

Syllabus : Crystal systems and X-rays: Crystal systems-Bravais lattice; Miller indices– Spacing between lattice planes of cubic crystals, Continuous and characteristic X-ray spectra; Moseley's law, Scattering of X-rays - Compton effect, Bragg's law.

Introduction : A solid material has two basic properties, namely rigidity and elasticity. Thus, solids have definite shape and size. The following tabular column gives the types of solids

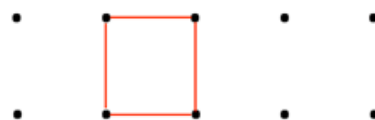
Types of solids	Definition	Examples
single crystals	Are solids having a regular, repetitive arrangement of atoms or molecules. They have Long range order and 3 – dimensional periodicity. Here the crystal lattice of the entire sample is continuous and unbroken to the edges of the sample	Quartz, salt, Iceland spar, diamond, topaz etc..
polycrystalline crystals	Or multicrystalline materials (microscopic crystals) are solids that are composed of many crystallites or grains of varying size and orientation.	Metals like copper, sodium, Magnesium etc..., some ceramics, rock, ice...
Quasicrystals	Long range order and no 3 –dimensional periodicity	Al ₇₂ Ni ₂₀ Co ₈
Amorphous materials	Are solids that lack long range order, i.e disordered or random atomic structure	Glass, plastic, silicon

Crystallography is a branch of science that deals with the geometric description of crystals and their internal atomic arrangement.

It is the symmetry of a crystal that has profound influence on its properties. Crystalline materials are solids with an atomic structure based on a regular repeated pattern across its whole volume. At long range length scales, each atom is related to every other equivalent atom in the structure by translational or rotational symmetry.

In crystallography, geometrical properties of the crystal are of interest. Thus an atom or a group of atoms are replaced by a geometric point.

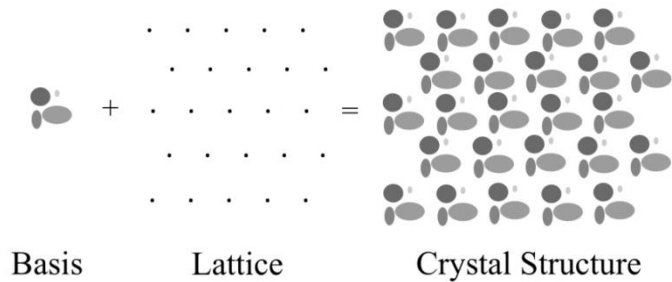
Crystal lattice : An infinite array of points in space is called the crystal lattice. Each point has an identical surroundings to all others as shown below.



Arrays are arranged in a periodic manner. The square shown represents a unit cell which is primitive. (This is in two dimension)

Basis and Crystal structure:

Every lattice point can be associated with one or more unit assembly of atoms or molecules identical in composition called **Basis**.

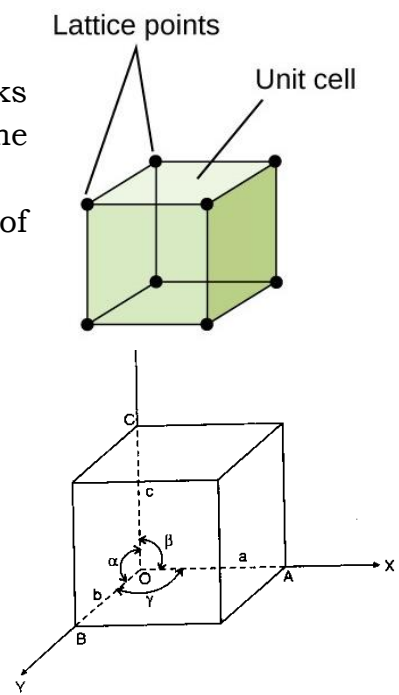


The regular periodic three-dimensional arrangement of Basis is called **Crystal Structure**. Thus lattice + basis = crystal structure.

Space lattice is imaginary. Crystal structure is real.

Unit cell and Lattice parameters

1. Atoms or groups of atoms forming building blocks of the smallest acceptable size of the whole volume of the crystal is defined as a **unit cell**
2. A unit cell is chosen to represent the symmetry of the crystal.
3. They are the basic building blocks of the crystal.
4. When these unit cells are translated in three dimensions, they will generate the crystal.
5. Each crystal lattice is described by a type of unit cell.
6. Each unit cell is described by three vectors a, b and c called the length of the sides and the interfacial angles α, β, γ between them. They are called **lattice parameters**



Primitive Cell

Primitive cell is defined as a geometrical shape which, when repeated indefinitely in three dimensions, will fill all space and it consists of **lattice points only at corners**. A unit cells may be primitive (simple) or Non-primitive (body centered, base centered, face centered).

Bravais lattice

A Bravais lattice is one in which all lattice points are identical in composition. Bravais showed that identical points can be arranged spatially to produce 14 types of regular pattern. These 14 space lattices are called Bravais lattices. According to Bravais, there are 14 lattices corresponding to seven crystal structures. They are cubic, tetragonal, orthorhombic, monoclinic, triclinic, trigonal (rhombohedral) and hexagonal.

SL.No.	Crystal system	Types of Bravais lattices	Number of Bravais lattices	Lattice parameters
1	Cubic	P, I, F	3	$a = b = c$ $\alpha = \beta = \gamma = 90$
2	Tetragonal	P, I	2	$a = b \neq c$ $\alpha = \beta = \gamma = 90$
3	Orthorhombic	P, I, F, C	4	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90$
4	Monoclinic	P, C	2	$a \neq b \neq c$ $\alpha = \gamma = 90 \neq \beta$
5	Triclinic	P	1	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
6	Rhombohedral (Trigonal)	P	1	$a = b = c$ $\alpha = \beta = \gamma \neq 90$
7	Hexagonal	P	1	$a = b \neq c$ $\alpha = \beta = 90, \gamma = 120$

In the above structures it is observed that the types of lattices are four.

(1) Simple denoted by P having lattice points only at the edges of the unit cell.

(2) Body centred denoted by I having a lattice point at the centre of the unit cell along with the edges.

(3) Face centred denoted by F having lattice points at the centres of all the faces of the unit cell along with edges.

(4) Base centred denoted by C having lattice points at the centres of the bases of the unit cell along with the edges.

Coordination number : It is defined as the number of particle immediately adjacent to each particle in the crystal lattice.

It is characteristic of a given space lattice and is determined by an inspection of the model. In a simple cubic lattice, each particle is adjoined by six other particles and so the coordination number is six. The coordination number for body centred and face centred cubic lattice are 8 and 12 respectively.

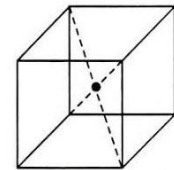
Crystal symmetry :The definite ordered arrangement of faces and edges of a crystal is known as crystal symmetry. Study of symmetry is a powerful tool for the understanding the crystal structure.

A crystal possess different symmetry elements. They are described by the symmetry operations. A symmetry operation is one that leaves the crystal and its environment invariant or unchanged after the operation.

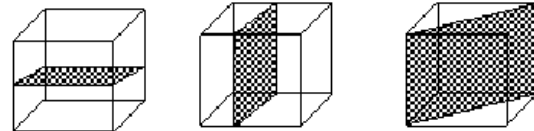
Symmetry operations performed about a point, line or a plane in a crystal are called **point group symmetry operation**. Symmetry operation performed by translation as well as rotation are called **space group symmetry operations**.

The point group symmetry elements are

(1) centre of symmetry or inversion centre – A cube has a centre called centre of symmetry from where all edges are of the same distance.



(2) Plane of symmetry or reflection symmetry – Here the crystal is said to have plane of symmetry if the crystal remains unchanged even after reflection about a plane. A cube has nine such symmetries. Some examples are shown here.



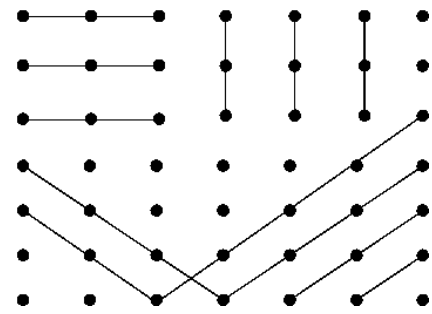
(3) Rotation symmetry – Here a crystal is said to possess rotational symmetry about an axis if the body after rotation by an angle remains the same as before. The axis said to be n – fold if the angle of rotation is given by $\frac{360}{n}$. For example, a cubic crystal has four fold rotation axis, as rotation by 90 degree of the crytsl leaves it invariant. Other possibilities are 60° (n = 6), 90° (n = 4), 120° (n = 3) and 180° (n = 2).

Miller indices :

- **Miller indices** is defined as the reciprocal of the intercepts made by the plane on the crystallographic axes when reduced to smallest numbers
- Notation system in crystallography to indicate the **internal planes of a crystal**.
- The crystal planes are a set of parallel planes used to determine the shape and structure of the unit cell and crystal lattice.
- The miller indices identify the set of planes in the crystal with which the crystal structure can be studied
- Denoted by three integers (***h k l***)

The crystal lattice may be regarded as made up of an aggregate of a set of parallel equidistant planes, passing through lattice points.

It can be chosen in different ways as shown in the diagram. (2 dimensional).



Miller devised a method to designate a set of parallel planes by three numbers called h , k and l called Miller indices.

Procedure to determine miller indices of a crystal plane

1. To determine the **intercepts** of a crystal plane along the three crystallographic directions (along the x, y, and z axes)
2. To express the intercepts as **multiples of unit cell dimensions**, or lattice parameters along the axes
3. To take the **reciprocal** of the intercepts
4. To reduce these numbers to smallest set of integral numbers by taking least common multiplier (**LCM**) of these and **multiplying** with the reciprocal values
5. The set of three integers are called miller indices denoted by **(h, k, l)** values

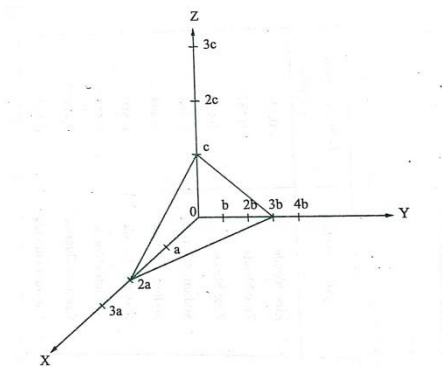
Example

Consider the diagram shown.

(1) The coordinates of the intercepts made by the planes along the crystallographic axes (x, y, z) is given by

$$\begin{matrix} x & y & z \\ 2a & 3b & c \\ pa & qb & rc \end{matrix}$$

where $p = 2, q = 3, r = 1$



(2) To express the intercepts as multiples of unit cell dimensions, or lattice parameters along the axes,

$$\begin{matrix} \frac{2a}{a} & \frac{3b}{b} & \frac{c}{c} \\ 2 & 3 & 1 \end{matrix}$$

(3) To determine the reciprocals of these numbers, $\frac{1}{2}, \frac{1}{3}, \frac{1}{1}$.

(4) To reduce these numbers to smallest set of integral numbers by taking least common multiplier of these and multiplying with LCM,

$$6 \times \frac{1}{2} \quad 6 \times \frac{1}{3} \quad 6 \times \frac{1}{1} . \text{ This results in } (3 \ 2 \ 6)$$

In general these are denoted by $(h \ k \ l)$ called Miller indices. It is also observed that $\frac{1}{p} : \frac{1}{q} : \frac{1}{r} = h : k : l$.

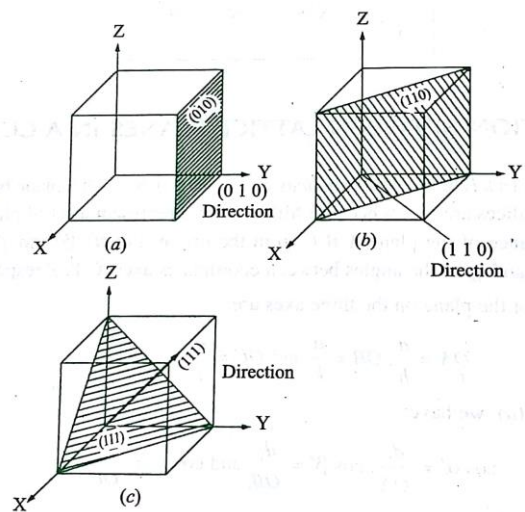
Important features of Miller indices of crystal planes :

- (1) All parallel equidistant planes have the same Miller indices. Thus miller indices define a set of parallel planes.
- (2) A plane parallel to one of the coordinate axis has an intercept of infinity.
- (3) If the Miller indices of two planes have the same ratio, i.e. (8, 4, 4) and (4, 2, 2) or (2, 1, 1) then the planes are parallel to each other.
- (4) If (h, k, l) are the Miller indices of a plane, then the planes cuts the axes into h, k and l equal segments respectively.

Important planes and directions in a cubic crystal

In the diagram (a), the plane cuts the Y axis at a, X axis at ∞ and Z axis at infinity. Thus the intercepts are $(\infty, 1, \infty)$.

The reciprocals are $\frac{1}{\infty} \ \frac{1}{1} \ \frac{1}{\infty}$ or $(0 \ 1 \ 0)$. These are the Miller indices. Similarly the Miller indices for the planes in the diagram (b) and (c) are $(1 \ 1 \ 0)$ and $(1 \ 1 \ 1)$ respectively



Separation between lattice planes in a cubic crystal.

Consider a cubic crystal of side a as shown. Let $(h \ k \ l)$ represent the Miller indices of the plane ABC. Let $ON = d$ be the distance of the plane ABC from the origin as shown in diagram (a). which is the interplanar spacing assuming a plane parallel to ABC at O.

Let α', β' and γ' be the angles by the three axes with the line ON respectively as shown in diagram (b). These are not interfacial angles of the unit cell.

The intercepts of the plane on the three axes are

$$OA = \frac{a}{h}, OB = \frac{a}{k} \text{ and } OC = \frac{a}{l} \dots(1)$$

From the diagram (b) we have $\cos \alpha' = \frac{d_1}{OA}$, $\cos \beta' = \frac{d_1}{OB}$ and $\cos \gamma' = \frac{d_1}{OC}$... (2)

From diagram (c)

$$(ON)^2 = x^2 + y^2 + z^2 \dots(3)$$

$$d^2 = [d^2 \cos^2 \alpha' + d^2 \cos^2 \beta' + d^2 \cos^2 \gamma']$$

$$\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1 \dots(4)$$

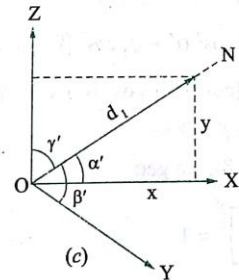
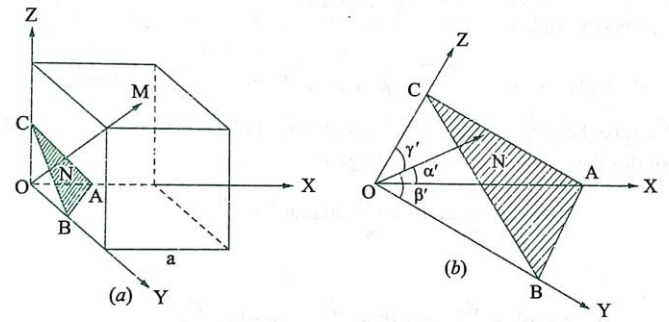
Substituting corresponding cosine terms from (2) in (4), we get

$$\left[\frac{d}{OA}\right]^2 + \left[\frac{d}{OB}\right]^2 + \left[\frac{d}{OC}\right]^2 = 1 \dots(5)$$

Substituting for OA, OB and OC from (1) in (5)

$$\left[\frac{dh}{a}\right]^2 + \left[\frac{dk}{a}\right]^2 + \left[\frac{dl}{a}\right]^2 = 1 \quad \text{or} \quad \frac{d^2}{a^2}(h^2 + k^2 + l^2) = 1$$

the interplanar spacing is
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \dots(6)$$



Relation between the cell constant and density of the material in cubic crystal

Consider a cubic crystal of cell constant a . Let the number of atoms per unit cell be n and the density of the material be ρ . The atomic weight of the material is M_A and the Avogadro number is N_A .

Then $\left(\frac{M_A}{\rho}\right) \text{ m}^3$ volume of the material will contain N_A atoms. Hence n atoms per unit cell will occupy a volume given by $V = \frac{M_A n}{\rho N_A}$.

As the volume of a cubic crystal is $V = a^3$. Thus $a^3 = \frac{M_A n}{\rho N_A}$

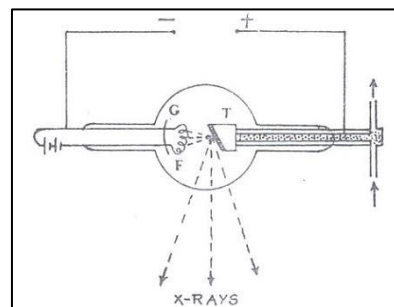
Or the cell constant is
$$a = \left[\frac{M_A n}{\rho N_A}\right]^{\frac{1}{3}}$$

X – Rays : X – rays are electromagnetic radiation of shorter wavelengths of the order of 0.001 to 10 nm. X-rays are produced when rapidly moving electrons that have been accelerated through a potential difference of order 1 kV to 1 MV strikes a metal target.

X-rays were discovered in 1895 by Wilhelm Röntgen. He was interested in the cathode rays (beams of electrons) developed in discharge tubes. By chance he noticed that a fluorescent screen ($\text{ZnS} + \text{Mn}^{++}$) lying on a table some distance from the discharge tube emitted a flash of light each time an electrical discharge was passed through the tube. Realizing that he had come upon something completely new, he devoted his energies to investigating the properties of the unknown ray “X” which produced this effect.

Production of X – Rays

The Coolidge tube - The X-ray tube consists of a glass envelope containing a high vacuum of the order of 10^{-5} mm of mercury. A cathode or negative electrode having a tungsten filament (F), which when heated emits electrons in a process called '*thermionic emission*'. The cathode also has a focussing cup (G) to direct the emitted electrons across the vacuum to hit the target. The anode or positive electrode is a thick copper rod with a small tungsten target (T) at the end. Tungsten is required as it has a high atomic number and a high melting point to improve the efficiency of bremsstrahlung X-ray production. A cooling system with water circulating around the anode is provided to conduct enormous heat generated away from the tube effectively.



Working - A potential difference (around 50, 000V) is applied between the cathode and anode. The tungsten filament is heated by an independent battery and the thermionically emitted electrons are accelerated across the potential difference to a high velocity before striking the tungsten target. When the electrons are suddenly decelerated on impact, some of the kinetic energy is converted into EM energy, as X-rays. Less than 1 % of the energy supplied is converted into X-radiation during this process. The rest is converted into the internal energy of the target which is taken out using cooling system.

1. The intensity of X – rays depends on the number of electrons striking the target per second. The number of electrons given out by the filament is proportional to the temperature of the filament which is controlled by the current in the filament circuit.
2. The frequency of X – rays depend on the potential difference between the cathode and the anode. If V is the pd and e the charge on the electron, the work

done on the electron in moving from cathode to the anode = eV. The electrons that acquire kinetic energy is converted to X – rays when they strike the target. If ν_{max} is the maximum frequency of X – rays produced, then

$$h\nu_{max} = eV.$$

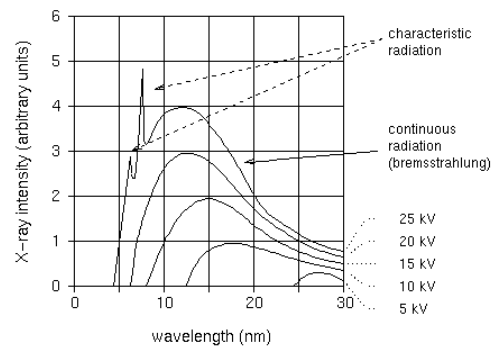
If λ_{min} is the minimum wavelength of X – rays produced, then $\lambda_{min} = \frac{c}{\nu_{max}} = \frac{hc}{eV}$.

Properties of X – rays

1. X-rays travel in straight lines and cannot be deflected by electric field or magnetic field.
2. They have a high penetrating power.
3. They effect photographic plates.
4. Fluorescent materials glow when X-rays are directed at them.
5. Photoelectric emission can be produced by X-rays. Ionization of a gas results when an X-rays pass through the gas.
6. They can be absorbed by tissues and reflected or scattered by bones in the human body.
7. X-rays can cause chemical and biologic damage to living tissue.

X – ray spectra

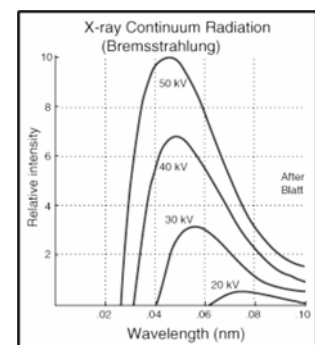
It was first studied by Urey and his coworkers. X – Ray spectra is the variation of Intensity of X – ray beam emitted by an X – ray tube with wavelength for different applied potential difference for a given substance.



The X – ray spectra consists of two types (1) Continuous spectra and (2) Characteristic X – ray spectra.

Continuous X – ray spectrum

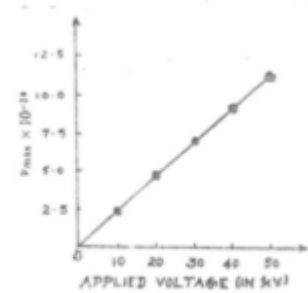
1. For a given applied voltage, the intensity of X – rays varies smoothly with wavelength. The intensity reaches a maximum value as the wavelength increases, then the intensity falls at greater wavelengths.
2. When the applied potential is increased, the intensity of X – rays also increases. The minimum wavelength which depends on the tube voltage decreases with increase in voltage.



3 Duane and Hunt showed that the λ_{min} is inversely proportional to the applied voltage V or ν_{max} is directly proportional to the applied voltage V. The graph shows this variation. This is mathematically indicated by the relation

$$\lambda_{min} = \frac{c}{\nu_{max}} = \frac{hc}{eV}, \text{ ie. } \lambda_{min} \propto \frac{1}{V} \quad \text{or} \quad h\nu_{max} = eV \quad \text{ie. } \nu_{max} \propto V.$$

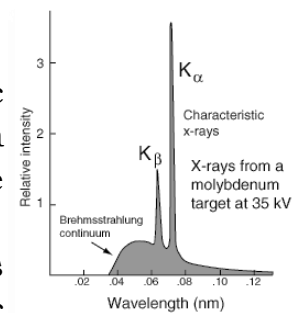
4. Most of the electrons that generate X – ray photons give up only a part of their energy in this way. Thus most of the X – rays are of wavelength longer than λ_{min} .
5. Thus a continuous spectrum is the result of the inverse photoelectric effect, with electron kinetic energy (eV) being transformed into X –ray photon energy (h ν).
6. Fast moving electrons are decelerated by the atoms of the target due to electrostatic forces and collisions emitting X – ray photons.



Note “Bremsstrahlung” means "braking radiation" and is retained from the original German to describe the radiation which is emitted when electrons are decelerated or "braked" when they are fired at a metal target. Accelerated charges give off electromagnetic radiation, and when the energy of the bombarding electrons is high enough, that radiation is in the x-ray region of the electromagnetic spectrum. It is characterized by a continuous distribution of radiation which becomes more intense and shifts toward higher frequencies when the energy of the bombarding electrons is increased.

Characteristic X – ray spectrum

1. It is the spectrum that indicates sharp lines at a specific applied voltage against the continuous X – ray spectra background which is the characteristic of the substance responsible for the spectrum.
2. The peaks seen in the diagram at specific wavelengths indicating the line spectrum which is the characteristic of the element used in the target of the Coolidge tube.
3. These peaks occur at different applied voltages for different elements.



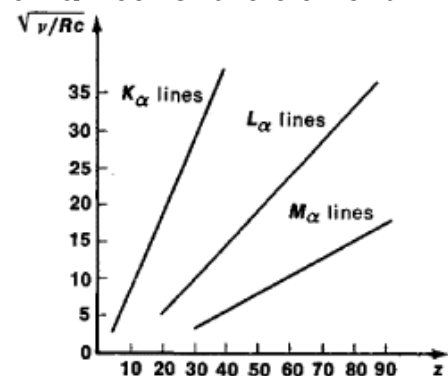
Origin of characteristic X – ray spectrum

1. The bombarding electrons on the target can eject electrons from the inner shells of the atoms of the metal target.
2. Those vacancies will be quickly filled by electrons dropping down from higher levels, emitting x-rays with sharply defined frequencies associated with the difference between the atomic energy levels of the target atoms.
3. Thus characteristic x-rays are emitted from heavy elements when their electrons make transitions between the lower atomic energy levels (ie. between K, L, M.. shells).
4. The characteristic x-rays emission which shows as two sharp peaks occur when vacancies are produced in the n=1 or K-shell of the atom and electrons drop down from above to fill the gap.
5. The x-rays produced by transitions from the n=2 to n=1 levels are called K_{α} x-rays, and those for the n=3 to n = 1 transition are called K_{β} x-rays.

6. Transitions to the $n=2$ or L-shell are designated as L x-rays ($n=3$ to $n = 2$ is L_α , $n=4$ to $n = 2$ is L_β , etc.).
7. The frequencies of the characteristic x-rays can be predicted from the Bohr model.
8. Moseley measured the frequencies of the characteristic x-rays from a large number of the elements of the periodic table and a plot of them which is now called a "Moseley plot" was drawn.
9. Characteristic x-rays are used for the investigation of crystal structure by x-ray diffraction.
10. Crystal lattice dimensions may be determined with the use of Bragg's law in a Bragg spectrometer

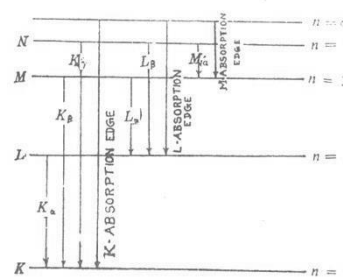
Moseley's law : Moseley had done experiments on the characteristic X-rays and this led to the development of the concept of atomic number.

1. The periodic table was made according to the atomic weight in earlier days. But some anomalies were found in such an arrangement.
2. Moseley measured the frequencies of characteristic X-rays from large number of elements for a particular line (like K_α line) and he studied the relationship between frequency and the atomic number of the element in the periodic table.
3. A graph between square root of frequency $\sqrt{\nu}$ Vs atomic number Z in the periodic table is found to be a linear graph.
4. This suggested that, elements are to be arranged based on atomic number and not on atomic weight. Hence, Moseley re-arranged the periodic table based on atomic number.
5. **Statement of Moseley's law** – The frequency of a spectral line in the X – ray spectrum, varies as the square of the atomic number of the element emitting it. $\nu \propto Z^2$. He expressed his observations mathematically as $\sqrt{\nu} = a(Z - b)$ where a and b are the constants depending on the particular line, ν is the frequency and Z is the atomic number.



Explanation of Moseley’s law according to Bohr’s theory

Bohr’s theory of hydrogen spectrum gives the frequency of a spectral line as $\nu = Z^2Rc \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$ where R is the Rydberg constant and c is the speed of light. For K_α line $n_1 = 1$ and $n_2 = 2$ for the electron making transition from second to first orbit. Thus $\nu = Z^2Rc \left(\frac{1}{1^2} - \frac{1}{2^2} \right) = \frac{3}{4} cRZ^2$.



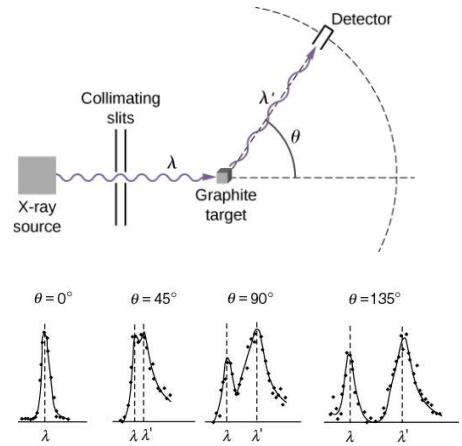
This shows $\nu \propto Z^2$ which approximately corresponds to Moseley’s law.

Distinction between Continuous and characteristic X ray spectra

SL. No.	Continuous spectra	Characteristic spectra
1	They consist of all possible of wavelengths	They consist of specific wavelengths superimposed on the continuous spectra.
2	The intensity increases with increase in applied voltage	They occur at specific applied voltages which depends on the nature of the material
3	They are produced due to bremsstrahlung	They are produced by inner shell (usually K shell) transitions.
4	When a metal target is bombarded with electrons, some electrons are scattered by the atoms, whose acceleration causes them to radiate. This mechanism is called bremsstrahlung.	Some electrons kick the inner shell electrons out of the target atom. These atoms which have one electron less in their inner shell will then rearrange its electronic configuration to fill the inner shell vacancy, emitting characteristic x rays.
5	Continuous spectrum depends very little on the metal used as target. The height of the curve increases with the increase of the Z of the metal, but the shape of the curve is independent of Z	It is the line spectrum that depends mainly on the material from which the X-rays originates, either the anticathode of the X-ray tube or absorbing material used in a fluorescence experiment.
6	The maximum frequency ν_{max} of the emitted X rays completely independent of metal used for the anticathode or the target	The frequencies of the spectral lines are independent of the voltage which accelerates the electrons and independent of the frequency of the incident radiation. Depends only on the chemical elements of which the material is composed.

Compton effect

1. The change in the wavelength of scattered X – rays after incident on a material due loss of energy of incident X – rays is **called Compton effect**.
2. Compton discovered that when X – rays of sharply defined wavelength were incident on a material of low atomic number like carbon, they suffered a change of wavelength on scattering.
3. The scattered X rays observed by a detector at different angles.
4. The scattered X – rays have two wavelengths one same as incident ray and the other of longer wavelength at angles other than 0° i.e. direct rays as shown.
5. This effect was explained by Compton on the basis of quantum theory of radiation. The whole process is treated as collision between a X – ray photon and an electron of the scatterer in which both momentum and energy are conserved.



Expression for Compton shift

Consider an X – ray photon of energy $h\nu$ and momentum $h\nu/c$ striking an electron at rest.

The scattered photon of energy $h\nu'$ and momentum $h\nu'/c$ moves in a direction making an angle θ to the original direction.

The electron acquires a momentum mv and moves an angle ϕ to the original direction.

The initial energy of electron is m_0c^2 and initial momentum is zero. Final energy due to recoil is mc^2 . Considering the x and y components of momentum and applying the principle of conservation of momentum we get

$$\frac{h\nu}{c} = \frac{h\nu'}{c} \cos \theta + mv \cos \phi \quad \dots\dots\dots(1) \quad (\text{along X axis})$$

$$0 = \frac{h\nu'}{c} \sin \theta - mv \sin \phi \quad \dots\dots\dots(2) \quad (\text{along Y - axis})$$

$$\text{From equation (1) } mvc \cos \phi = h(\nu - \nu' \cos \theta) \quad \dots\dots\dots(3)$$

$$\text{From equation (2) } mvc \sin \phi = h\nu' \sin \theta \quad \dots\dots\dots(4)$$

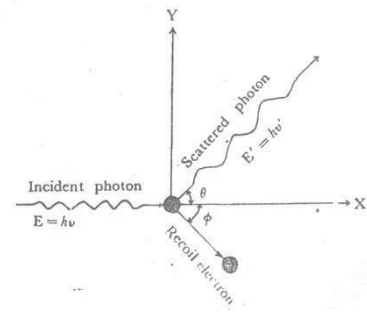
Squaring and adding equations (3) and (4)

$$m^2v^2c^2 = h^2(\nu^2 - 2\nu\nu' \cos \theta + \nu'^2 \cos^2 \theta) + h^2\nu'^2 \sin^2 \theta$$

$$m^2v^2c^2 = h^2(\nu^2 - 2\nu\nu' \cos \theta) + h^2\nu'^2$$

$$m^2v^2c^2 = h^2(\nu^2 - 2\nu\nu' \cos \theta + \nu'^2) \quad \dots\dots\dots(5)$$

According to the principle of conservation of energy



$$hv + m_0c^2 = hv' + mc^2 \quad \dots\dots\dots(6)$$

$$ormc^2 = h(v - v') + m_0c^2$$

$$\text{squaring the above equation } m^2c^4 = (h(v - v') + m_0c^2)^2$$

$$orm^2c^4 = h^2(v^2 - 2vv' + v'^2) + 2h(v - v') m_0c^2 + m_0^2c^4 \quad \dots\dots\dots(7)$$

subtracting equation (5) from (7)

$$m^2c^2(c^2 - v^2) = -2h^2vv'(1 - \cos \theta) + 2h(v - v') m_0c^2 + m_0^2c^4 \quad \dots\dots(8)$$

The value of $m^2c^2(c^2 - v^2)$ is obtained from the relativistic formula $m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$,

squaring this equation $m^2 = \frac{m_0^2}{1 - \frac{v^2}{c^2}} = \frac{m_0^2c^2}{c^2 - v^2}$. Multiplying both sides by c^2

$$\text{we get } m^2c^2 = \frac{m_0^2c^4}{c^2 - v^2} \quad \text{or } m^2c^2(c^2 - v^2) = m_0^2c^4 \quad \dots\dots\dots(9)$$

comparing equations (8) and (9)

$$m_0^2c^4 = -2h^2vv'(1 - \cos \theta) + 2h(v - v') m_0c^2 + m_0^2c^4$$

Simplifying $2h(v - v') m_0c^2 = 2h^2vv'(1 - \cos \theta)$

$$\text{Or } \frac{v - v'}{vv'} = \frac{h}{m_0c^2} (1 - \cos \theta) \quad \text{or } \frac{1}{v'} - \frac{1}{v} = \frac{h}{m_0c^2} (1 - \cos \theta)$$

Multiplying both sides by $c \frac{c}{v'} - \frac{c}{v} = \frac{h}{m_0c} (1 - \cos \theta)$

$$\text{Or } \lambda' - \lambda = \frac{h}{m_0c} (1 - \cos \theta) \quad \dots\dots\dots(10)$$

The change in wavelength is $d\lambda = \frac{h}{m_0c} (1 - \cos \theta)$ called the **Compton shift**

The change in wavelength is independent of the wavelength of the incident radiation as well as the nature of the scattering material. $d\lambda$ depends on the angle of scattering only.

Case 1 : When $\theta = 0$, $\cos \theta = 1$ and hence $d\lambda = 0$.

Case 2 : When $\theta = 90^\circ$, $\cos \theta = 0$ and

$$\text{Hence } d\lambda = \frac{h}{m_0c} = \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-31} \times 3 \times 10^8} = 0.0243 \times 10^{-10}m = 0.0243 \text{ \AA}$$

This is called the Compton wavelength.

Case 3 : When $\theta = 180^\circ$, $\cos \theta = -1$ and hence $d\lambda = \frac{2h}{m_0c} = 0.0485 \text{ \AA}$. Thus $d\lambda$ has the maximum value at $\theta = 180^\circ$.

X – Ray diffraction

- X – rays are electromagnetic rays like light and thus exhibit interference and diffraction. The wavelength of X rays are of the order 0.1nm.
- The diffraction grating produce diffraction of light as the condition to produce diffraction is, the wavelength of light (500 nm) is comparable to the size of the obstacle or the slit. Thus grating cannot produce X- ray diffraction.
- In 1912 Laue suggested that a crystal which consisted of a three dimensional array of regularly spaced atoms could serve the purpose of a

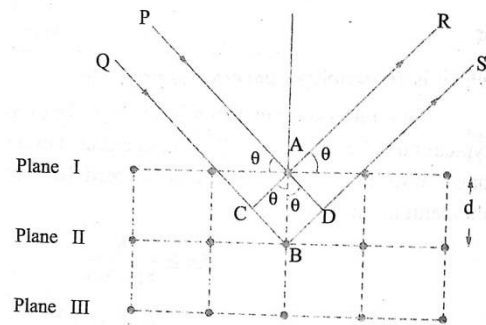
grating. Thus crystal acts as a space grating for X rays to undergo diffraction. Here the interplanar spacing is of the order of wavelength of X rays.

- The diffraction pattern consists of a bright central spot and a series of spots arranged in a regular pattern around the central spot.
- According to Bragg, the spots are produced due to the reflection of incident X rays from various sets of parallel crystal planes (called Bragg planes) with each plane having a large number of lattices points of equal spacing.

Bragg's law :

Consider a X ray PA reflected at atom A from plane I in the direction AR and another ray QB reflected at another atom B from plane II in the direction BS.

Now from the atom A two perpendiculars AC and AD are drawn to QB and BS respectively. The two reflected rays will be in phase or out of phase depending on the path difference.



When the path difference (CB + BD) is a whole wavelength (λ) or multiples of whole wavelength ($n\lambda$), then the two rays will superpose constructively to produce a intense spot.

Thus the condition for this reinforcement or superposition is

$$CB + BD = n\lambda \quad \dots(1)$$

In the diagram, from the right angle triangles, ACB and ADB,

$$CB = d \sin\theta \quad \text{and} \quad DB = d \sin\theta \quad \dots(2)$$

where d is the interplanar spacing and θ is the angle between the incident ray and the plane of reflection called glancing angle.

Substituting (2) in (1) $d \sin\theta + d \sin\theta = n\lambda$

Thus the condition for reinforcement is **$2d \sin\theta = n\lambda$** where n is the integer taking values 1, 2, 3, which correspond to first order, second order, third order.... Maxima respectively.

The above equation is called the **Bragg's law**.

For first maximum $\sin\theta_1 = \frac{\lambda}{2d}$, for second maximum, $\sin\theta_2 = \frac{2\lambda}{2d}$ and for third maximum $\sin\theta_3 = \frac{3\lambda}{2d}$ etc.... The intensity of the maxima decreases as the order of spectrum increases.

PART A

- 1 Distinguish between crystalline and amorphous states of matter and hence define lattice, basis, crystal structure, unit cell and cell parameters.
- 2 What are Bravais lattices? Mention all the Bravais lattices along with the crystal system they belong to and the corresponding cell parameters.
- 3 (a) What are symmetry elements in crystallography? Explain the various point group operations.
(b) What is coordination number? Explain.
- 4 (a) What are Miller indices? Explain the procedure of finding these Miller indices with an example.
(b) Arrive at the interplanar spacing between lattice planes of a cubic crystal.
- 5 (a) State and explain Moseley's law. Mention any two importance of Moseley's law.
(b) Distinguish between continuous and characteristic X ray spectra.
- 6 What is Compton effect? Derive an expression for the Compton shift.
- 7 (a) What are X rays? Mention the characteristics of X rays.
(b) Explain continuous and characteristic X ray spectra.
- 8 (a) Arrive at the relation between the cell constant and density of the material in a cubic crystal
(b) With a neat diagram explain the Bragg's law of X ray diffraction.

PART B

1. In a crystal, a plane cuts intercepts of $3a$, $2b$ and $6c$ along the three crystal axes. Determine the Miller indices of the plane.
Hint : Take the intercepts and then reciprocal and multiply by LCM $(hkl) = (231)$
- 2 Find the Miller indices of a plane which is parallel to y axis and intercepts 2 and $1/3$ along x and z axes respectively.
Hint : Intercept along y axis is infinity. $(hkl) = (1,0,6)$
- 3 Find the inter planar spacing for the lattice planes of Miller indices $(3\ 2\ 1)$ $(2\ 1\ 0)$ and $(1\ 1\ 1)$ for the cubic lattice with $a = 5.62\text{\AA}$.
Hint : $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$.
4. Compute the Miller Indices for a plane intersecting at $x = \frac{1}{4}$, $y = 1$, and $z = 1/2$,
Answer: $(4, 1, 2)$
5. Calculate the miller indices for the plane with intercepts $2a$, $-3b$ and $4c$ the along the crystallographic axes.
Answer $(6, \bar{4}, 3)$
6. The lattice constant for a unit cell of aluminum is 4.031\AA Calculate the interplanar space of $(2\ 1\ 1)$ plane. Answer: $d = 1.6456\text{\AA}$
- 7 Calculate the minimum voltage that should be applied to the X ray tube to produce photons of wavelength 0.1\AA .
Hint : $V = \frac{hc}{\lambda e}$
- 8 Monochromatic X rays of wavelength 0.15\AA undergoes Compton effect from a carbon block. Calculate the wavelength scattered through i) 45° , (ii) 135° and (iii) 180°
Hint : $d\lambda = \frac{h}{m_0c}(1 - \cos\theta)$ and $\lambda - \lambda' = d\lambda$, find λ
- 9 The anode voltage in an X ray tube is 80kV and the wavelength of the X ray produced is 0.15\AA . Find the planck's constant.

Hint : $V = \frac{hc}{\lambda e}$

- 10 Find the smallest glancing angle at which K_{α} line of Molybdenum of wavelength 0.5 \AA will be reflected from calcite crystal of spacing 3 \AA . At what angle will the third order reflection occur?

Hint : $\sin\theta_1 = \frac{\lambda}{2d}$, find θ_1 and $\sin\theta_3 = \frac{3\lambda}{2d}$, find θ_3

- 11 Calculate the glancing angle on the plane (1 1 0) of a cube rock salt ($a = 2.81\text{ \AA}$) corresponding to second order diffraction maximum for the X rays of wavelength 0.71 \AA .

Hint : $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$ and $\sin\theta_2 = \frac{2\lambda}{2d}$, find θ_2 .

- 12 X rays of wavelength of 1.54 \AA are used to calculate the spacing of (200) plane in platinum. The Bragg angle for this reflection is 22.4° . What is the size of unit cell of the platinum crystal?

Hint : $d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{a}{2}$, $(hkl) = (200)$ and $2d \sin\theta = n\lambda$ where $n = 1$, find a

- 13 The wavelength of prominent X ray line from a copper target is 1.54 \AA . This radiation when diffracted from (111) plane of a crystal with fcc structure, correspond to Bragg angle of 19.2° . If the density of the crystal is 2698 kgm^{-3} , and atomic weight $26.98 \text{ kg mol}^{-1}$, Calculate the Avogadro number.

Hint : $d = \frac{n\lambda}{\sin\theta}$, $n = 1$, find d , $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$ find a ,

number of atoms per unit cell for fcc = $n = 4$ and $N_A = \frac{M_A n}{\rho a^3}$

- 14 X rays of wavelength 0.3 \AA undergoes 60° Compton scattering. Find the wavelength of the photon after scattering.

Hint : $\lambda - \lambda' = \frac{h}{m_0 c} (1 - \cos\theta)$

- 15 Find the perpendicular distance between the two planes indicated by the Miller indices (1 2 1) and (2 1 2) in a unit cell of a cubic lattice with a lattice constant parameter 'a'. Answer : $d = d_1 - d_2 = 0.0749 a$

16. What is the distance between the adjacent Miller planes if the first order reflection from X-rays of wavelength 2.29 \AA occurs at $27^\circ 8'$? Ans 2.51 \AA

17. X-rays of wavelength $\lambda = 1.5 \text{ \AA}$ are reflected from the (2 2 2) planes of a cubic crystal with unit cell $a = 5 \text{ \AA}$. Calculate the Bragg angle, θ , for $n=1$.

18. X - rays of wavelength 0.71 \AA are incident on a sodium chloride crystal. Calculate the first order reflection angle from the (100), (110) and (111) planes. The d spacing for (100) plane is 2.84 \AA .

19. In Compton effect, the wavelength of the X - rays scattered at an angle of 45° is 0.022 \AA . Calculate the wavelength of X - rays.

20. The molecular weight of NaCl is 58.448 and its density 2.165 g cm^{-3} . What is the edge length of a cube that contains one mole of NaCl ?

Free electron theory of metals

Properties of Metals

1. Metals have high electrical and high thermal conductivities.
2. In steady state Ohm's law is obeyed. ($J \propto E$ or $I \propto V$)
3. Electrical resistivity above Debye temperature (it is the temperature of a crystal's normal mode of vibration i.e. highest temperature that can be achieved due to a single normal vibration) is directly proportional to the absolute temperature. ($\rho \propto T$)
4. At very low temperatures, the resistivity of the metal is directly proportional to the fifth power of absolute temperature. ($\rho \propto T^5$)
5. For most metals resistivity is inversely proportional to the pressure ($\rho \propto \frac{1}{P}$)
6. Wiedemann - Franz's law is obeyed. ($\frac{K}{\sigma} \propto T$) where K is thermal conductivity and σ is electrical conductivity.
7. At absolute zero temperature, the value of resistivity tends to zero - Superconductivity.

Classical theory of metals - Drude and Lorentz free electron theory of metals

Postulates :

1. Metals are composed of positive metal ions with the valence electrons moving freely among the positive ions.
2. The electrons are in random motion. They are confined to remain within the boundaries of the metal. They can move from one place to another within the metal without loss of energy and occasionally collide with the positive ions.
3. The free electrons are bound to the positive metal ions by the electrostatic force of attraction.
4. The random motion of electrons within the metal can be imagined to be similar to molecules in a gas. (Electron gas) Thus classical kinetic theory of gases can be applied to the electrons.
5. Classical Maxwell - Boltzmann distribution law is applied to electron gas.

Expression for the Electrical conductivity - Ohm's law

Consider a large number of free electrons each of charge e , moving in random motion in a metal and constantly colliding with the other electrons.

If the average time taken by electrons between two successive collisions called relaxation time be τ and the random velocity of the electrons along any one direction be u , then $\tau = \frac{\lambda}{u}$ (1)

Where λ is the mean free path which is the average distance travelled by the electrons between any two successive collisions.

If an electric field E is applied to such a metal, the force F exerted on an electron is $F = -eE$ where $F = ma$ and a is the acceleration of the electron $a = \frac{d^2x}{dt^2}$.

Thus $m \frac{d^2x}{dt^2} = -eE$ or $\frac{d^2x}{dt^2} = -\frac{e}{m} E$

Integrating the above equation $\int \frac{d^2x}{dt^2} dt = -\int \frac{e}{m} E dt$. Thus $\frac{dx}{dt} = \dot{x} = -\frac{eE}{m} t + C$

At $t = 0, \dot{x} = 0 \therefore C = 0$. Thus $\dot{x} = -\frac{eE}{m} t$ (2)

The average velocity of electrons between two successive collisions is found by integrating eqn. (2)

$$\bar{\dot{x}} = \frac{1}{\tau} \int_0^{\tau} -\frac{eE}{m} t dt = -\frac{1}{\tau} \left(\frac{eE}{m} \frac{\tau^2}{2} \right)$$

Thus $\bar{\dot{x}} = -\frac{eE\tau}{2m}$. The average velocity of electrons is called **drift velocity v_d** .

Thus the drift velocity is given by $v_d = -\frac{eE\tau}{2m}$ (3)

From the above expression, relaxation time is given by $\tau = \frac{2m v_d}{eE}$(4)

If the current through the metal of area of cross section A is I and n is the number of electrons per unit volume, then $I = -neAv_d$

If J is the current density which is the current per unit area, then

$$J = -n e v_d = -n e \left(-\frac{eE\tau}{2m} \right) = \frac{n e^2 E \tau}{2m}$$
 Thus $J = \frac{n e^2 E \tau}{2m}$ (5)

Substituting for τ from eqn. (1) in the above equation, we get $J = \frac{n e^2 E \lambda}{2m u}$

Multiplying and dividing the above equation by u we get $J = \frac{n e^2 E \lambda u}{2m u^2}$

From the kinetic theory $\frac{1}{2} m u^2 = \frac{3}{2} k T$ or $m u^2 = 3 k T$ where k is the Boltzmann constant

Thus $J = \frac{n e^2 E \lambda u}{2(3 k T)} = \frac{n e^2 E \lambda u}{6 k T}$ (6)

The current density $J = \sigma E$ (7)

Comparing (6) and (7) where $\sigma E = \frac{n e^2 E \lambda u}{6 k T}$ or $\sigma = \frac{n e^2 \lambda u}{6 k T}$

The expression for the electrical conductivity is $\sigma = \frac{n e^2 \lambda u}{6 k T}$

Verification of Ohm’s law :

If the metal is of length is l and area of cross section A , V is the applied potential, then $E = \frac{V}{l}$. (as the electric field is negative potential gradient)

The current density $J = \frac{I}{A}$,

Substituting for J and E from the above equations in the equation

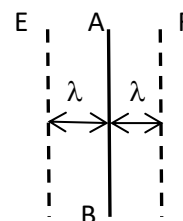
$$J = \sigma E \text{ we get } \frac{I}{A} = \sigma \frac{V}{l} \text{ or } V = \left(\frac{l}{\sigma A} \right) I \text{ where } \frac{l}{\sigma A} = R$$
 Thus **$V = R I$**

where R is the resistance of the metal and $\frac{1}{\sigma} = \rho$ called resistivity of the metal.

This verifies Ohm’s law.

Expression for Thermal conductivity

Consider a metal assumed to be made of a number of layers. Consider any three such layers as shown with layer E at temperature T_1 and F at temperature T_2 . Consider λ as the mean free path which is the distance between the layers E and A and also A and F.



If n is the number of electrons per unit volume, u is the average velocity of electrons, then the number of electrons crossing from layer E to F through A per unit area per unit time is $\frac{1}{6} n u$. (As the system is in three dimensions, the electrons can move in any of the three directions x , y and z . Thus $1/3^{\text{rd}}$ of electrons move along each axis. Also half of $1/3^{\text{rd}}$ moves in one direction and remaining in the opposite direction of that axis. Thus $1/6^{\text{th}}$ is considered along a specific direction).

If $T_1 > T_2$, from the kinetic theory of gases, the heat energy transferred from E to F per unit area per unit time is $Q_1 = \frac{1}{6} n u \times \frac{1}{2} m u_1^2$ (1)

where, $\frac{1}{2} m u_1^2$ is the energy of each electron

$$Q_1 = \frac{1}{6} n u \times \frac{3}{2} k T_1. \quad (\text{Since } \frac{1}{2} m u_1^2 = \frac{3}{2} k T_1)$$

$$Q_1 = \frac{1}{4} n u k T_1 \quad \dots\dots\dots(2)$$

The energy transferred from F to E is $Q_2 = \frac{1}{4} n u k T_2$

Hence the net heat energy transferred from E to F per unit area per unit time is $Q = Q_1 - Q_2$

$$Q = \frac{1}{4} n u k (T_1 - T_2) \dots\dots\dots(3)$$

If K is the thermal conductivity of the metal, then the energy transfer per unit area per unit time by definition is

$$Q = \frac{K (T_1 - T_2)}{2 \lambda} \dots\dots\dots(4) \quad (\text{where } 2 \lambda \text{ is the distance between layers E and F})$$

Comparing equations (3) and (4) we get

$$\frac{1}{4} n u k (T_1 - T_2) = \frac{K (T_1 - T_2)}{2 \lambda}$$

$$\text{Or } K = \frac{1}{2} \lambda n u k$$

Wiedemann – Franz law

Statement : The ratio of thermal conductivity to that of the electrical conductivity of a metal is directly proportional to the absolute temperature of the metal.

$$\text{The thermal conductivity } K = \frac{1}{2} \lambda n u k \quad \dots\dots\dots(1)$$

$$\text{The electrical conductivity } \sigma = \frac{n e^2 \lambda u}{6 k T} \quad \dots\dots\dots(2)$$

Taking the ratio of the above equations we get $\frac{K}{\sigma} = 3 \left(\frac{k}{e}\right)^2 T$

Or $\frac{K}{\sigma T} = L$ or $\frac{K}{\sigma} = L T$ where $L = \frac{3K^2}{e^2}$ is called the Lorentz number.

Hence $\frac{K}{\sigma} \propto T$ which is the Wiedemann – Franz law.

Merits of Classical Free Electron Theory:

1. It is used to verify Ohm's law.
2. The electrical and thermal conductivities of metals can be explained.
3. It is used to derive Wiedemann- Franz law
4. It is used to explain the optical properties of metals.

Drawbacks of Classical Free Electron Theory:

1. It is a macroscopic theory.
2. It cannot explain the electrical conductivity of semiconductors and insulators properly.
3. Dual nature is not explained.
4. It cannot explain the Compton effect and Photo-electric effect.
5. The theoretical and experimental values of specific heat do not agree with each other.
6. Atomic fine spectra could not be accounted.
7. Different types of magnetisms could not be explained satisfactorily by this theory.

Quantum theory of metals

Sommerfeld and Pauli applied quantum mechanics and modified the free electron theory.

- 1 Instead of classical Maxwell – Boltzmann distribution law that is applied to electrons in the classical theory, the distribution of energy in electron gas is said to obey Fermi – Dirac distribution law according to the quantum theory.
- 2 The energy of electrons in a metal are quantized. The energy levels in the metal are filled with electrons on the basis of Pauli exclusion principle.
- 3 According to this principle, an energy level can take only two electrons one with spin up and the other with spin down. Thus the electrons, depending on the energy values are filled from the lowest energy upwards.
- 4 The energy of the highest occupied level at absolute zero temperature is called Fermi energy.

Expression for density of states for free electrons

Density of states is defined as the number of electronic states present in a unit energy range. It is represented by $g(E)$.

$$g(E) = \frac{dN}{dE}$$

where dN is the number of electron quantum energy states present in the energy interval E and $E + dE$.

The number of quantum states in the energy state dE can be determined using quantum mechanical analysis of particle in a box. According to this analysis, the energy of an electron in the n th state is $E = \frac{n^2 h^2}{8 m L^2}$

Here n is an integer that takes values 1,2,3.... Also, n is treated like vectors representing the distance from the lowest energy line. Then one can use Pythagoras theorem to combine them into one single vector. i.e. $R = \sqrt{n_x^2 + n_y^2 + n_z^2}$

Thus the energy is represented as $E = \frac{R^2 h^2}{8 m L^2}$, or $R = \left[\frac{8 m L^2 E}{h^2} \right]^{\frac{1}{2}}$.

The number of states with energy E_n will just be the number of states inside the sphere of radius R .

The n - space associated with particle in a box involves only positive values of n , so that volume must be divided by 8. It is then multiplied by 2 to account for two possible spin values of electron.

Thus the number of quantum states

$$N = 2 \times \frac{1}{8} \times \frac{4}{3} \pi R^3 = \frac{1}{3} \pi \left[\frac{8 m L^2 E}{h^2} \right]^{\frac{3}{2}} = \frac{1}{3} \pi [8 m E]^{\frac{3}{2}} \frac{L^3}{h^3}$$

$$\text{or } N = \frac{1}{3} \pi [2 \sqrt{2 m E}]^3 \frac{L^3}{h^3} = \frac{1}{3} \pi \frac{8 (2 m E)^{3/2} L^3}{h^3}$$

$$N = \frac{8 \pi (2 m)^{3/2} V E^{3/2}}{3 h^3} \quad \text{where } V = L^3 = \text{volume}$$

$$\text{Thus the density of states } g(E) = \frac{dN}{dE} = \frac{d}{dE} \left(\frac{8 \pi (2 m)^{3/2} V E^{3/2}}{3 h^3} \right) = \frac{8 \pi (2 m)^{3/2} V}{3 h^3} \frac{3}{2} \sqrt{E}$$

$$\text{or } g(E) = \frac{8 \sqrt{2} \pi V m^{3/2}}{h^3} \sqrt{E}$$

Thus the number of energy states per unit volume per unit energy E is

$$g(E) = \frac{8 \sqrt{2} \pi m^{3/2}}{h^3} \sqrt{E}. \quad \text{or } g(E) \propto \sqrt{E}.$$

Fermi – Dirac distribution function : Fermi energy (E_F)

Fermi energy is the maximum energy occupied by a free electron at absolute zero temperature.

The electron gas in a metal obeys Fermi – dirac statistics (called fermions). In an assembly of fermions, if there are $g(E)$ allowed quantum states in an energy range E and $E + dE$ and $n(E)$ is the number of particles, then $n(E)$ states are filled and $g(E) - n(E)$ are vacant.

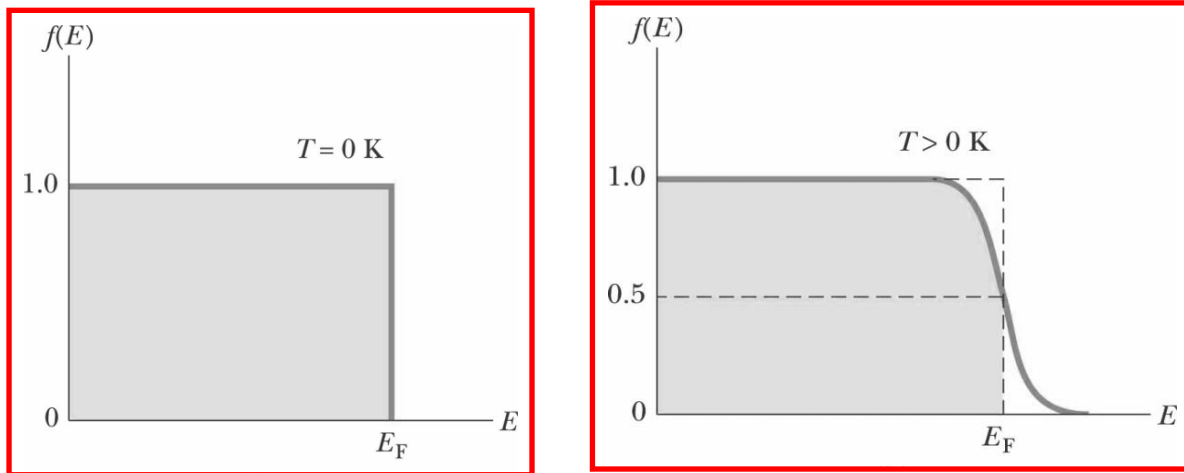
The Fermi dirac distribution function $f(E)$ is defined as

$$f(E) = \frac{n(E)}{g(E)} = \frac{1}{1 + e^{(E - E_F)/kT}} \quad \dots\dots(1)$$

It indicates the fraction of quantum states occupied or the probability that the level E is occupied by an electron.

$f(E) = 1$ for $E < E_F$ ie. all quantum states are filled.

$f(E) = 0$ for $E > E_F$ ie. quantum states above E_F are empty. This function is plotted as shown



All levels below E_F are completely filled and all levels above E_F are empty at absolute temperature. As the temperature is increased, $f(E)$ changes from 1 to 0 more and more gradually. For $E = E_F$, $f(E) = 1/2$ at all temperatures.

Expression for Fermi energy

The number of electrons between the energy E and $E + dE$ is

$$n(E) dE = g(E) dE f(E) \quad \dots\dots(1)$$

where $g(E)$ is the density of states given by $g(E) = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \sqrt{E} \quad \dots\dots(2)$

and $f(E)$ is the Fermi distribution function $f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} \quad \dots\dots(3)$

Substituting (2) and (3) in equation (1) we get

$$n(E)dE = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \sqrt{E} \frac{1}{1 + e^{(E-E_F)/kT}} \quad \dots\dots(4)$$

The total number of electrons in the system is given by integrating the above equation

$$N = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \int_0^\infty \frac{\sqrt{E} dE}{1 + e^{(E-E_F)/kT}} \quad \dots\dots(5)$$

At absolute zero temperature, the maximum energy of the electron is the Fermi energy E_F

Thus $N = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \int_0^{E_F} \sqrt{E} dE$, ($\because 1 + e^{(E-E_F)/kT} = 1$ As $E < E_F$ thus $E - E_F$ is negative and at absolute zero temperature $e^{(E-E_F)/k \times 0} = e^{-\infty} = 0$)

Integrating, we get $N = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \frac{2}{3} E_F^{3/2}$ or $N = \frac{8\pi V}{3} \left(\frac{2m}{h^2}\right)^{3/2} E_F^{3/2}$

Rising the power of the above equation to $2/3$, $N^{2/3} = \left(\frac{8\pi V}{3}\right)^{2/3} \frac{2m}{h^2} E_F$

Simplifying the above equation, the expression for Fermi energy is given by

$$E_F = \frac{h^2}{2m} \left(\frac{3N}{8\pi V}\right)^{2/3} \quad \dots\dots(6)$$

From the above equation it is observed that E_F depends only on the density of electrons given by $n = N/V$

Thus $E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3}$ This is the expression for fermi energy at absolute zero temperature.

E_F is independent of size of the metal. The values of E_F for few metals are given by 4.72 eV for lithium, 3.12 eV for sodium, 7 eV for copper at absolute zero temperature.

The value of Fermi energy at any other high temperature is

$E_F = E_{F(0)} \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{E_{F(0)}} \right)^2 \right]$ where $E_{F(0)}$ is Fermi energy at absolute zero temperature. At room temperature, the change in Fermi energy is very small compared to that at absolute temperature.

Electron energy distribution

The number of electrons in an electron gas that have energies between E and $E + dE$ is $n(E) dE = g(E)dE f(E)$

$$n(E)dE = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \sqrt{E} \frac{1}{1+e^{(E-E_F)/kT}} \dots(1)$$

As $E_F = \frac{h^2}{2m} \left(\frac{3N}{8\pi V} \right)^{2/3}$

or $N^{2/3} = \left(\frac{8\pi V}{3} \right)^{2/3} \frac{2m}{h^2} E_F$

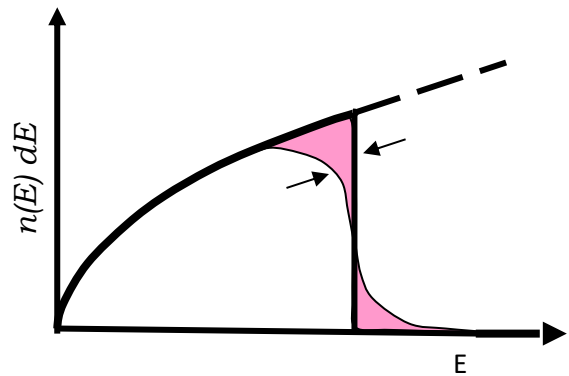
or $N = \frac{8\pi V}{3} \left(\frac{2m}{h^2} \right)^{3/2} E_F^{3/2}$ or $\frac{8\pi V 2\sqrt{2}}{3} \left(\frac{m}{h^2} \right)^{3/2} = \frac{N}{E_F^{3/2}}$

This implies that $\frac{8\sqrt{2}\pi V m^{3/2}}{h^3} = \frac{3N}{2E_F^{3/2}} = \frac{3N}{2} E_F^{-3/2} \dots(2)$

Thus, substituting for the terms of LHS of (2) in (1) we get

$$n(E)dE = \frac{3N}{2} E_F^{-3/2} \frac{\sqrt{E} dE}{1+e^{(E-E_F)/kT}} \text{ where } n(E)dE \propto \sqrt{E}$$

The above equation is plotted for $T = 0$ K and for temperature greater than 0 K.



Expression for average kinetic energy of electrons at absolute zero temperature

The number of electrons in an electron gas that have energies between E and $E + dE$ is $n(E) dE = g(E)dE f(E) \dots\dots(1)$

where $g(E)$ is the density of states given by $g(E) = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \sqrt{E}$

and $f(E)$ is the Fermi distribution function $f(E) = \frac{1}{1+e^{(E-E_F)/kT}}$

Substituting above expressions in equation (1) we get

$$n(E)dE = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \sqrt{E} \frac{1}{1+e^{(E-E_F)/kT}} \dots(2) \quad (\because 1 + e^{(E-E_F)/kT} = 1 \text{ As } E < E_F \text{ thus } E - E_F \text{ is negative and at absolute zero temperature } e^{(E-E_F)/k \times 0} = e^{-\infty} = 0)$$

Also $E_F = \frac{h^2}{2m} \left(\frac{3N}{8\pi V} \right)^{2/3}$ or $N^{2/3} = \left(\frac{8\pi V}{3} \right)^{2/3} \frac{2m}{h^2} E_F$

Or $N = \frac{8\pi V}{3} \left(\frac{2m}{h^2} \right)^{3/2} E_F^{3/2}$

This implies that $\frac{8\sqrt{2}\pi V m^{3/2}}{h^3} = \frac{3N}{2E_F^{3/2}} = \frac{3N}{2} E_F^{-3/2}$ (3)

Thus equation (2) after substituting from (3) is given by

$n(E) dE = \left(\frac{3N}{2} \right) E_F^{-3/2} E^{1/2} dE$

Total energy at absolute temperature is given by

$E_0 = \int_0^{E_F} E n(E) dE = \frac{3N}{2} E_F^{-3/2} \int_0^{E_F} E E^{1/2} dE$

$E_0 = \int_0^{E_F} E n(E) dE = \frac{3N}{2} E_F^{-3/2} \int_0^{E_F} E^{3/2} dE$

$E_0 = \frac{3N}{2} E_F^{-3/2} \frac{E_F^{5/2}}{5/2} = \frac{3}{5} N E_F$

The average electron energy at absolute zero temperature is given by

$\bar{E}_0 = \frac{E_0}{N} = \frac{3}{5} E_F$ Thus $\bar{E}_0 = \frac{3}{5} E_F$

Note :The expression for Fermi momentum is $p_F = \sqrt{2mE_F}$

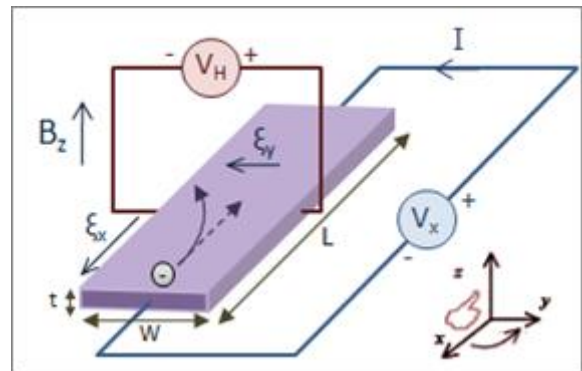
Fermi velocity is the average velocity of an electron in an atom at absolute

temperature given by $v_F = \sqrt{\frac{2E_F}{m}}$.

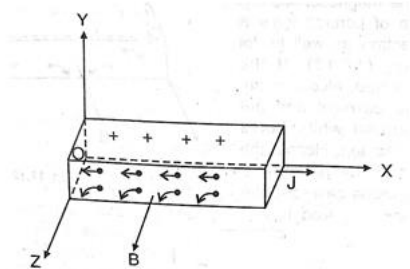
Fermi temperature is given by $T_F = \frac{E_F}{k}$ where k is the Boltzmann constant.

Hall effect

When a metal or a semiconductor carrying an electric current is placed in a magnetic field, an electric field is produced inside the material in a direction which is at right angles to both the current and the magnetic field. This was discovered by Edwin H Hall and is called the **Hall effect**.



Hall effect in a metal : Consider a metal in the form of a rectangular slab as shown. Let the current be I flowing along the positive X direction. J is the current density (ratio of current to area) also along the + X direction. Let a magnetic field of strength B be applied along the + Z direction. The electrons which are moving along the negative X direction will experience a Lorentz force given by $F = evB$ (1) (since $F = evB \sin\theta$ with $\theta =$



90°) where e is the charge on the electron, v is the velocity with which electron is moving. This force acts along the negative Y direction (Fleming left hand rule).

Under the action of the Lorentz force, the electrons collect at the bottom surface of the metal slab making it negative and the top surface becomes positive. Thus an electric field is created called the Hall field E_H along the negative Y axis.

Now the electrons experience a force due to electric field given by $F = eE_H$ (2)

This force is opposite to the Lorentz force and at equilibrium the two are equal given by $eE_H = evB$ or $E_H = vB$ (3)

The current in the conductor is given by $I = neAv$.

The current density $J = \frac{I}{A} = \frac{neAv}{A} = nev$ where n is the number of electrons per unit volume. From the above equation $v = \frac{J}{ne}$ (4)

Substituting for v from (4) in (3) $E_H = \frac{JB}{ne} = R_H BJ$ (5) where $R_H = \frac{1}{ne}$

R_H is called the Hall coefficient which depend on the nature of the conductor. In case of a metal as electrons are the charge carriers, the Hall coefficient is negative i.e. $R_H = -\frac{1}{ne}$.

If V_H is the Hall voltage generated in the metal of thickness d , then $E_H = \frac{V_H}{d}$.

Thus from equation (5) $\frac{V_H}{d} = R_H BJ$ or $V_H = R_H B J d$ or $V_H = \frac{B J d}{ne}$

Importance of Hall effect

1. The sign of the current carrying charge can be determined by the Hall effect.
2. The electron concentration (number of electrons per unit volume) can be calculated by measuring Hall coefficient.
3. The mobility of electrons can be measured directly.
4. Hall effect can used to find the electronic structure of the material.
5. Knowing R_H , the magnetic field can be measured from Hall voltage.

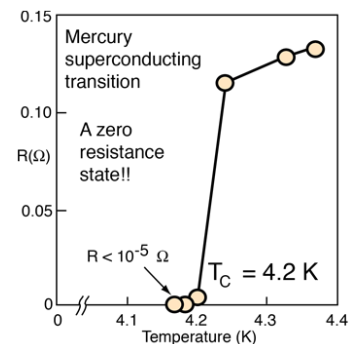
Superconductivity

Introduction : In general the electrical resistivity ρ of metals and alloys decreases when they are cooled (i.e. temperature is decreased). When the temperature is lowered the thermal vibrations of the atoms decrease and the conduction electrons are less frequently scattered. For a perfectly pure metal, the resistivity must approach zero as the temperature approaches absolute zero. This is not real as any metal will always possess impurity. Thus there is always some residual resistivity ρ_0 or electrical resistance even at absolute zero temperature.

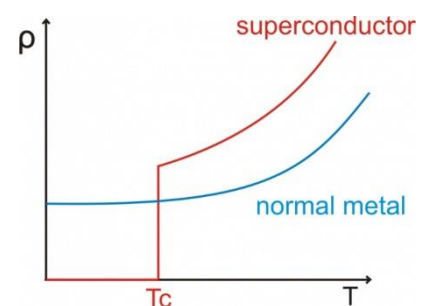
Certain metals, however, show a remarkable behaviour when they are cooled. As the temperature is lowered the resistivity decreases as usual, but at a certain low temperature close to absolute zero, the resistivity suddenly reduces to zero. Then they are said to have passed into superconducting state.

Superconductivity is a phenomenon of certain materials attaining exactly zero electrical resistance and expulsion of magnetic flux fields, when cooled below a characteristic critical temperature.

It was discovered by Dutch physicist Kamerlingh Onnes in the year 1911. Onnes, after having successfully liquified helium in 1908, investigated the low temperature resistivity of mercury in 1911. The mercury could be made very pure by distillation, and this was important because the resistivity at low temperatures tends to be dominated by impurity effects. He found that the resistivity suddenly dropped to zero at 4.2K, a phase transition to a zero resistance state. This phenomenon was called superconductivity, and the temperature at which it occurred is called its critical temperature.



Critical temperature T_c : The critical temperature or transition temperature for superconductors is the temperature at which the electrical resistivity of a metal drops to zero as shown in the graph. The transition is so sudden and complete that it appears to be a transition to a different phase of matter. This superconducting phase is described by the BCS theory. Several materials exhibit superconducting phase transitions at low temperatures. The highest critical temperature was about 23 K until the discovery in 1986 of some high temperature superconductors.



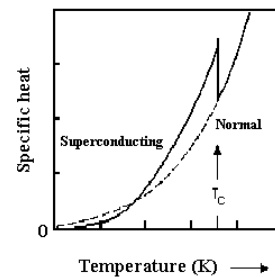
Materials with critical temperatures in the range 120 K have received a great deal of attention because they can be maintained in the superconducting state with liquid

nitrogen (77 K). Eg. Gallium $T_C = 1.1 K$, Aluminium $T_C = 1.2 K$, Indium $T_C = 3.4 K$ Tin $T_C = 3.7 K$, Lead $T_C = 7.2 K$, Niobium $T_C = 9.3 K$ La-Ba-Cu-oxide $T_C = 17.9 K$ and Y-Ba-Cu-oxide $T_C = 92 K$.

Experimental Facts

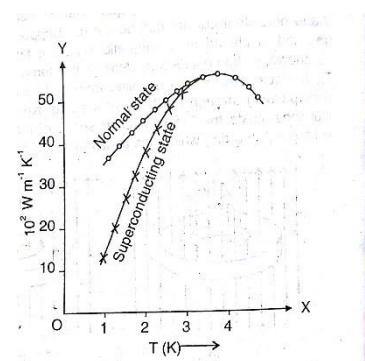
1. When impurities are added to superconducting elements, the superconducting property is not lost but the transition temperature is lowered.
2. **Isotope effect** : It has been observed that the critical temperature of superconductors varies with isotopic mass. In Mercury T_C varies from 4.185 K to 4.146 K as the average atomic mass M varies from 199.5 to 203.4 amu. They obey a relation $T_C\sqrt{M} = constant$. The variation of critical temperature with isotopic mass is called isotope effect.
3. The thermal properties such as the specific heat capacity and thermal conductivity of a substance change abruptly, when it passes over to superconducting state.

(a) Specific heat : The specific heat of a normal metal at low temperature is of the form $C_n(T) = \gamma T + \beta T^3$. The first term on the right hand side is the specific heat of electrons in the metal and the second term is the contribution of lattice vibrations. But from the graph it is seen that a superconductor shows a jump at critical temperature T_C . Since the superconductivity affects electrons mainly, the second contribution βT^3 almost remains the same in the superconducting state. The variation of electronic specific heat C_{es} is nonlinear with temperature. It is given by $C_{es}(T) = A e^{-\frac{\Delta}{k_B T}}$.



An exponential dependence implies that it requires a finite energy Δ to excite an individual electron in a superconductor.

(b) Thermal conductivity : The thermal conductivity of superconductors undergo a continuous change between the two phases (normal and superconducting) and is usually lower in the superconducting phase. This suggests that the electronic contribution drops and possibly the superconducting electrons playing no part in the heat transfer. The thermal conductivity of tin at 2K is $3400 \text{ Wm}^{-1}\text{K}^{-1}$ for normal phase and $1600 \text{ Wm}^{-1}\text{K}^{-1}$ for the superconducting phase. The variation is as shown in the graph.



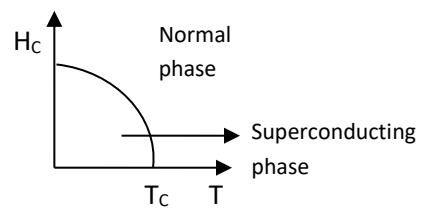
4 **Persistent currents** : The fact that the resistance is zero has been demonstrated by sustaining currents or persistent currents in superconducting lead rings for many years with no measurable reduction. An induced current in an ordinary metal ring would decay rapidly from the dissipation of ordinary resistance, but superconducting rings had exhibited a decay constant of over a billion years. Thus currents persists in a superconducting ring over very long time.

In a superconducting state, since the dc electrical resistance is practically zero, persistent current is observed to flow in superconducting rings. The current flowing in a ring at any time t due to changing magnetic flux density B is given by Lenz law according to which $-A \frac{dB}{dt} = R(t) + L \frac{dI}{dt}$ where A is the area, R is the resistance of the ring and L is the inductance of the ring. If there is no external magnetic field applied to the ring $B = 0$.

Thus $R(t) + L \frac{dI}{dt} = 0$ The solution of this equation can be written as

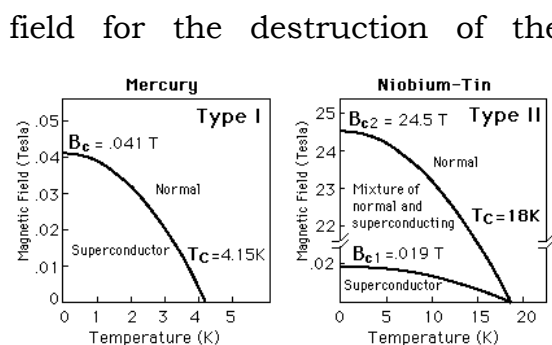
$I(t) = I(0)e^{-\frac{R}{L}t}$. The current decays in the ring exponentially in the absence of the external magnetic field. But if the ring is a superconductor, then resistance is zero i.e. $R = 0$, thus $I(t) = I(0)$. Thus the current does not decay with time and remains the same called the persistent current.

5 **Critical magnetic field** : Destruction of superconductivity by magnetic fields : If a strong magnetic field called critical magnetic field is applied to a superconducting specimen, it becomes normal conductor and recovers normal resistivity even at $T < T_C$. The critical value of the applied magnetic field for the destruction of the superconductivity is denoted by $B_C(T)$ and is a function of temperature. It is called **critical field**. For a given substance, the value of H_C decreases as the temperature increases from $T = 0 K$ to $T = T_C$. The variation can be expressed by the formula



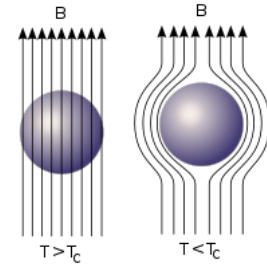
$$B_C(T) = B_C(0) \left[1 - \left(\frac{T}{T_C} \right)^2 \right]$$

where $B_C(0)$ is the critical field at 0 K. At the critical temperature T_C the critical field is zero, $B_C(T_C) = 0$. This result is expected, because at $T = T_C$, the specimen is already normal and field is necessary for this transition. The variation of critical field with temperature is as shown in the graph for mercury. Generally for all substances the variation is the same.



Meissner effect

In 1933, Meissner and Ochsenfold measured the magnetic flux distribution outside Tin and Lead specimen which has been cooled below their transition temperature while in the magnetic field. They found that at their transition temperatures the specimens spontaneously became perfectly diamagnetic, cancelling all the flux even though they are inside the magnetic field.



When a conductor is cooled in a magnetic field to temperature below the critical temperature then, at the critical temperature the magnetic field lines are expelled from the interior of the superconductor. This phenomenon is called the **Meissner effect**. Thus at $T \leq T_c$ when magnetic field is expelled from the material the superconductor is said to exhibit diamagnetism. Thus in the superconducting state, the magnetic flux density inside it is zero. i.e. $B = 0$.

The magnetic flux density B along a specific direction within a material is given by

$B = \mu_0(H + I)$ (1) where H is the applied magnetic field and I is the intensity of magnetization,

$\frac{B}{H} = \mu_0 \left(1 + \frac{I}{H}\right)$ But $\frac{I}{H} = \chi$ called the volume magnetic susceptibility of the specimen.

Thus $\frac{B}{H} = \mu_0 (1 + \chi)$ For a superconductor $B = 0$, thus the equation reduces to $\chi = -1$.

The negative sign indicates that the specimen is a diamagnet.

The superconducting state is a characteristic thermodynamic phase of a substance in which the material cannot sustain steady electric and magnetic fields. Thus the two mutually independent properties of a superconductor are : (1) zero resistivity ($\rho = 0$ and $E = 0$) and (2) perfect diamagnetism ($B = 0$ and $\chi = -1$). They are essential properties that characterize the superconducting state.

Critical current density

The magnetic field which causes the superconductor to become normal from a superconducting state need not necessarily be an external magnetic field. It may arise as a result of electric current flow in the conductor. If the field produced by the current in the conductor exceeds critical field H_c , the superconductivity disappears. The maximum current density J at which the superconductivity disappears is called the critical current density J_c .

For a ring of radius r carrying a current I , the magnetic field is given by $H_i = \frac{I}{2\pi r}$.

If H_i exceeds H_C , the superconductor becomes normal. If a transverse magnetic field is also applied to the ring, then the critical magnetic field is given by

$H_C = H_i + 2H$ or $H_C = \frac{I_C}{2\pi r} + 2H$ or $I_C = (H_C - 2h)2\pi r$. This is called Sisbee's rule. If the applied field is zero, $H = 0$, then the critical current is

$I_C = 2\pi r H_C$. Thus a superconductor loses to be so if the current is critical current given by the above expression in a ring. This puts a limit to the current that can flow in a ring for the material to remain as a superconductor.

Types of superconductors

Type I and Type II superconductors

Depending upon their behaviour in an external magnetic field, superconductors are divided into two types: a) Type I superconductors and b) Type II superconductors

1) Type I superconductors:

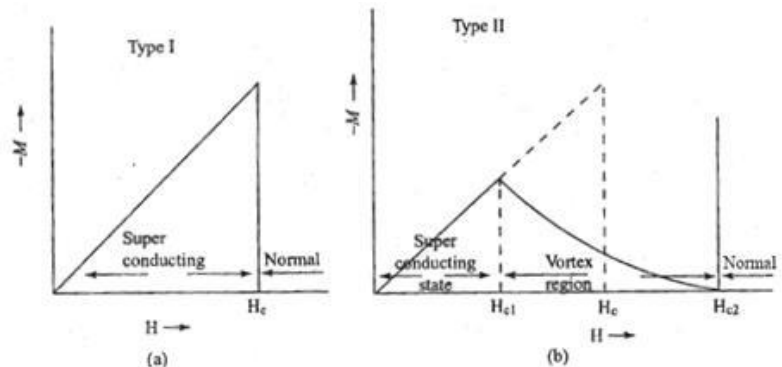
a). Type I superconductors are those superconductors which lose their superconductivity very easily or abruptly when placed in the external magnetic field. As can be seen from the graph of intensity of magnetization (M) versus applied magnetic field (H), when the Type I superconductor is placed in the magnetic field, it suddenly or easily loses its superconductivity at critical magnetic field H_C .

After H_C , the Type I superconductor will become normal conductor.

b). Type I superconductors are also known as **soft superconductors** because of the reason that they lose their superconductivity easily.

c) Type I superconductors perfectly obey Meissner effect.

d) Example of Type I superconductors: Aluminum ($H_C = 0.0105$ T), Zinc ($H_C = 0.0054$ T)



2) Type II superconductors:

a). Type II superconductors are those superconductors which lose their superconductivity gradually but not easily or abruptly when placed in the external magnetic field. As you can see from the graph of intensity of magnetization (M) versus applied magnetic field (H), when the Type II

superconductor is placed in the magnetic field, it gradually loses its superconductivity. Type II superconductors start to lose their superconductivity at lower critical magnetic field (H_{C1}) and completely lose their superconductivity at upper critical magnetic field (H_{C2}).

b) The state between the lower critical magnetic field (H_{C1}) and upper critical magnetic field (H_{C2}) is known as vortex state or intermediate state.

After H_{C1} , the Type II superconductor will become conductor.

c). Type II superconductors are also known as **hard superconductors** because of reason that is they lose their superconductivity gradually but not easily.

c) Type II superconductors obey Meissner effect but not completely.

d) Example of Type II superconductors: NbN ($H_C = 8 \times 10^6$ T), $BaBi_3$ ($H_C = 59 \times 10^3$ T)

e) Application of Type II superconductors: Type II superconductors are used for strong field superconducting magnets.

Differences between Type I and Type II superconductors

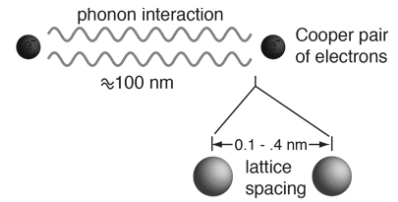
S. No.	Type I superconductor	Type II superconductor
1	They are Soft superconductors that can tolerate the impurities without affecting the superconducting properties	They are Hard superconductors that cannot tolerate the impurities. The presence of impurities affect the superconducting properties
2	They have low critical magnetic field	They have high critical magnetic field
3	They exhibit complete Meissner effect	They trap magnetic flux and hence Meissner effect is not complete
4	The current flows through the surface only	The current flows throughout the material
5	Eg. Tin, Aluminium	Eg. Tantalum, Niobium

BCS theory :

The properties of Type I superconductors were modelled successfully by the efforts of John Bardeen, Leon Cooper, and Robert Schrieffer in what is commonly called the BCS theory. A key conceptual element in this theory is the pairing of electrons close to the Fermi level into Cooper pairs through interaction with the crystal lattice. This pairing results from a slight attraction between the electrons related to lattice vibrations; the coupling to the lattice is called a phonon interaction.

Cooper pairs : The behavior of superconductors suggests that electron pairs are coupling over a range of hundreds of nanometers, three orders of magnitude

larger than the lattice spacing. Called Cooper pairs, these coupled electrons can take the character of a boson and condense into the ground state.



This pair condensation is the basis for the BCS theory of superconductivity. The effective net attraction between the normally repulsive electrons

produces a pair binding energy on the order of milli-electron volts, enough to keep them paired at extremely low temperatures.

Pairs of electrons can behave very differently from single electrons which are fermions and must obey the Pauli exclusion principle. The pairs of electrons act more like bosons which can condense into the same energy level. The electron pairs have a slightly lower energy and leave an energy gap above them on the order of 0.001 eV which inhibits the kind of collision interactions which lead to ordinary resistivity. For temperatures such that the thermal energy is less than the band gap, the material exhibits zero resistivity.

Bardeen, Cooper, and Schrieffer received the Nobel Prize in 1972 for the development of the theory of superconductivity.

High temperature superconductors:

It was generally believed that Superconductivity is exhibited only by materials at very low temperatures. The alloy Nb_3Ge had the highest known T_c equal to 23.2 K. In the year 1986 George Bednorz and Karl Alex Muller discovered that an oxide of lanthanum, barium and copper (La-Ba-Cu-O) became superconducting at 30 K. Then it was thought that superconductivity could be achieved even at higher temperature. This led to the production of materials with higher and higher values of T_c . Some examples of high temperature superconductors are $\text{Ti}_2\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ with $T_c = 125\text{K}$ and $\text{Hg Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ at $T_c = 134\text{K}$.

Applications of superconductors:

- (1) Superconductors are used in making magnets that can produce very strong magnetic fields.
- (2) The ability of superconductors to conduct electricity with zero resistance leads to its application in efficient transmission and distribution of electrical power.
- (3) SQUIDS (superconducting quantum interference devices) are used to detect magnetic fields as low as 10^{-14}T .
- (4) The Meissner effect exhibited by superconductors is used in magnetic levitation. That is, a small permanent magnet can be made to float above a superconductor.
- (5) Superconducting magnets are used in MRI (magnetic resonance imaging) scanning devices.

- (6) A current generated once in a circular ring of superconductor remains for infinite time. This property can be used as memory device or information storage in a computer.

SQUIDS : A superconducting quantum interference device (SQUID) is a very sensitive device for measuring weak magnetic fields. It is capable of measuring magnetic fields as low as 5 aT (5×10^{-18} T). Due to their sensitivity, SQUIDS are widely used in research, biological studies and other ultrasensitive electronic and magnetic measurements where faint signals cannot be sensed using conventional measurement instruments.

There are two types of SQUID, the radio frequency (RF) SQUID consisting of only one Josephson junction, and the direct current (DC) SQUID with two or more junctions. The RF is cheaper in construction but less sensitive compared to the DC.

A typical DC SQUID has two parallel junctions inserted in a superconducting loop. Without a magnetic field, the input current splits equally between the branches. This maintains an externally connected tank circuit at resonance. Any external magnetic field causes a change in the resonant frequency in the tank circuit, and a current imbalance that leads to a voltage across the Josephson junction. The voltage is a function of the magnetic flux and can therefore be measured and used to calculate the magnetic flux.

The superconducting materials used for low-temperature SQUIDS are pure niobium or lead alloys. The device is cooled with liquid helium to maintain superconductivity. High-temperature SQUIDS are made from high-temperature superconductors such as yttrium barium copper oxide (YBCO) and cooled with the cheaper and readily available liquid nitrogen. However, they are not as sensitive as the low-temperature models, but are good enough for certain applications.

A SQUID is very sensitive in detection of magnetic energy fields, as low as 100 billion times smaller in magnitude than the energy that moves a compass needle. This extreme sensitivity makes them ideal for highly sensitive applications in research, biological studies and medical tests where the magnetic fields present cannot be measured using conventional instruments.

For example, SQUIDS are used in measuring faint signals in the human brain or heart by sensing the magnetic fields created by the neurological currents. Other applications include the construction of highly sensitive gradiometers, magnetometers and voltmeters.

Josephson junction : Two superconductors separated by a thin insulating layer can experience tunneling of Cooper pairs of electrons through the junction. The Cooper pairs on each side of the junction can be represented by a wavefunction similar to a free particle wavefunction. In the DC Josephson effect, a current proportional to the phase difference of the wavefunctions can flow in the junction in the absence of a voltage. In the AC Josephson effect, a Josephson junction will oscillate with a characteristic frequency which is proportional to the voltage across the junction. Since frequencies can be measured with great accuracy, a Josephson junction device has become the standard measure of voltage.

PART A

1. (a) Mention the basic properties of metals.
(b) Derive an expression for electrical conductivity of a metal based on free electron theory. Hence establish Ohm's law.
2. (a) Derive the expression for thermal conductivity of the metal based on free electron theory.
(b) State and explain Weidman-Franz law.
3. (a) Define the density of states for free electron. Derive an expression for density of states for free electron.
(b) Explain Fermi distribution function.
4. (a) What is Fermi energy?
(b) Obtain the expressions for Fermi energy of a metal.
5. (a) Explain electron energy distribution with the help of a graph in case of metals.
(b) Arrive at the average kinetic energy of electrons at absolute zero temperature.
6. (a) Define Hall effect. Derive an expression for Hall voltage and Hall field in the case of metals and hence derive an expression for Hall co-efficient.
(b) Write a note on importance of Hall effect.
7. (a) What is superconductivity? Explain.
(b) Explain critical field, critical temperature and critical current density.
8. (a) Explain Meissner effect. Explain any three experimental facts about superconductivity.
(b) Explain the Type I and type II superconductors.
9. (a) Write a note on BCS theory.
(b) What is SQUID? Explain. Explain any three applications of superconductivity.

PART B

- 1 Calculate the drift velocity of the free electrons in a conductor of area $10^{-4}m^2$ given the electron density to be $8 \times 10^{28}m^{-3}$ when a current of 5 A flows in it.
[Hint : $v_d = \frac{I}{neA}$]
- 2 The drift velocity of free electrons in a metal wire of diameter 5 mm is $6 \times 10^{-4}ms^{-1}$. The current is 10 A. Calculate the electron density.
[Hint : $n = \frac{I}{eAv_d}$ where $A = \pi r^2$]
- 3 Calculate the relaxation time of free electrons in copper of atomic weight 63.5. Density of copper is $8.94 \times 10^3 kgm^3$ and electrical conductivity is $6 \times 10^7 mho m^{-1}$.
[Hint : $J = \frac{ne^2E\tau}{2m}$, As $\sigma = \frac{J}{E} = \frac{ne^2\tau}{2m}$ or $\tau = \frac{2\sigma m}{ne^2}$ where $n = \frac{N_A}{V} = \frac{\rho N_A}{M} = \frac{8.94 \times 10^3 \times 6.02 \times 10^{26}}{63.5}$]
- 4 Calculate the electrical conductivity of copper from the following data : atomic weight of copper = 63.5, density of copper = $8.94 \times 10^3 kgm^3$ and relaxation time = $2.48 \times 10^{-14}s$. [Hint: $\sigma = \frac{ne^2\tau}{2m}$]
- 5 Find the Fermi energy in copper on the assumption that each copper atom contributes one free electron to the electron gas. The density of copper is $8.94 \times 10^3 kgm^3$ and its atomic mass = 63.5 amu Given 1 amu = $1.66 \times 10^{-27}kg$.

[Hint : $n = \frac{\text{density}}{\text{total mass}} = \frac{8.94 \times 10^3}{63.5 \times 1.667 \times 10^{-27}}$, $E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3}$ J, to convert eV divide by 1.6×10^{-19} $E_F(\text{Cu}) = 7.04 \text{ eV}$]

6 Calculate the fermi energy for lithium and sodium given their densities to be 534 and 971 kgm^{-3} and their atomic weights to be 6.931 and 22.99 amu respectively.

[Hint: $E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3}$ J, to convert eV divide by 1.6×10^{-19} $E_F(\text{Li}) = 4.7 \text{ eV}$, $E_F(\text{Na}) = 3.152 \text{ eV}$]

7 The fermi energy of silver is 5.5 eV. Calculate the fermi temperature and fermi velocity.

[Hint : $T_F = \frac{E_F}{k}$ and $v_F = \sqrt{\frac{2E_F}{m}}$. Convert eV to J by multiplying with 1.6×10^{-19}]

8 The fermi energy of copper is 7.1 eV. Calculate the number of electrons per unit volume, given the density of copper is $8.94 \times 10^3 \text{ kgm}^3$.

[Hint : $E_F = \frac{h^2}{2m} \left(\frac{3n}{8\pi} \right)^{2/3}$ to calculate n]

9 A copper wire of cross sectional area $5 \times 10^{-6} \text{ m}^2$ carries a steady current of 50 A. Assuming one free electron per atom, calculate the (1) density of free electrons, (2) drift velocity of the electrons and (3) relaxation time given resistivity of copper is $1.7 \times 10^{-8} \Omega \text{ m}$.

[Hint : $n = \frac{\rho N_A}{M}$, $v_d = \frac{I}{neA}$, $\rho = \frac{2m}{ne^2\tau}$, to find τ]

10 A current of 50 A is established in a copper slab 0.5 cm thick and 2cm wide. The slab is placed in a magnetic field of 1.5 T. The magnetic field is perpendicular to the plane of the slab and to the current. The free electron concentration in copper is 8.48×10^{28} electron/ m^3 . What is the magnitude of Hall voltage across the width of the slab? [Hint : $V_H = \frac{BJd}{ne}$ where $J = \frac{I}{A}$ and $A = \text{width}(w) \times \text{thickness}(d)$]

11 Calculate the Hall coefficient of sodium, if the number of free electrons per unit volume is $2.55 \times 10^{28} \text{ m}^{-3}$.

[Hint : $R_H = -\frac{1}{ne}$]