1.What are the postulates of classical free electron theory?

Postulates of classical free electron theory are –

1. A solid metal has a nucleus with revolving electrons. The electrons move freely like molecules in gas.

2. The free electrons move in a uniform potential field due to the ions fixed in the lattice.

3. In the absence of an electric field (E=0), The free electrons move in random directions and collide with each other. During this collision no loss of energy is observed since the collisions are elastic.

4. In the presence of an electric field (E not equal to 0), electrons are accelerated in the direction opposite to the direction of the applied electric field.

5. Since the electrons are assumed to be perfect gas, they obey laws of classical theory of gasses.

6. Classical free electrons in metal obey Maxwell-Boltzmann statistics.

2. Write the success of classical free electron theory.

Success of classical free electron theory are –

1. It verifies Ohm's law.
2. It explains the electrical and thermal conductivities of metals.
3. It derives from Wiedemann – Franz law (The relation between electrical conductivity and thermal conductivity).

4. It explains optical properties of metals.

3. Write any three failures of classical free electron theory.

Three drawbacks of classical free electron theory –

1. The phenomena such as photoelectric effect, Compton effect and black body radiation couldn't be explained by classical free electron theory.
2. It cannot explain the electrical conductivity of semiconductors and Insulators.
3. Ferromagnetism cannot be explained by theory.

4. What are the postulates of quantum free electron theory?

Assumptions (Postulates) of Quantum free electron theory

1. In a metal the available free electrons are fully responsible for electrical conduction.
2. The electrons move in a constant potential inside the metal. They cannot come out from the metal surface and have very high potential barriers.
3. Electrons have wave nature; the velocity and energy distribution of the electron is given by the Fermi-Dirac distribution function.
4. The loss of energy due to interaction of the free electron with the other free electron.

5. Electrons are distributed in various energy levels according to the Pauli Exclusion Principle.

5. Write the success of quantum free electron theory.

Success of quantum electron theory-

1. It successfully explains the electrical and thermal conductivity of metals.
2. We can explain the Thermionic phenomenon.
3. Temperature dependence of conductivity of metals can be explained by this theory.
4. It can explain the specific heat of metals.
5. It explains magnetic susceptibility of metals.

EX1 - Write any three failures of classical free electron theory.

Failures of classical free electron theory are –

1. It is unable to explain why certain crystals have metallic properties and others do not.
2. Failed to give difference of metals/semiconductors/ insulators
3. It is unable to explain why the atomic arrays in metallic crystals should prefer certain structures only.

6. Write a short note on Band theory of solids.

Bloch initiated this theory in which the electrons move in a periodic potential provided by periodicity of the crystal lattice and developed by Kronig-penney and others.

It explains the mechanisms of conductivity, semiconductivity on the basis of energy bands and hence band theory.

In band theory of solids, Every molecule comprises various discrete energy levels, there are many energy bands but the following are the three most important energy bands in solids:

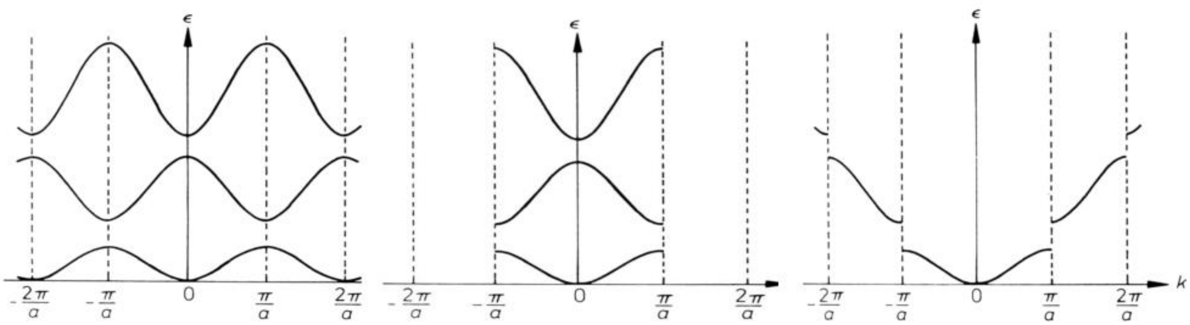
- Valence Band
- Conduction Band
- Forbidden Band

7.Explain three types of E-K diagrams.

E-K diagram is the diagram of energy of electron on the wave number ‘k’ is given by E-K diagram where E is directly proportional to K^2

There are three types of E-K diagrams:

Extended, reduced and periodic Brillouin zone schemes



Periodic Zone **Reduced Zone** **Extended Zone**

All allowed states correspond to k-vectors in the first Brillouin Zone.

Can draw E(k) in 3 different ways

24

1. Periodic zone scheme -

   The periodic repetition of allowed energy values corresponding to each allowed band can be represented as being obtained by the periodic repetition of religion -PIE/a<k<PIE/a through whole K-space.

   The representation Ek = Ek + G shows all energy levels in all regions of the wave vector space. It is called the **periodic zone scheme.**

2. Extended Zone scheme :

In this scheme, Different bands are drawn in different zones in K-space. Hence a discontinuous is observed at k = +-n*pie/a where n=+-1,+-2,.....

The representation $Ek = h^2k^2 / 2m$ shows all bands in the first Brillouin zone only. It is called the **reduced zone scheme.**

3. Reduced zone scheme :

   In this scheme, from right to left to k axis through distance which are integral multiples of 2*pie/a so that they all fit within the interval -pie/a<k<pie/a in the first brillouin zone.

   Their **extended zone scheme** shows different bands in different Brillouin zones with discontinuities at zone edges.

8.What is meant by the Brillouin Zone? Explain.

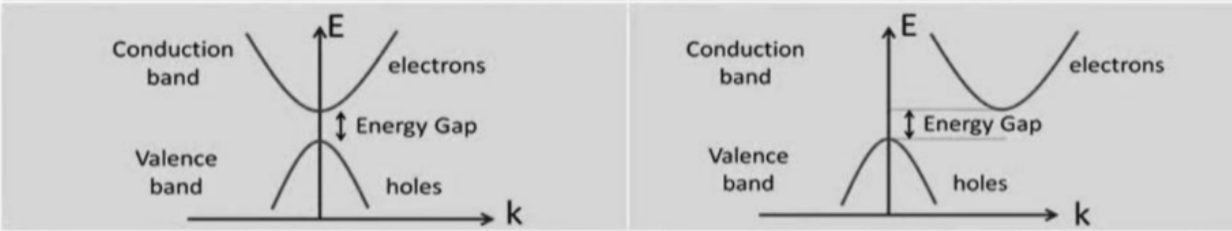
Brillouin zones are the specific regions in reciprocal space of a given Bravais lattice space, where the properties of Bloch electrons are usually studied.

First brillouin zone- Region in space that you can reach from the origin of the reciprocal space without crossing any Bragg plane.

Second brillouin zone- Region in space that you will reach by crossing only one Bragg plane and no more.

Third brillouin zone- Region in space that we will reach by crossing 2 Bragg planes without crossing 3rd Bragg plane .

9.Write any three differences between direct and indirect band gap semiconductors.



Direct bandgap Semiconductors	Indirect bandgap Semiconductors
Maximum of valence band and minimum of conduction band occur at same momentum values	Maximum of valence band and minimum of conduction band occur at two different momentum values.
Electron making a transition from valence band to conduction band need not undergo any change in its momentum.	In order to make a transition from maximum point in valence band to minimum point in conduction band, the electron requires energy for the change in momentum in addition to the energy gap E_g
The compound semiconductors such as GaAs, are direct gap semiconductors	All elemental semiconductors such as Si, Ge, are indirect gap semiconductors
These direct gap semiconductors are used in LED and Semiconductor Lasers.	Not useful for LEDs and Semiconductor Lasers

10. Write a short note on Phonons.

A packet of these waves can travel throughout the crystal with a definite energy and momentum, so in quantum mechanical terms the waves can be treated as a particle, called a **Phonon**.
A phonon is a definite discrete unit or quantum of vibrational mechanical Energy, just as a photon is a quantum of electromagnetic or light energy. It is named phonons because at high energy levels long wavelength phonons give rise to sound. According to quantum mechanics, similar particles have wave nature, waves must also have particle nature. So, phonons are also treated as quasi particles. Similar to particles, these waves can carry throughout the crystal, heat, energy and momentum.

11. What is effective mass? Obtain the expression for effective mass of electrons.

Effective mass is that mass which a particle seems to have when it is present in a crystal of periodic potential.

Its given by the expression m* = h^2(d^2E/dk^2)^-1 where E and K are energy of particle and crystal momentum.

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

Now $$\frac{dE}{dk} = \frac{d}{dk}\left[\frac{(\hbar k)^2}{2m}\right] = \frac{2\hbar^2 k}{2m} = \frac{\hbar^2 k}{m}$$

and $$\frac{d^2E}{dk^2} = \frac{d}{dk}\left(\frac{dE}{dk}\right) = \frac{d}{dk}\left(\frac{\hbar^2 k}{m}\right) = \frac{\hbar^2}{m}$$

Thus, the effective mass, m*, is defined to be

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

and $$m^* = \frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)}$$

12. Explain probability of occupation in a given energy level using Fermi-Dirac distribution?

At temperature T>0K, the distribution of electrons over a range of allowed energy levels at thermal equilibrium is given by fermi-dirac distribution function

$$f(E) = \frac{1}{1+e^{\left(\frac{E-E_F}{kT}\right)}}$$

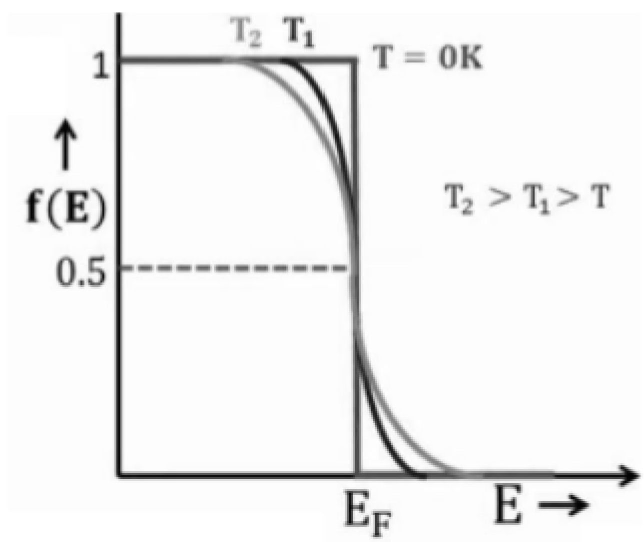
f(E) is the probability of occupancy for energy level E

E_F is Fermi energy

T is temperature in ^{0}K and

$k = 1.38 \times 10^{-23} J/K = 8.625 \times 10^{-5} eV/K$

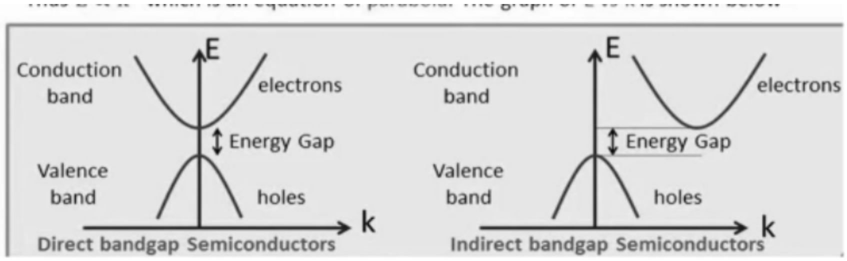
As the temperature increases, empty levels will be created below the fermi level and filled levels above the fermi levels. Probability of occupancy below fermi level is no longer one and above fermi level is no longer zero. As we increase the temperature more empty levels occur below the fermi level and more filled levels above the fermi level. Probability of occupancy reduces below the fermi level and probability of occupancy increases above the fermi levels.



13. Write any three differences between N-type and P-type semiconductors

N-type semiconductor	P-type semiconductor
1. It is an extrinsic semi-conductor which is obtained by doping the impurity pentavalent impurity atoms such as antimony, phosphorous, arsenic etc. to the pure germanium or silicon semiconductor.	1. It is an extrinsic semiconductor which is obtained by doping trivalent impurity atoms such as boron, gallium, indium etc. to the pure germanium or silicon semiconductor.
2. The impurity atoms added, provide extra electrons in the structure, and are called donor atoms.	2. The impurity atoms added, create vacancies of electrons (i.e., holes) in the structure and are called acceptor atoms.
3. The electrons are majority charge carriers and holes are minority charge carriers.	3. The holes are majority charge carriers and eletrons are minority carriers.

14. Explain direct band gap and indirect band gap in materials with the help of E-K diagram.

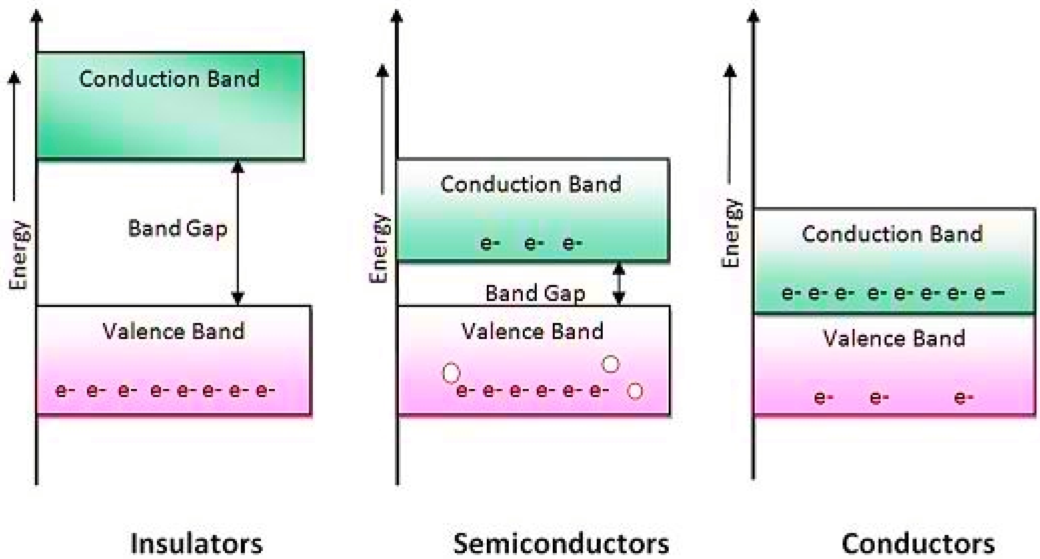


Maximum of valence band minimum of conduction band occurs at the same momentum value/k value it is called direct band gap semiconductors
Maximum of valence band minimum of conduction band occurs at different momentum value/k value it is called indirect band gap semiconductors

Upper parabola-- energy of electrons
Lower parabola- energy of holes

7

15. Write the classification of electronic materials on the basis of band theory.



- In the case of metallic conductors, the conduction band overlaps on the electrons in the valence band.
- In insulators, there is a large gap between both these bands. Hence, the electrons in the valence band remain bound and no free electrons are available in the conduction band.
- Semiconductors have a small gap between both these bands. Some valence electrons gain energy from external sources and cross the gap between the valence and conduction bands. By this movement, they create a free electron in the conduction band and a vacant energy level in the valence band for other valence electrons to move. This creates the possibility of conduction.

16. Evaluate the Fermi function for energy K B T above the Fermi energy.

2 . **Evaluate the Fermi function for energy K_BT above the Fermi energy.**

Solution:

We know Fermi Function $F(E) = \dfrac{1}{1+e^{(E-E_F)K_BT}}$

For an energy K_BT aboveFermi energy

$$E-E_F = K_BT$$

$$F(E) = \frac{1}{1+e^1} = \frac{1}{1+2.7183}$$

Fermi distribution function $F(E) = 0.2689$

17. What is meant by density of states? Derive expression for density of states and plot the 'energy' versus 'density of states' graph.

Density of states is defined as the number of available electrons states per unit volume in an energy interval between E and E + dE.

Number of electrons in an energy state =

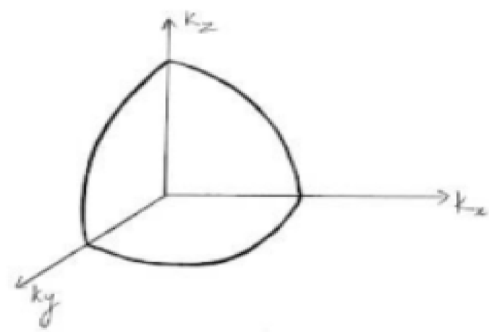
$$\int Z(E)\, P(E) dE$$

The density of state for 3D is defined as the number of electronic or quantum states per unit energy range per unit volume and is usually defined as $D(E)_{3D}$

$$D(E)_{3D} = \frac{1}{V}\frac{dN}{dE} \quad ...(12)$$

Volume

$$V = \left(\frac{\pi}{L}\right)^3$$



Volume of the 8th part of the sphere in K-space

$$= \frac{1}{8} \times \frac{4}{3}\pi K^3$$

$$\therefore\ N = 2 \times \frac{1}{8} \times \frac{4}{3}\pi K^3 \left(\frac{L}{\pi}\right)^3 \quad ...(13)$$

Here factor 2 comes because each quantum state contains two electronic states, one for spin up and other for spin down.

Eq. (12) can be written as

$$D(E)_{3D} = \frac{1}{V}\frac{dN}{dK} \times \frac{dK}{dE} \quad ...(14)$$

From eq. (13) we have

$$\frac{dN}{dK} = \pi K^2 \left(\frac{L}{\pi}\right)^3 \quad ...(15)$$

As we know

$$E = \frac{\hbar^2 K^2}{2m}$$

So

$$\frac{dE}{dK} = \frac{\hbar^2 K}{m}$$

And

$$\frac{dK}{dE} = \frac{m}{\hbar^2 K} \quad ...(16)$$

By using Eqs. (15)and (16), eq. (14) becomes

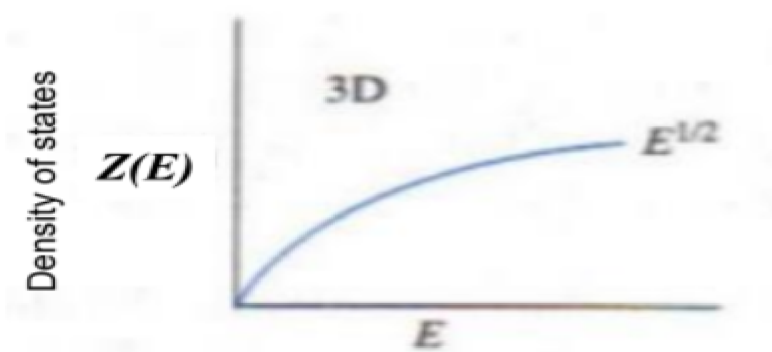
$$D(E)_{3D} = \frac{1}{L^3} \times \pi K^2 \left(\frac{L}{\pi}\right)^3 \times \frac{m}{\hbar^2 K}$$

$$D(E)_{3D} = \frac{mK}{\pi^2 \hbar^2}$$

$$D(E)_{3D} = \frac{m}{\pi^2 \hbar^2}\frac{\sqrt{2mE}}{\hbar} \quad (\hbar = \frac{h}{2\pi})$$

$$D(E)_{3D} = \frac{\sqrt{2} m^{\frac{3}{2}}}{\pi^2 \hbar^2} E^{\frac{1}{2}}$$

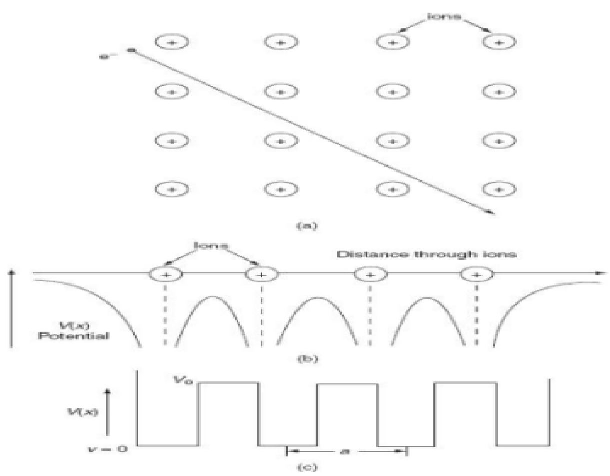
$$D(E)_{3D} \propto E^{\frac{1}{2}}$$



18. What is the Kronig Penney model and explain the band formation in solids using the Kronig Penney model.

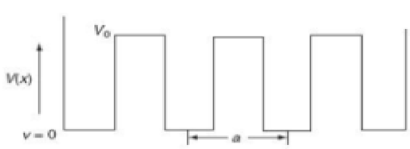
Kronig Penney model :

- According to Kronig and Penney the electrons move in a periodic square well potential.
- This potential is produced by the positive ions (ionized atoms) in the lattice.
- The potential is zero near to the nucleus of positive ions and maximum between the adjacent nuclei. The variation of potential is shown in figure.

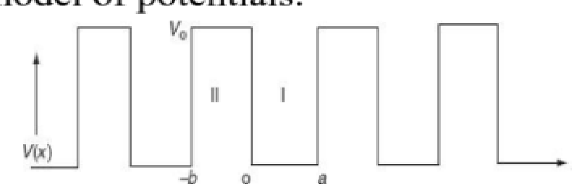


4

It is not easy to solve Schrödinger's equation with Bloch potentials. So, Kronig and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in Fig. (c). This model is called Kroning-Penney model of potentials.



(c)



The energies of electrons can be known by solving Schrödinger's wave equation in such a lattice. The Schrödinger time-independent wave equation for the motion of an electron along X-direction is given by: $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi = 0$

The energies and wave functions of electrons associated with this model can be calculated by solving time-independent one-dimensional Schrödinger's wave equations for the two regions I and II as shown in Fig

5

The Schrödinger's equations are:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$ for $0<x<a$.............(2)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V_o]\,\psi = 0$$ for $-b<x<0$.............(3)

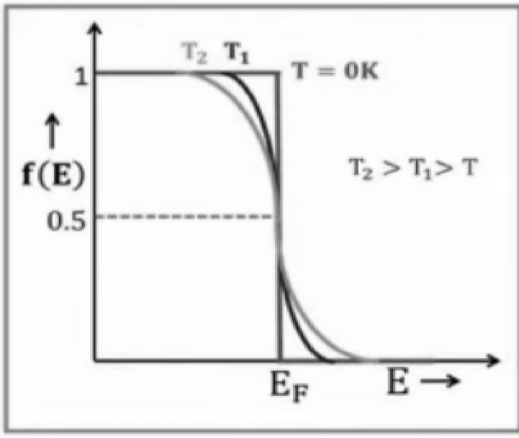
We define two real quantities (say) α and β such that:

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad \beta^2 = \frac{2m}{\hbar^2}(V_0 - E) \quad \text{———— (5.43)}$$

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0$$ for $0<x<a$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0$$ for $-b<x<0$

19. Prove that the probability of finding an electron at Fermi level is 0.5 at a temperature above absolute zero.



$$f(E) = \frac{1}{1 + e^{\left(\frac{E-E_F}{kT}\right)}}$$

At $T > 0$ K, For $E = E_F$

$$e^{\left(\frac{E-E_F}{kT}\right)} = e^{\frac{0}{kT}} = e^0 = 1$$

$$\therefore f(E) = \frac{1}{1 + e^{\left(\frac{E-E_F}{kT}\right)}} = \frac{1}{1+1} = \frac{1}{2}$$

At $T > 0$ K, probability of occupancy for Fermi level is always half

At any temperature, the probability of occupancy at fermi evel is always 0.5

20. Compare a direct band gap and an indirect band gap semiconductor material with an example for each.

Sr. No	Direct Band gap semiconductor	Indirect band gap semiconductor
1	A direct band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band aligns with the minimum energy level of the conduction band with respect to momentum.	A indirect band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band are misaligned with the minimum energy level of the conduction band with respect to momentum.
2	In a DBG semiconductor, a direct recombination takes place with the release of the energy equal to the energy difference between the recombining particles.	Due to a relative difference in the momentum, first, the momentum is conserved by release of energy and only after both the momenta align themselves, a recombination occurs accompanied with the release of energy.
3	The efficiency factor of a DBG semiconductor is much more than that of an IBG semiconductor.	The probability of a radiative recombination, is much less in comparison to that in case of DBG semiconductors
4	The most thoroughly investigated and studied DBG semiconductor material is Gallium Arsenide (GaAs).	The two well-known intrinsic semiconductors, Silicon and Germanium are both IBG semiconductors.
5	DBG semiconductors are always preferred over IBG for making optical sources.	The IBG semiconductors cannot be used to manufacture optical sources.

21. Calculate the minimum energy of an electron bound in a one-dimensional well of width 5 nm.

$l = 5\times10^{-9}\,m$

$$E_1 = \frac{h^2}{8ml^2} \rightarrow \frac{(6.63\times10^{-34})^2}{8\times9.1\times10^{-31}\times5\times10^{-9}\times5\times10^{-9}}\,J$$

$$\Rightarrow 0.0241\times10^{-17}\,J$$

(or) $$\frac{0.0241\times10^{-17}\,J}{1.6\times10^{-19}} = 1.509\,eV$$

MCQs

1. Density of states for a given material is __________.

a. Directly proportional to square root of energy
b. Inversely proportional to square root of energy
c. Directly proportional to cube root of energy

d. inversely proportional to cube root of energy

$$D(E)_{3D} \propto E^{\frac{1}{2}}$$

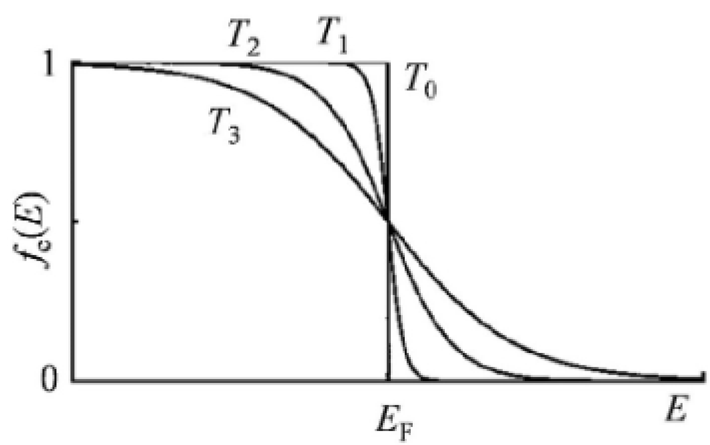
Soln - A

2. ______________ is defined as a “quantum of lattice ________”.

a. Photon, vibration
b. Phonon,vibration
c. Fermion,Oscillation
d. Boson,Vibration

Soln -(B)- The Phonos are vibrations of the atomic lattice.

3. The figure given below shows the variation of Fermi function (f(E)) with temperature. Analyze and identify the trend of temperature variation.



As the temperature increases, empty levels will be created
below the fermi level and filled levels above the fermi levels
Probability of occupancy below fermi level is no longer one and
above fermi level is no longer zero. As we increase the temperature
more empty levels occur below the
fermi level and more filled levels above the fermi level. Probability of
occupancy reduces below the fermi level and probability of
occupancy increases above the fermi levels

Here T3>T2>T1

ALTISM OP……

ALTISM OP…….