Semiconductor Physics

Syllabus code: BSC-PHY-103G

Introduction to subject

A semiconductor is a material that has a resistivity value in between that of a conductor and an insulator. A semiconductor material is a device that allows the passage of electric current through it.

Consider the device CPU, it consists of many numbers of transistors within it and these transistors contain the semiconductor material which allows the passage of current and all these are controlled by a switch.

Here in a transistor, the passage of electric current is controlled by the actions based on the state of the switch whether it is on or off. Hence such a device, which allows the current to pass through them partially is called a semiconductor device.

Examples of Semiconductor Devices

- These devices are said to be neither good insulators nor good conductors, hence the name 'Semi Conductors'.
The semiconductor examples include the following:

- op-amps

- resistors

- capacitors

- diodes

- Transistors

Syllabus

UNIT – I: Electronic Materials

Free electron theory, Density of states and energy band diagrams, Kronig-Penny model (to introduce origin of band gap), Energy bands in solids, E-k diagram, Direct and indirect band gaps, Types of electronic materials: metals, semiconductors, and insulators, Density of states, Occupation probability, Fermi level, Effective mass, Phonons.

UNIT – II: Semiconductors

Intrinsic and extrinsic semiconductors, Dependence of Fermi level on carrier-concentration and temperature (equilibrium carrier statistics), Carrier generation and recombination, Carrier transport: diffusion and drift, p-n junction, Metal-semiconductor junction (Ohmic and Schottky), Semiconductor materials of interest for optoelectronic devices.

UNIT – III : Light-Semiconductor Interaction

Optical transitions in bulk semiconductors: absorption, spontaneous emission, and stimulated emission; Joint density of states, Density of states for photons, Transition rates (Fermi's golden rule), Optical loss and gain; Photovoltaic effect, Exciton, Drude model.

UNIT – IV: Measurements & Engineered Semiconductor Materials

Four-point probe and van der Pauw measurements for carrier density, resistivity, and hall mobility; Hot-point probe measurement, capacitance-voltage measurements, parameter extraction from diode I-V characteristics, DLTS, band gap by UV-Vis spectroscopy, absorption/transmission. Densityofstatesin2D, 1D and 0D (qualitatively). Practical examples of low-dimensional systems such as quantum wells, wires, and dots: design, fabrication, and characterization techniques. Heterojunctions and associated band diagram.

Future scope

Study of semiconductor physics is important from the viewpoint of its technological applications. The knowledge of Semiconductors will help in understanding the mechanisms of various electronic devices used in day to day life.

Applications of Semiconductor Devices

- They are used in the designing of logic gates and digital circuits.

- These are used in microprocessors.

- They are also used in analog circuits such as oscillators and amplifiers.

- Used in high voltage applications.

Unit 1: Electronic Materials

Table of Contents

- Basics of quantum mechanics

- Free electron theory

- Density of states and energy band diagrams

- Kronig-Penny model (to introduce origin of band gap)

- Energy bands in solids

- E-k diagram, Direct and indirect band gaps

- Types of electronic materials: metals, semiconductors, and insulators,

- Density of states, Occupation probability,

- Fermi level, Effective mass, Phonons

Basics of quantum mechanics

- De-broglie Hypothesis
- Wave function and its physical significance
- Time dependent Scrodinger Equation
- Time independent Scrodinger Equation
- Particle in rigid one-dimensional box

De-broglie Hypothesis

- The de Broglie hypothesis states that particles of matter can behave as both waves and particles, just like light.

- In quantum mechanics, matter is believed to behave both like a particle and a wave at the sub-microscopic level. The particle behavior of matter is obvious. When you look at a table, you think of it like a solid, stationary piece of matter with a fixed location. At this macroscopic scale, this holds true. But when we zoom into the subatomic level, things begin to get more complicated, and matter doesn't always exhibit the particle behavior that we expect.

Wave function and its physical significance

- A wave function in quantum physics is a mathematical description of the quantum state of an isolated quantum system. The wave function is a complex-valued probability amplitude, and the probabilities for the possible results of measurements made on the system can be derived from it. The most common symbols for a wave function are the Greek letters ψ or Ψ.

- Properties:
  - ψ and d ψ /dt should be Single valued.
  - ψ and d ψ /dt should be continuous.
  - ψ and d ψ /dt should be finite.

Schrödinger Equations

- The Schrödinger equation is a linear partial differential equation that describes the wave function or state function of a quantum-mechanical system.

- **Time-dependent equation**

The most general form is the time-dependent Schrödinger equation (TDSE), which gives a description of a system evolving with time:

Time-dependent Schrödinger equation *(general)*

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

Where $\hbar = \dfrac{h}{2\pi}$ is reduced Planck constant. Ψ is state of quantum system.

Time-dependent Schrödinger equation in position basis
(single nonrelativistic particle)

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t)$$

Time-independent equation

The time-dependent Schrödinger equation described above predicts that wave functions can form standing waves, called stationary states. These states are particularly important as their individual study later simplifies the task of solving the time-dependent Schrödinger equation for any state. Stationary states can also be described by a simpler form of the Schrödinger equation, the time-independent Schrödinger equation (TISE).

Time-independent Schrödinger equation *(general)*

$$\hat{H} |\Psi\rangle = E |\Psi\rangle$$

Time-independent Schrödinger equation *(single nonrelativistic particle)*

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Particle in rigid one-dimensional box

A particle in a one-dimensional box is the name given to a hypothetical situation where a particle of mass m is confined between two walls, at x=0 and x=L. In the infinite square well that we will consider, the potential energy is zero within the box but rises instantaneously to infinity at the walls.

Potential
Energy

Wall

Wall

Particle may
only be found
in this region

0

0

L

X
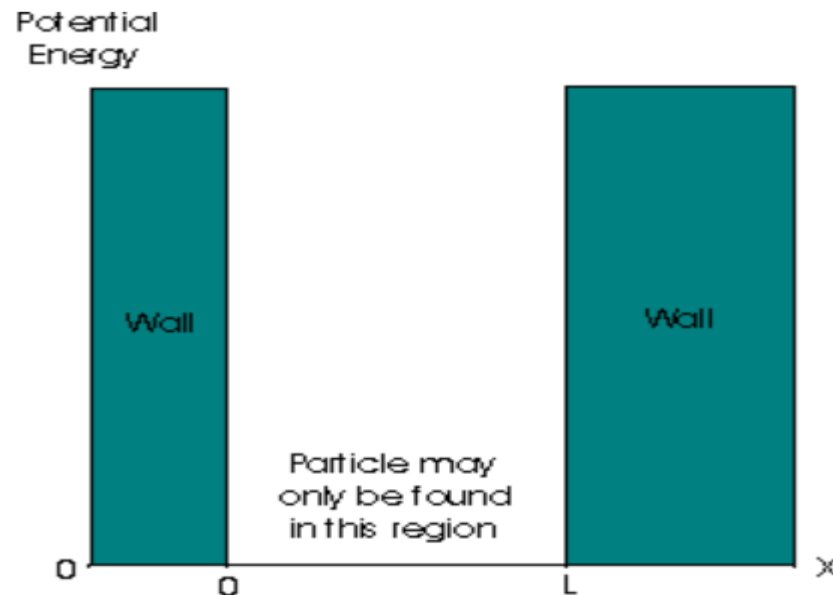
the solution in this form.

where C and D are two more arbitrary constants, and $0 \leq x \leq L$.

Now, because of the presence of the potential walls, we shall see that further restrictions upon the permitted wavefunctions arise. For x > L or x < 0 , the wavefunction may bWithin the box, the Schrodinger equation for the particle is precisely the same as that for a particle in free space (V = 0), which was solved on this page.

- If we use the first of the boundary conditions we obtain 0 = C (as cos 0 = 1 and sin 0 = 1) which implies that the wavefunction for the particle in a one-dimensional box reduces to

- If we then put x = L and apply the second boundary condition, we obtain: DsinkL=0

$$\psi_k(0) = 0 \quad \text{and} \quad \psi_k(L) = 0$$

The boundary condition may thus only be satisfied if kL is an integer multiple of π, as the sine of any integer multiple of pi is zero. Thus we may write:

$$kL = n\pi \quad \text{where} \quad n = 1, 2, 3....\text{etc}$$

Note that n = 0 is not an acceptable solution, as it implies k = 0, which again makes the wavefunction zero everywhere. Note that the above equation tells us that the energy of the particle is now quantised, limited to discrete values. This quantisation arises due to the restriction of n to discrete values, and this arises out of a need to fulfil the boundary conditions imposed on the system.

It is a general observation that quantisation of a physical property such as the energy arises due to boundary conditions, as it is these conditions that render some solutions unacceptable. Note also that the gaps between adjacent energy levels decrease as the integer n increases.

Thus the complete, normalised wavefunction for the particle in a one-dimensional box is:

$$\Psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

- The wavefunctions and energies are labeled with a quantum number, n.
- A quantum number is a number (an integer, or in some cases a half-integer) which labels the state of the system. For a particle in a box, there are an infinite number of acceptable wavefunctions (and thus an infinite numbers of states in which the system may found) , and the quantum number n specifies which state the system.
- The fact that n cannot be zero means that the lowest amount of energy the particle may possess (when n is 1) is not zero, as would be permitted in classical mechanics (and would imply a completely stationary particle) but is in fact,This minimum, irremovable energy of the particle is called its zero-point energy.

Classical free electron theory: Drude-Lorentz theory

- Metals consist of large number of free electrons that behaves like a molecules of perfect gas.

- Assembly of free electrons in a metal: free electron gas

- Random motion of free electron gas: speed is function of temperature, no practical contribution to conductivity

- On application of external field, random motion is modified, e- have some drift velocity

- All valence electrons can absorb energy. Average K.E.= 3/2 KT

- Follows Maxwell-Boltzman statistics

- Potential is uniform everywhere inside the crystal

- P.E. of electron inside the metal is neglected. Therefore, Total Energy= K.E.

Failure of Classical free electron theory

- Could not explain heat capacity of free electron gas

- Could not explain paramagnetic susceptibility of free elelctrons

- Could not explain variation in electrical conductivity with temperature

- Could not explain Wiedemann-Frenz law

- Could not explain long mean free path at low temperatures

Need of Quantum theory

- Fermi- Dirac Statistics
- Pauli exclusion principle
- Sommerfield free electron theory

Postulates of Quantum free electron theory (Sommerfield Theory)

- Free electrons in metal are free particle in box
- Electrons obey Pauli exclusion principle
- Electrons have high K.E. than classical K.E
- Electrons move in constant potential field

Fermi-Dirac Statistics: Occupation Probability

$$F(E) = \frac{1}{1+\exp\left(\dfrac{E-E_F}{kT}\right)}$$

(a) $T \rightarrow 0$ K

$T=0$ K
600 K
6000 K

Fermi–Dirac

$E_F = 2.5$ eV
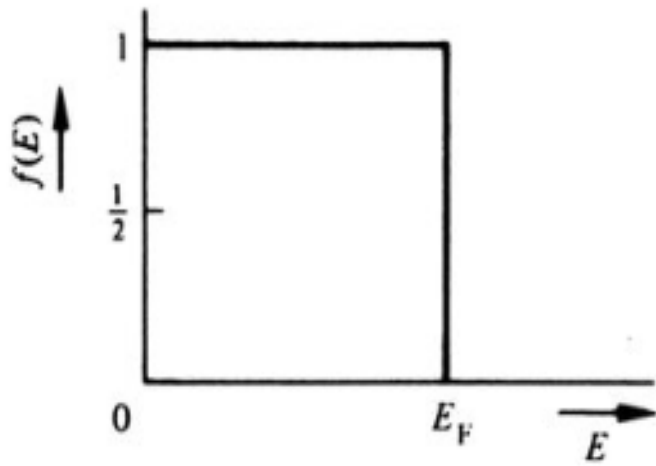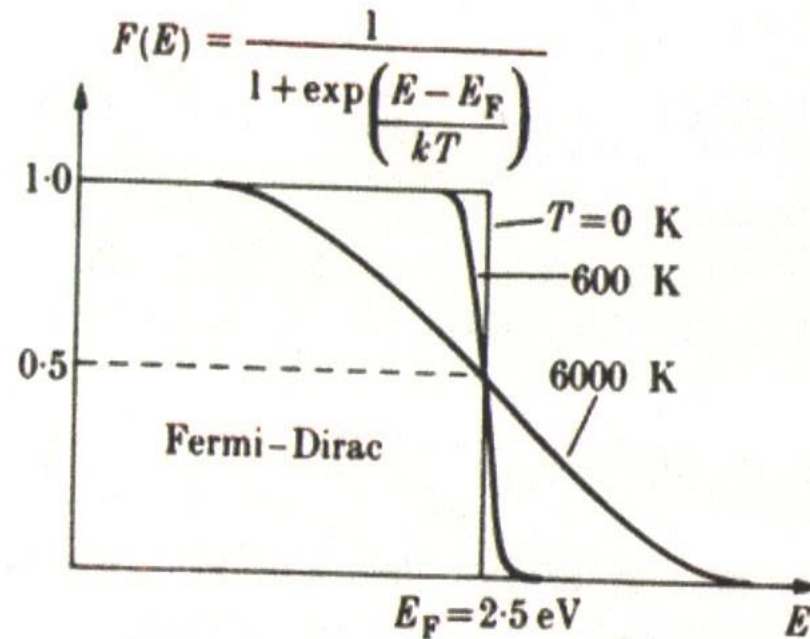
Density of states

The density of states (DOS) is essentially the number of different states at a particular energy level that electrons are allowed to occupy, i.e. the number of electron states per unit volume per unit energy.

Now that we have seen the distribution of modes for waves in a continuous medium, we move to electrons. The calculation of some electronic processes like absorption, emission, and the general distribution of electrons in a material require us to know the number of available states per unit volume per unit energy.
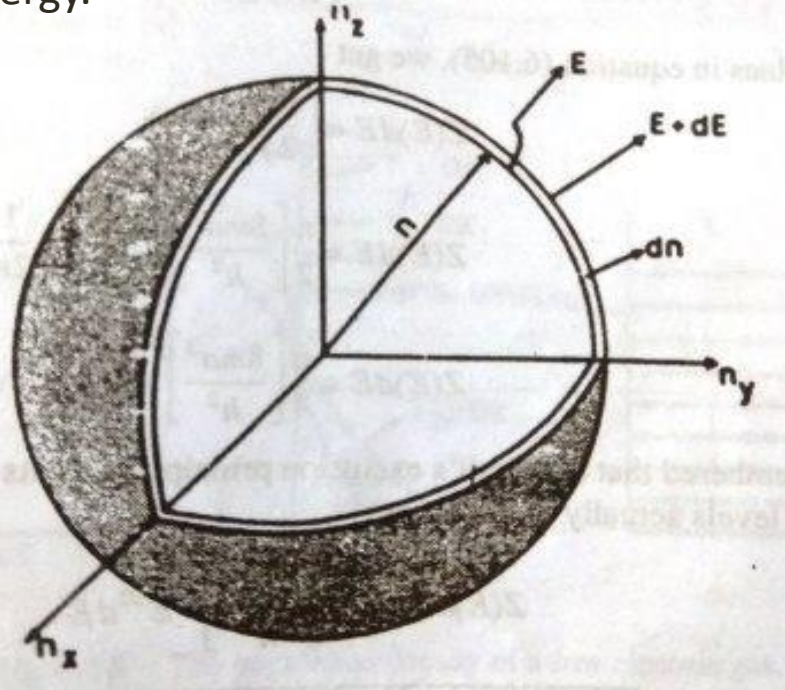
The density of states is once again represented by a function $g(E)$ which this time is a function of energy and has the relation $g(E)dE$ = the number of states per unit volume in the energy range: $(E, E+dE)$.

Failures of Quantum free electron theory

- This theory did not include mean free path.
- Could not explain conductivity of divalent and trivalent atoms
- Relaxation time is assumed to be same for thermal and electrical conductivity but they are not same. Phonons also carry thermal energy.
- Fermi surface considered spherical but it is not spherical
- Could not explain metallic properties of crystals

Material	Valency	ρ ($\Omega \bullet$m) at 20 °C Resistivity	σ (S/m) at 20 °C Conductivity
Silver	1	1.59×10^{-8}	6.30×10^{7}
Copper	1,2	1.68×10^{-8}	5.96×10^{7}
Gold	1,3	2.44×10^{-8}	4.10×10^{7}
Aluminum	3	2.82×10^{-8}	3.5×10^{7}
Zinc	2	5.90×10^{-8}	1.69×10^{7}

Band theory of solids

❑ In the free electron theory a constant potential was assumed inside the solid.

❑ In reality the presence of the positive ion cores gives rise to a varying potential field. In a simple model the potential as in Fig.1 can be assumed ('a' is the lattice spacing and 'w' is the width of the potential). If 'w' $\rightarrow$ 0, we get 'δ' functions.

❑ The travelling electron wave interacts with this periodic potential (for a crystalline solid).

❑ The electron wave can be Bragg diffracted.

Kronig- Penney Model

$$a$$

Actual Potential

$$V \qquad \text{Kronig-Penny Model} \qquad V_0 \qquad X$$

$$w$$
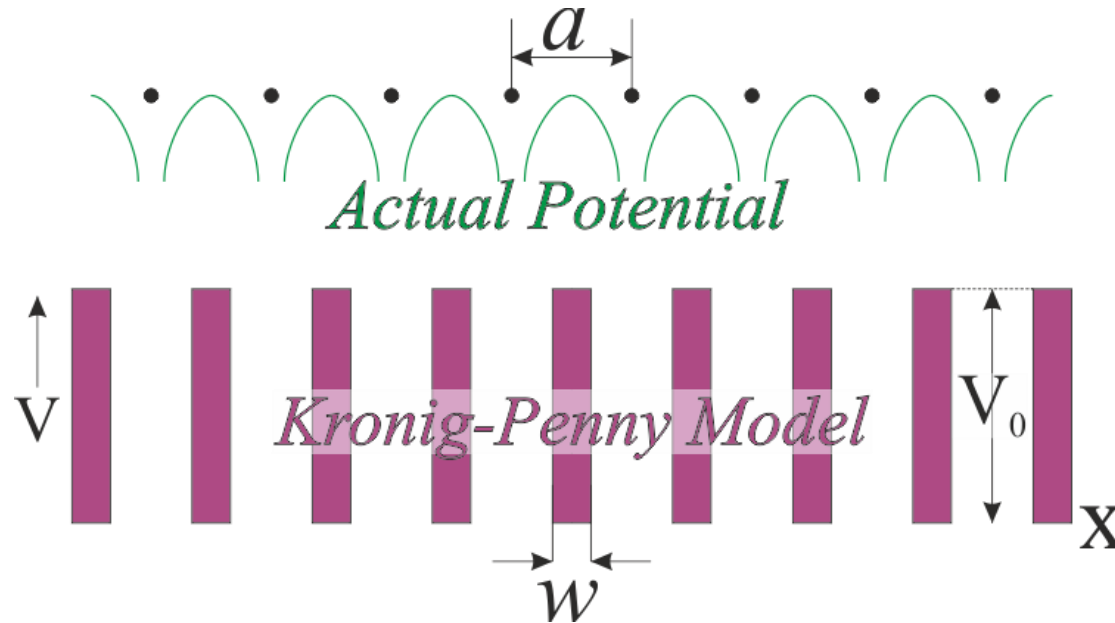
Bragg diffraction from a 1D solid

$n\lambda = 2d \, Sin\theta$

$1D \Rightarrow \theta = 90^{\circ}$

$n\lambda = 2a$

$n2\pi/k = 2a$

$$k = \frac{n\pi}{a}$$

$$\lambda_{Critical} \in \left[2a, \ a, \ \frac{2a}{3}, \ ... \right]$$

$$k_{Critical} \in \left[\pm\frac{\pi}{a}, \ \pm\frac{2\pi}{a}, \ \pm\frac{3\pi}{a}, \ ... \right]$$

$$E = \frac{h^2 k^2}{8\pi^2 m}$$

$-\frac{2\pi}{a}$ $-\frac{\pi}{a}$ $+\frac{\pi}{a}$ $+\frac{2\pi}{a}$

Band gap

E →
k →

First Brillouin Zone
Second Brillouin Zone
Third Brillouin Zone
Fourth Brillouin Zone

E
k

Band Gap
Band Gap
Band Gap

0   π/a   2π/a   3π/a   4π/a
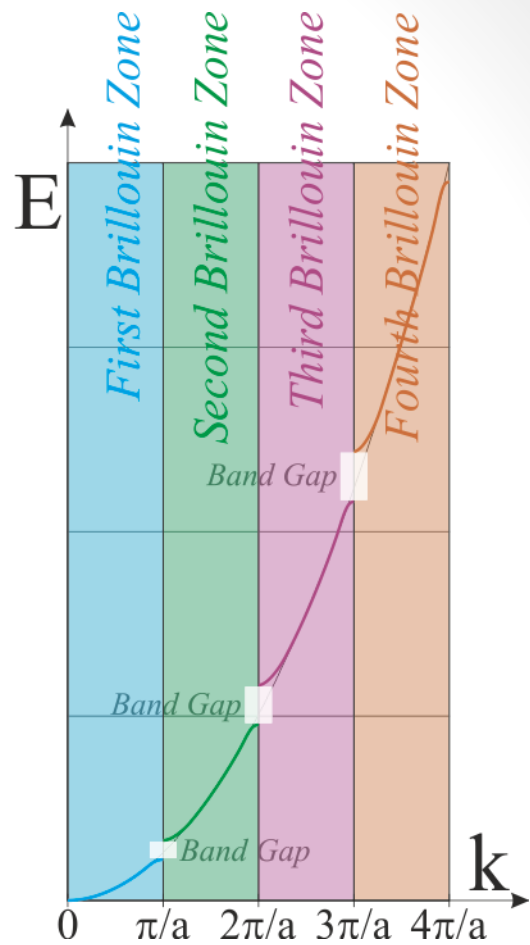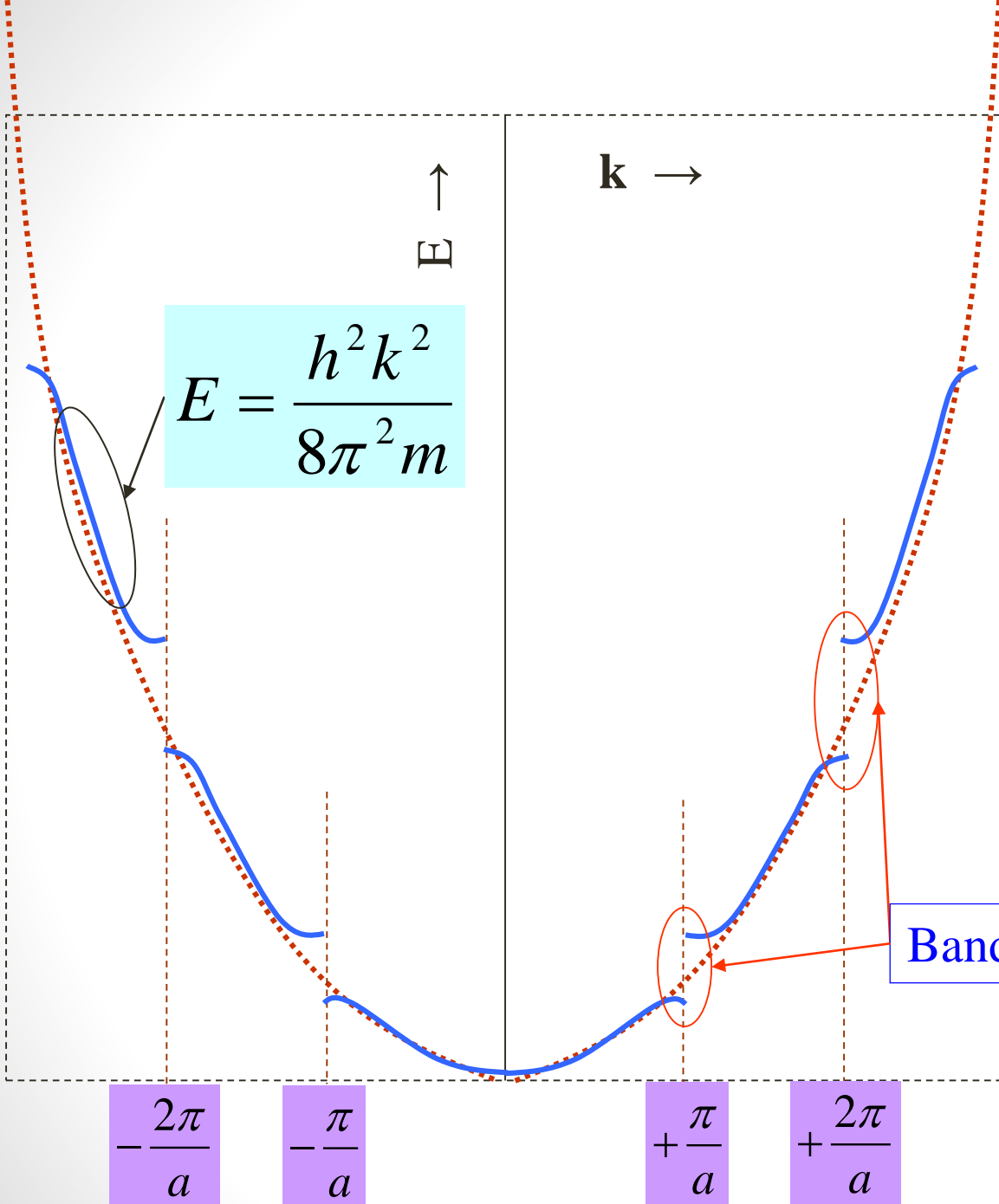
- The Velocity of electrons for the above values of k are zero.

- These values of k and the corresponding E are forbidden in the solid.

- The waveform of the electron wave is two standing waves.

- The standing waves have a periodic variation in amplitude and hence the electron probability density in the crystal.

- The potential energy of the electron becomes a function of its position

(cannot be assumed to be constant (and zero) as was done in the free electron model).
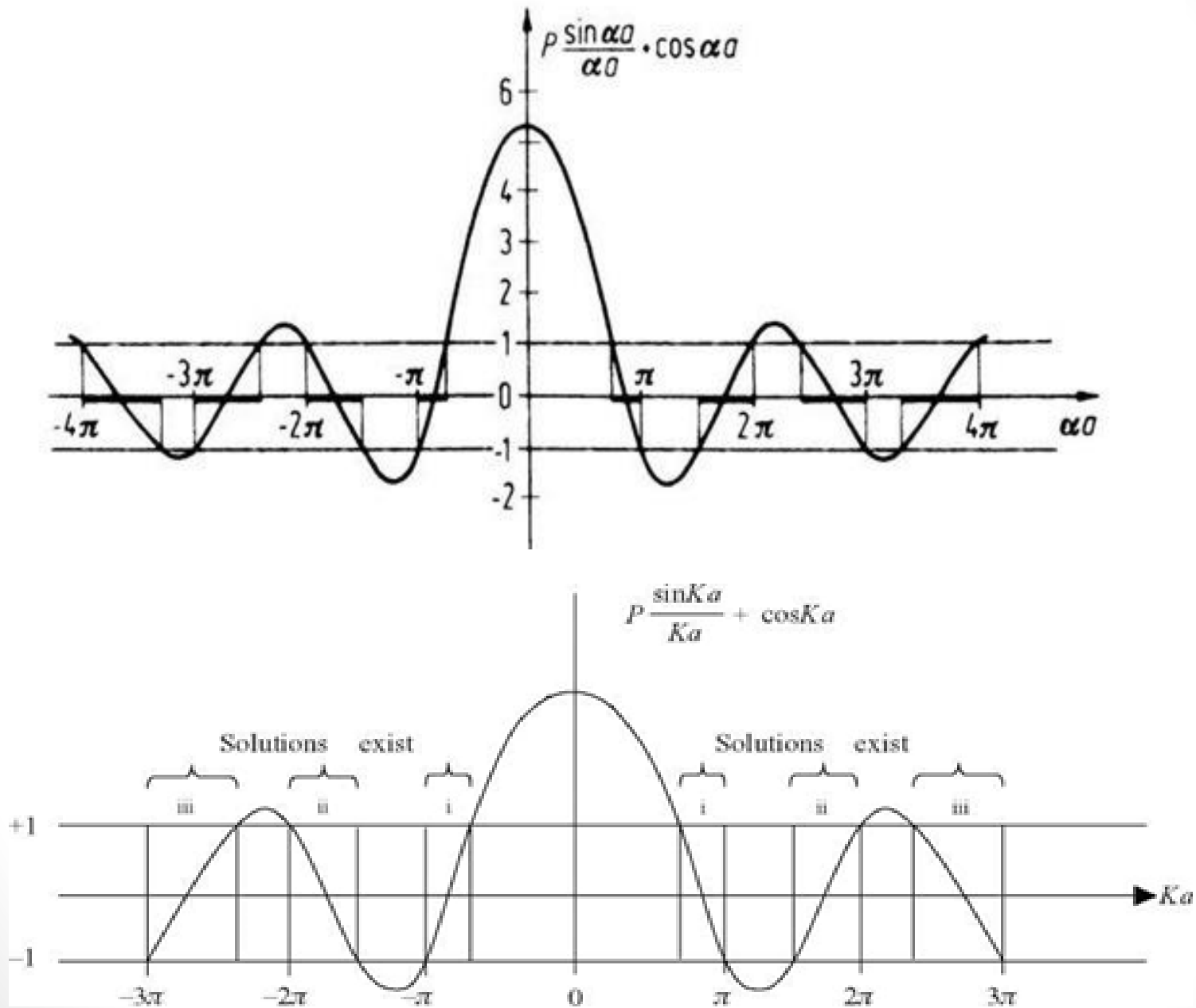
Figure 1.2 Graph of right hand side of Equation 1.8 as a function of P for P = 2

E-K diagrams: Energy is periodic in K

1) Periodic Zone
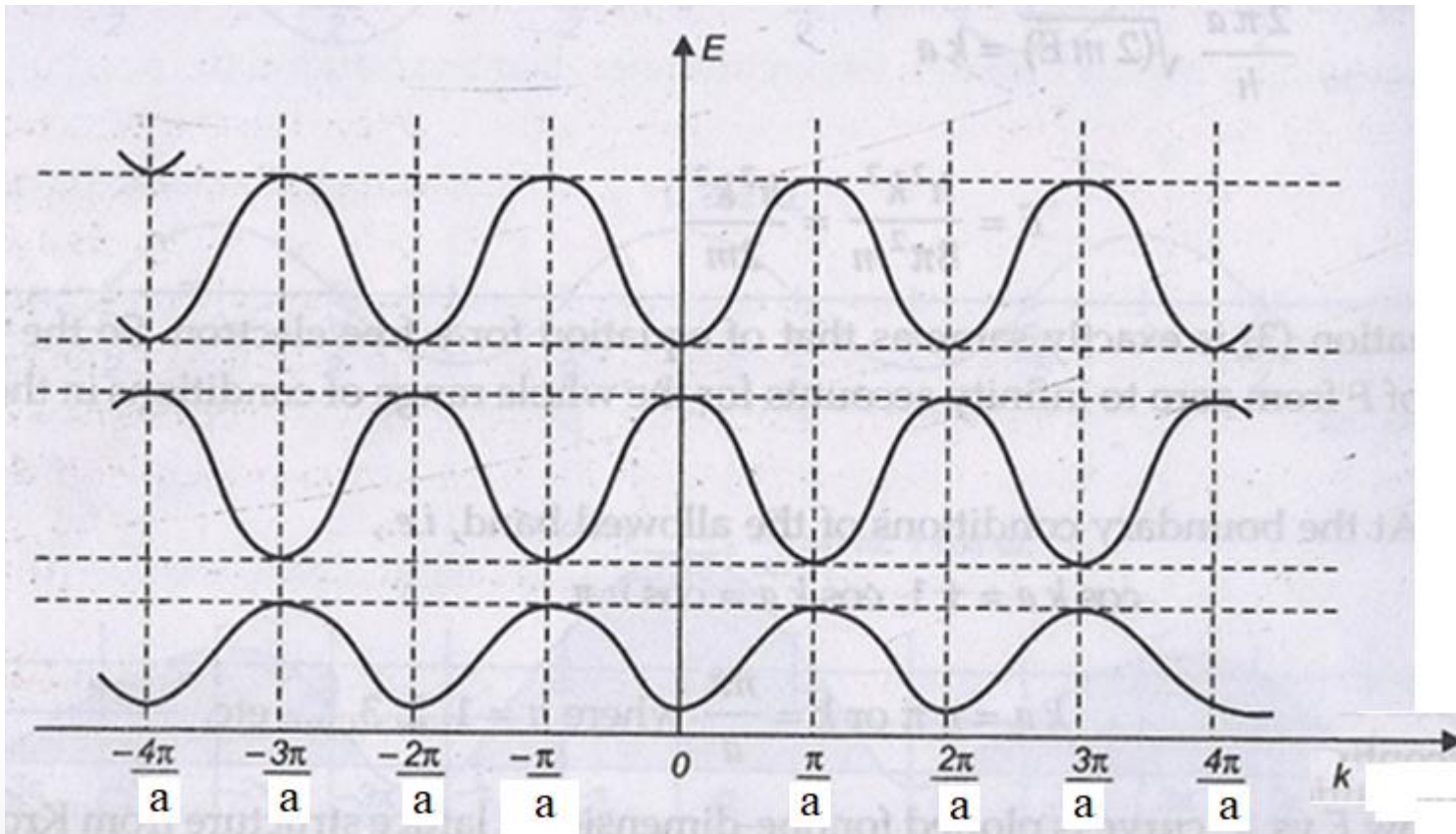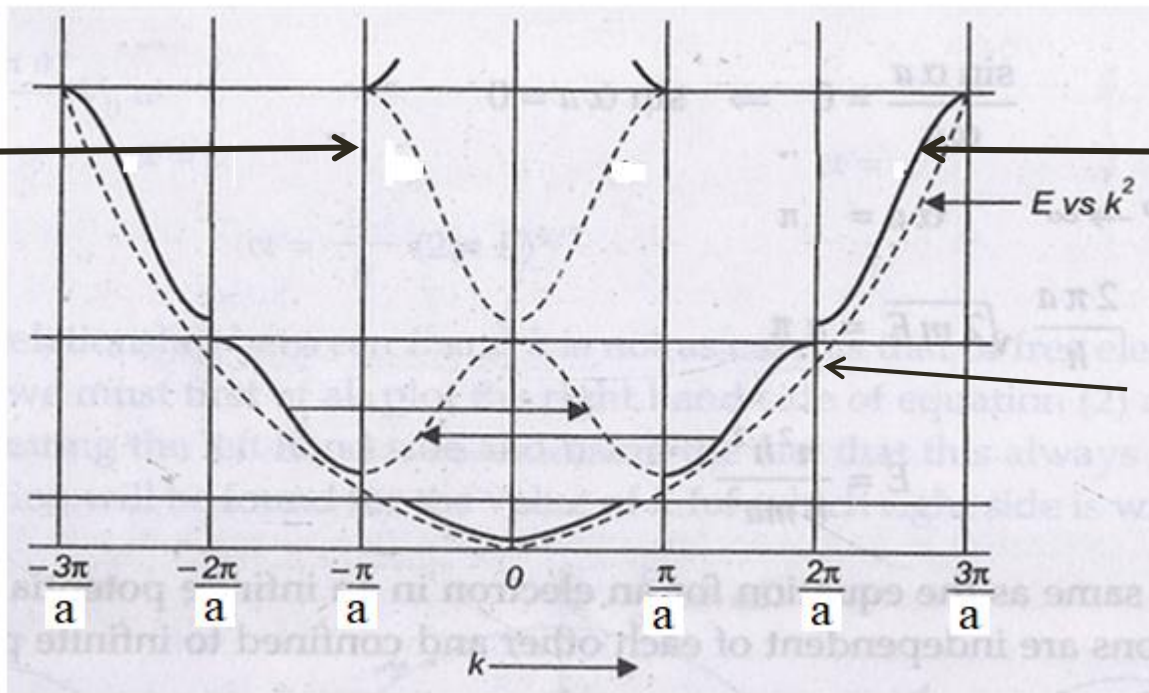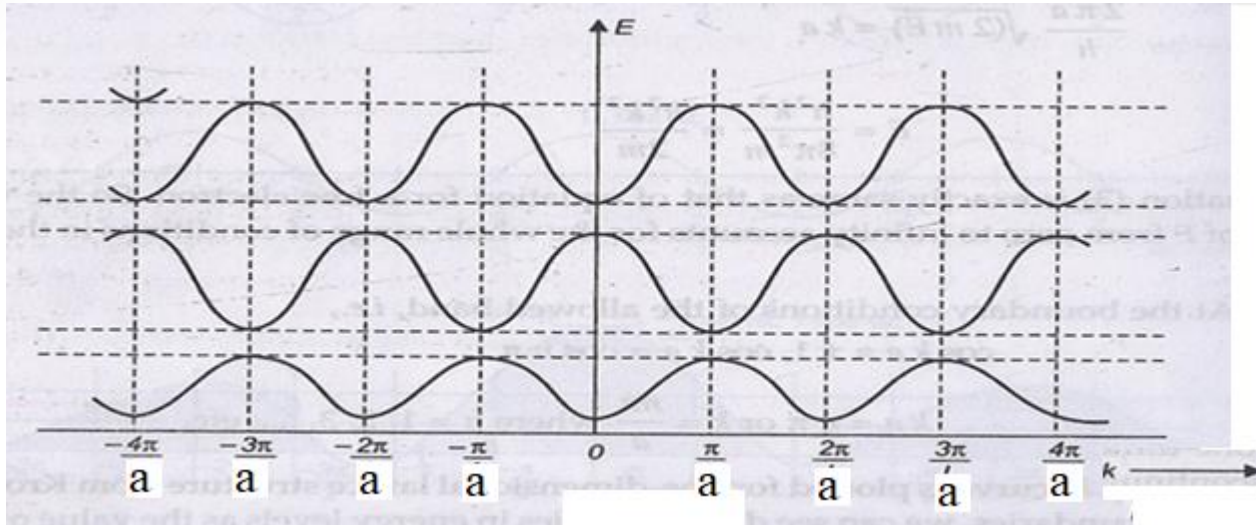
Reduced Zone

Extended Zone

E vs k^2

E - k curve for-free electron.

Effective mass of electron

❑ The magnitude of the Energy gap between two bands is the difference in the potential energy of two electron locations.

❑ The effective mass of an electron (m*) in a solid could be different from the rest mass (m_0). The effective mass can be larger or smaller than the rest mass.

❑ Collisions with atoms increases the rest mass, while enhanced propagation in the crystal gives a reduced effective mass.

❑ From the concept of group velocity the effective mass can be deduced. It is related to the curvature of the E-k curve. Close to band edges, m^* can be negative.

$$m^* = \frac{h^2}{4\pi^2} \frac{1}{\left(d^2 E / dk^2 \right)}$$

K.E of the electron increasing
Decreasing velocity of the electron
−ve effective mass (m*) of the electron

Within a band
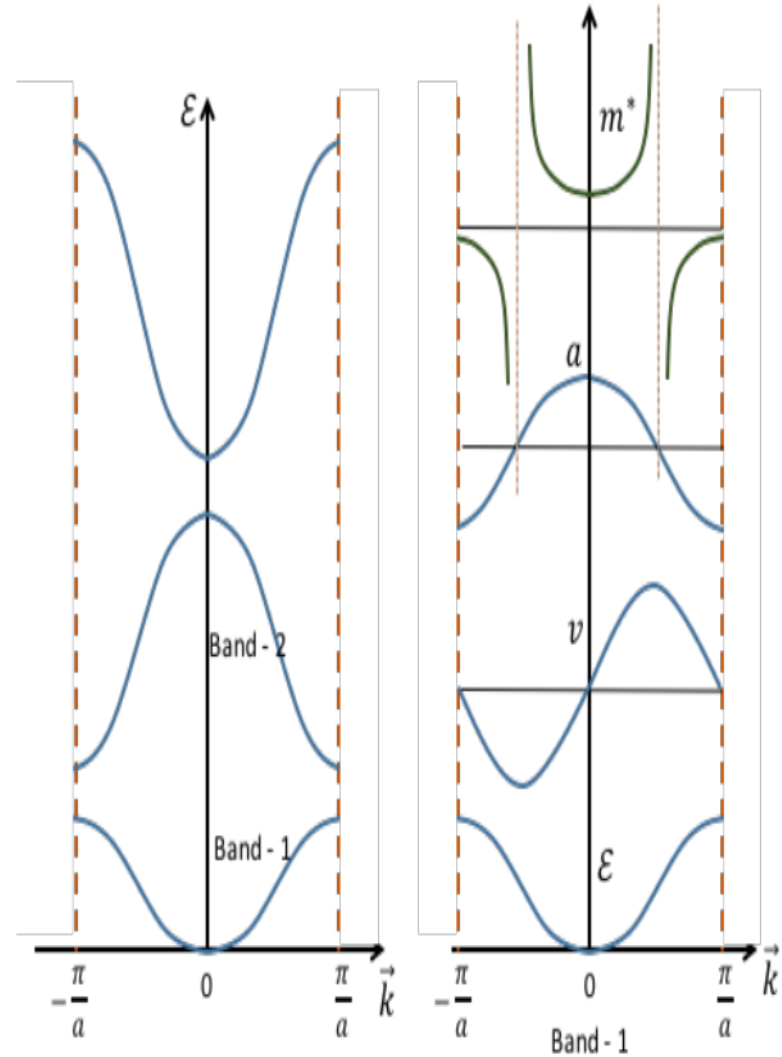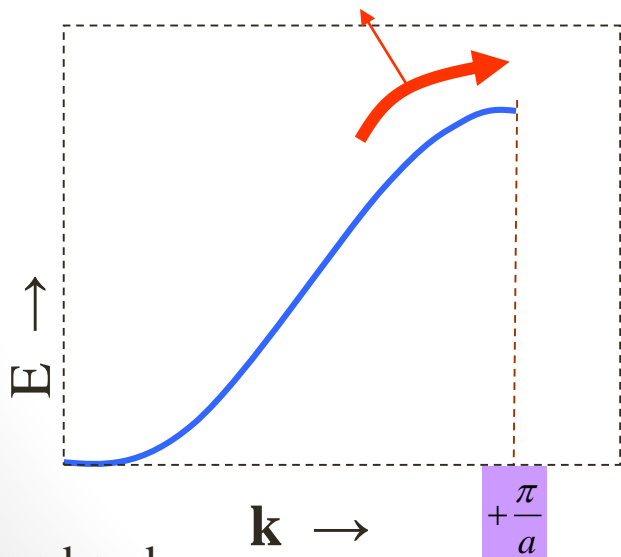
Direct indirect band gap
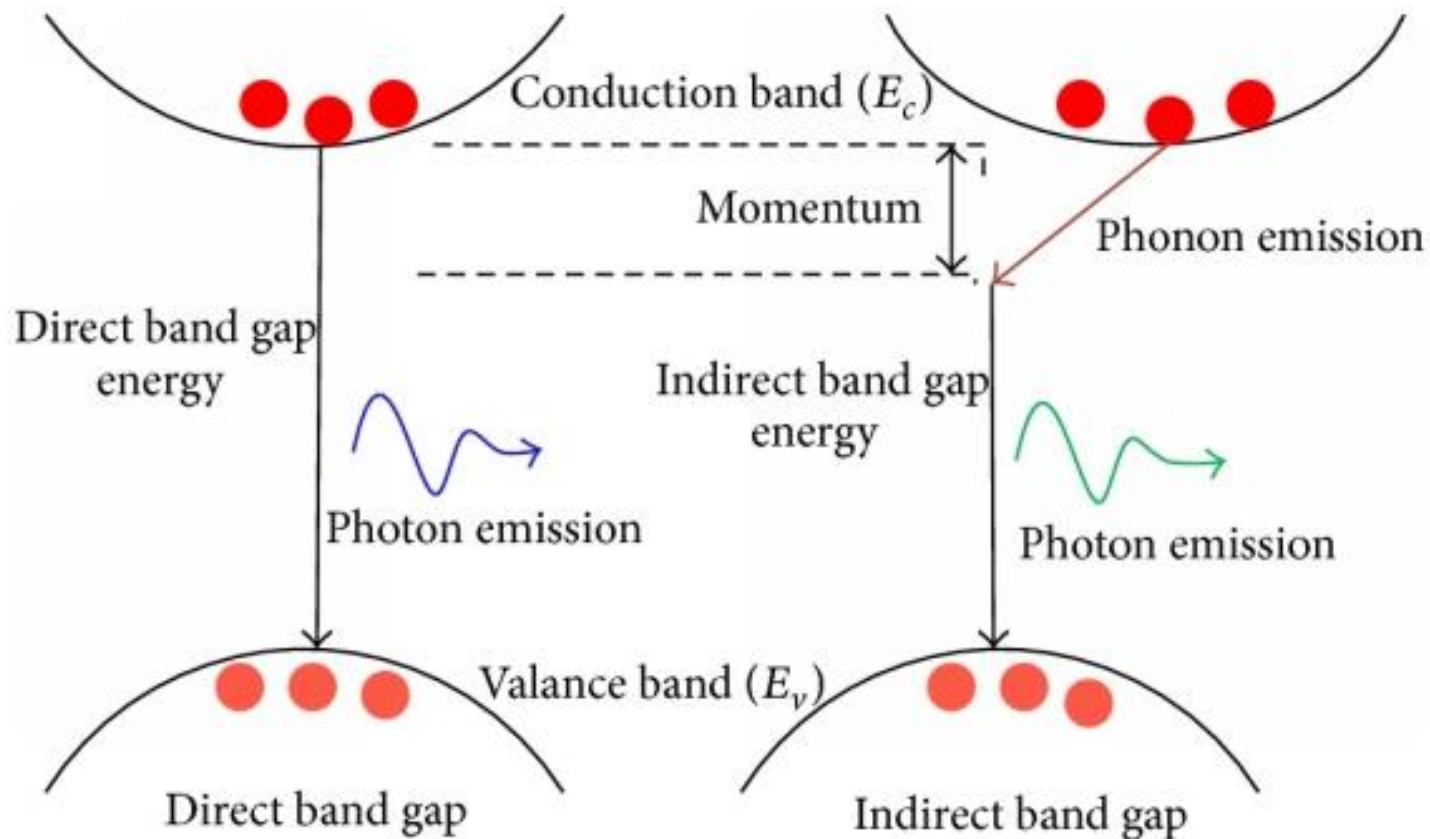
Types of electronic materials: metals, semiconductors, and insulators

Monovalent metals

Divalent metals

❑ Monovalent metals: Ag, Cu, Au → 1 e⁻ in the outermost orbital
⇒ outermost energy band is only half filled

❑ Divalent metals: Mg, Be → overlapping conduction and valence bands
⇒ they conduct even if the valence band is full

❑ Trivalent metals: Al → similar to monovalent metals!!!
⇒ outermost energy band is only half filled !!!

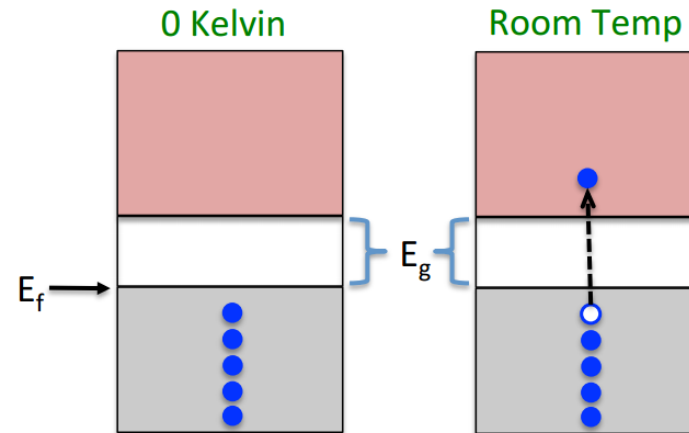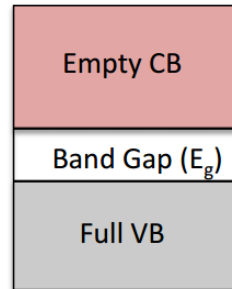# Energy band diagram: SEMICONDUCTORS

Semiconductor

Conduction Band

2-3 eV
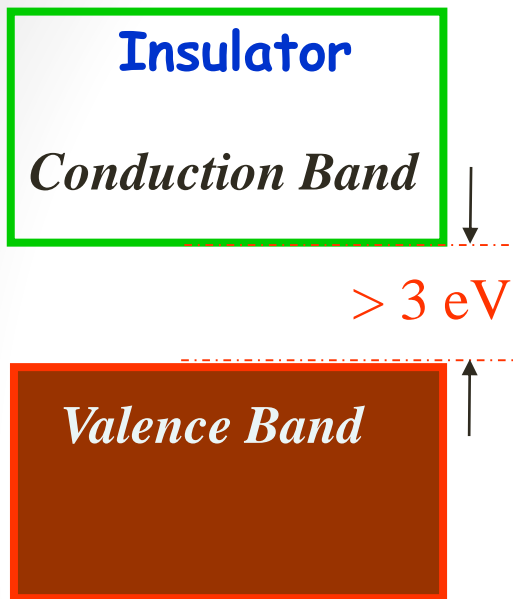
Valence Band

Band Gaps of some intrinsic semiconductors							
Material	Si	Ge	GaP	GaAs	InSb	CdS	ZnTe
Band Gap (eV)	1.11	0.67	2.25	1.42	0.17	2.4	2.26

Energy Band Diagram at 0K

Empty CB

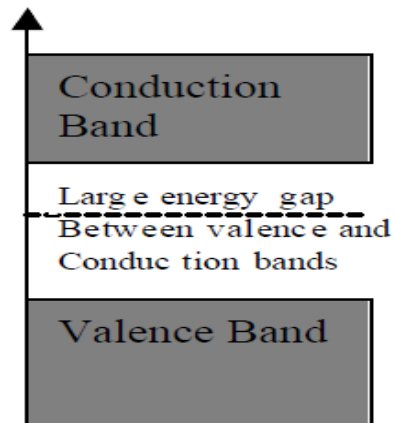Band Gap (E_g)

Full VB

0 Kelvin

Room Temp

E_f

E_g

❑ Elements of the 4th column (C, Si, Ge, Sn, Pb) → valence band full but no overlap of valence and conduction bands

❑ Diamond → PE as strong function of the position in the crystal
⇨ Band gap is 5.4 eV

❑ Down the 4th column the outermost orbital is farther away from the nucleus and less bound ⇒ the electron is less strong a function of the position in the crystal ▶ reducing band gap down the column
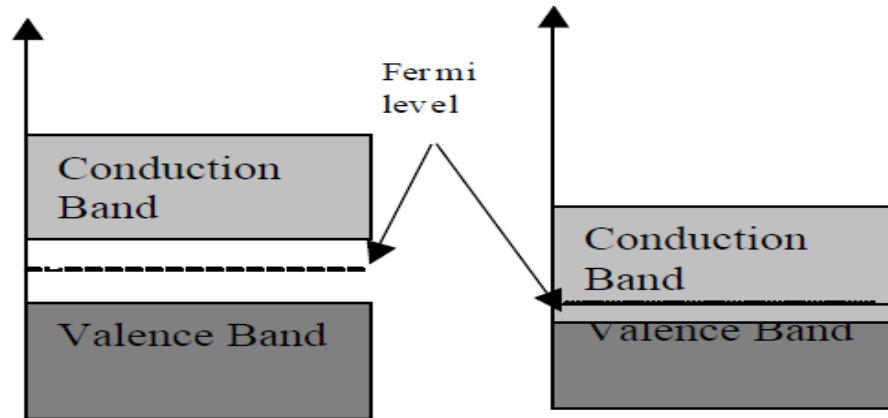
Insulator

Conduction Band

> 3 eV

Valence Band

Insulators does not have any feevetive free electron. Therefore, transition of electron from valence band to conduction band is not posiible.

Conduction Band

Large energy gap Between valence and Conduction bands

Valence Band

Insulator

Conduction Band

Valence Band

Semiconductor

Fermi level

Conduction Band

Valence Band

Conductor