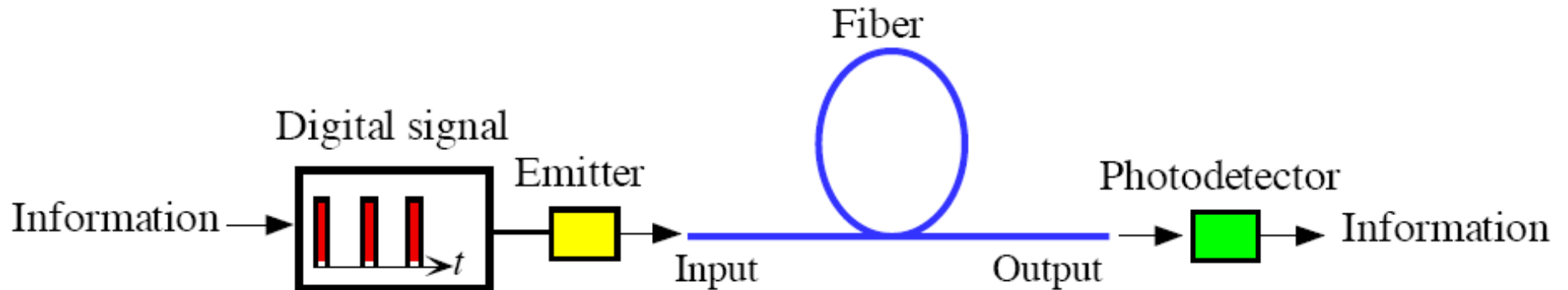# Communications with Optical Fibers

In digital communications, signals are generally sent as light pulses along an optical fiber. Information is first converted to an electrical signal in the form of pulses that represent bits of information. The electrical signal drives a laser diode whose light output is coupled into a fiber for transmission. The light output at the destination end of the fiber is coupled to a photodetector that converts the light signal back to an electrical signal. The information bits are then decoded from this electrical signal.

Chapter 4: Semiconductor Physics

Crystal structures of solids

Energy band structures of solids

Charge carriers in semiconductors

Carrier transport

Semiconductors

- **Semiconductors** are a group of materials having conductivities between those of **metals** and **insulators**.

- Two general classifications of semiconductors are elemental semiconductor materials (e.g., Si and Ge) and compound semiconductor materials (e.g., AlP, AlAs, GaP, GaAs, InP).

- **Silicon** is by far the most common semiconductor used in integrated circuits.

- **Gallium arsenide** is the most common of compound semiconductors. Its good optical properties make it useful in optical devices. It is also used in specialized applications, for example, when high speed is required.

- There are more complex compound semiconductors, for example, $Al_xGa_{1-x}As$, which provide flexibility when choosing material properties.

Semiconductors

Periodic Table of the Elements 2005

Molecular Research Institute

Types of Solids

There are three general types of solids: **amorphous**, **polycrystalline**, and **single crystal**. They are characterized by the size of ordered regions within the material. An ordered region is a spatial volume in which atoms or molecules have a regular geometric arrangement or periodicity.

Amorphous materials: order within a few atomic or molecular dimensions.

Polycrystalline materials: a number of regions with order over many atomic or molecular dimensions. These ordered regions are called **grains**, which are separated from one another by **grain boundaries**.

Single crystal materials: a high degree of order or regular geometric periodicity throughout the entire volume of the material.
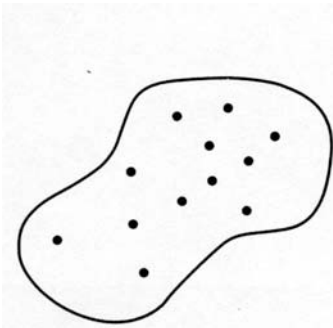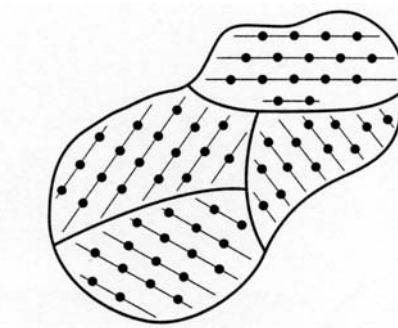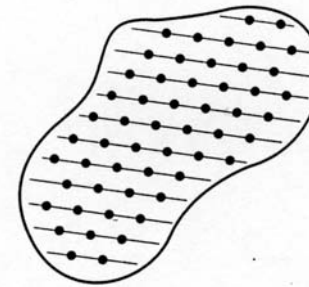
amorphous   polycrystalline   single crystal

Lattices and Unit Cells

A representative unit, or group of atoms in single-crystal materials is repeated at regular intervals in each of the three dimensions. The periodic arrangement of the unit or group in the crystal is called the **lattice**. Each unit or group can be represented by a dot, which is called **a lattice point**.

Single crystal lattices have translational symmetries (<u>assuming each crystal is infinitely large in space</u>). They can be characterized by three non-colinear directions. These translation directions need not be perpendicular to each other.
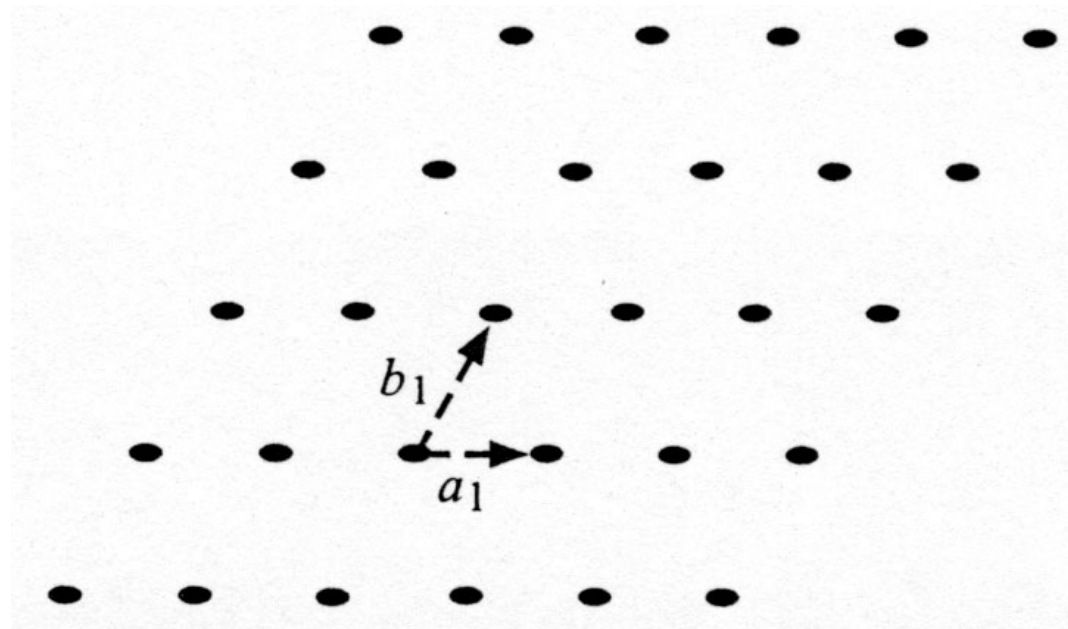
Lattices and Unit Cells

Because a three-dimensional lattice is a periodic repetition of a group of atoms, we need consider only a fundamental unit that is being repeated. A **unit cell** is a small volume of the crystal that can be used to reproduce the entire crystal.

A unit cell is not a unique entity. There exist various possible unit cells.

A **primitive cell** is the smallest unit cell that can be repeated to form the lattice.

In many cases, it is more convenient to use a unit cell that is not a primitive cell. Unit cells may be chosen to have orthogonal sides.
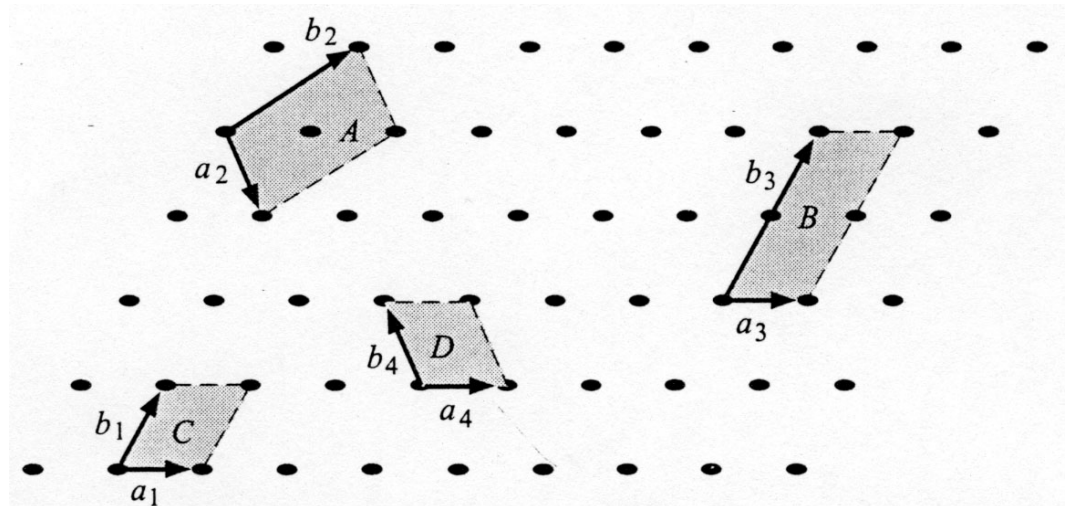
A Generalized Primitive Cell
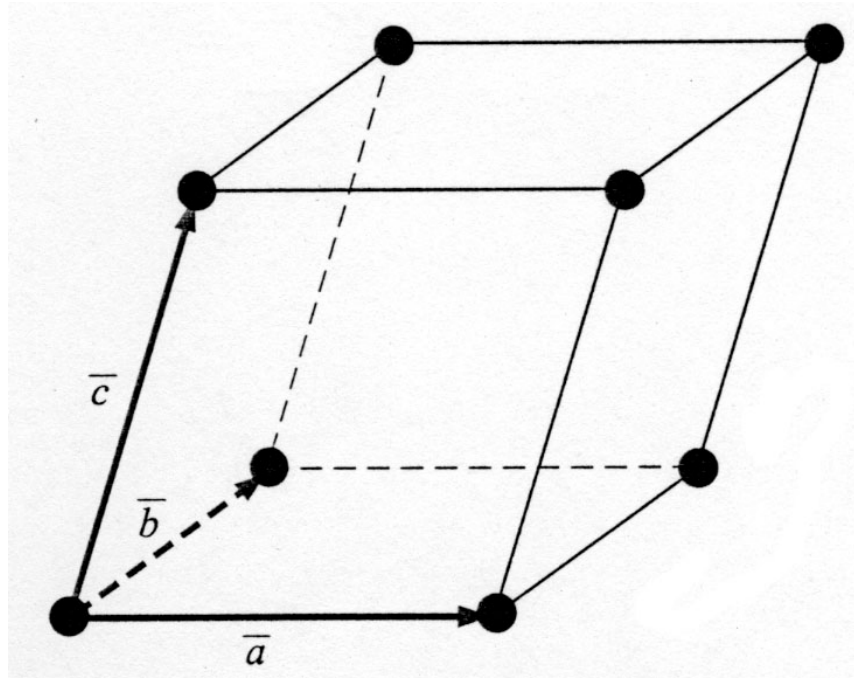
The lattice is characterized by three vectors **a**, **b**, and **c**, which need not be perpendicular and which may or may not be equal in length. Every equivalent lattice point in the three-dimensional crystal can be found using the vector

$$\mathbf{r} = p\mathbf{a} + q\mathbf{b} + s\mathbf{c}$$

where p, q, and s are integers.
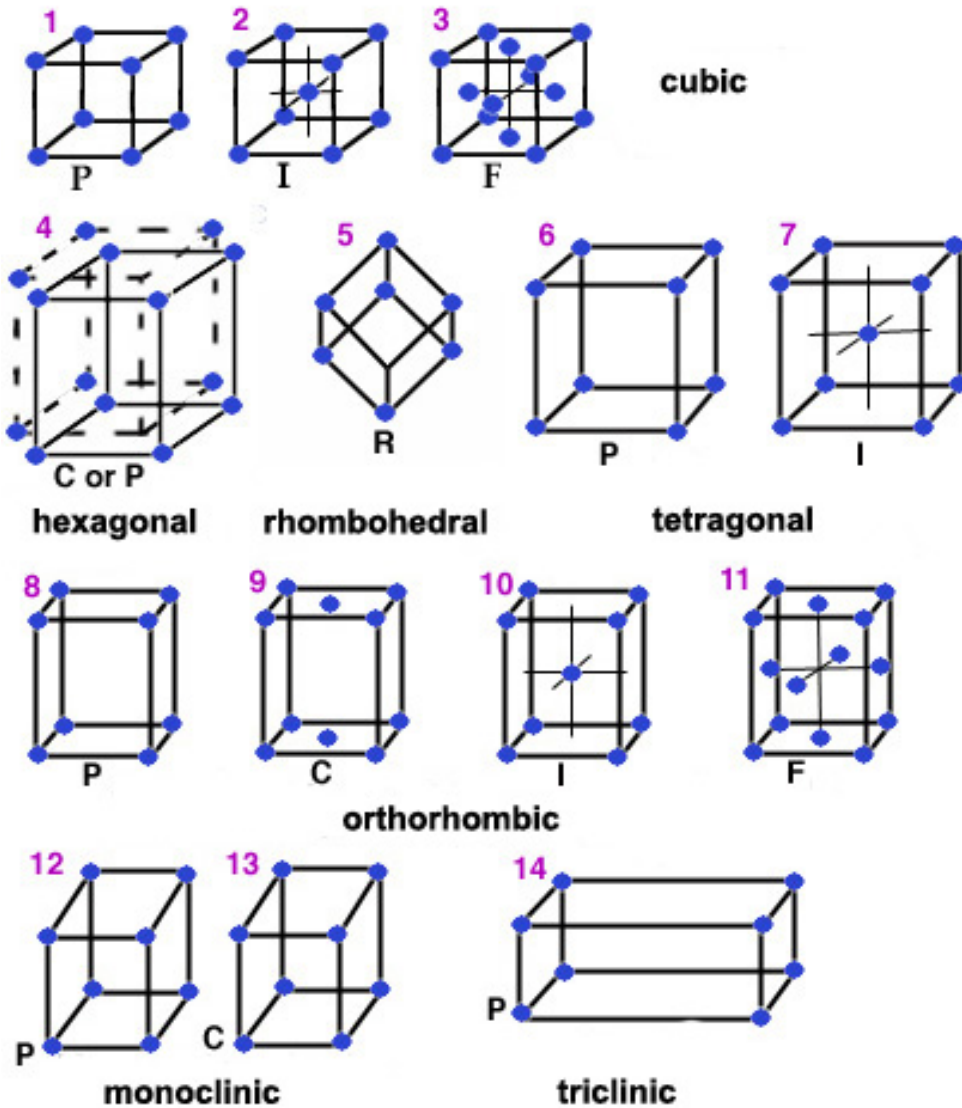
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$ (1st setting) $\alpha = \gamma = 90° \neq \beta$ (2nd setting)
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°; \gamma = 120°$
Trigonal (Rhombohedral)	same as hexagonal $(a = b = c; \alpha = \beta = \gamma)$

7 crystal classes, 14 Bravais lattices.
P: primitive; I: body-centered; F: face-centered; C: side-centered

Examples of Some Basic Crystal Structures
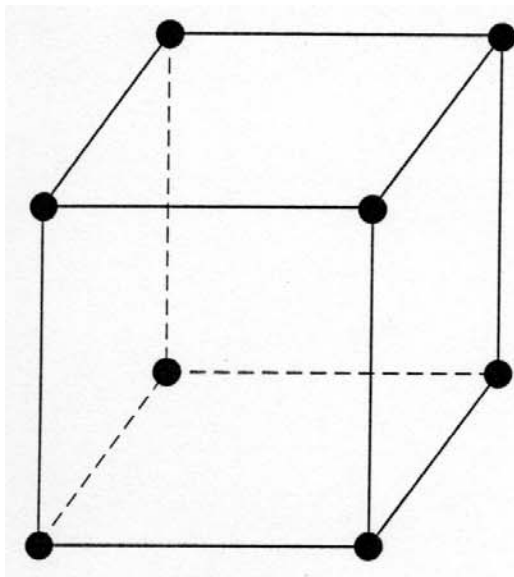
simple cubic (sc)   **body-centered cubic (bcc)**   **face-centered cubic (fcc)**
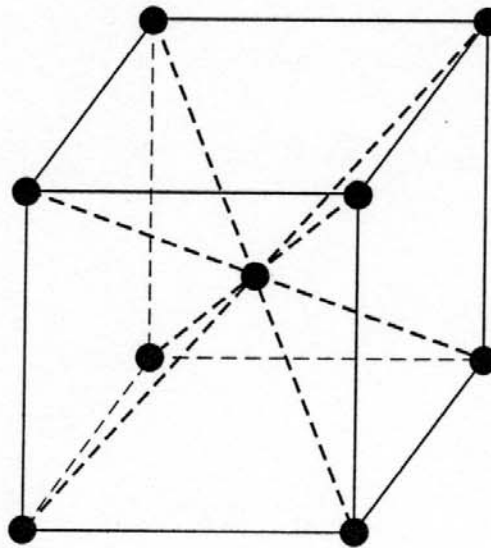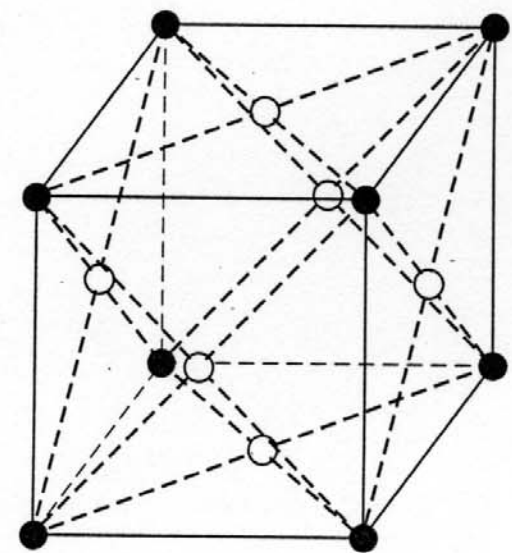
For these structures, we can choose three vectors a, b, and c that are perpendicular to each other and equal in length.

The sc structure has an atom located at each corner. The bcc structure has an additional atom at the center of the cube. The fcc structure has additional atoms on each face plane.

Crystal Planes and Miller Indices

Real crystals are not infinitely large. They have surfaces. Crystal surfaces are often related to different lattice planes. Lattice planes are characterized with **Miller indices (hkl)**, which are a set of integers with no common factors, inversely proportional to the intercepts of the crystal plane along the crystal axes:

$$h : k : l = \frac{1}{p} : \frac{1}{q} : \frac{1}{s}$$
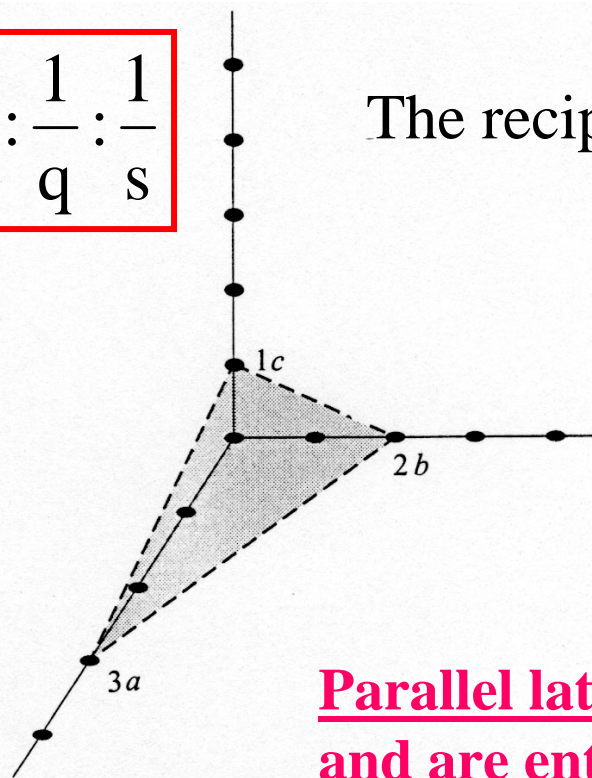
$$p = 3, \ q = 2, \ s = 1$$

The reciprocals of the intercepts are $\left(\dfrac{1}{3}, \dfrac{1}{2}, \dfrac{1}{1} \right)$

Multiply the smallest common denominator, which is 6 in this case, to obtain (hkl) = (2,3,6)

Parallel lattice planes have same Miller indices and are entirely equivalent to each other.

Common Lattice Planes in Cubic Crystals

(100)   (110)   (111)
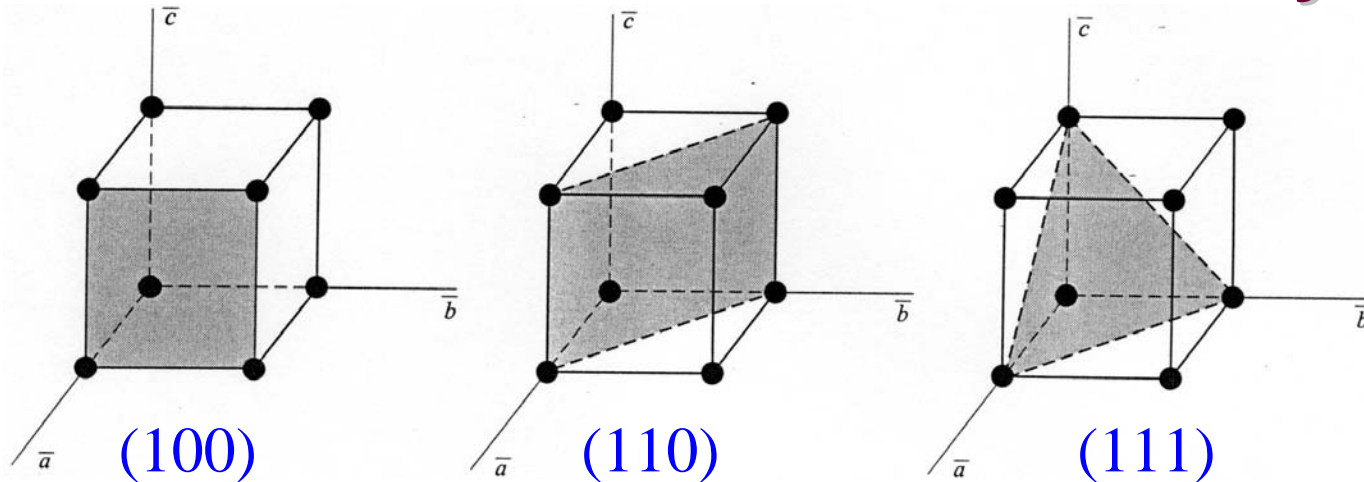
- When planes are parallel to certain axes, the corresponding intercepts will be ∞ and thus the reciprocals will be zeros.

- If a plane passes through the origin, we would obtain infinity as one or more of the Miller indices. However, we can avoid the use of infinity by translating the origin to another equivalent lattice point since the location of the origin is entirely arbitrary.

- Each face plane of the sc structure is entirely equivalent. These planes are grouped together and referred to as the {100} set of planes.

- The distance between parallel lattice planes and the concentrations of atoms in specific planes are important parameters.

Surface Density of Atoms on a Particular Plane

Example: consider the bcc structure. Assume the atoms can be represented as hard spheres with the closest atoms toughing each other and the lattice constant is 0.5 nm. Calculate the surface density of atoms on the (110) plane.
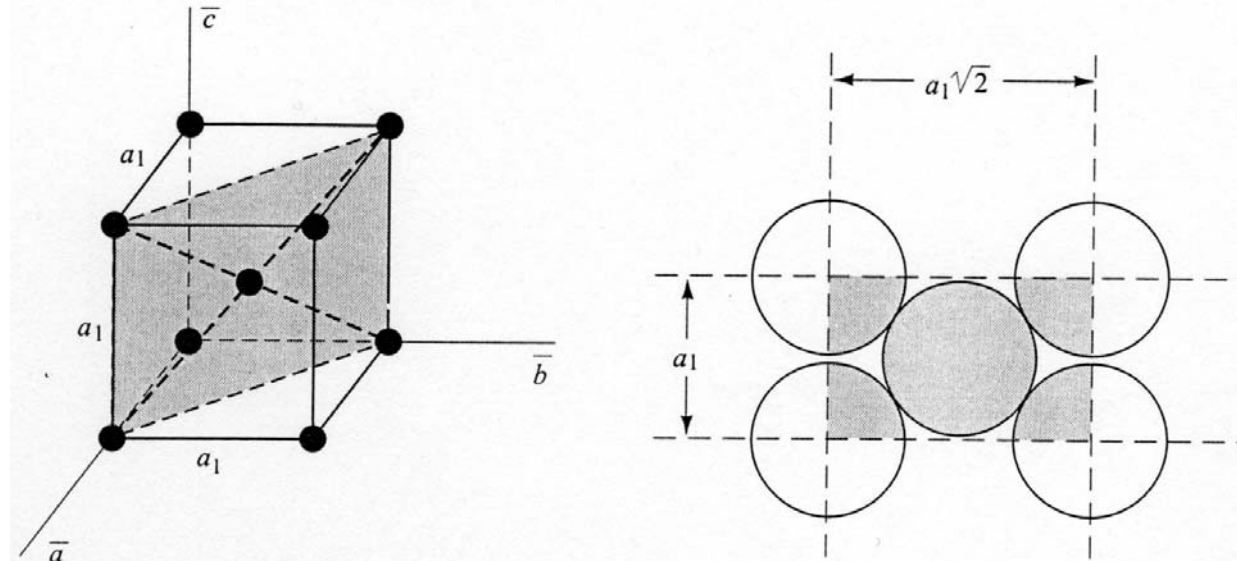
Consider the atoms on the (110) plane. The atom at each corner is shared by four similar rectangles. So one fourth of each atom at the corner contributes to the shaded rectangle. <u>The four corner atoms effectively contribute one atom to the shaded rectangle.</u> The atom at the center is not shared by any other rectangle. It is entirely included in the shaded rectangle. Therefore, the shaded rectangle contains two atoms.

Surface Density of Atoms on a Particular Plane

Solution: the surface density is found by dividing the number of lattice atoms by the surface area.

$$\text{Surface density} = \frac{2}{(a_1)(a_1\sqrt{2})} = \frac{2}{(5\times10^{-8})^2(\sqrt{2})} = 5.66\times10^{14} \text{ atoms per cm}^2$$

The surface density of atoms is a function of the particular crystal plane and generally varies from one crystal plane to another.

Description of directions in a lattice:

In addition to lattice planes, we also want to describe a particular direction in the crystal. The direction can be expressed as a set of three integers that are the components of a vector in that direction. For example, the body diagonal in the sc lattice has vector components of 1,1,1. The body diagonal is then described as the **[111]** direction. <u>The brackets are used to designate direction as distinct from the parentheses used for crystal planes.</u>

The Diamond Structure

Silicon is the most common semiconductor material. Both silicon and germanium have a diamond crystal structure. (Of course diamonds also have such a crystal structure!)
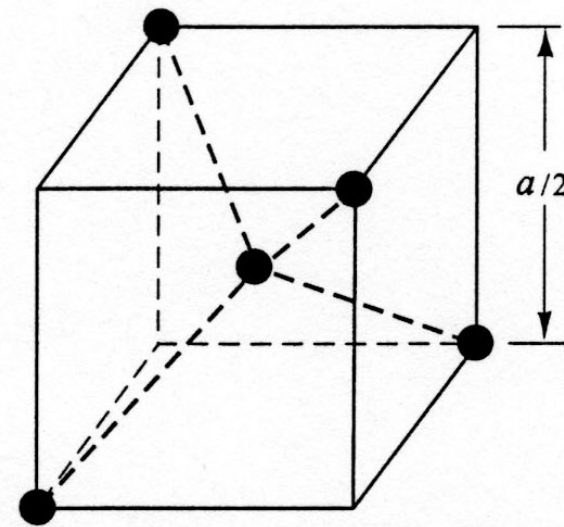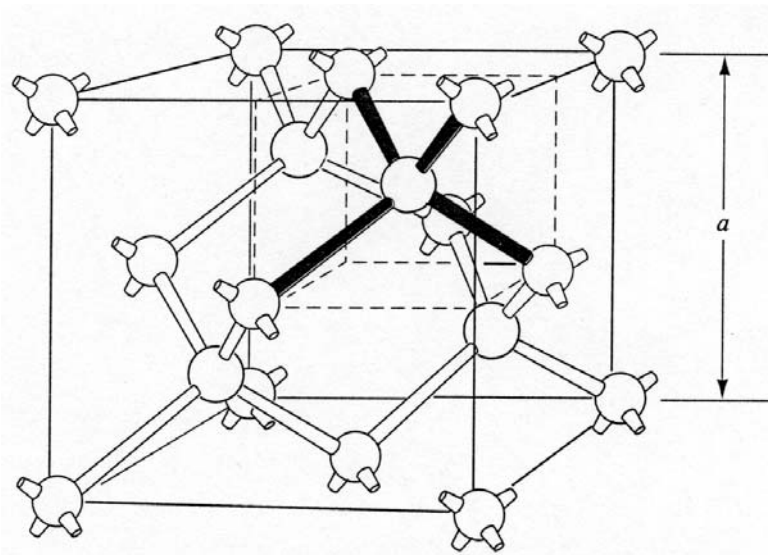
There are totally eight Si atoms in the unit cell. The basic building block of the diamond structure is the tetrahedral structure.

The Diamond Structure
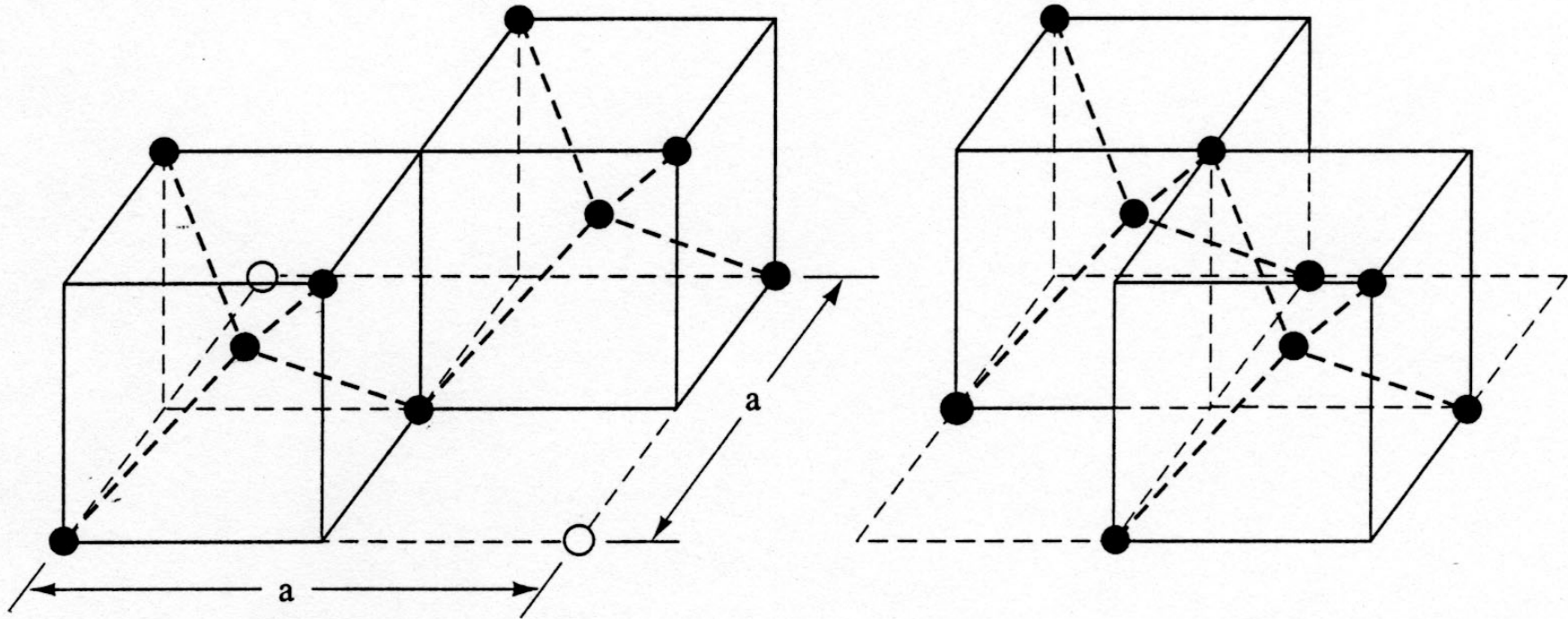
An important characteristic of the diamond structure is that <u>any atom in the structure has four nearest-neighbor atoms</u>.

All atoms in the diamond structure are of the same species, such as silicon or germanium.

The Zincblende (Sphalerite) Structure
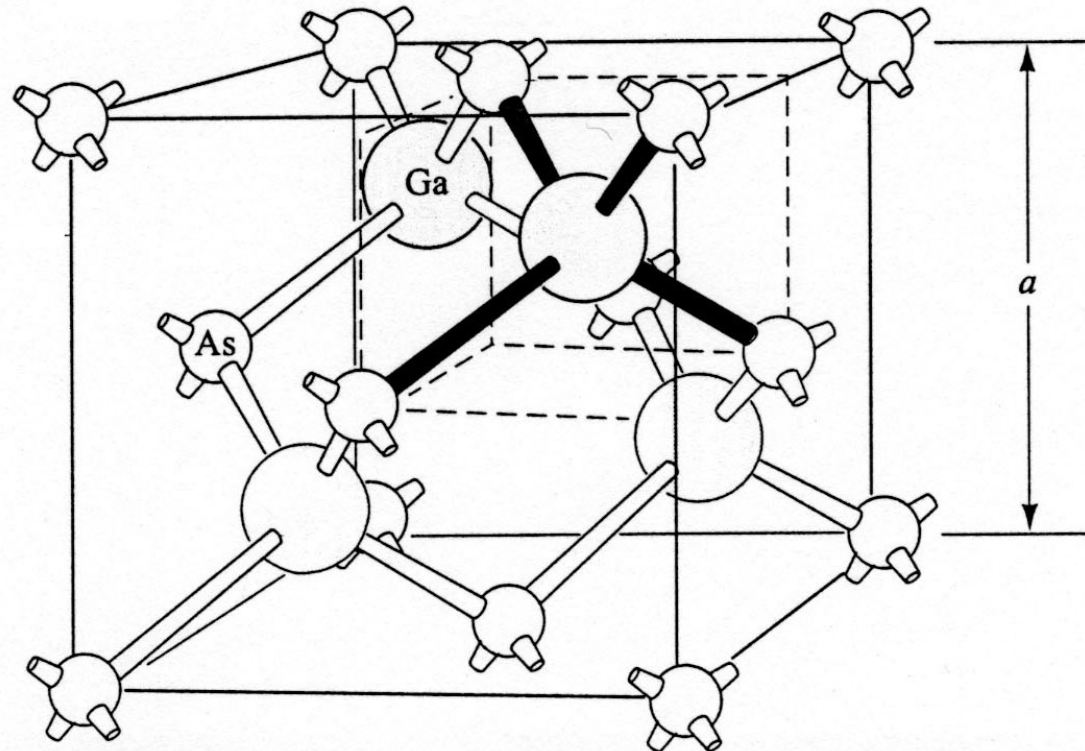
The zincblende (sphalerite) structure differs from the diamond structure only in that there are two different types of atoms in the structure.

Compound semiconductors, such as GaAs, have the zincblende structure.

The important feature of both the diamond and zincblende structure is that each atom has four nearest-neighbor atoms.

Atomic Bonding

The formation of one particular crystal structure depends on the interaction, or the type of bond, between atoms in the crystal.

The interaction between atoms can be described by quantum mechanics.

The interaction of atoms tends to form closed valence shells. The elements (e.g., Na, K) in group I tend to lose their one electron and become positively charged. The elements (e.g., Cl, Br) in group VII tend to gain one electron and become negatively charged. These oppositely charged ions experience a Coulomb attraction to form a bond referred to as an **ionic bond**. Some examples of ionic bonding are NaCl and KBr.

Another atomic bond that tends to achieve closed valence shells is **covalent bonding**. For example, in the hydrogen molecule, a hydrogen atom has one electron and needs one more electron to complete the valence shell. Covalent bonding results in electrons being shared between atoms so that in effect the valence shell of each atom is full.

H•   **•H**

H:H

Atomic Bonding

Si has four valence electrons. Each Si atom needs four more electrons to complete the valence shell. Therefore, each Si atom forms four covalent bonds with four neighboring Si atoms, which results in the formation of diamond structure.

The third major type of atomic bonding is referred to as **metallic bonding**. Group I elements have one valence electron. They tend to lose one electron to become positively charged. For example, when a large number of Na atoms are brought into close proximity, qualitatively, we may think of positive sodium ions being surrounded by a sea of negative electrons, the solid being held together by the electrostatic forces.

The fourth type of atomic bond is called the **van der Waals bond**, which is the weakest of atomic bonds. It results from weak dipole interactions between molecules. Solids formed by this type of bond have low melting temperatures.
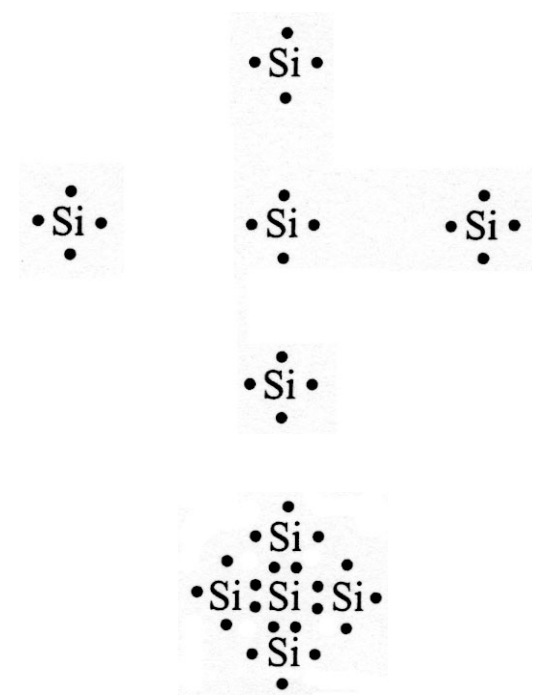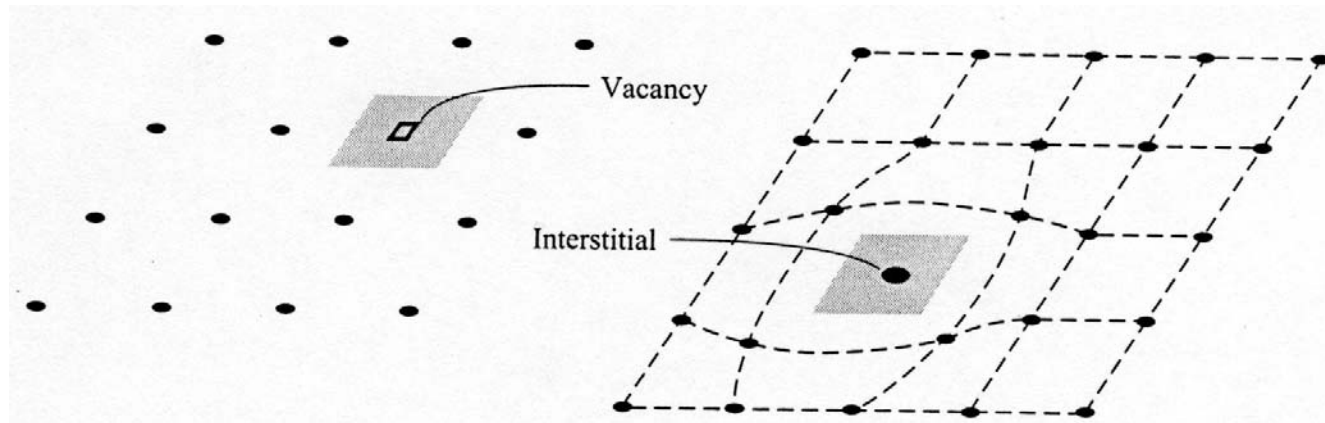
Imperfections in Solids

In real crystals, lattices are not perfect. They contain imperfections and impurities, which can alter the electrical properties of solid materials.

One type of imperfections that all crystals have in common is called **lattice vibration**, which is induced by the thermal energy. The thermal motion causes the distance between atoms to randomly fluctuate, slightly disrupting the perfect geometric arrangement of atoms.

Another type of defects is called **point defect**, including **vacancy** and **interstitial**. Vacancy and interstitial not only break the perfect geometric arrangement, but also disrupt the ideal chemical bonding between atoms.

Imperfections in Solids
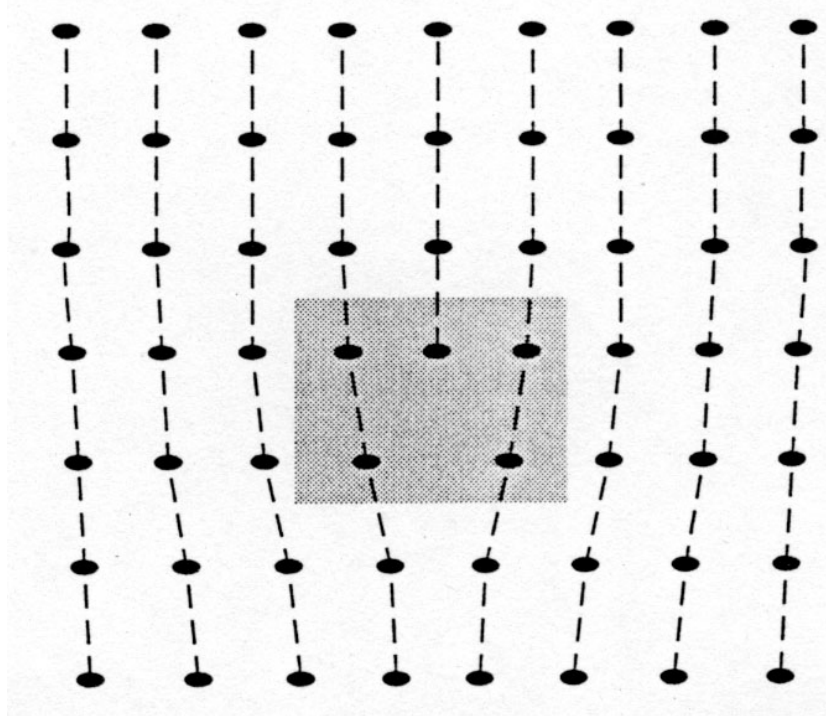
A two-dimensional representation of a line dislocation

A line defect occurs when an entire row of atoms is missing from its normal site. This defect is referred to as a line dislocation. As with a point defect, a line dislocation disrupts both the normal geometric periodicity of the lattice and the ideal atomic bonds in the crystal.

Impurities in Solids
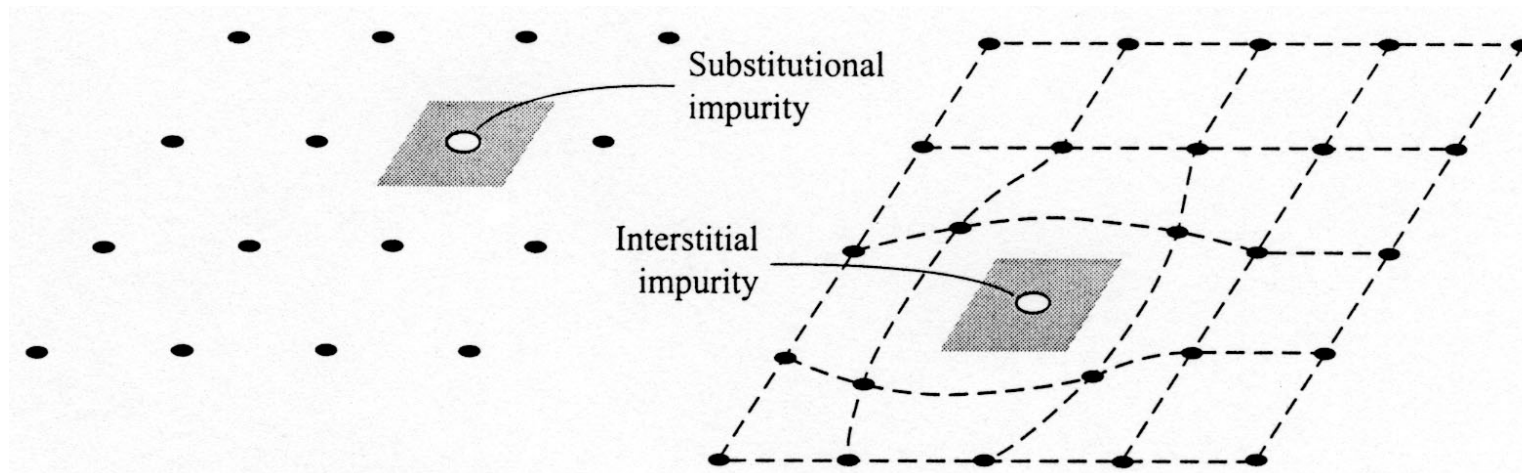
Impurity atoms may be present in a crystal. Impurity atoms may be located at normal lattice sites, in which case they are called **substitutional impurities**. Impurity atoms may also be located between normal lattice sites, in which case they are called **interstitional impurities**.

Controlled amounts of particular impurity atoms can favorably alter the electrical properties of semiconductors. The technique of introducing impurity atoms into a semiconductor in order to alter its conductivity is called **doping**. Two general methods of doping are **impurity diffusion** and ion **implantation**.

Doping Si by Diffusion and Ion Implantation
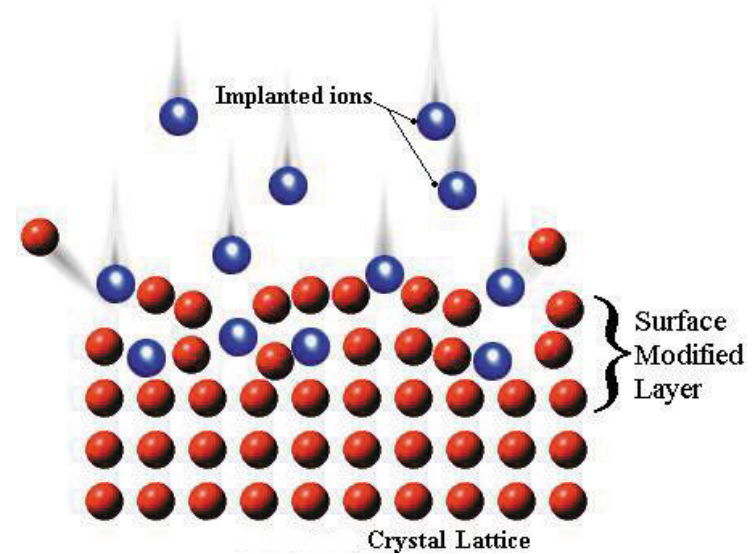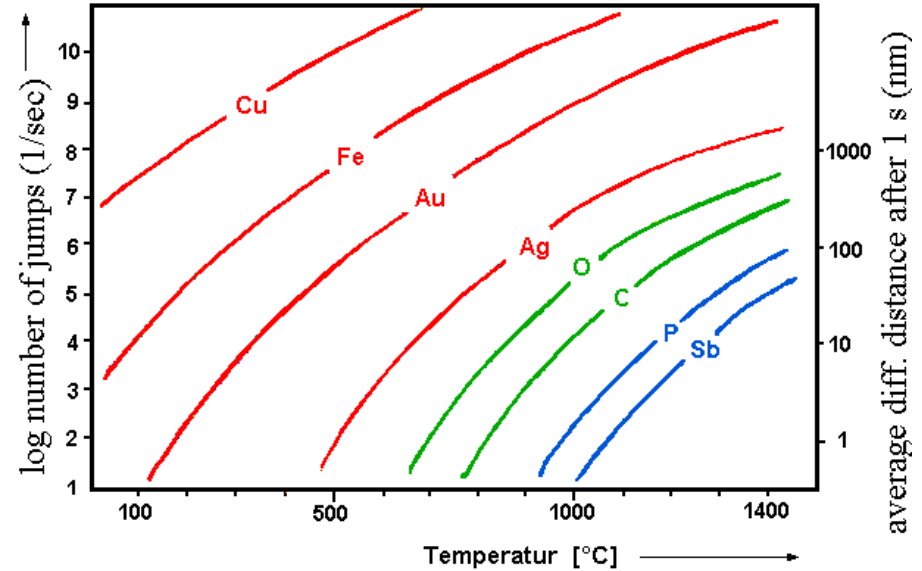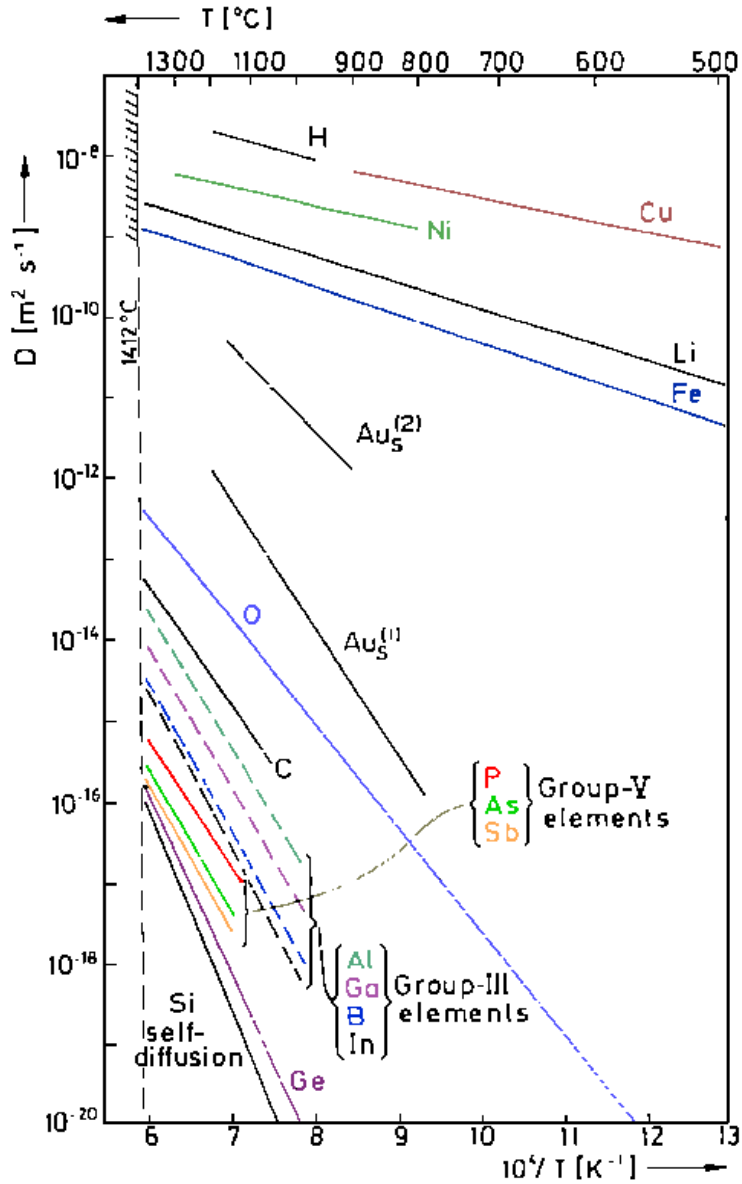
Growth of Semiconductors

The success in fabricating very large scale integrated (VLSI) circuits is a result, to a large extent, of the development of and improvement in the formation or growth of pure single-crystal semiconductor materials. Si, for example, has concentrations of most impurities less than 1 part in 10 billion.
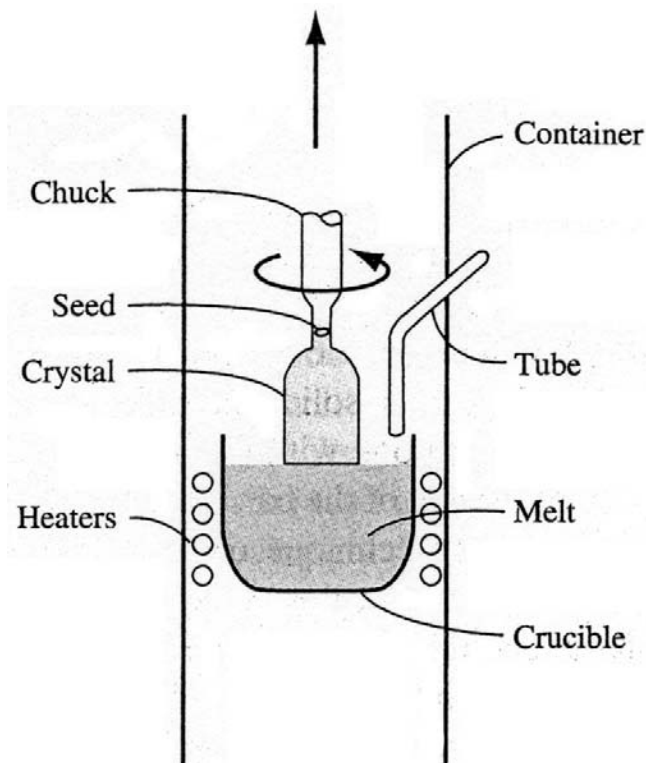
Czochralski crystal puller
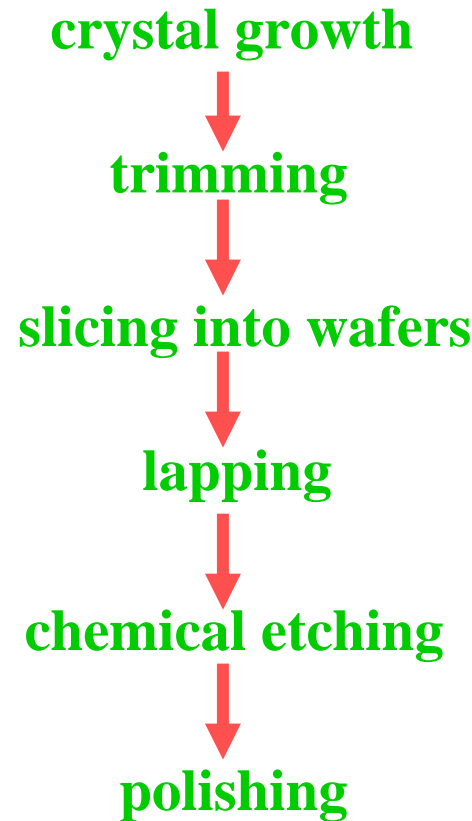
crystal growth

↓

trimming

↓

slicing into wafers

↓

lapping

↓

chemical etching

↓

polishing

Reading Materials

D. A. Neamen, "Semiconductor Physics and Devices: Basic Principles", Irwin, Boston, MA 02116, 1992, Chapter 1, "the Crystal Structure of Solids".

Chapter 4: Semiconductor Physics

Crystal structures of solids

Energy band structures of solids

Charge carriers in semiconductors

Carrier transport

Formation of Energy Bands

From quantum mechanics, we know that the energy of the bound electron of the hydrogen atom is quantized with associated radial probability density functions.

When two hydrogen atoms are brought in close proximity, their wave functions will overlap , which means the two electrons will interact. This interaction results in the quantized energy level splitting into two discrete energy levels.

The wave function for the lowest electron energy state
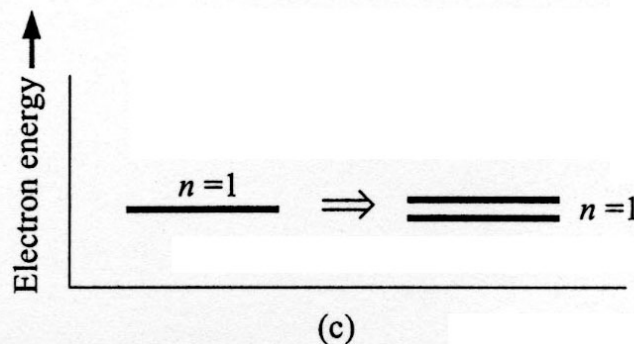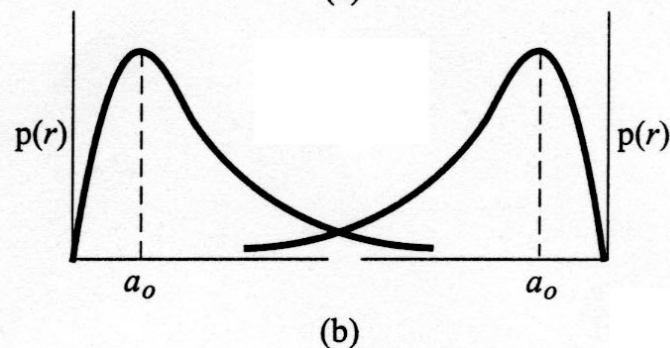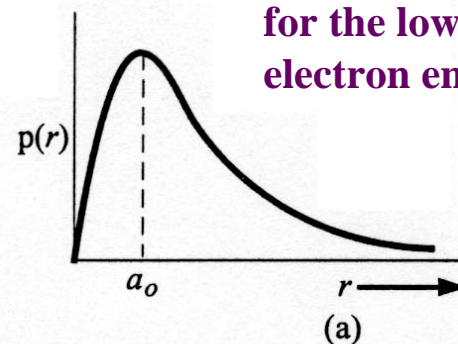
Formation of Energy Bands

Similarly, when a number of hydrogen-type atoms that are arranged in a periodic lattice and initially very far apart are pushed together, the initial energy level will split into a band of discrete energy levels.

According to the **Pauli exclusion principle**, the total number of quantum states will remain the same after the joining of atoms to form a system (crystal).

There will be many energy levels within the allowed band in order to accommodate all of the electrons in a crystal.

As an example, suppose that we have a system of 10^{19} one-electron atoms and the width of the energy band at the equilibrium inter-atomic distance is 1 eV. If the spacing between neighboring levels is the same, the difference in neighboring levels will be 10^{-19} eV, which is extremely small so that we have a quasi-continuous energy distribution through the allowed energy band.
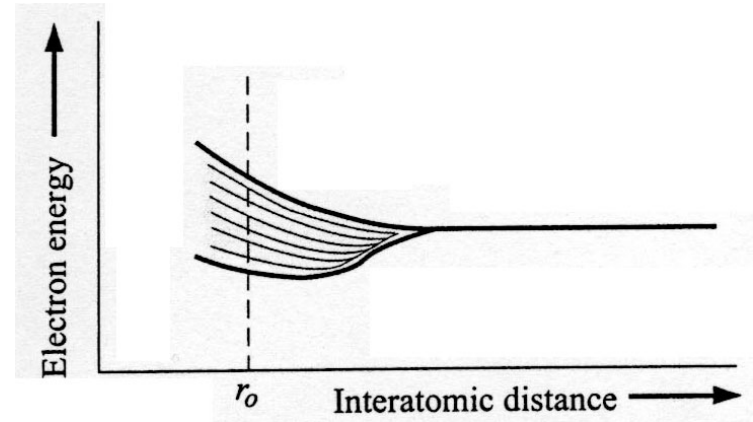
Example: consider an electron traveling at a velocity of 10^7 cm/sec. if the velocity increases by 1 cm/sec, calculate the change in its kinetic energy.

Solution:

$$\Delta E = \frac{1}{2}mv_2^2 - \frac{1}{2}mv_1^2 = \frac{1}{2}m\left(v_2^2 - v_1^2\right)$$

$$v_2 = v_1 + \Delta v$$

$$\Delta v << v_1$$

$$v_2^2 = \left(v_1 + \Delta v\right)^2 = v_1^2 + 2v_1\Delta v + \left(\Delta v\right)^2 \approx v_1^2 + 2v_1\Delta v$$

$$\Delta E \approx \frac{1}{2}m\left(2v_1\Delta v\right) = mv_1\Delta v$$

$$\Delta E = \left(9.11\times10^{-31}\right)\left(10^5\right)\left(0.01\right) = 9.11\times10^{-28}\,\text{J}$$

$$\Delta E = \frac{9.11\times10^{-28}}{1.6\times10^{-19}} = 5.7\times10^{-9}\,\text{eV}$$

Comment: the kinetic energy change is orders of magnitude larger than the energy spacing in the allowed energy band, which suggests that the discrete energies within an allowed energy band can be treated as a quasi-continuous distribution.

Allowed and Forbidden Energy Bands

Consider again a periodic arrangement of atoms. Each atom contains electrons up to $n = 3$ energy level. If these atoms are brought together, the outermost electrons in the $n = 3$ energy shell will begin to interact and split into a band of allowed energies. As the atoms move closer, the electrons in the $n = 2$ shell, and finally the innermost electrons in the $n = 1$ shell, will also form two bands of allowed energies.
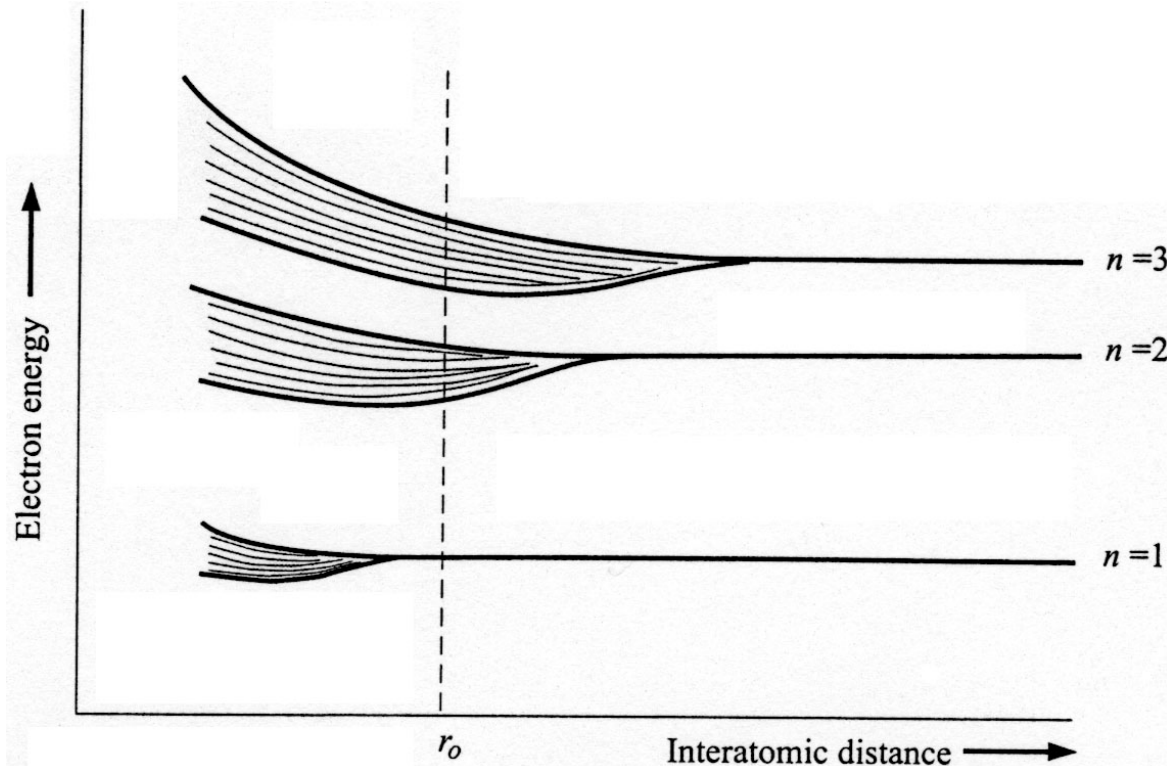
Allowed and Forbidden Energy Bands
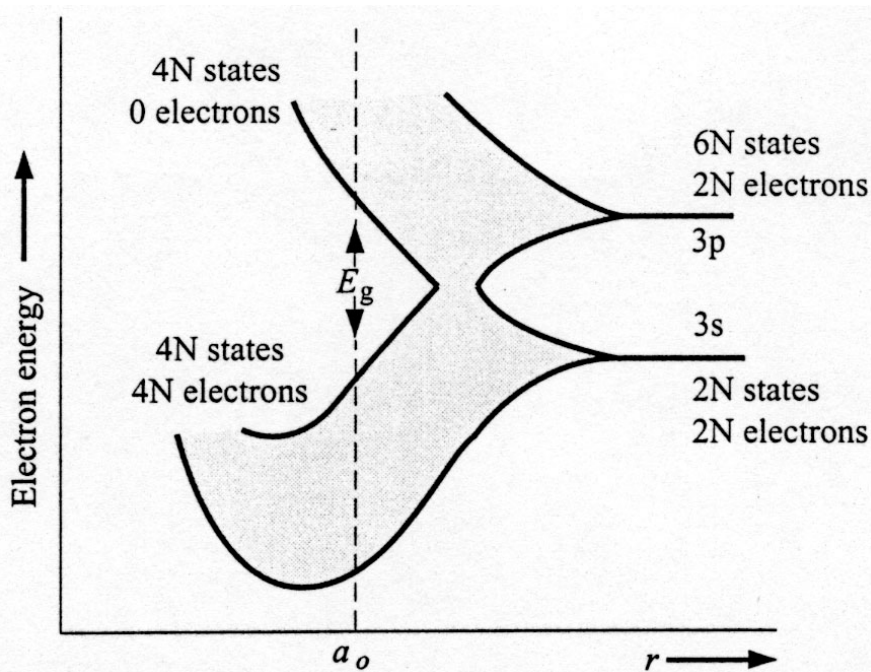
For silicon, we need only consider the $n = 3$ level because the first two energy shells are completely full and are tightly bound to the nucleus.

The 3s state contains two quantum states per atom, and the 3p state contains six quantum states per atom.

At the equilibrium inter-atomic distance, the 3s and 3p bands mix together and split to form two new bands with four quantum states per atom in the lower band and four quantum states per atom in the upper band. At absolute zero degrees, all the states in the lower band (**the valence band**) will be occupied by electrons and are full. All the states in the upper band (**the conduction band**) will be empty. The energy difference between the top of the valence band and the bottom of the conduction band is **the bandgap energy**.

The Kronig-Penney Model

The band structure can be developed more rigorously by considering quantum mechanics.

We will consider a one-dimensional single-crystal lattice.

The potential functions of adjacent atoms overlap to form a one-dimensional periodic potential function.
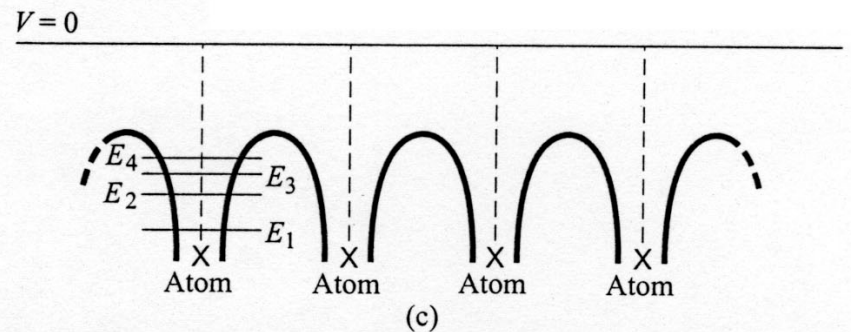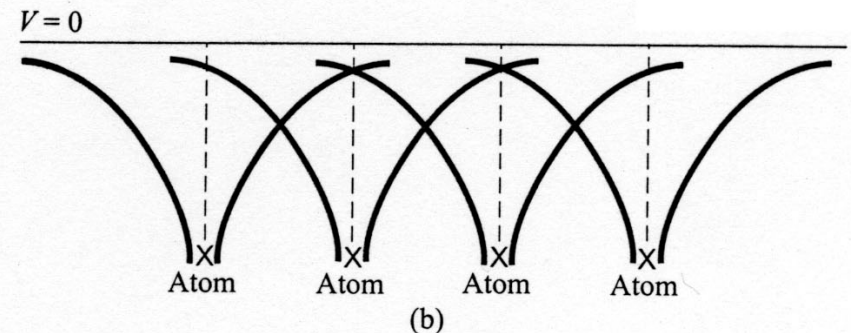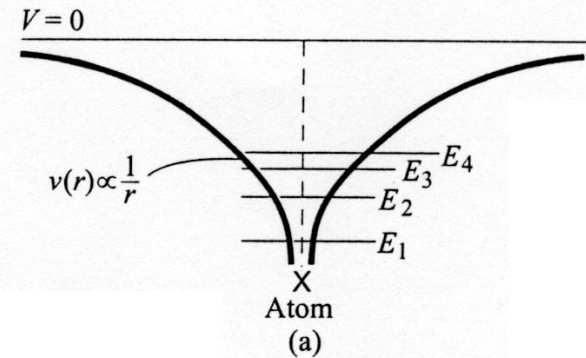
The Kronig-Penney Model

We will consider a simplified potential function, which is called the one-dimensional Kronig-Penney model of the periodic potential function, and solve Schrodinger's wave equation. The Kronig-Penney model is an idealized potential, but the results will reveal many of the important features of the quantum theory of solids.
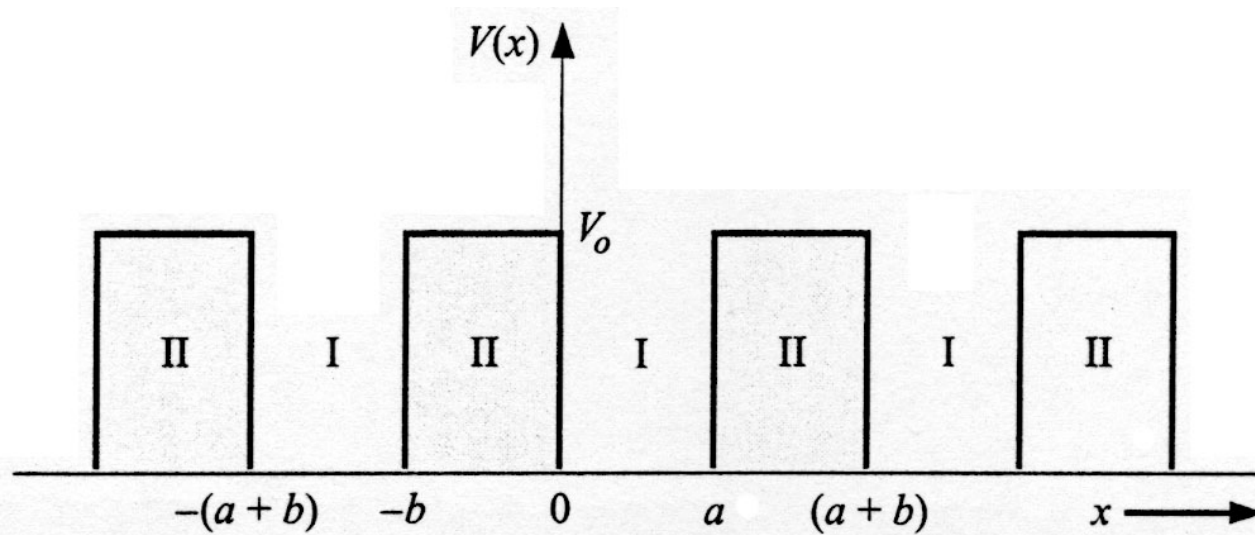
Bloch theorem: all one-electron wave functions for periodically varying potentials is of the form

$$\psi(x) = u(x)e^{jkx}$$

k is called a constant of motion.
$u(x)$ is a periodic function.

The total solution to the wave equation is the product of the time-independent solution and the time-dependent solution.

$$\Psi(x,t) = \psi(x)\phi(t) = u(x)e^{jkx}e^{-j(E/\hbar)t}$$

$$\Psi(x,t) = u(x)e^{j[kx-(E/\hbar)t]}$$

k **is also called a wave number.**

We need to determine the relation between k, E, and V_0.
The time-independent wave equation is

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

Consider the region I ($0 < x < a$) in which $V(x) = 0$. We obtain:

$$\frac{d^2 u_1(x)}{dx^2} + 2jk\frac{du_1(x)}{dx} - \left(k^2 - \alpha^2\right)u_1(x) = 0 \qquad \alpha^2 = \frac{2mE}{\hbar^2}$$

Consider the region II ($-b < x < 0$) in which $V(x) = V_0$. We obtain:

$$\frac{d^2 u_2(x)}{dx^2} + 2jk\frac{du_2(x)}{dx} - \left(k^2 - \alpha^2 + \frac{2mV_0}{\hbar^2}\right)u_2(x) = 0$$

We may define

$$\frac{2m}{\hbar^2}\left(E - V_0\right) = \alpha^2 - \frac{2mV_0}{\hbar^2} = \beta^2$$

The equation for region II becomes

$$\frac{d^2 u_2(x)}{dx^2} + 2jk\frac{du_2(x)}{dx} - \left(k^2 - \beta^2\right)u_2(x) = 0$$

The solution for region I is of the form

$$u_1(x) = Ae^{j(\alpha - k)x} + Be^{-j(\alpha + k)x} \qquad \text{for } 0 < x < a$$

The solution for region II is of the form

$$u_2(x) = Ce^{j(\beta - k)x} + De^{-j(\beta + k)x} \qquad \text{for } -b < x < 0$$

The wave function and its first derivative must be continuous. This means that the wave amplitude function $u(x)$ and its first derivative $\partial u(x)/\partial x$ must be continuous.

If we consider the boundary at $x = 0$, we have $u_1(0) = u_2(0)$

$$A + B = C + D$$

By applying the condition that

$$\left.\frac{du_1}{dx}\right|_{x=0} = \left.\frac{du_2}{dx}\right|_{x=0}$$

We obtain

$$A(\alpha - k) - B(\alpha + k) = C(\beta - k) - D(\beta + k)$$

Because the wave amplitude function $u(x)$ is periodic, we have

$$u_1(a) = u_2(-b)$$

$$\left.\frac{du_1}{dx}\right|_{x=a} = \left.\frac{du_2}{dx}\right|_{x=-b}$$

Then

$$Ae^{j(\alpha-k)a} + Be^{-j(\alpha+k)a} = Ce^{-j(\beta-k)b} + De^{j(\beta+k)b}$$

$$A(\alpha - k)e^{j(\alpha-k)a} - B(\alpha + k)e^{-j(\alpha+k)a} = C(\beta - k)e^{-j(\beta-k)b} - D(\beta + k)e^{j(\beta+k)b}$$

Now we have four homogeneous equations:

$$A + B - C - D = 0$$

$$(\alpha - k)A - (\alpha + k)B - (\beta - k)C + (\beta + k)D = 0$$

$$Ae^{j(\alpha-k)a} + Be^{-j(\alpha+k)a} - Ce^{-j(\beta-k)b} - De^{j(\beta+k)b} = 0$$

$$(\alpha - k)Ae^{j(\alpha-k)a} - (\alpha + k)Be^{-j(\alpha+k)a} - (\beta - k)Ce^{-j(\beta-k)b} + (\beta + k)De^{j(\beta+k)b} = 0$$

We have four homogeneous equations for four unknowns. There is a nontrivial solution if, and only if, the determinant of the coefficients is zero. The result is

$$\frac{-(\alpha^2 + \beta^2)}{2\alpha\beta}(\sin \alpha a)(\sin \beta b) + (\cos \alpha a)(\cos \beta b) = \cos k(a + b)$$

The most interesting solutions occur for $E < V_0$, which applies to the electron bound within the crystal. The parameter β is thus imaginary. We can define

$$\beta = j\gamma$$

Then
$$\frac{\gamma^2 - \alpha^2}{2\alpha\gamma}(\sin \alpha a)(\sinh \gamma b) + (\cos \alpha a)(\cosh \gamma b) = \cos k(a+b)$$

Hyperbolic functions:

$$\sinh \alpha = \frac{1}{2}\left(e^\alpha - e^{-\alpha}\right)$$
$$\cosh \alpha = \frac{1}{2}\left(e^\alpha + e^{-\alpha}\right)$$

$$\sinh \alpha = -j \sin j\alpha$$
$$\cosh \alpha = \cos j\alpha$$

The above equation cannot be solved analytically. We have to use numerical or graphical methods to obtain **the relation between k, E, and V_0**. The solution will result in a band of allowed energies.

In order to illustrate the nature of the results, we make further simplification to let $b \to 0$ and the barrier height $V_0 \to \infty$, but with the product bV_0 remaining finite. We then have

$$\left(\frac{mV_0 ba}{\hbar^2} \right) \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

$$\cosh(0) = 1$$

$$\sinh(x \to 0) = x$$

$$\frac{\gamma^2 - \alpha^2}{2\alpha} b = \frac{(\gamma^2 - \alpha^2) ba}{2} \frac{1}{\alpha a} = \frac{\left[\frac{2m}{\hbar^2}(V_0 - E) - \frac{2m}{\hbar^2} E \right] ba}{2} \frac{1}{\alpha a}$$

$$= \frac{\left[\frac{2m}{\hbar^2}(V_0 - 2E) \right] ba}{2} \frac{1}{\alpha a} \approx \frac{mV_0 ba}{\hbar^2} \frac{1}{\alpha a}$$

The *k*-Space Diagram

We define a parameter as

$$P' = \frac{mV_0 ba}{\hbar^2}$$

We then have

$$P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

We need remember that the above equation is not a solution to the wave equation. It only gives the conditions for which Schrodinger's wave equation will have a solution.

We first consider the special case for which $V_0 = 0$. In this case, $P' = 0$, which corresponds to a free particle since there are no potential barriers. We then have

$$\cos \alpha a = \cos ka$$

$$\alpha = k$$

$$\boxed{\text{\textbf{\textit{k} is related to the particle momentum for the free electron.}}}$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2m\left(\frac{1}{2}mv^2\right)}{\hbar^2}} = \frac{p}{\hbar} = k$$

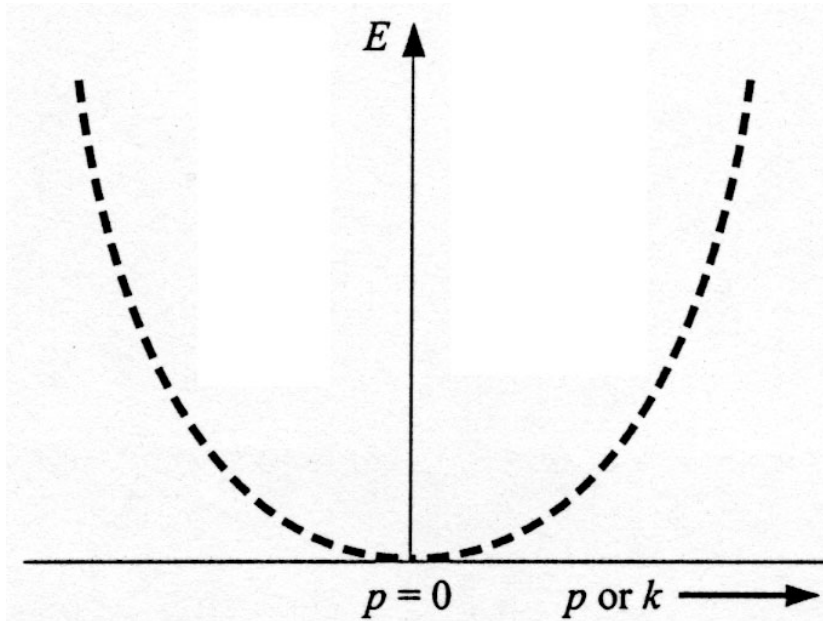$$E = \frac{p^2}{2m} = \frac{k^2\hbar^2}{2m}$$

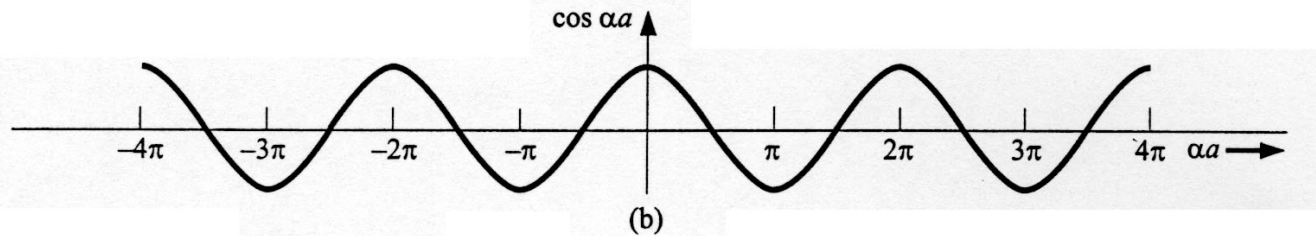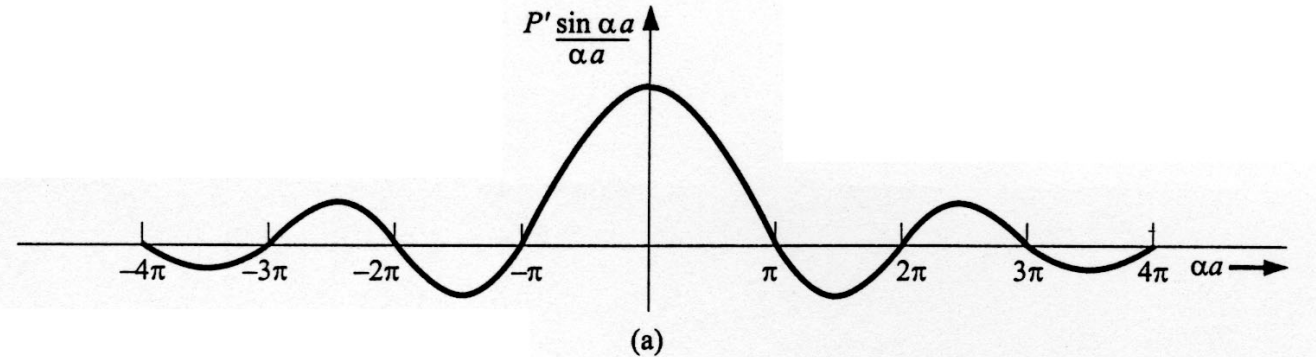# The k-Space Diagram

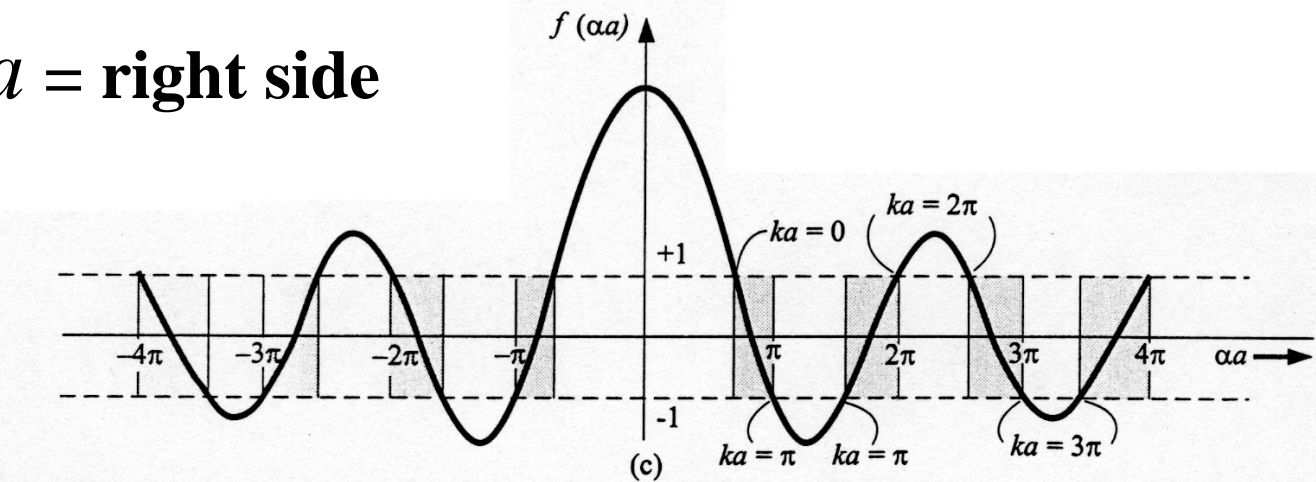**The case of the free electron**

E **is a parabolic function of** *k*.

We now consider the case for which $V_0 > 0$. We use the graphical method to solve the equation on the previous slide.

$$\text{left side} = f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$$
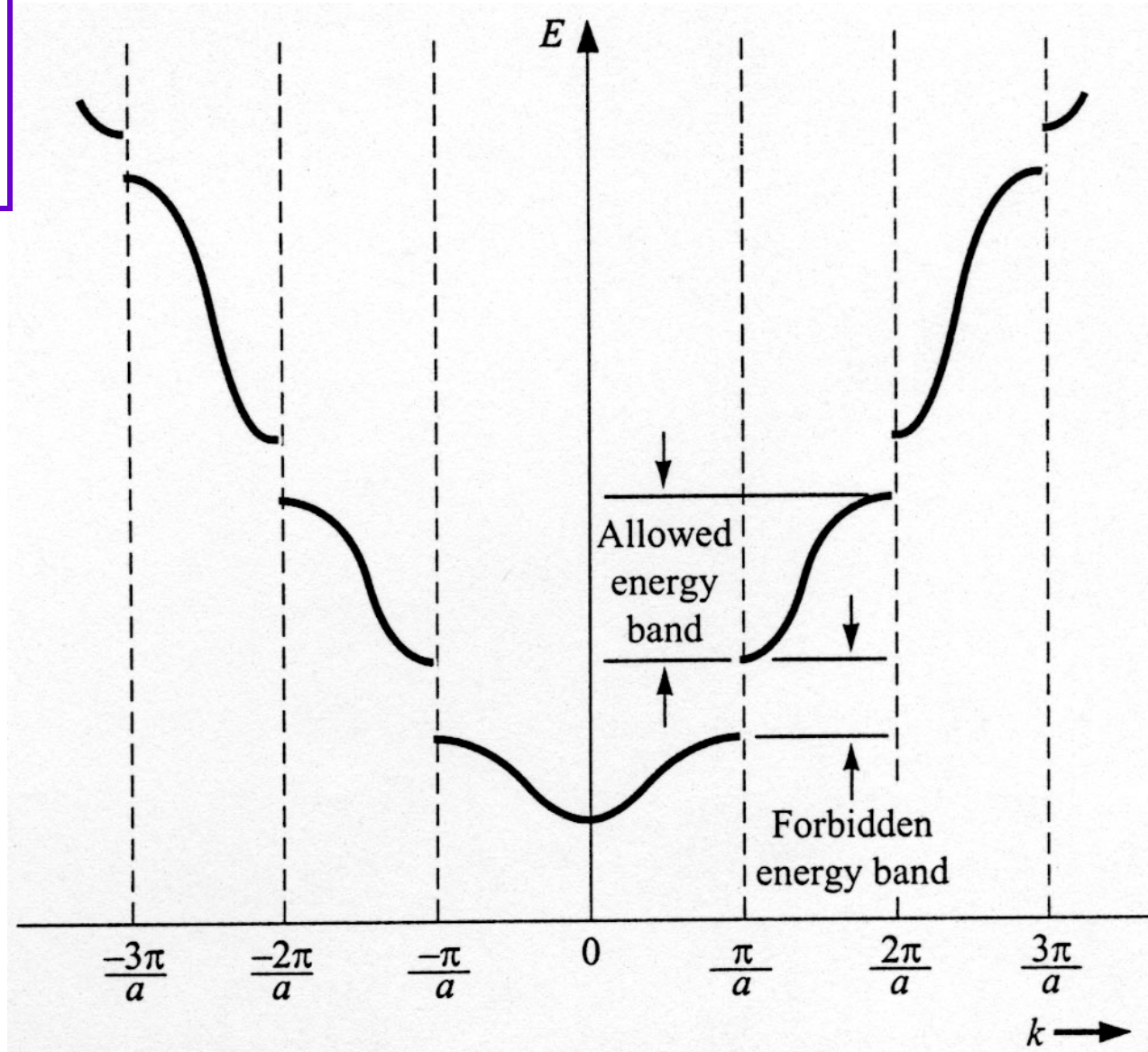
The k-Space Diagram

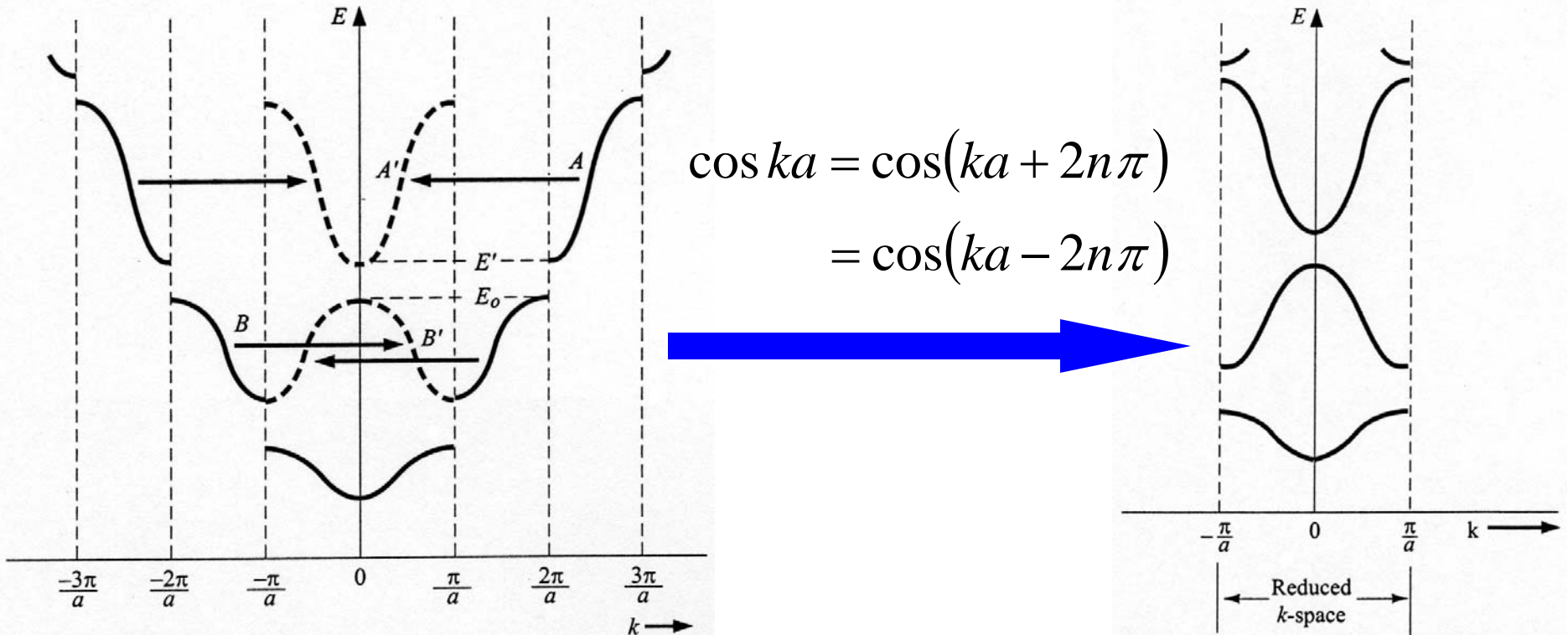$$f(\alpha a) = \cos ka = \text{right side}$$

The k-Space Diagram

$$\alpha^2 = \frac{2mE}{\hbar^2}$$

The k-Space Diagram

Displace portions of the curve by multiples of 2π so that the entire E versus k is contained within $-\pi/a < k < \pi/a$.

$$\cos ka = \cos(ka + 2n\pi)$$
$$= \cos(ka - 2n\pi)$$

$\hbar k$ in a single crystal is referred to as the **crystal momentum**.

The basic features of one-dimensional single-crystal lattice can be extended to three-dimensional single-crystal materials.

The Energy Band and the Bond Model

The performance of many semiconductor devices is related to the current-voltage (*I-V*) characteristics. We will need to consider electrical conduction in solids, which is related to the band theory.
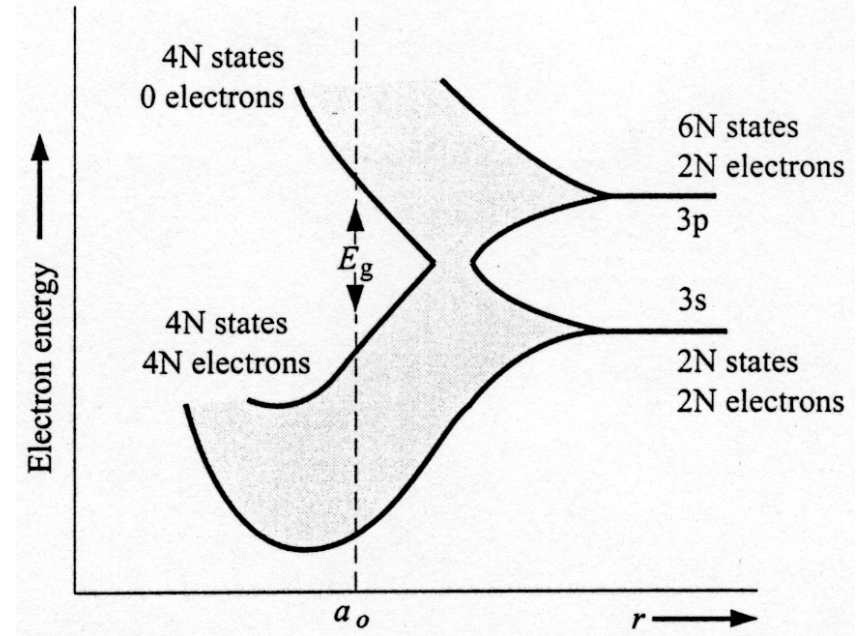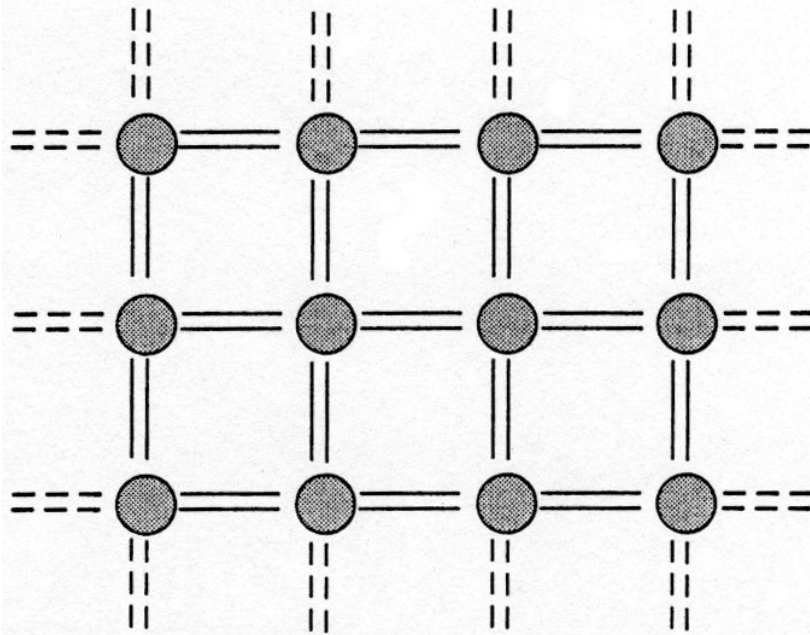
Consider Si. At $T = 0$ K, each silicon atom is surrounded by eight valence electrons that are in their lowest energy state. In terms of the band theory, the 4N states in the valence band are completely occupied by electrons, and the conduction band is completely empty.
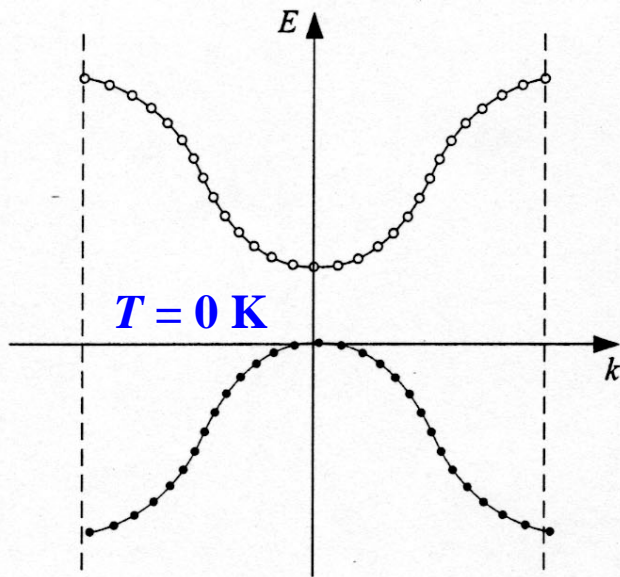
The Energy Band and the Bond Model
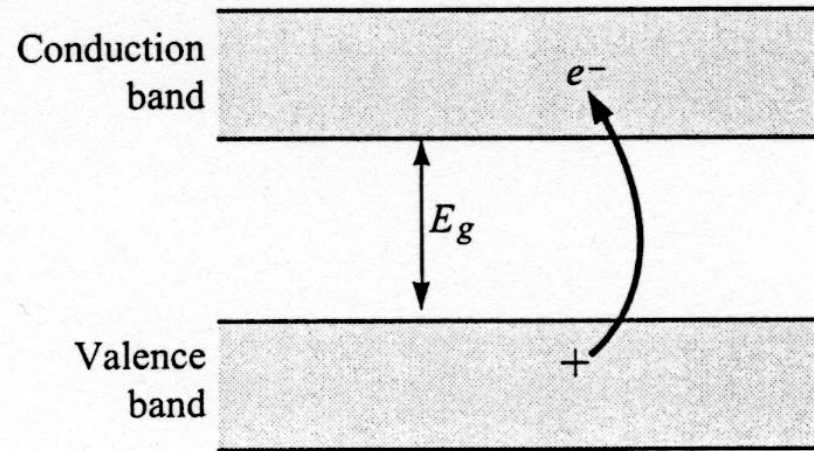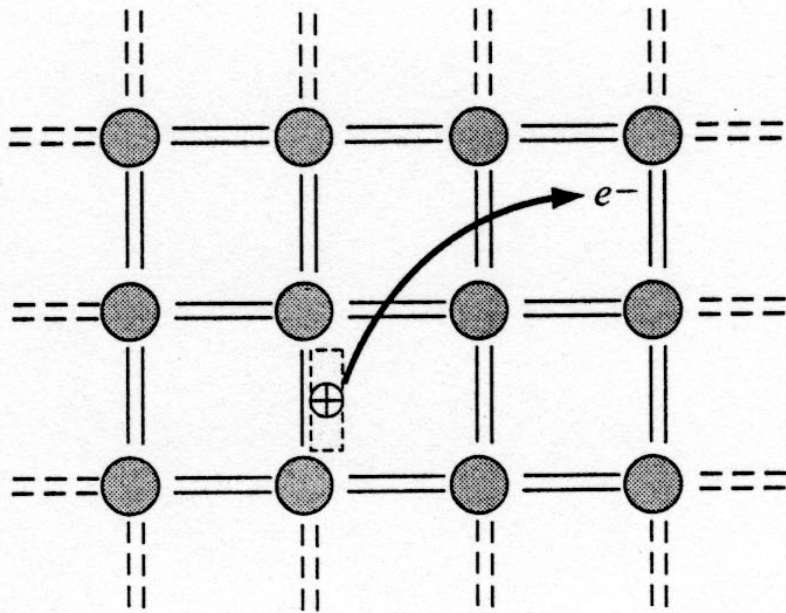
At $T > 0$ K, a few electrons may gain enough thermal energy to break the covalent bond and jump into the conduction band.
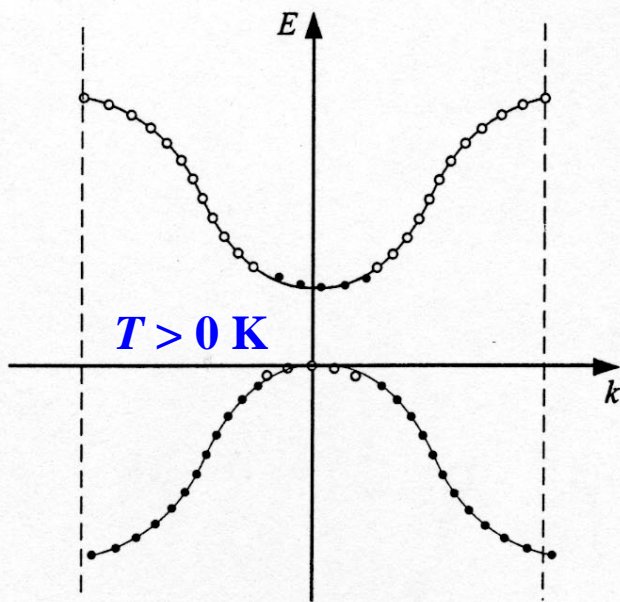
As a negatively charged electron breaks away from its covalent bonding position, a positively charged "empty state" is created in the original covalent bonding position in the valence band. As T further increases, more electrons jump into the conduction band and more positive "empty states" are created in the valence band.

The Energy Band and the Bond Model

This bond breaking can also be related to the E versus k energy bands.

At $T = 0$ K, the valence band is completely full and the conduction band is completely empty. At $T > 0$ K, some electrons have gained enough energy to jump to the conduction band and have left empty states in the valence band.

We assume at this point that there is no external forces. The electron and "empty state" distributions are symmetrical with k.
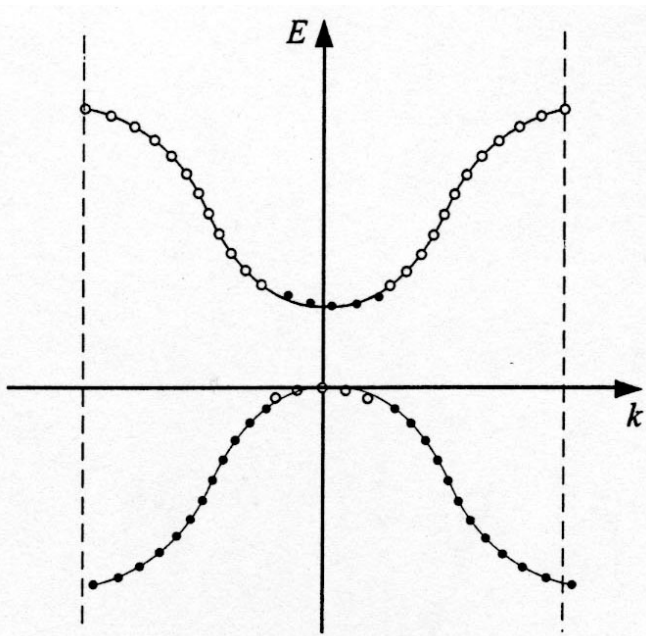
Drift Current

If we have a collection of positively charged ions (q) with a volume density N (cm^{-3}) and an average drift velocity v_d (cm/sec), then the drift current density is

$$J = qNv_d \left(\text{A/cm}^2\right)$$

If we consider the individual ion velocities with v_i being the velocity of the ith ion and take the summation over a unit volume, then we have

$$J = q \sum_{i=1}^{N} v_i$$

Electrons are negatively charged. A net drift of electrons **in the conduction band** will give a current. However, the electron distribution in the conduction band is an even function of k. Recall that $p = \hbar k$ for a free electron is related to the momentum. The number of the electrons with $+|k|$ value is equal to that with $-|k|$ value. The net drift current density due to these electrons is zero.

Drift Current

If an external force is applied, electrons will gain energy and momentum and the distribution **in the conduction band** will become asymmetric.

$$dE = Fdx = Fvdt$$
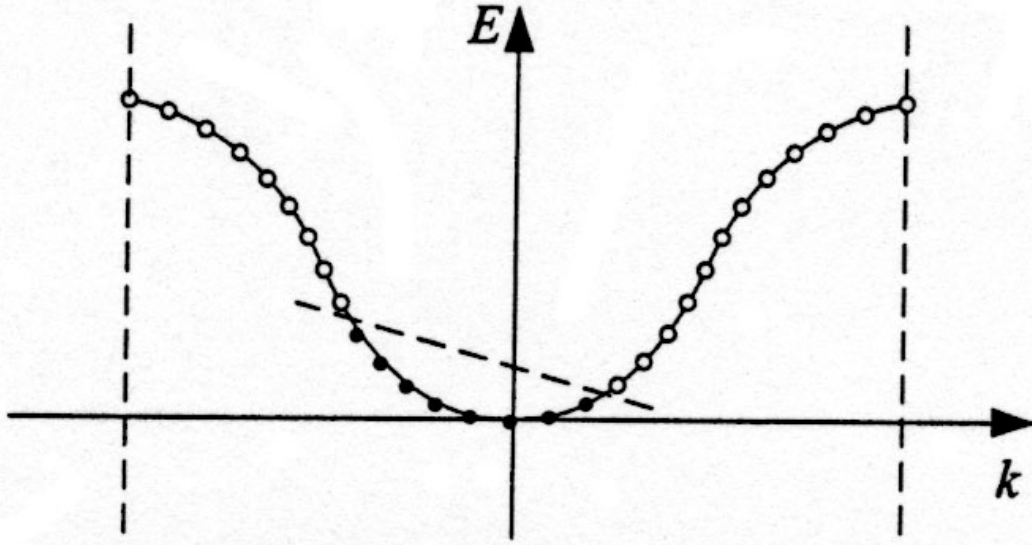
We can write the drift current density due to the motion of electrons as

$$J = -e \sum_{i=1}^{n} v_i$$

where n is the number of electrons per unit volume. The summation is taken over a unit volume so that the current density is A/cm^2.

Electron Effective Mass

The movement of an electron in a crystal lattice will, in general, be different from that of an electron in free space. In addition to an externally applied force, there are internal forces in the crystal due to positively charged ions and negatively charged electrons.

$$F_{total} = F_{ext} + F_{int} = ma$$

We use an **effective mass** m^* to take into account both the electron mass and the effect of the internal forces.
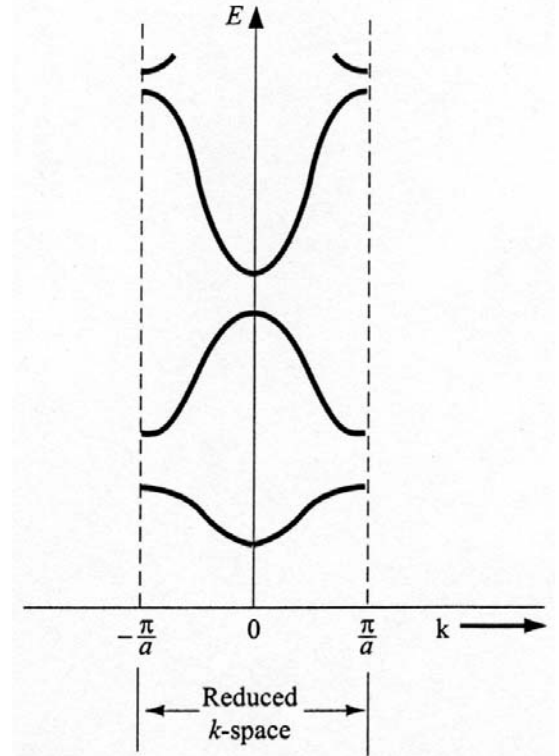
$$F_{ext} = m^* a$$

We can also relate the effective mass of an electron in a crystal to the E versus k curves. Consider the case of a free electron:

$$p = \hbar k$$

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

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} = \frac{\hbar p}{m}$$

$$\frac{1}{\hbar}\frac{dE}{dk} = \frac{p}{m} = v$$

$$\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m}$$

$$\frac{1}{\hbar^2}\frac{d^2 E}{dk^2} = \frac{1}{m}$$

Apply the result from the Kronig-Penney model to the electron in the bottom of an energy band. The energy near the bottom of the energy band may be approximated by a parabola:

$$\left(E - E'\right) = C_1\left(k - k_0\right)^2$$

$$\frac{d^2 E}{dk^2} = 2C_1$$

$$\frac{1}{\hbar^2}\frac{d^2 E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m_n^*}$$

Electron Effective Mass

$$F = ma = -eE$$

$$a = \frac{-eE}{m_n^*}$$

The effective mass is a parameter that relates the quantum mechanical results derived from the Kronig-Penney model to the classical force equations. In most instances, the electrons **in the bottom of the conduction band** can be thought of as a classical particle whose motion can be modeled using Newtonian mechanics, provided that the internal forces and quantum mechanical properties are taken into account through the effective mass m_n^*.

Concept of the Hole
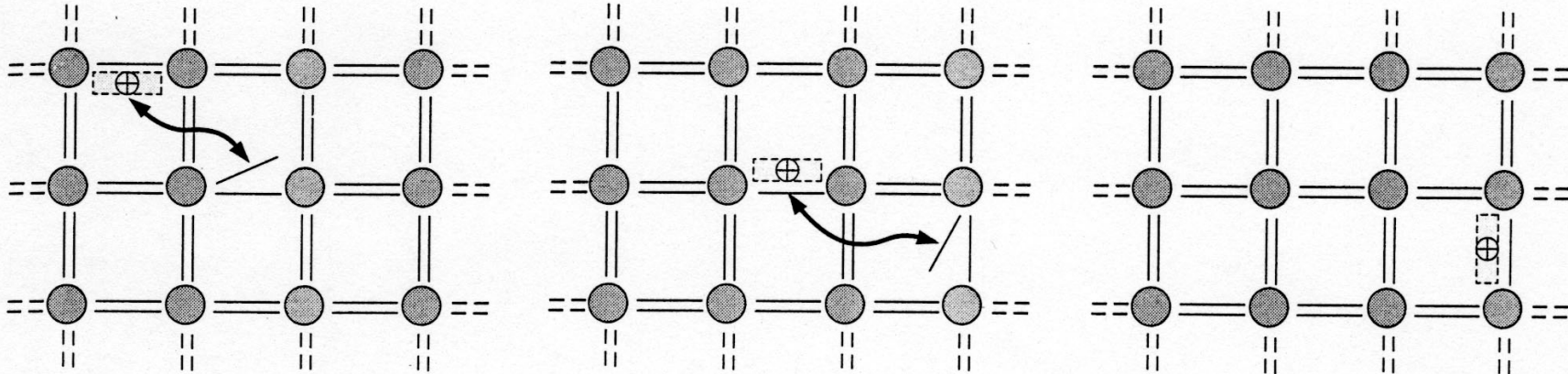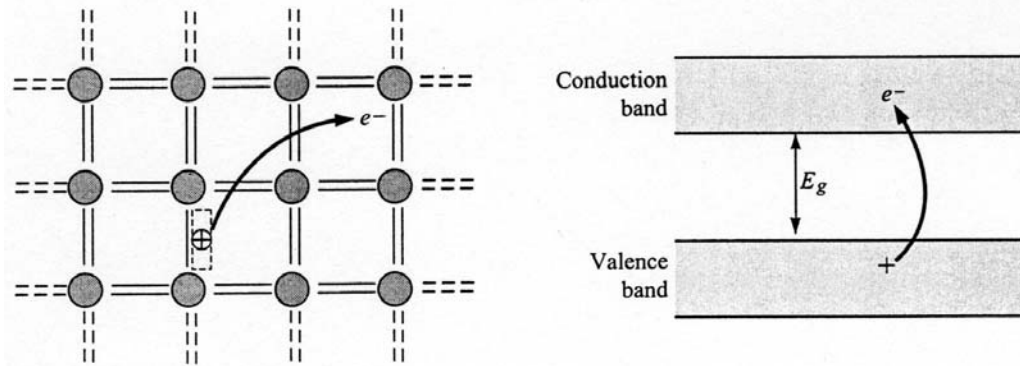
If valence electrons gain a certain amount of energy, they can hop into the "empty state". The movement of a valence electron into the "empty state" is equivalent to the movement of the positively charged "empty state" itself.

This charge carrier is called **a hole** and can also be thought of as a classical particle whose motion can be modeled using Newtonian mechanics.

Concept of the Hole

Consider the electrons **in the valence band** and their drift current density:

$$J = -e \sum_{i(\text{filled})} v_i \qquad\qquad J = -e \sum_{i(\text{total})} v_i + e \sum_{i(\text{empty})} v_i$$

Remember that we have:

$$v(E) = \left(\frac{1}{\hbar} \right)\left(\frac{dE}{dk} \right)$$

The band is symmetric with k. For every electron with a velocity $|v|$, there is a corresponding electron with a velocity $-|v|$. Because the band is full, the distribution of electrons with respect to k cannot be changed by an external force. Then we have

$$-e \sum_{i(\text{total})} v_i = 0$$

$$\boxed{J = +e \sum_{i(\text{empty})} v_i}$$

The v_i in the summation is associated with the empty state.
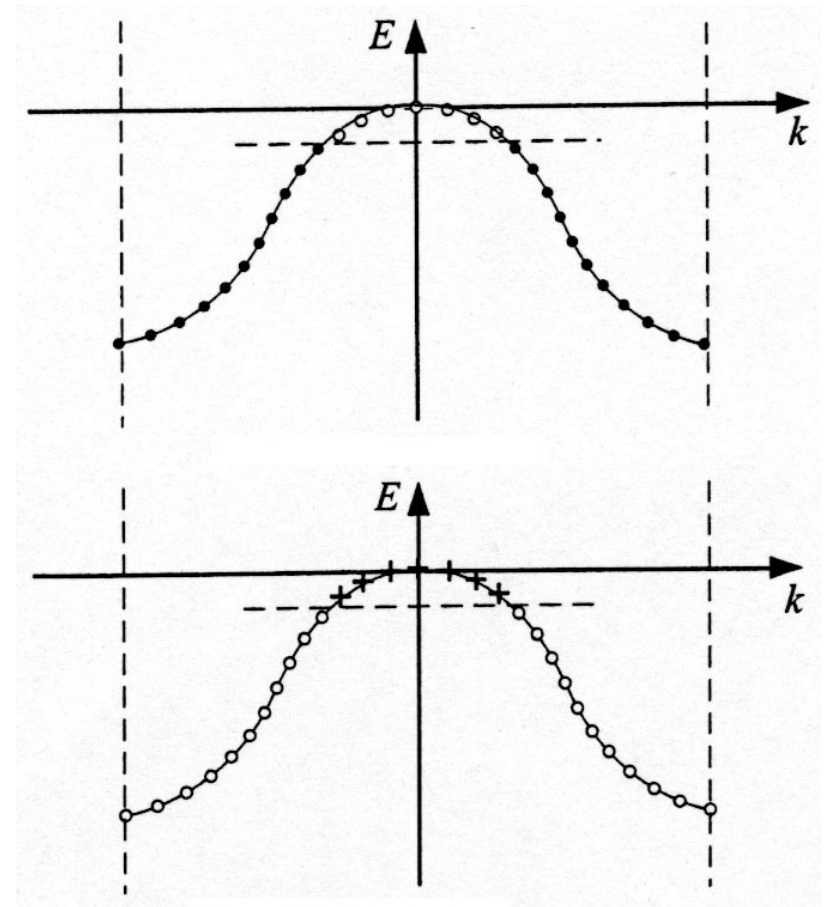
Concept of the Hole

It is equivalent to placing positively charged particles in the empty states and assuming all other states **in the valence band** are empty, or neutrally charged.

Consider **an electron** near the top of a **valence band**:

$$(E - E_0) = -C_2(k - k_0)^2$$

$$\frac{d^2 E}{dk^2} = -2C_2$$

$$\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$$

C_2 is a positive quantity and thus m^* is a negative quantity.

Hole Effective Mass

If we consider **an electron** near the top of **a valence band** and use Newton's force equation for an applied electric field, we will have

$$F = m^* a = -eE$$

$$a = \frac{-eE}{m^*} = \frac{+eE}{-m^*}$$

$$a = \frac{+eE}{m_p^*}$$

The motion of electrons in a nearly full band can be described by considering just the empty states. The band can be modeled as having particles with a positive electronic charge and a positive effective mass. The density of these particles in the valence band is the same as the density of empty electronic energy states. This new particle is called the **hole**. The hole has a positive electronic charge and a positive effective mass denoted by m_p^*. This quantity is used to relate quantum mechanics to classical mechanics.
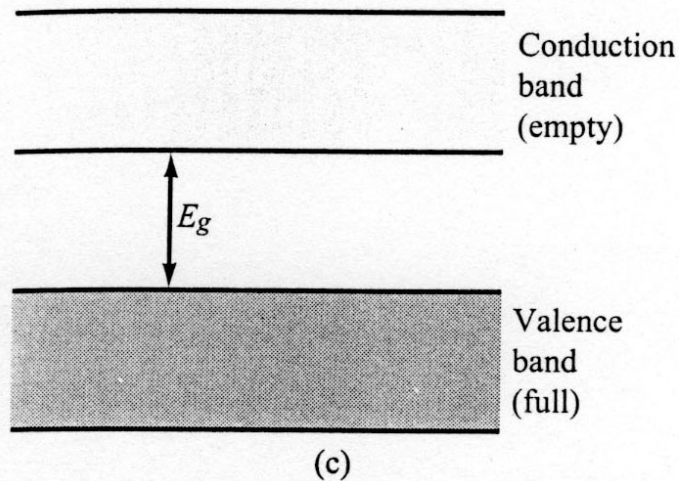
Metals, Insulators, and Semiconductors in terms of Energy Band Structures

Allowed energy band (empty)

(a)
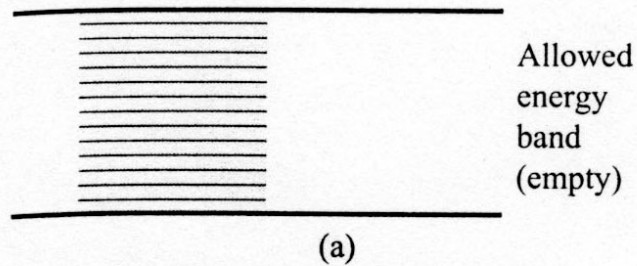
There will be no current for a completely empty band because there are no particles to move.

Allowed energy band (full)

(b)
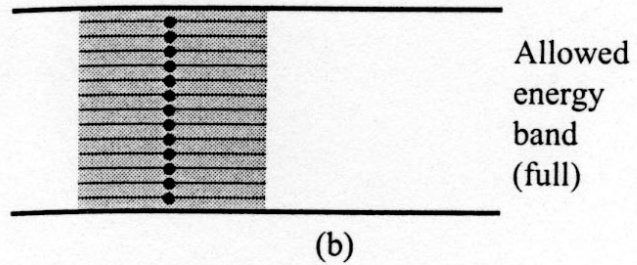
There will also be no current for a completely full band because of the band symmetry with respect to k.

Conduction band (empty)

E_g

Valence band (full)

(c)

Insulators have energy bands either completely filled or completely empty and bandgap energies in the range of 3.5 to 6 eV or larger. For comparison, the kT at room temperature (25 °C) is 25.7 meV.
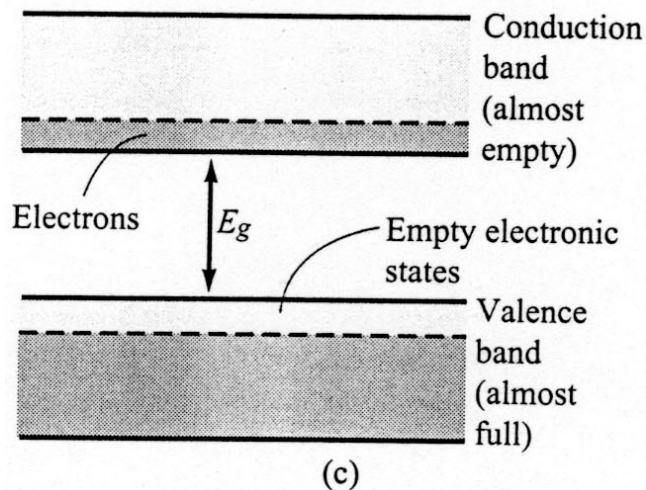
Metals, Insulators, and Semiconductors in terms of Energy Band Structures

Allowed energy band (almost empty)

(a)
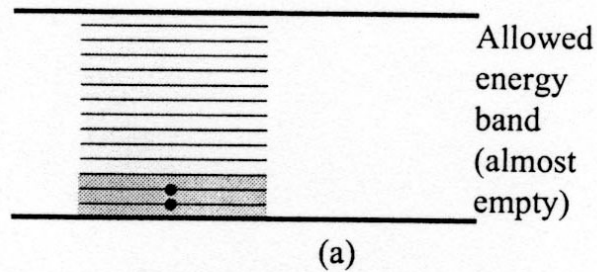
A band with relatively few electrons. If an electric field is applied, the electrons can move to higher energy states to generate a current.

Allowed energy band (almost full)

(b)
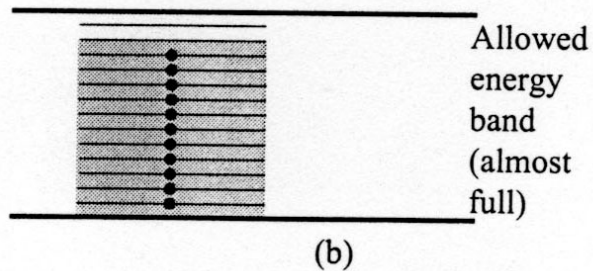
An almost full band. We can consider the holes, which move under an electric field to generate a current.

Conduction band (almost empty)

Electrons E_g

Empty electronic states

Valence band (almost full)

(c)

A representative energy band for a semiconductor at $T > 0$ K. The bandgap energy of a semiconductor is on the order of 1 eV. The conductivity of a semiconductor can be varied over many orders of magnitude.

Metals, Insulators, and Semiconductors in terms of Energy Band Structures

Partially filled band

Full band
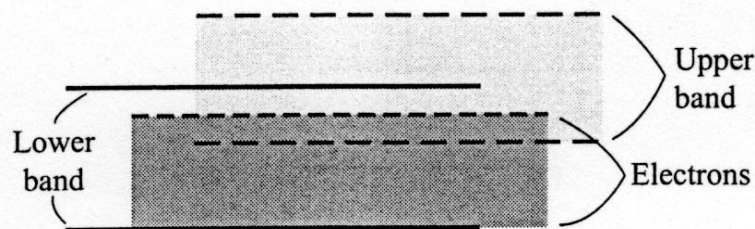
(a)

Upper band

Lower band

Electrons

(b)
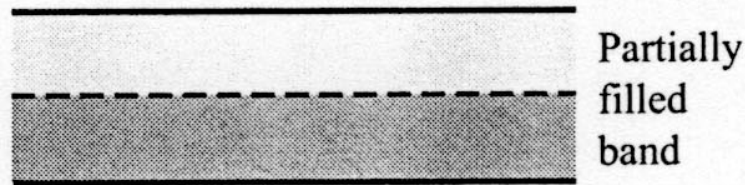
Metals have low resistivity values. The energy band diagram for a metal can be in one of two forms.
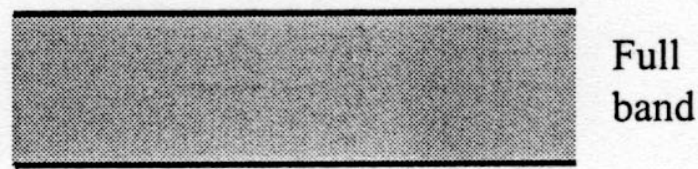
One case is a partially filled band in which there are many electrons available for conduction.
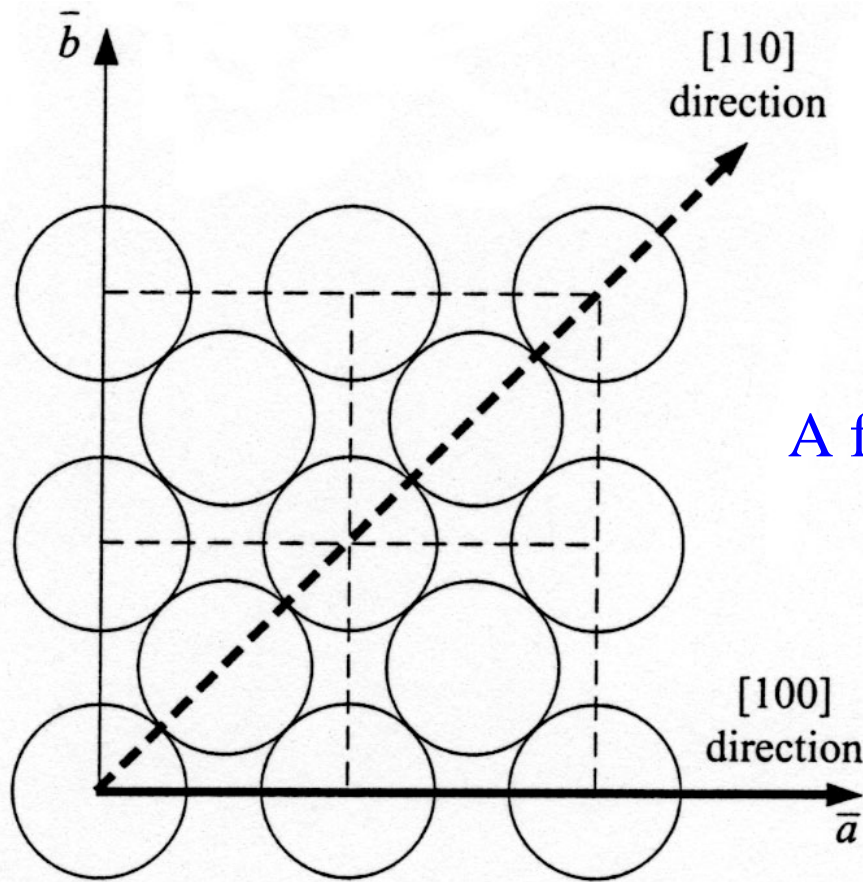
The other case is that the conduction band overlaps with the valence band. There are a large number of electrons as well as a large number of holes for conduction.
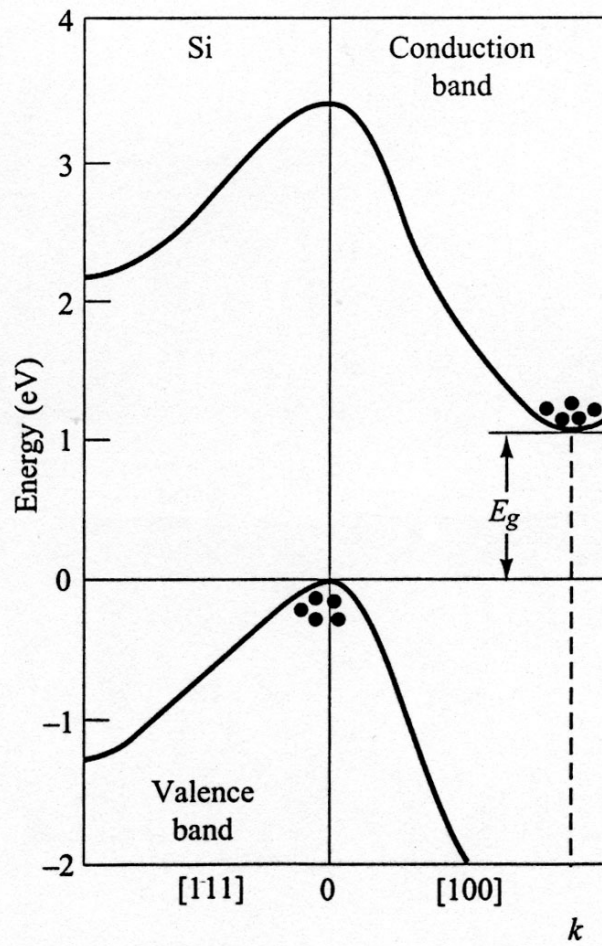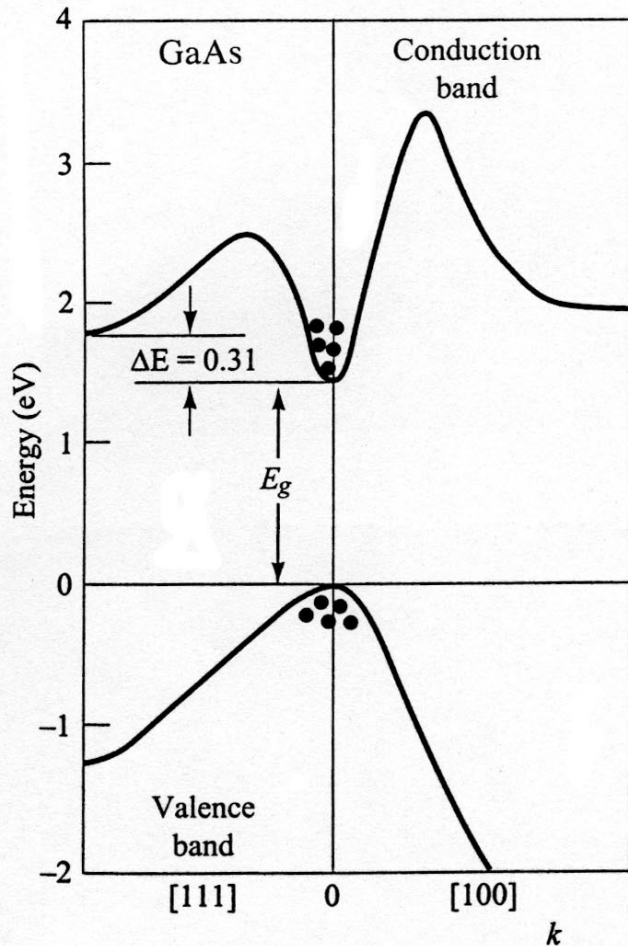
Extension to Three Dimensions

A face-centered cubic crystal

Electrons traveling in different directions encounter different potential patterns and therefore different k-space boundaries. The E versus k diagrams are in general a function of the k-space direction in a crystal.

Energy band diagrams are symmetric in k so that only the positive axis is displayed. GaAs is a **direct bandgap** semiconductor. Si is an **indirect bandgap** semiconductor. The electron transitions in indirect bandgap semiconductors must involve changes of crystal momentum, and thus the emission efficiency of indirect bandgap semiconductors is much smaller than that of direct bandgap semiconductors.

The curvature is related to the effective masses of electrons and holes, which are different along different directions. Usually a statistical average is used for device calculations.

Density of States

We are eventually interested in the current-voltage characteristics in semiconductor devices, which depend on the number of electrons and holes available for conduction. The number of carriers is in turn a function of the number of available energy or quantum states.

Electrons are allowed to move relatively freely in the conduction band of a semiconductor, but they are confined in a crystal. As a first step, consider a free electron confined to a three-dimensional infinite potential well:

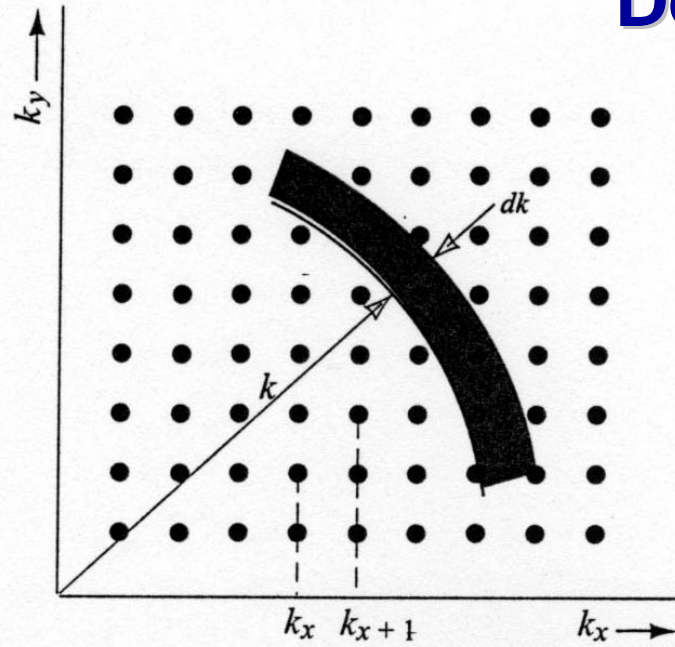$$V(x,y,z) = 0 \text{ for } 0 < x < a$$
$$0 < y < a$$
$$0 < z < a$$

$$V(x,y,z) = \infty \quad \text{elsewhere}$$
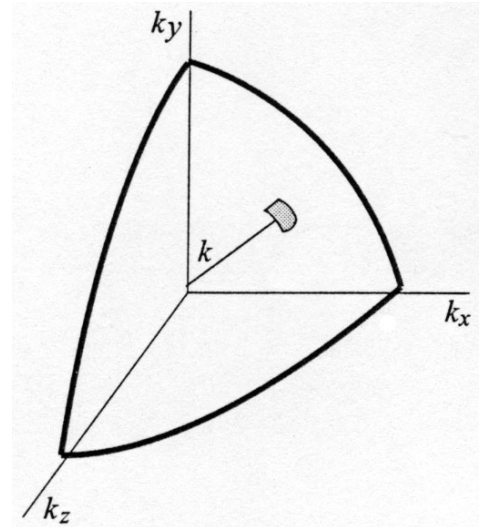
Solving Schrodinger's wave equation in three dimensions leads to:

$$\frac{2mE}{\hbar^2} = \left(n_x^2 + n_y^2 + n_z^2\right)\left(\frac{\pi^2}{a^2}\right) = k_x^2 + k_y^2 + k_z^2 = k^2$$

n_x, n_y, and n_z, are positive integers.

Density of States

Schematic showing allowed quantum states in *k*-space.

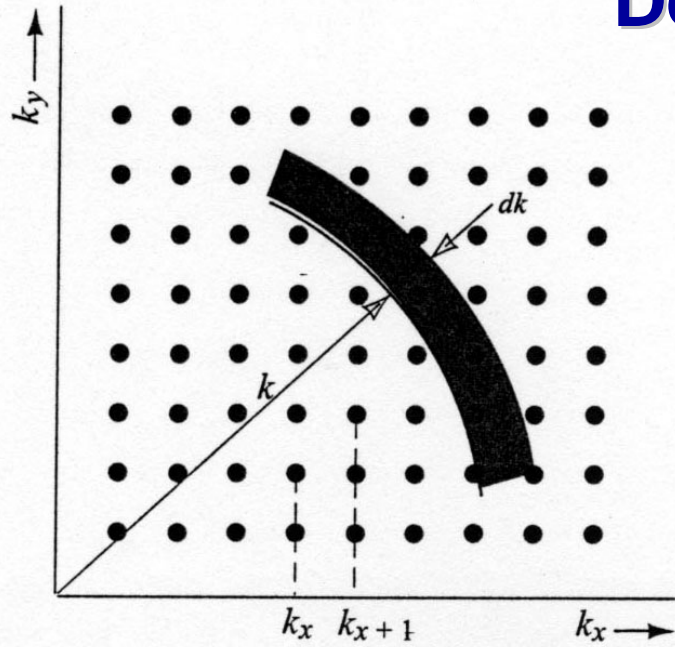Only the positive one eighth of the spherical *k*-space should be considered.

The distance between two states in the k_x direction is

$$k_{x+1} - k_x = (n_x + 1)\left(\frac{\pi}{a}\right) - n_x\left(\frac{\pi}{a}\right) = \frac{\pi}{a}$$

Generalizing this result to three dimensions gives the volume V_k of a single quantum state:

$$V_k = \left(\frac{\pi}{a}\right)^3$$

Density of States

We now determine the density of quantum states in k-space:

$$g_T(k)dk = 2\left(\frac{1}{8}\right)\frac{4\pi k^2 dk}{\left(\dfrac{\pi}{a}\right)^3}$$

$$g_T(k)dk = \frac{\pi k^2 dk}{\pi^3}a^3$$

The above formula gives the number of quantum states between k and $k + dk$. We can use this formula to determine the number of quantum states between E and $E + dE$ using the relationship between E and k for a free electron:

$$k^2 = \frac{2mE}{\hbar^2} \qquad k = \frac{1}{\hbar}\sqrt{2mE} \qquad dk = \frac{1}{\hbar}\sqrt{\frac{m}{2E}}dE$$

Density of States

$$g_T(E)dE = \frac{\pi a^3}{\pi^3}\left(\frac{2mE}{\hbar^2}\right)\frac{1}{\hbar}\sqrt{\frac{m}{2E}}dE$$

$$g_T(E)dE = \frac{4\pi a^3}{h^3}(2m)^{3/2}\sqrt{E}\,dE$$

The density of quantum states per unit volume of the crystal is:

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

The unit is in terms of states per unit energy per unit volume.

Example: calculate the density of states with energies between 0 and 1 eV for a free electron.

Solution:

$$N = \int_0^E g(E)dE = \frac{4\pi(2m)^{3/2}}{h^3} \int_0^E \sqrt{E}\,dE$$

$$= \frac{4\pi(2m)^{3/2}}{h^3} \frac{2}{3} E^{3/2} = \frac{8\pi(2mE)^{3/2}}{3h^3}$$

$$N = \frac{8\pi\left[2(9.11\times10^{-31})(1.6\times10^{-19})\right]^{3/2}}{3(6.625\times10^{-34})^3}$$

$$= 4.5\times10^{27}\,\text{m}^{-3} = 4.5\times10^{21}\,\text{cm}^{-3}$$

Extension to Semiconductors

The E versus k curve near $k = 0$ at the bottom of the conduction band can be approximated as a parabola, which is the same as a free electron, except that the mass is replaced by the electron effective mass.
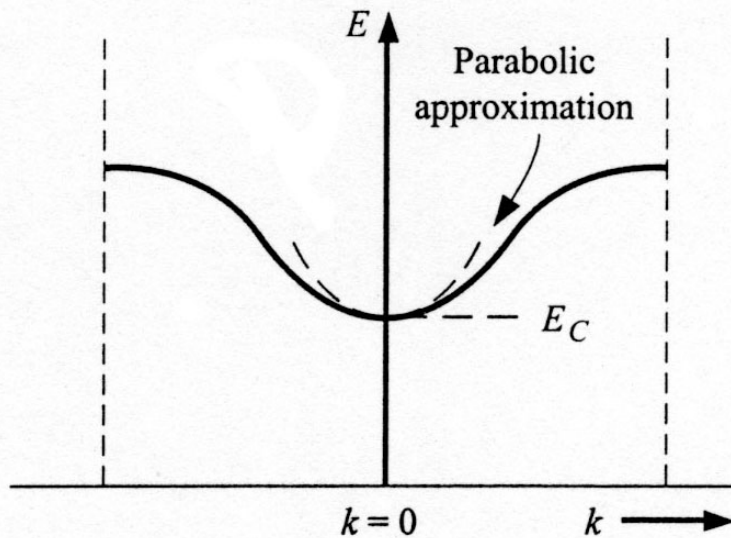
$$E = E_c + \frac{\hbar^2 k^2}{2m_n^*}$$

$$E - E_c = \frac{\hbar^2 k^2}{2m_n^*}$$

$$g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c} \qquad \text{Valid for } E \geq E_c.$$
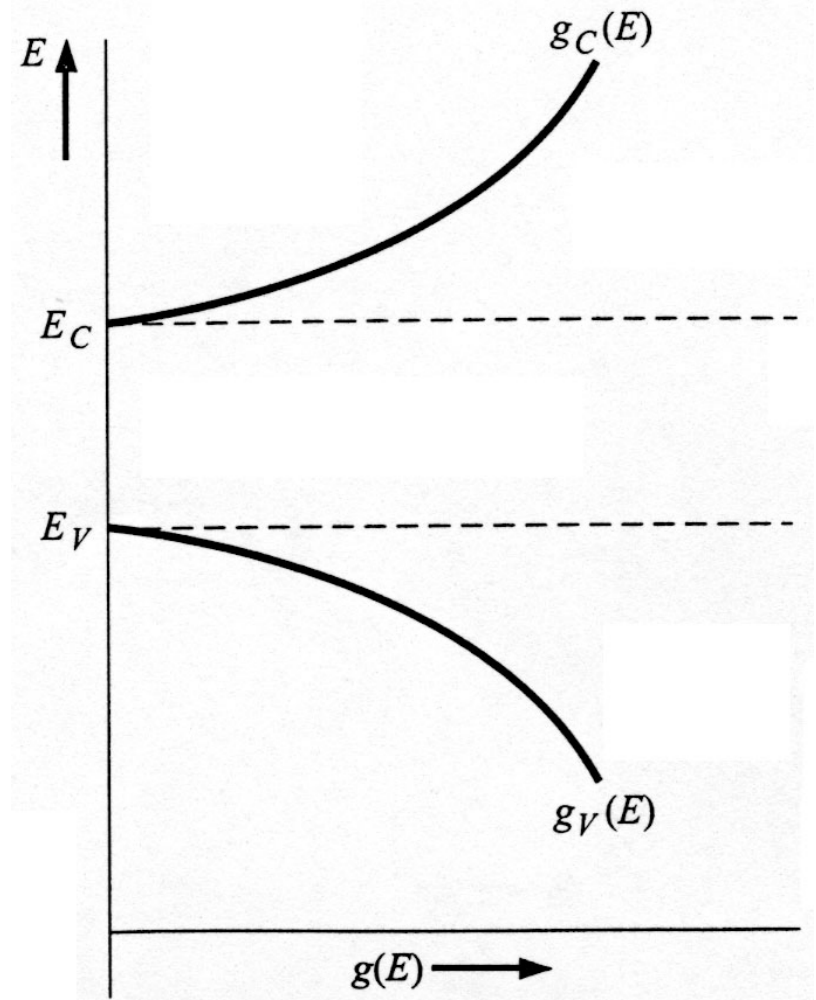
Extension to Semiconductors

We can obtain similar equations for the region close to the top of the valence band:

$$E = E_v - \frac{\hbar^2 k^2}{2m_p^*}$$

$$E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$$

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

Valid for $E \leq E_v$.

Statistical Laws

We are interested only in the statistical behavior of electrons as a whole rather than in the behavior of each individual electron because the electrical characteristics in a crystal are determined by the statistical behavior of a large number of electrons.

Maxwell-Boltzmann distribution: the particles are distinguishable and there is no limit to the number of particles allowed in each energy state.

Bose-Einstein distribution: the particles are indistinguishable and there is no limit to the number of particles permitted in each energy state.
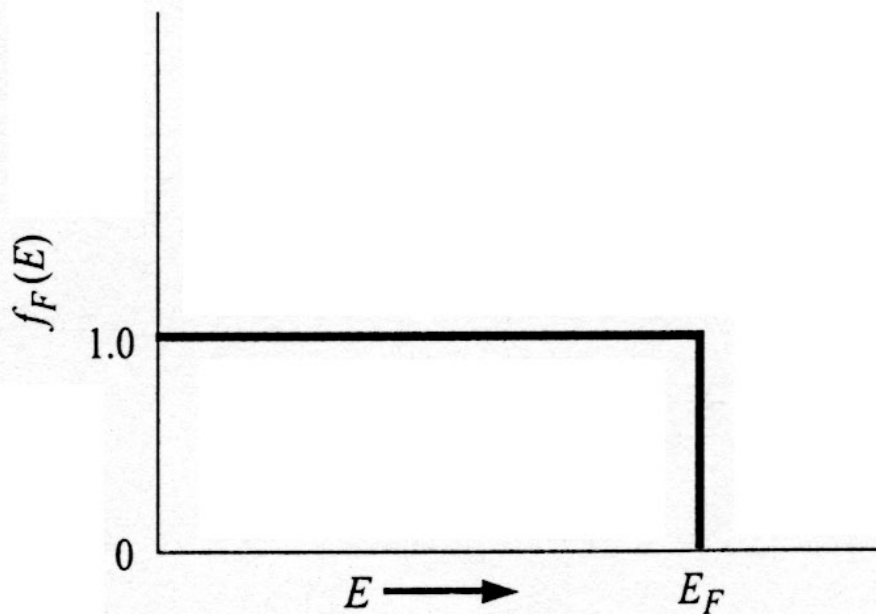
Fermi-Dirac distribution: the particles are indistinguishable and only one particle is allowed in each quantum state. Electrons in a crystal obey Fermi-Dirac distribution.

Fermi-Dirac Probability Function

$$f_F(E) = \cfrac{1}{1 + \exp\left(\cfrac{E - E_F}{kT}\right)}$$

At $T = 0$ K,
when $E < E_F$, $f_F(E) = 1$,
when $E > E_F$, $f_F(E) = 0$.

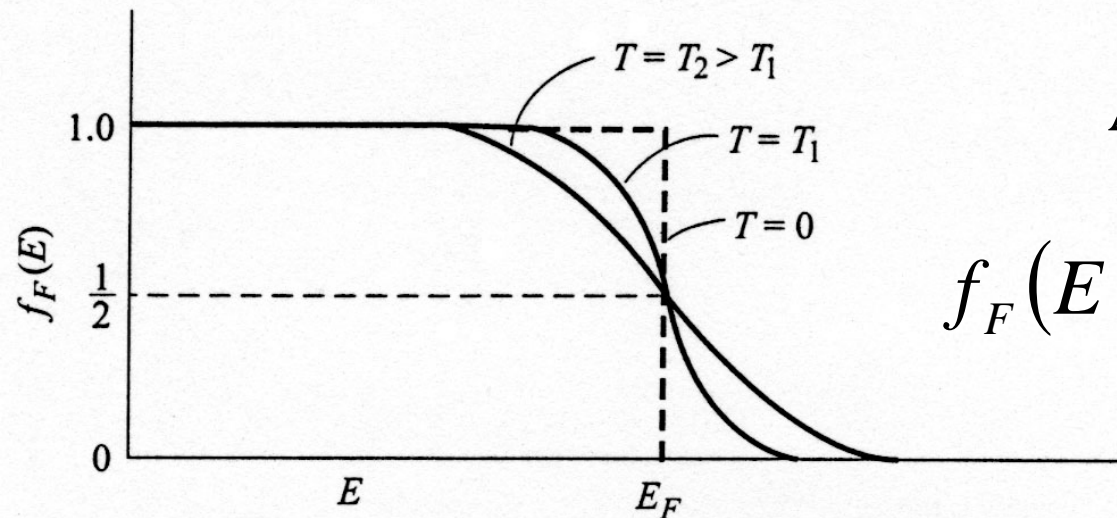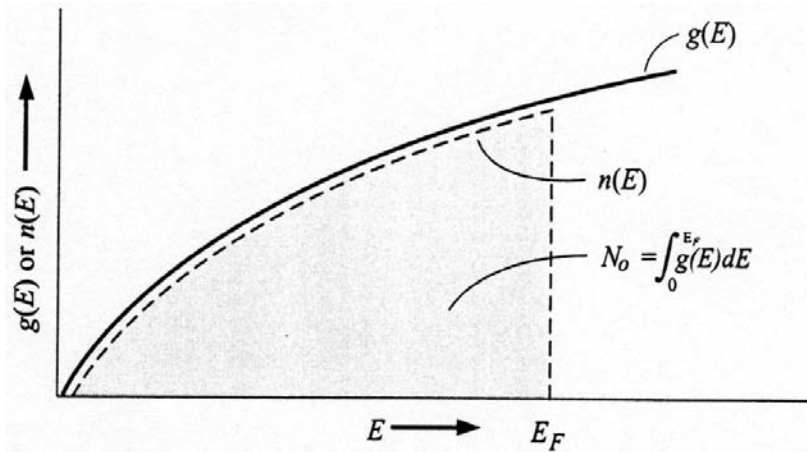E_F is called the Fermi energy.

The probability of a quantum state being occupied is unity for $E < E_F$ and the probability of a state being occupied is zero for $E > E_F$. All electrons have energies below the Fermi energy at $T = 0$ K.

Fermi-Dirac Probability Function

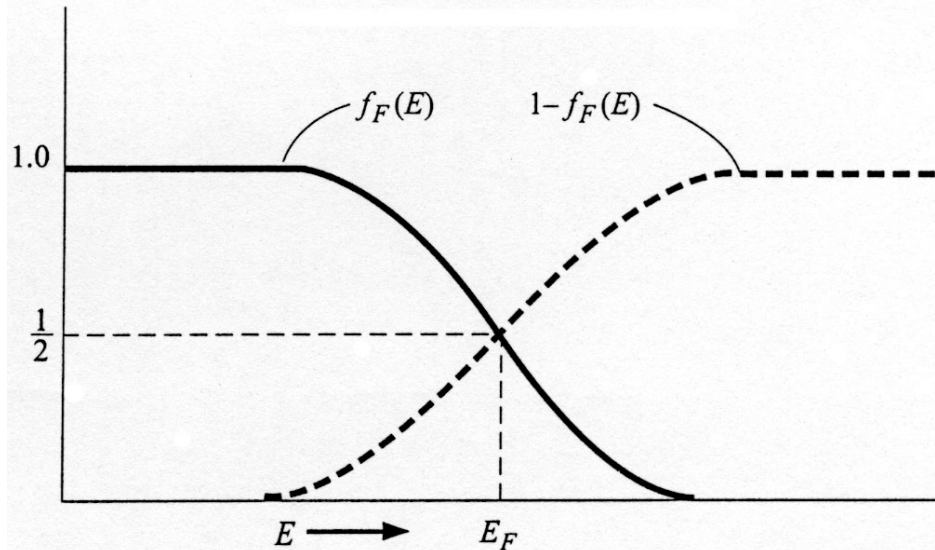If $g(E)$ and N_0 are known for a system, then the Fermi energy E_F can be determined.
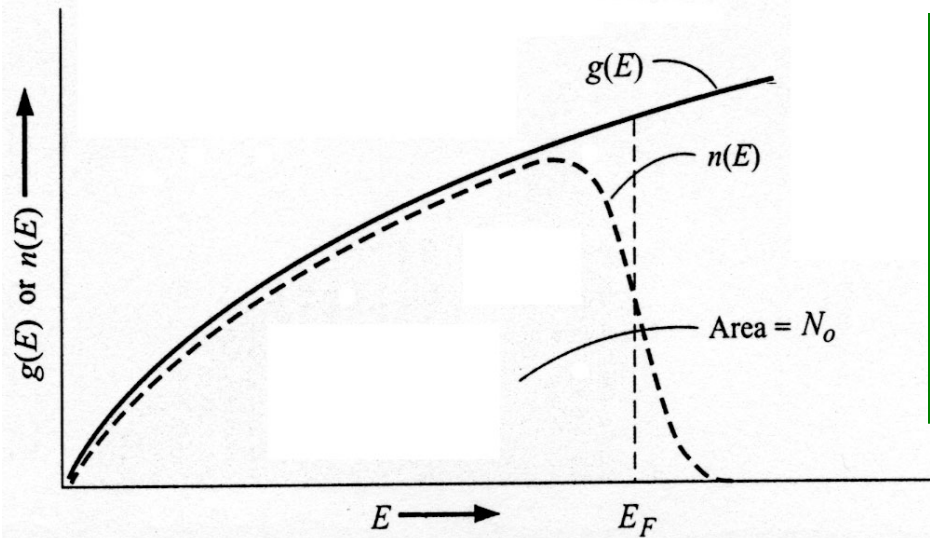
At $T > 0$ K and $E = E_F$,

$$f_F(E = E_F) = \frac{1}{1 + \exp(0)} = \frac{1}{2}$$

At $T > 0$ K, there is a probability that some energy states above E_F will be occupied by electrons and some energy states below E_F will be empty.
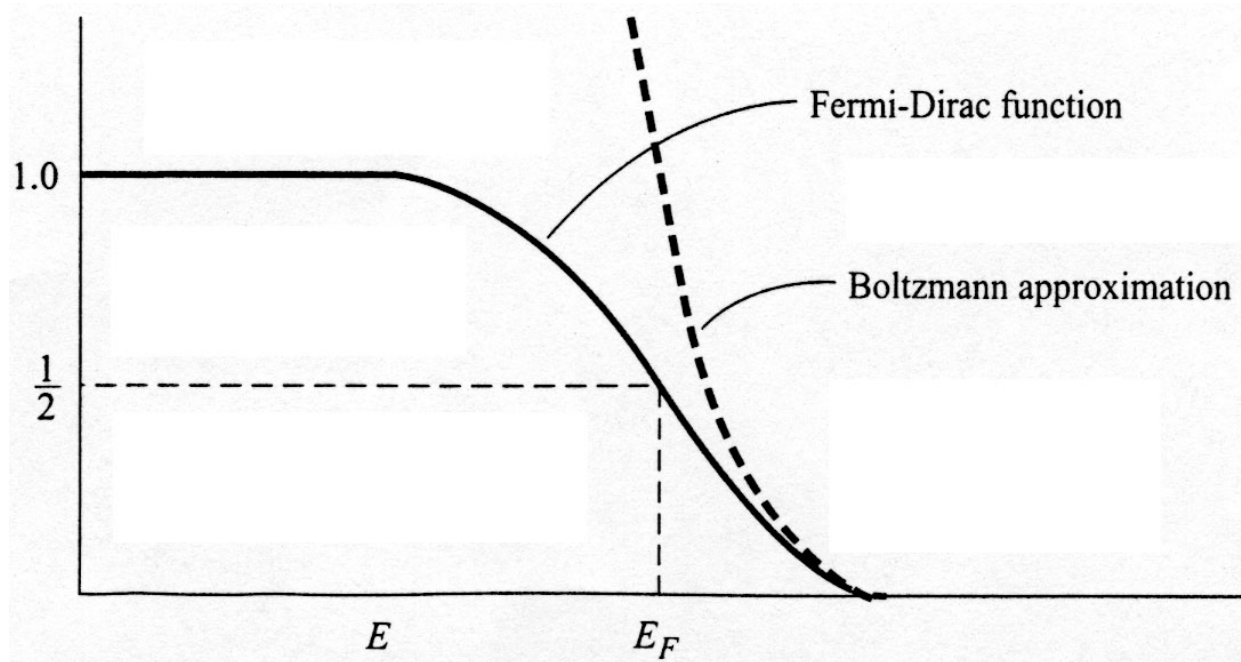
Fermi-Dirac Probability Function

The function $f_F(E)$ is symmetrical with the function $1-f_F(_E)$ about the Fermi energy E_F.

The total number of electrons in the system remains constant, and the distribution of these electrons among the available states changes with temperature.

Maxwell-Boltzmann Approximation

When $E - E_F \gg kT$,

$$f_F(E) \approx \exp\left[\frac{-(E - E_F)}{kT}\right]$$

Reading Materials

D. A. Neamen, "Semiconductor Physics and Devices: Basic Principles", Irwin, Boston, MA 02116, 1992, Chapter 3, "Introduction to the Quantum Theory of Solids".