UNIT-2 BAND STRUCTURE OF SOLIDS

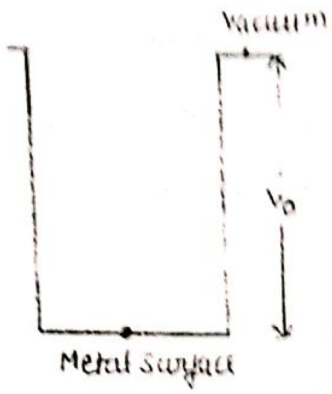
FREE ELECTRON THEORY (QUALITATIVE IDEA) AND ITS FEATURES

In Drude in 1900, postulated that the metals consist of positive ion cores with the valence electrons moving freely among these cores. The electrons are however, bound to move within the metal due to electrostatic attraction between the positive ion cores and electrons. The potential field of these ion cores, which is responsible for such an interaction, is assumed to be constant throughout the metal and the mutual repulsion among the electrons is neglected. The behaviour of the electrons moving inside the metal is considered to be similar to that of atoms or molecules in perfect gas. These free electrons are also referred to as free electron gas and the theory is accordingly named as free electron gas model. However, the free electron gas differ from an ordinary gas in some respects.

(1) The free electron gas is negatively charged whereas the molecules of an ordinary gas are most neutral.

(2) The concentration of electrons in an electron gas is quite large as compared to the concentration of molecules in an ordinary gas.

The valence $\bar{e}^{ns}$ or conduction electrons obey Pauli's exclusion principle. These $\bar{e}^{ns}$ are responsible for conduction of electricity through metals. Since the electrons move in a uniform electrostatic field of ion cores, their potential energy is constant and normally taken as zero ie the existence of the +ve ion cores is ignored. Thus the total energy of a conduction electron is equal to its K.E. Since the movement of conduction electrons is restricted to within the crystal only the potential energy of a stationary electron inside a metal is less than the potential energy of an identical electron just outside it. This energy difference V_0 serves as a potential barrier and stops the inner electrons from leaving the surface of the metal. Thus in free electron gas model, the movement free electrons in a metal is equivalent to the movement of a gas ... tron gas inside a potential energy box which is taken as one is shown in figure.



...tric surface bounded potential barrier Vo, ...h represent difference potential energy of a ...ionary e present at surface of the metal and ...st outside in vacuum.

Based on the Drude's consideration that the electron gas behaves as a perfect gas, H.A Lorentz postulated in 1909 that the electrons constituting the electron gas obey Maxwell Boltzmann statistics under equilibrium conditions. The combined ideas of Drude and Lorentz constitute the Drude-Lorentz theory. As the theory is based on the classical ideas of Maxwell Boltzmann statistics, it is called the classical theory.

· The theory has been successfully applied to explain the various properties of metals:

(i) Validity of Ohm's law

) Since the electrons move freely inside the metals irrespective of ...e crystal structure, the ratio of the electrical conductivity σ to ...e thermal conductivity K should be constant for all metals at constant temprature

$$\frac{\sigma}{K} = \text{const}$$

This is called the widemann-Franz model.

) This theory also explains the high lustre and complete opacity ...f metals. The opacity is due to the absorption of all the incident ...e m radiations by free $\bar{e}^{ns}$ which are then set into forced oscillations. The electrons return to their normal states by emitting the same ...mount of energy in all direction thus producing metallic lustre.

FAILURE

The theory predicted that resistivity varies as $\sqrt{T}$ whereas actually it is found to vary linearly with temprature. The theory failed to explain the heat capacity and paramagnetic susceptibility of the

... properties are based on interactions of free electrons with the external sources of energy which may be thermal or magnetic in nature. The application of Maxwell-Boltzmann statistics of this theory allows all the free electrons to gain energy which results in much higher values of heat capacity and paramagnetic susceptibility. The use of the Fermi-Dirac or quantum statistics allows only a fraction of the total number of free electrons to gain energy, and the values of heat capacity and paramagnetic susceptibility thus obtained matched with the observed values.

The classical theory is also unable to account for the occurrence of long mean free paths (~ 10^8 to 10^9 interatomic spacings or more than one cm) at low temperature.

SOMMERFELD'S QUANTUM THEORY

Considering the free nature of valence electrons are assumed in the classical theory, Sommerfeld treated the problem quantum mechanically using Fermi-Dirac statistics rather than the classical Maxwell-Boltzmann statistics. The possible electronic energy states in the potential energy box and the distribution of electrons in these states are determined using quantum statistics.

FREE ELECTRON GAS IN ONE-DIMENSIONAL BOX.

Consider an electron of mass 'm' which is bound to move in one dim crystal of length 'L'. The electron is prevented from leaving the crystal by the presence of a large potential energy barrier at its surface. Although the barriers extend over a few atomic layers near the surface, these are taken infinitely large for the sake of simplicity. The problem is identical to that of an electron moving in a one-dimensional potential box which is represented by a