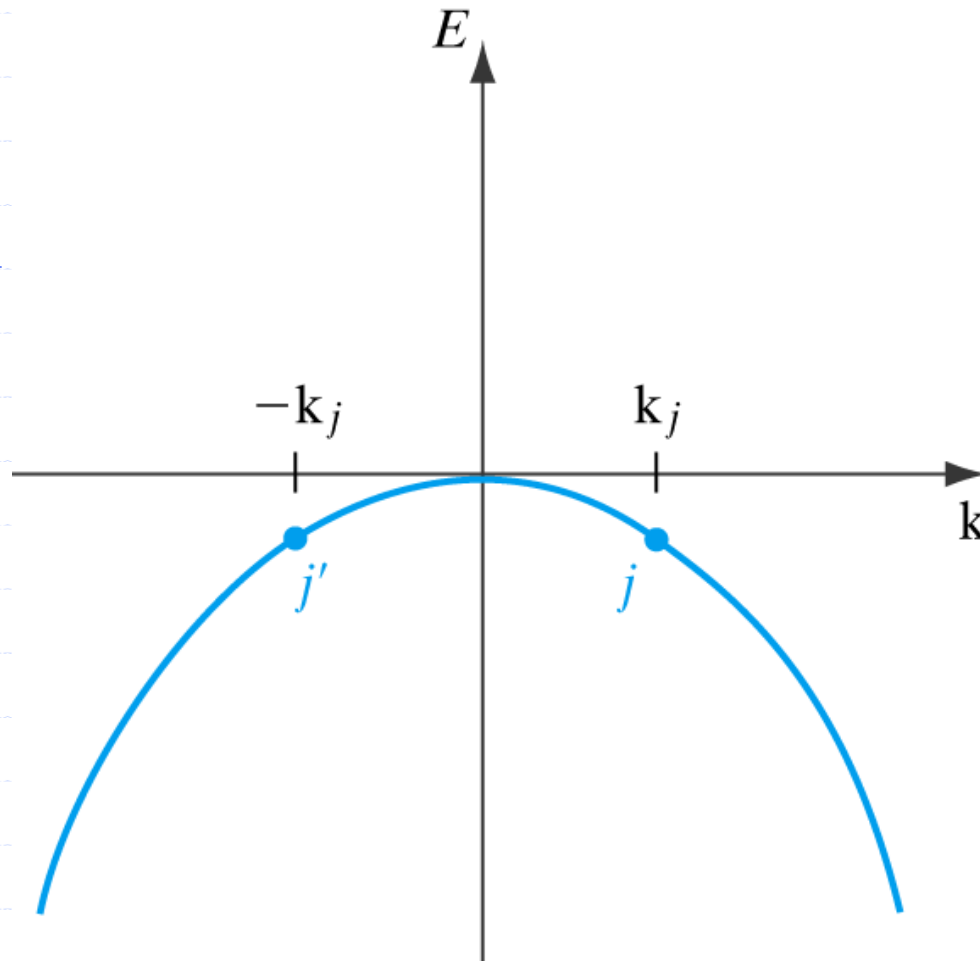
Figure 3—8
A valence band with all states filled, including states j and j9, marked for discussion. The jth electron with wave vector k j is matched by an electron at j9 with the opposite wave vector 9k j . There is no net current in the band unless an electron is removed. For example, if the jth electron is removed, the motion of the electron at j9 is no longer compensated.
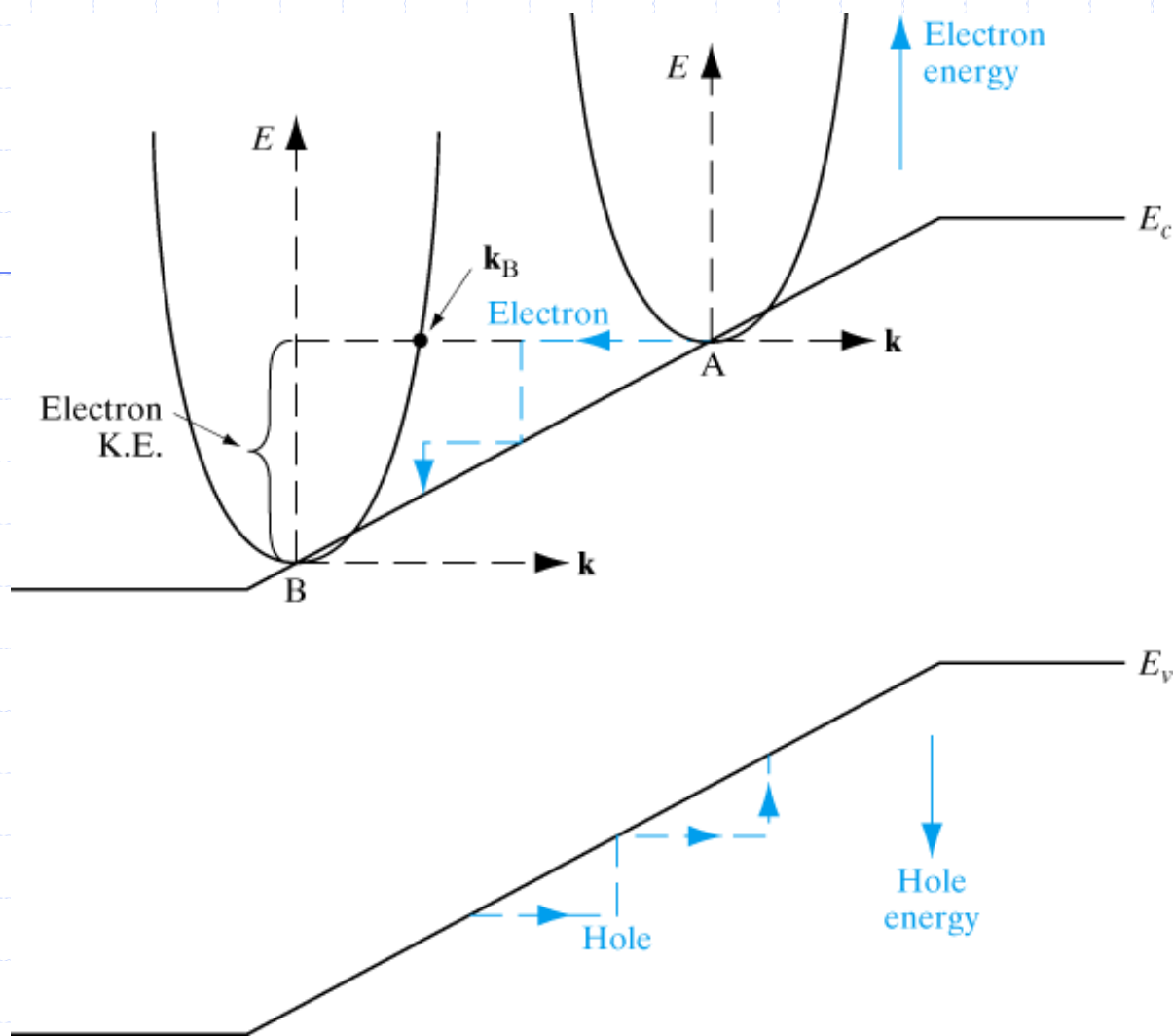
Figure 3—9
Superimposition of the (E,k) bandstructure on the E-versus-position simplified band diagram for a semiconductor in an electric field. Electron energies increase going up, while hole energies increase going down. Similarly, electron and hole wavevectors point in opposite directions and these charge carriers move opposite to each other, as shown.