

# **DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY SRM INSTITUTE OF SCIENCE AND TECHNOLOGY**

**21PYB102J – SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS**

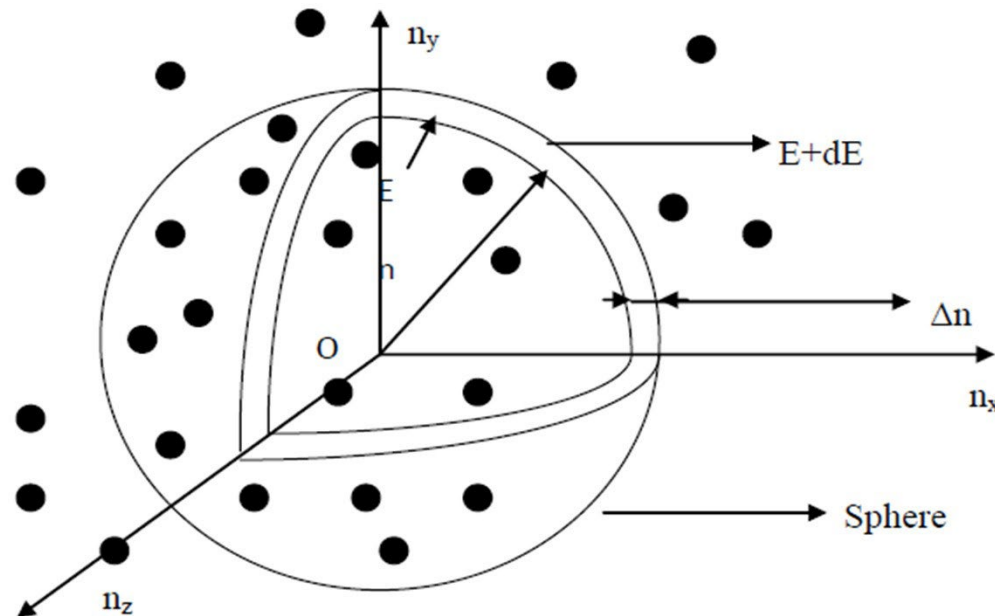
## **LECTURE 2**

# **DENSITY OF STATES ENERGY BANDS IN SOLIDS**

## DENSITY OF STATES



**Definition:** Density of States  $Z(E) dE$  is defined as the number of available electron states per unit volume in an energy interval ( $dE$ ).



To find the number of energy levels in a cubical metal piece and to find number of electrons that can be filled in a given energy level, let us construct a sphere of radius 'n' in the space.

The **sphere** is further divided in to many shells and each of this shell represents a particular combination of quantum numbers ( $n_x$ ,  $n_y$ , and  $n_z$ ) and therefore represents a particular energy value.

Let us consider two energy values **E** and **E + dE**. The number of energy states between E and E + dE can be found by finding the number of energy states between the shells of the radius **n** and **n + Δn**, from the origin.

The number of energy states within the sphere of radius n =  $\frac{4}{3} \pi n^3$  Since  $n_x$ ,  $n_y$ , and  $n_z$  will have only positive values, **we have to take only one octant of the sphere (i.e) 1/8 th of the sphere volume**.

The number of available energy states within the sphere of radius

$$n = 1/8 [4/3 \pi n^3]$$

Similarly the number of available energy states within the sphere of radius

$$n + dn = 1/8 [4/3 \pi (n+dn)^3]$$

The number of available energy states between the shells of radius  $n$  and  $n + dn$  (or) between the energy levels

$$E \text{ and } E + dE = 1/8 [4/3 \pi (n+dn)^3 - 4/3 \pi n^3]$$

The number of available energy states between the energy interval

$$Z(E)dE = 1/8 \times 4/3 \pi [n^3 + dn^3 + 3n^2dn + 3dn^2n - n^3]$$

Since the higher powers of  $dn$  is very small,  $dn^2$  and  $dn^3$  terms can be neglected.

$$Z(E)dE = \pi / 6 (3n^2 dn)$$

$$Z(E)dE = \pi / 2 (n^2 dn) \longrightarrow (1)$$

We know the energy of the electron in a cubical metal piece of sides  $\ell$

$$E = \frac{n^2 h^2}{8m \ell^2}$$

$$n^2 = \frac{8m \ell^2 E}{h^2} \longrightarrow (2)$$

$$n = \left[ \frac{8m \ell^2 E}{h^2} \right]^{1/2} \longrightarrow (3)$$

Differentiating equation (2) we get

$$2n dn = \frac{8m \ell^2}{h^2} dE$$

→ (4)

$$n dn = \frac{8m \ell^2}{2 h^2} dE$$

Equation 1 can be written as

$$Z(E)dE = \pi / 2 (n^2 dn)$$

$$Z(E)dE = \pi / 2 n (n dn)$$

Substituting equation (3) and (4) in the above equation we have

$$Z(E)dE = \pi / 2 \left[ \frac{8m \ell^2 E}{h^2} \right]^{1/2} \left[ \frac{8m \ell^2}{2 h^2} dE \right]$$

$$Z(E)dE = \pi / 4 \left[ \frac{8m \ell^3}{h^2} \right]^{3/2} E^{1/2} dE$$

$$Z(E)dE = \pi / 4 \left[ \frac{8m}{h^2} \right]^{3/2} \ell^3 \cdot E^{1/2} dE$$

Here  $\ell^3$  represents the volume of the metal piece. If  $\ell^3 = 1$ , then we can write that

The number of available energy states per unit volume (i.e) Density of states

$$Z(E)dE = \pi / 4 \left[ \frac{8m}{h^2} \right]^{3/2} E^{1/2} dE \longrightarrow (5)$$

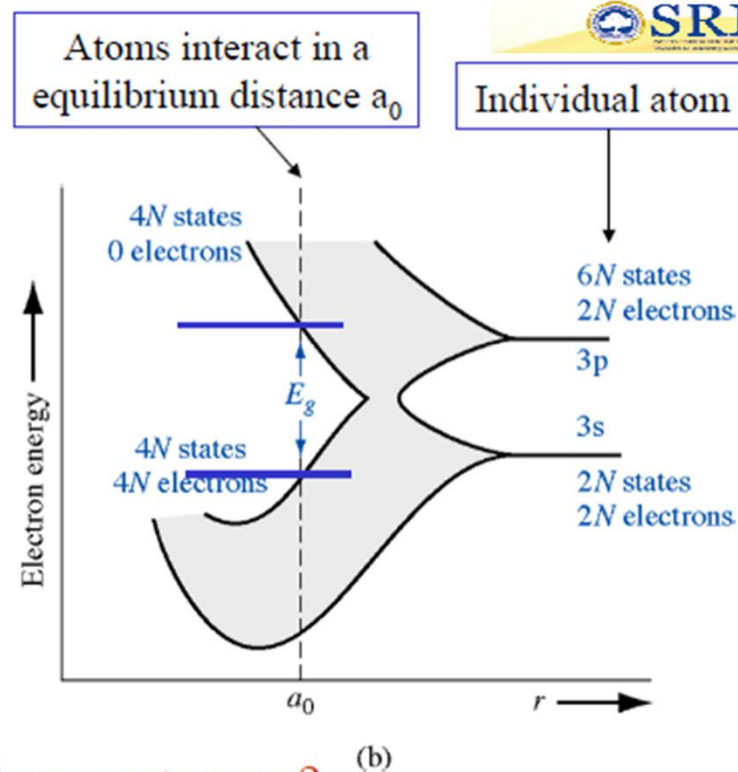
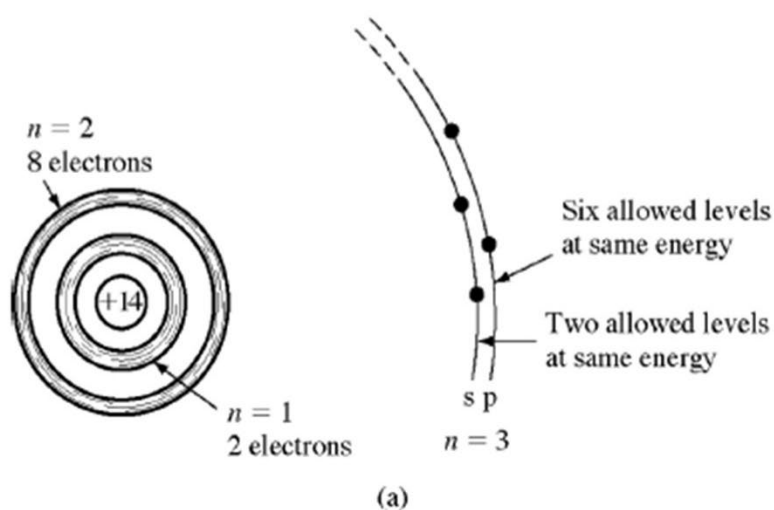
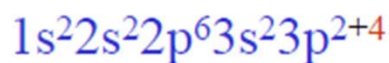
Since each energy level provides 2 electron states one with spin up and another spin down, we have

Density of states

$$Z(E)dE = 2 \times \pi / 4 \left[ \frac{8m}{h^2} \right]^{3/2} E^{1/2} dE$$

$$Z(E)dE = \pi / 2 \left[ \frac{8m}{h^2} \right]^{3/2} E^{1/2} dE \longrightarrow (6)$$





Temperature = ?

(a) Schematic of an isolated Si atom. (b) The splitting of the 3s and 3p states of silicon into allowed and forbidden energy bands.



# Additional Comments

The density of states has a functional dependence on energy.

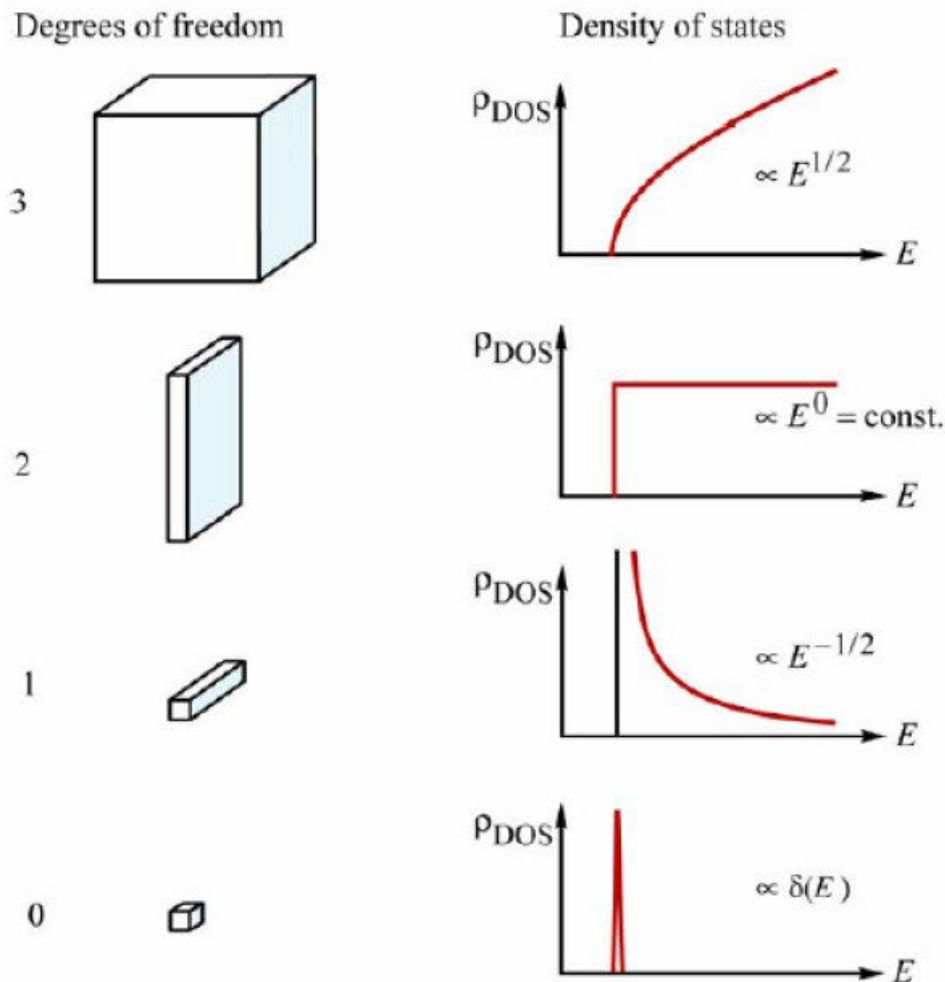


Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

# Additional Comments

Degrees of freedom	Dispersion (kinetic energy)	Density of states	Effective density of states
3 (bulk)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2)$	$\rho_{\text{DOS}}^{3\text{D}} = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{E - E_C}$	$N_c^{3\text{D}} = \frac{1}{\sqrt{2}} \left( \frac{m^* kT}{\pi \hbar^2} \right)^{\frac{3}{2}}$
2 (slab)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)$	$\rho_{\text{DOS}}^{2\text{D}} = \frac{m^*}{\pi \hbar^2} \sigma(E - E_C)$	$N_c^{2\text{D}} = \frac{m^*}{\pi \hbar^2} kT$
1 (wire)	$E = \frac{\hbar^2}{2m^*} k_x^2$	$\rho_{\text{DOS}}^{1\text{D}} = \frac{m^*}{\pi \hbar} \sqrt{\frac{m^*}{2(E - E_C)}}$	$N_c^{1\text{D}} = \sqrt{\frac{m^* kT}{2\pi \hbar^2}}$
0 (box)	–	$\rho_{\text{DOS}}^{0\text{D}} = 2\delta(E - E_C)$	$N_c^{0\text{D}} = 2$

**Table 12.1** Density of states for semiconductor with 3, 2, 1, and 0 degrees of freedom for propagation of electrons. The dispersion relations are assumed to be parabolic. The formulas can be applied to anisotropic semiconductors if the effective mass  $m^*$  is replaced by the density-of-states effective mass  $m_{\text{DOS}}^*$ . If the semiconductor has a number of  $M_c$  equivalent minima, the corresponding density of states must be multiplied by  $M_c$ . The bottom of the band is denoted as  $E_C$  and  $\sigma(E)$  is the step-function.

# Practical Applications

Quantum Wells (2D) - a potential well that confines particles in one dimension, forcing them to occupy a planar region

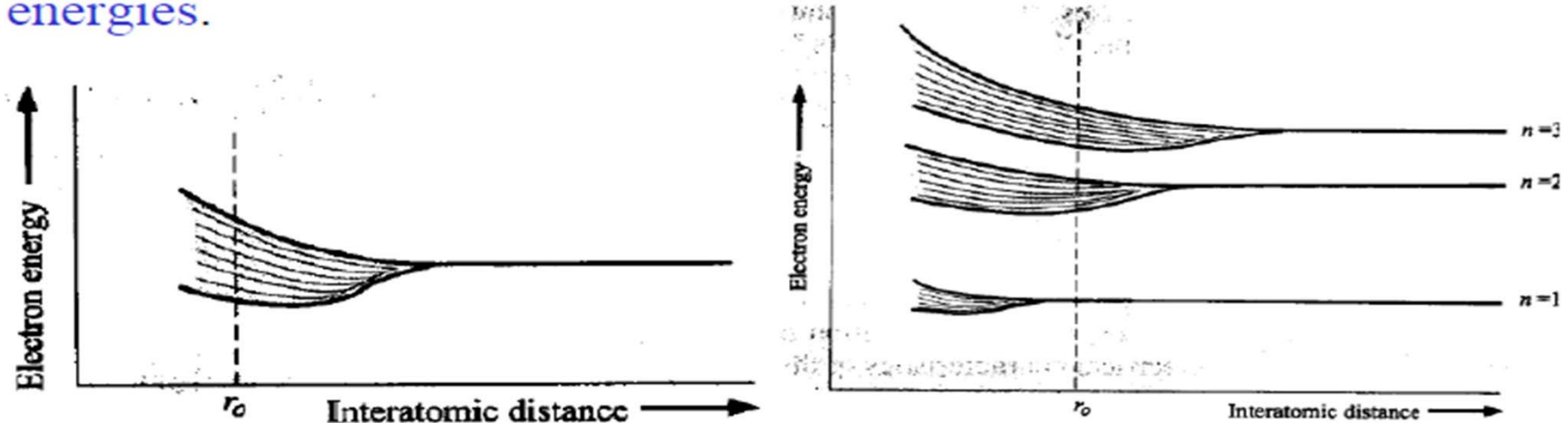
Quantum Wire (1D) - an electrically conducting wire, in which quantum transport effects are important

Quantum Dots (0D) - a semiconductor crystal that confines electrons, holes, or electron-pairs to zero dimensions.

## Energy bands in solids



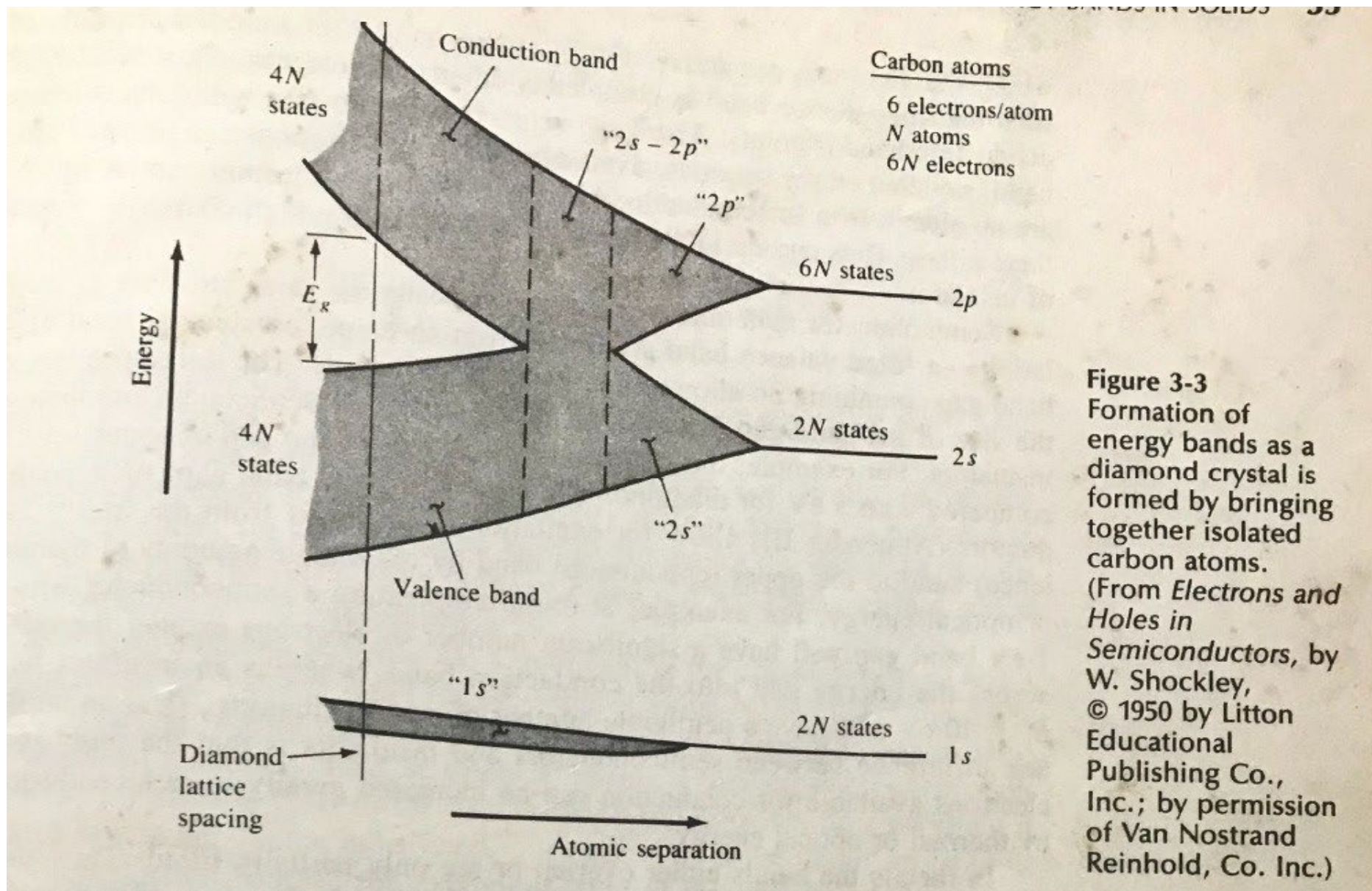
- Consider a regular periodic arrangement of atoms in which each atom contains more than one electron. If the atoms are initially far apart, the electrons in adjacent atoms will not interact and will occupy the discrete energy levels.
- If the atoms are brought closer enough, the outmost electrons will interact and the energy levels will split into a band of allowed energies.



The splitting of an energy state into a band of allowed energies.



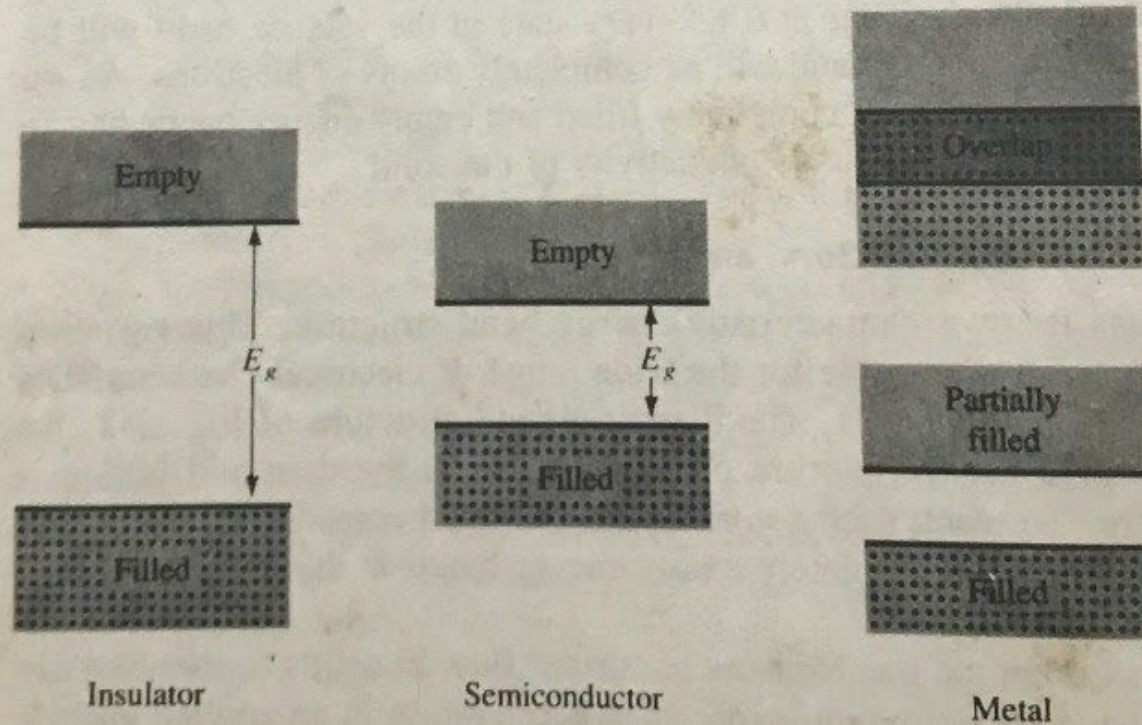
# Band structure of Carbon atoms



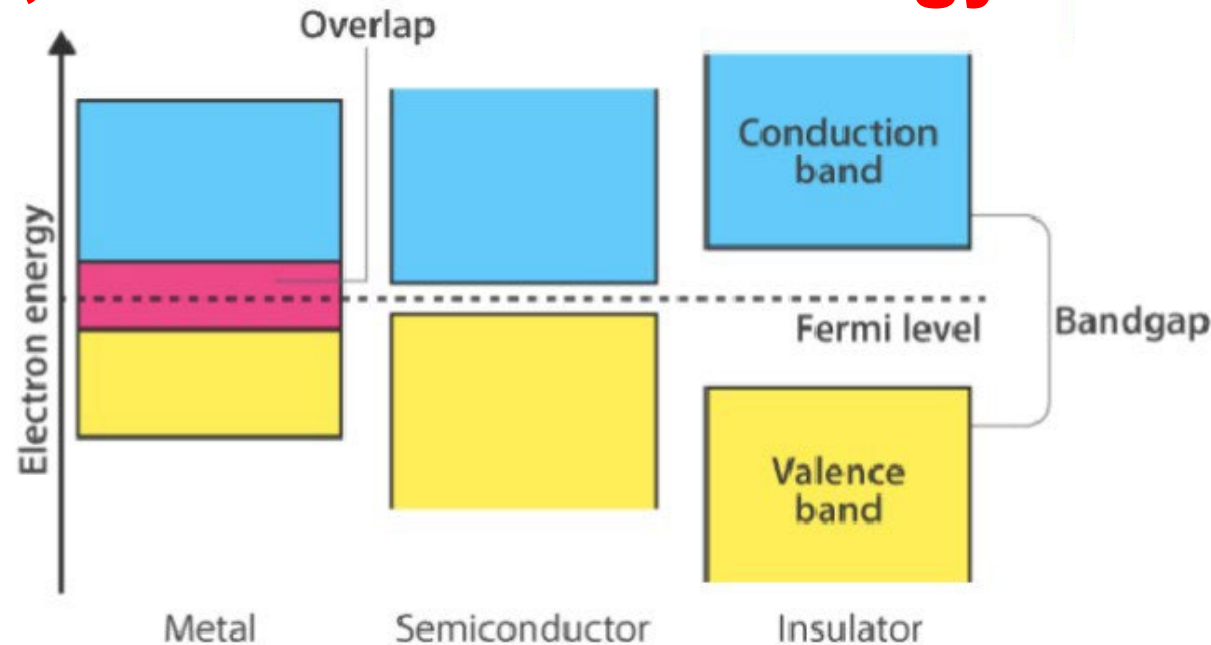
**Figure 3-3**  
Formation of energy bands as a diamond crystal is formed by bringing together isolated carbon atoms.  
(From *Electrons and Holes in Semiconductors*, by W. Shockley, © 1950 by Litton Educational Publishing Co., Inc.; by permission of Van Nostrand Reinhold, Co. Inc.)

# Band structure: Metal Semiconductor Insulators

Figure 3-4  
Typical band  
structures at 0 K.



# Valence, conduction and Energy Band Gap



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**Valence Band:** range of permissible energy values that are the highest energies an electron can have and still be associated with a particular atom of a solid material .  
Or The valence band is simply the outermost electron orbital of an atom of any specific material that electrons actually occupy.

**Conduction band:** band of electron orbitals that electrons can jump up into from the valence band when excited. When the electrons are in these orbitals, they have enough energy to move freely in the material. This movement of electrons creates an electric current.

**Energy Band Gap:** The energy difference between the highest occupied energy state of the valence band and the lowest unoccupied state of the conduction band is called the band gap and is indicative of the electrical conductivity of a material.



# Fermi energy and Fermi level

**Fermi energy** → value of energy for a Fermi level at absolute zero temperature (at 0 K). It is the maximum kinetic energy an electron can have at this temperature.

We can define the term Fermi energy as the highest occupied energy level of a material at absolute zero temperature. In other words, all the electrons of a solid tend to occupy energy states at or below the solid's Fermi energy at 0 K temperature.

**Fermi level** → chemical potential of electrons. It is an energy level in which the probability of finding an electron is 50%. **It is the highest occupied molecular orbital in the valence band at 0 K.** Therefore, there are many vacant states to accept electrons. The Fermi level is located at the bandgap, between the conduction band and valence band.

**Fermi energy is the energy of Fermi level whereas Fermi level is a measure of least tightly bound electrons within a solid.**

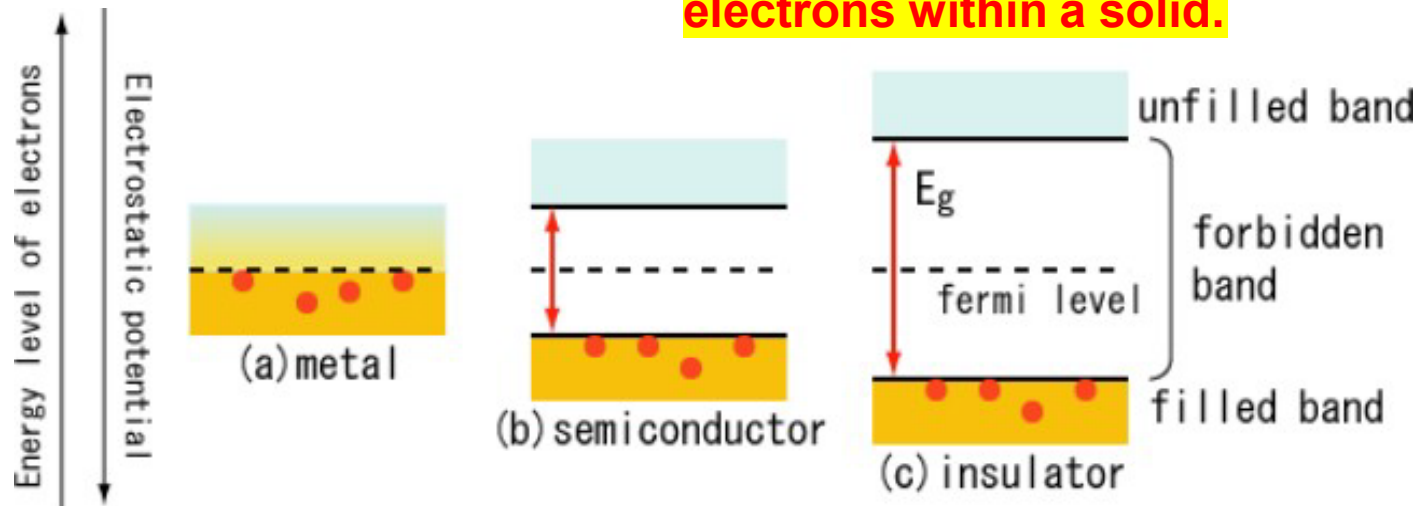
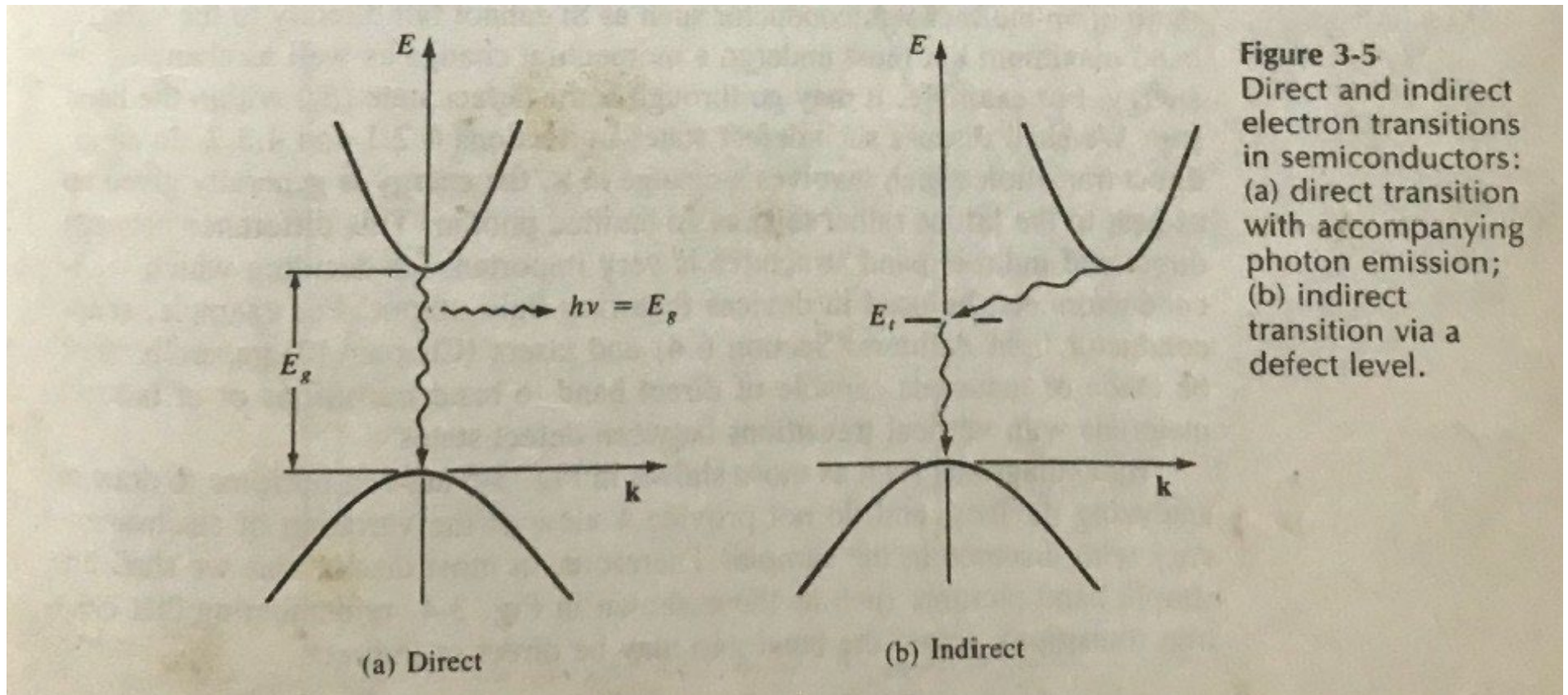


Figure 01: Comparing Band Gaps of Metal, Semiconductor and Insulator

# Direct and Indirect Band Gap



**Direct bandgap semiconductor:** the top of the valence band (VB) and the bottom of the conduction band (CB) occur at the same value of momentum.

**Indirect bandgap semiconductor:** the maximum energy of the valence band (VB) occurs at a different value of momentum to the minimum in the conduction band (CB) energy