DJK3A: MODERN PHYSICS

Unit I

Crystal Structure:

Lattice Translation Vectors- Basis And The Crystal Structure- Primitive Lattice Cell- Types Of Lattices- Two Dimensional Lattice Types- Three Dimensional Lattice Types -Index System For Crystal Planes- Sodium Chloride Structure- Cesium Chloride Str

Unit II

Dielectric Properties:

Local Field – Clausius - Mossotti Relation – Polarizability - Electronic Polarizability – Ionic Polarizability – Orientational Polarizability – Dielectric Constant – Frequency Dependence Of Dielectric Constant - Measurement Of Dielectric Constant – Ferro Electricity – Hysteresis – Piezoelectricity

Unit III

Superconductivity:

Statistical Mechanics - probability- principle of equal a priori probability -microstate and macro state- thermodynamic probability -constrains on a system -static and dynamic systems -most probable state (equilibrium state) -concept of a cell in a compartment -ensemble and average properties Degrees of freedom -position space -momentum space-phase space- the mu- space and gamma space-

UNIT IV

NUCLEAR PHYSICS AND RADIATION PHYSICS:

Nuclear Physics: Nuclear constituents, size, mass, spin and charge - binding energy - binding energy curve - nuclear fission - chain reaction – nuclear reactor - Radiation Physics: radioactive disintegration – half-life period - radiation hazards

UNIT V

RELATIVITY AND QUANTUM MECHANICS:

Relativity: Frames of references - postulates of special theory of relativity - Lorentz transformation equations - Wave mechanics: matter waves - de Broglie wavelength - properties of wave functions - Quantum mechanics: postulates of quantum mechanics - Schrödinger equation - time dependent form

Reference Book:

1. Introduction to Solid State Physics (8th Ed) - Charles Kittel
2. Solid State Physics – R.J. Singh – Pearson Education
3. Thermodynamics and statistical physics Brij Lal N.Subramanium P.S Hemne S.Chand publications
4. Atomic and Nuclear Physics: Brij Lal & Subramaniam, S Chand & Co., 2000
5. Quantum Mechanics: V. Devanathan, Narosa, Chennai, 2005.

Unit I : Crystal Structure

Lattice Translation Vectors- Basis And The Crystal Structure- Primitive Lattice Cell- Types Of Lattices- Two Dimensional Lattice Types- Three Dimensional Lattice Types -Index System For Crystal Planes- Sodium Chloride Structure- Cesium Chloride Structure

Introduction

Lattice Translation Vectors

Let us consider an ideal crystal. It is composed of atoms or groups of atoms arranged in a regular pattern so that the atomic arrangement at one location looks exactly the same in all respects to the arrangement at a corresponding locations. In the language of crystals ,we say that in a crystal there exits some smallest group of atoms that repeats itself in all direction in the crystal by means of the translation operation T defined as

$$T=n_1a+n_2b+n_3c \qquad \text{---------------} \ (1)$$

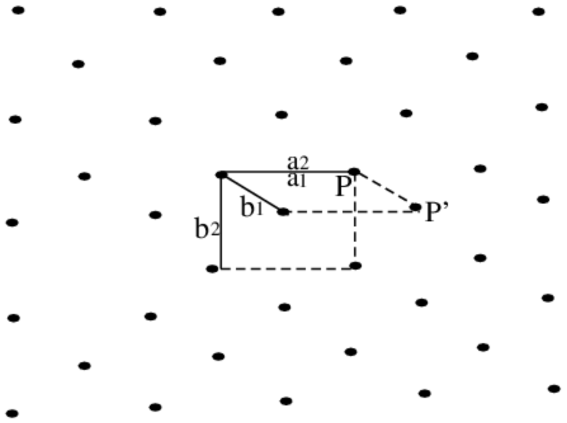


Figure : Translation vectors

Where n_1,n_2,n_3 are arbitrary integers and a,b,c are vectors defined as the fundamental translation vectors. Moreover, see that the application of this operation (1) to any point r (measured from some arbitrary origin) result in a point r′ :

$$r' = r + T = r+n_1a+n_2b+n_3c \qquad \text{-------------------} \ (2)$$

Which is identical in all respects to the original point r, and thus satisfies the essential features of a perfect crystal. This is not possible for an imperfect crystal , there r′ is not identical to r for any arbitrary choice of n_1,n_2,n_3 and the vectors a, b, c are not translational vectors. Thus in order for an assembly of atoms to be defined as crystal structure, it must be possible to find three translational vectors a,b,c which satisfies (2) such that r′ is identical to r. In other words, we can say that if no a, b, c exist according to the above prescription, the assembly cannot be classified to be a crystal. These translation vectors a, b, c are often called as crystal axes or basis vectors.

Now, with reference to a given crystal there may be many ways of choosing these translation vectors. However, a_1 and b_1 are such that every identical point in the crystal can be reached by an application of the translational operation

$T=a_1n_1+b_1n_2$

With some combination of n_1 and n_2. For example, we can get p, from p by using the operation $T=0.a_1+1.b_1$ and can write

$P'=P+0.a_1+1.b_1$.

Such translation vectors are called the primitive translation vectors. On the other hand, the vectors a_2 and b_2 cannot do it. When we try to do it using a_2 and b_2 we get

$$P'=P+\frac{1}{2}a_2+\frac{1}{2}b_2.$$

But this involves non-integer coefficients of a_2 and b_2 and thus is not in accord with the periodicity of the crystal. Such axes are called the non-primitive translation vectors. For the description of the crystal structures either type of the translational vectors may be used. Usually, one which is orthogonal is convenient, specially for calculating purposes. Further, they must be shortest in length. Keeping these factors in mind, the vectors a_2 and b_2 are regarded as convenient for the description of the lattice.

Basis and Crystal structure

In a perfect crystal there is a regular arrangement of atoms and the atomic arrangement in a crystal is called the crystal structure. The points in the space about which these atoms, ions or molecules are located and such points in space are called lattice points. The group of lattice points in a three dimensional pattern is known as crystal lattice or space lattice. In crystal lattice every point has its surroundings, identical to that of every other point. If all the atoms , molecules or ions at the lattice points are identical, then the lattice is called a Bravais lattice

The space lattice has been defined as an array of imaginary points that are arranged in space so that each points has identical surroundings. Thus in order to obtain a crystal structure an atom or group of atoms must be placed on each lattice points in a regular manner. Such an atom or group of atoms is called the basis and this acts as a building unit or a structural unit for the complete crystal structure. Obviously a lattice combined with a basis generates the crystal structure. This means there is an infinite number of basis-lattice combinations that describe the same crystal structure.

Space lattice + basis ----→ Crystal structure.

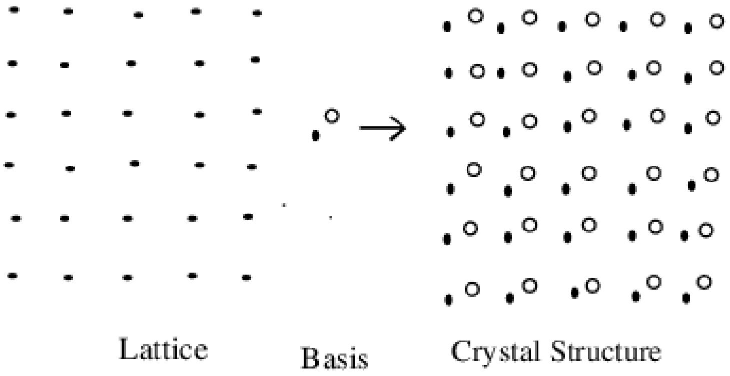


Figure: Crystal structure from lattice and basis

Primitive Lattice Cell

In describing crystal structures, it is convenient to divide the structure into repetitive building blocks called unit cells. Obviously a unit cell is the smallest component of the space lattice. The unit cell is defined as the smallest block of a geometrical figure, repeating again and again in a space lattice in the entire three dimensions, so as to build the whole crystal. A unit cell is described by the length a,b,and c called as translational vectors and the angles subtended by the lengths α,β and γ called as interfacial angles.

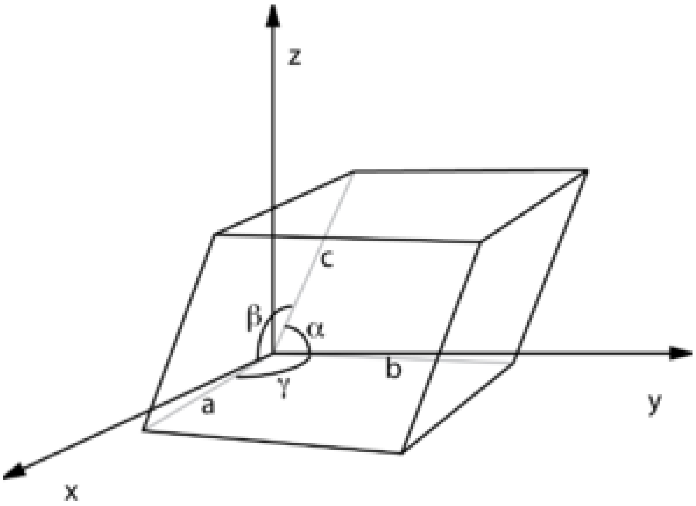


Figure: Lattice parameters of unit cell

If the values of translational vectors and interfacial angles are known, we can easily determine the actual size of the unit cell.

The unit cell that contains one lattice points only at their corners is called as primitive cell. The unit cell that contain more than one lattice point are called non primitive cells . The unit cells may be primitive cells but all the primitive cells are not unit cells. A unit cell formed using the primitive lattice vectors as sides is called a primitive unit cell. It can be shown that the volumes of all primitive unit cells are the same and the smallest among all possible unit cells.

Two-Dimensional Lattices

There are five types of two dimensional lattice . They are

1) Oblique lattice ; $a \neq b$, $\theta \neq 90^0$

2) Square lattice ; $a=b$, $\theta=90^0$

3) Rectangular lattice ; $a \neq b$, $\theta=90^0$

4) centered-rectangular ; $a \neq b$, $\theta=90^0$ with center of the atom

5) Hexagonal lttice ; $a=b$, $\theta=120^0$

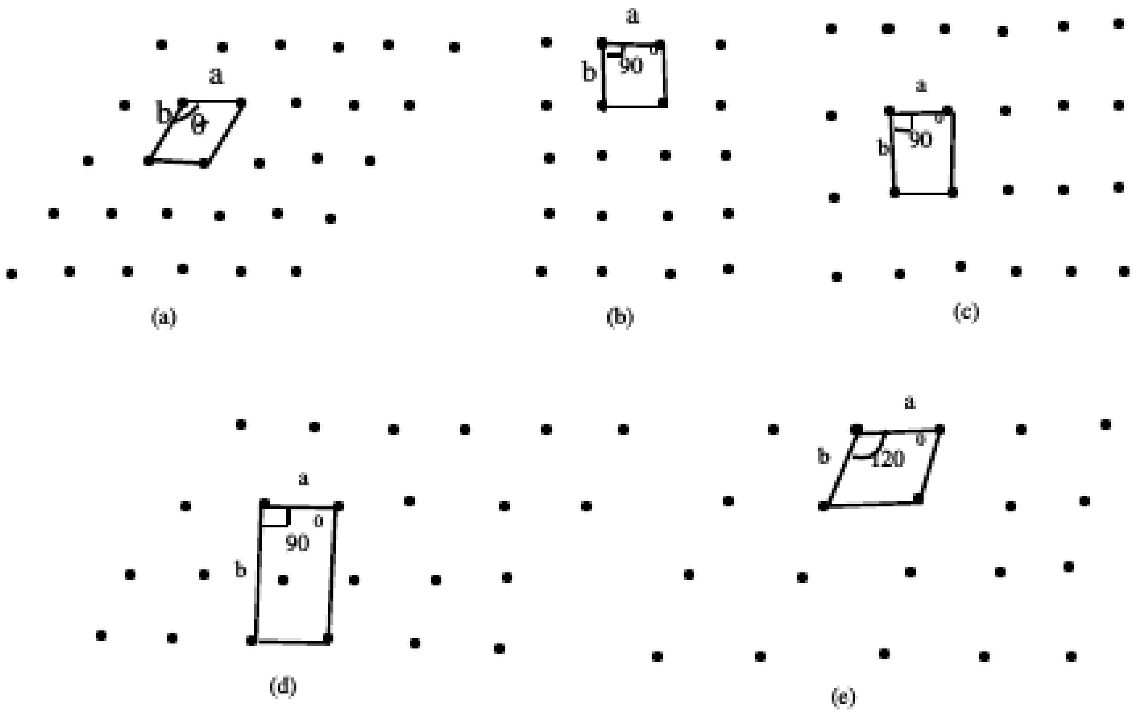


Figure : Two dimensional lattices

Three-Dimensional Bravais lattices

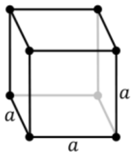
If all the atoms at the lattice points are identical, the lattice is said to be Bravais lattice. The seven classes of crystal lattices consists of 14 types of unit cells that are called as bravais lattice in three dimensions. In three dimensions the picture becomes complicated due to additional symmetry elements and due to the added dimensionality itself. The thirty-two permitted crystal point groups require fourteen different space lattices or Bravais lattices. The lattices are grouped into seven systems according to certain specifications about the lengths of edges and angles between them of a convenient unit cell. These fourteen Bravais lattices with seven crystal systems and these are illustrated in figures.

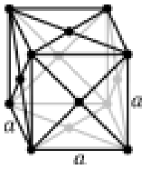
1. Cubic system

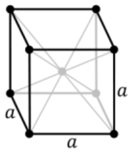
i) Simple cubic

ii) Face centerd cubic

iii) Body centered cubic





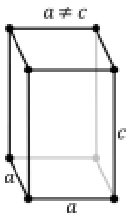


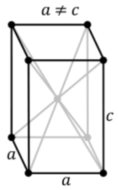
2. Tetragonal system (a≠ c)

i) Tetragonal simple

i) Tetragonal simple

ii) Tetragonal body





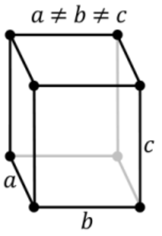
3. Orthorhombic system (a≠ b≠ c)

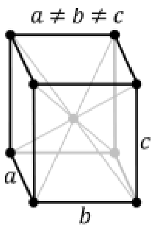
i) Orthorhombic simple

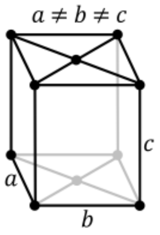
ii) Orthorhombic body

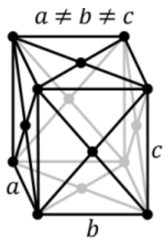
iii) Orthorhombic base

iv) Orthorhombic face





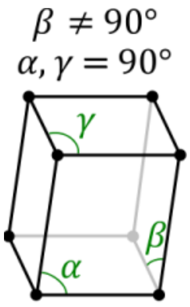


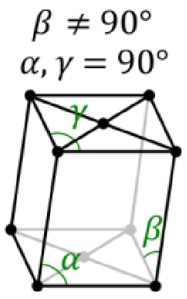


4. Monoclinic system($\alpha=\beta=90^0$)

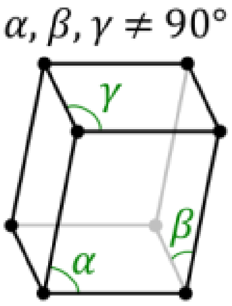
i) Monoclinic simple

ii) Monoclinic base

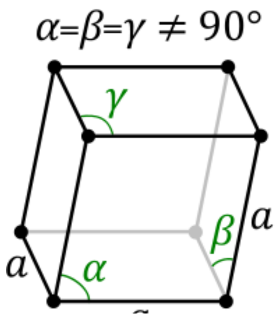




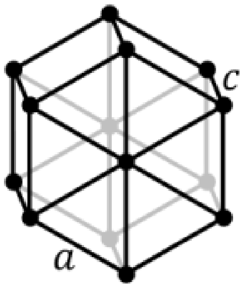
5. Triclinic simple ($\gamma \neq 90^0$)



6.Rhombohedral simple($\alpha=\beta=\gamma \neq 90^0$)



7. Hexagonal



Crystals Planes and Miller Indices

A crystal lattice is considered as a collection of a set of parallel equidistant planes passing through lattice points. These planes are known as lattice planes or crystal planes.

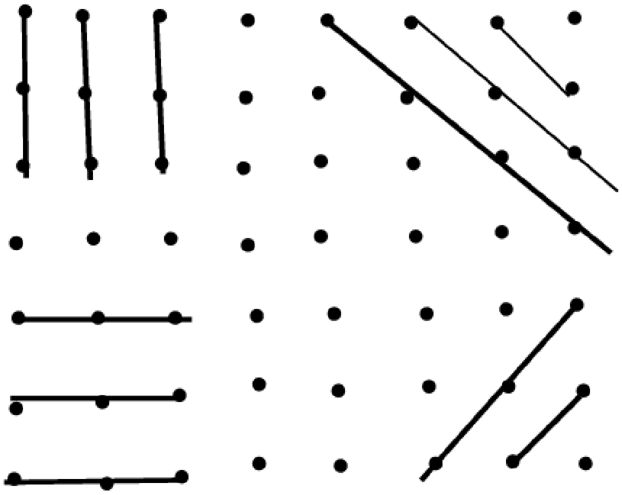


Figure: Crystal Planes

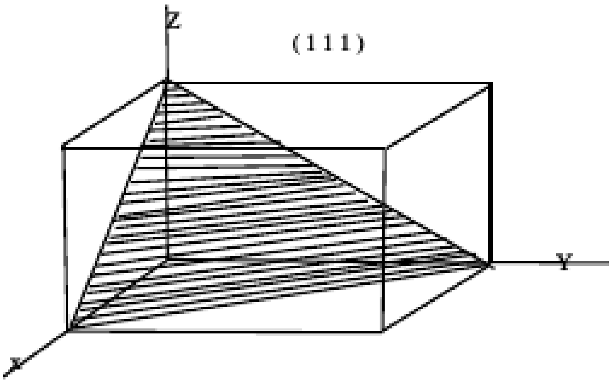
Miller evolved a method to designate a set of parallel planes in a crystal by three numbers h, k and ℓ usually written within brackets and thus *(h,k,ℓ)* is known as Miller indices. Miller indices are three possible integers that have the same ratios as the reciprocals of the intercepts on the three axes.

Procedure for finding Miller indices

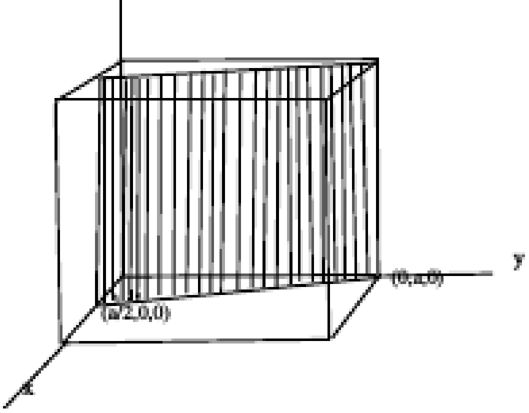
1. Take any atom as the origin in the crystal and erect co-ordinate axes from this atom in the directions of the basis vectors. The axes may be primitive or non-primitive.
2. Choose one plane of the set of interest and note its intercepts on the axes a,b,c in terms of the lattice constants. The plane must be chosen so that no intercept is at the origin. Since all the parallel planes are exactly alike, it is convenient always to consider the plane nearest to the origin.

3. Take the reciprocals of these intercepts and convert these into the smallest set of integers that can be obtained by multiplying each of the fractions by the same number.

The result is conventionally enclosed in parenthesis *(h,k,ℓ)*. By taking reciprocals, we bring all the planes inside a single unit cell, so that we can discuss all crystal planes in terms of planes passing through a single unit cell. The fractions are converted into smallest set of integers for convenience. The following examples illustrate these steps:



The figure, shows a plane whose intercepts are 1a,1b,1c. The Miller indices of the family to which this plane belongs are obtained by taking the reciprocals of these numbers: $\frac{1}{1},\frac{1}{1},\frac{1}{1}$; and reducing to the smallest set of integers. This can be done by multiplying each of the reciprocals by 1 in this case, giving 1,1,1. Thus the Miller indices of this plane are (1 1 1) plane.



If an intercept is at infinity *i.e*. the plane is parallel to one of the co-ordinate axis the corresponding index is zero. This is clearly understood by obtaining the Miller indices of a plane shown in figure. Here

Intercepts : ½ a , a , ∞
Reciprocals : ½ , 1 , ∞
Indices : **(210)**

Thus, the plane is a (2 1 0) plane. If a plane cuts an axis on the negative side of the origin, the corresponding index is negative and is indicated by placing a minus sign above the index :(h,k,ℓ).

Simple Crystal Structures

The three dimensional crystal structures are obtained by arranging the different atomic planes one above the other. The different methods of arrangements of the atomic planes give rise to different structures.

Cubic crystal structure is the simplest of the crystal structures. Cubic crystal system contains three Bravais lattices namely simple cubic (sc), body centered cubic (bcc) and face centered cubic(fcc)

Simple Cubic (sc) Structure

Figure: a) Simple cubic structure b) Atomic radius of SC structure

The simple cubic structure is the simplest and easiest crystal structure. Simple cubic structure is shown in the figure. We observe that this cell contains atoms only at the eight corners and thus there is only one atom associated with this cell. These atoms touch along the cube edges.

Assuming the atoms as the hard spheres, the radius in a close packing is

$r = \frac{1}{2}a$, and the packing factor (f) is the ratio of the Volume of atoms in the unit cell and the Volume of unit cell ie., $f = \frac{\frac{4}{3}\pi r^3}{a^3} = 0.52$

Thus, 52% of the volume is occupied by the atom and the remaining 48% volume is vacant.

Face-Centered Cubic (fcc) Structure

In face centered cubic structure the unit cell contains one atom at each of its corners and one atom each of its six faces. Thus there are eight corner atoms and six face centered atoms. However the atoms are in contact with the diagonal atoms. In fcc structure each corner of the unit cell contains one atom and each face contains one atom. Thus there are eight corner atoms and six face centered atoms. In this case the nearest neighbours of any corner atoms are the face centered atoms of the surrounding unit cells. Any corner atom has four such atoms in its own plane four in a plane above it and four in a plane below it, thus the coordination number of the fcc structure is twelve.

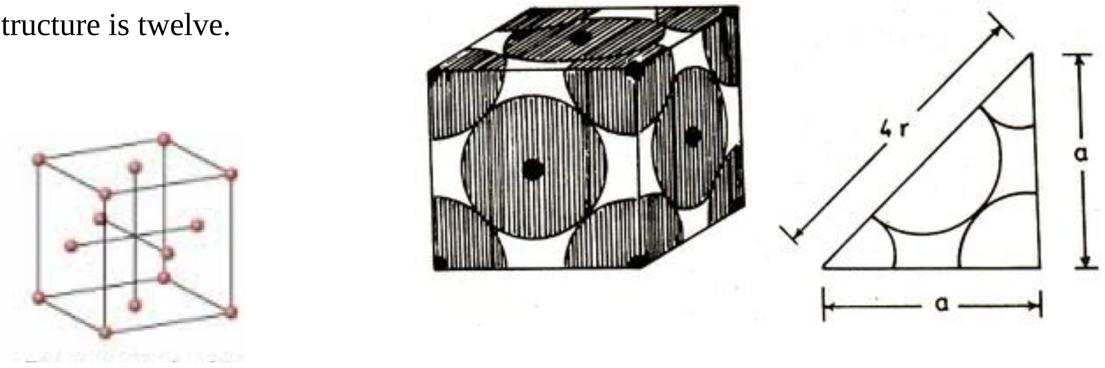


Figure: a) face centered structure b)unit cell of fcc c) Atomic radius of fcc structure

With reference to the above discussion, let us now consider the structure which is formed when the third layer is added to the stacking sequence AB in such a way that its atoms are in positions corresponding to C; that is, in the positions which are neither directly above those of layer A nor those of layer B. In this case the stacking sequence is thus ABCABC… This structure has cubic symmetry, the successive layers being (111) planes. A unit cell of this structure is shown in fig. We observe that in addition to the atoms at the eight corners, there are also atoms at the six face centers of this cubic cell: hence the name face-centered cubic (fcc). Now, since a corner atom is shared among eight cells which touch there and a face-centered atom is shared between two cells, there are $8\frac{1}{8}+6\frac{1}{2}=4$ atoms associated with this cell. From this we conclude that this cell is a non-primitive one because for simple structures containing atoms of one kind only, the primitive cell usually contains only one atom. The primitive cell for this structure is a 60° rhombohedra as is illustrated by the heavy drawing in the figure. It contains atoms only at the corners and thus there is only one atom associated with it.

Assuming them to be the hard spheres, the radius in a close packing is then determined by the condition. $(4r)^2=2a^2$

Therefore, $r = \frac{1}{4}\sqrt{2a}$ (4r = length of face diagonal).

In fcc structure each corner of the unit cell contains one atom and each face of the unit cell there is an atom. Thus there are eight corner atoms and six face centered atoms. We find that each corner atom is common to the corners of eight unit cells. So the contribution of each corner atom to a particular unit cell is only 1/8. As there are eight corner atoms in a unit cell the contribution of number of corner atoms per unit cell is $\frac{1}{8}x8=1$ Each face atom is common to the face of two unit cells. So the contribution of each face atom to a particular unit cell is only ½ . As there are six face atoms in a unit cell, contribution of the number of face per unit cell is $\frac{1}{2}x6=3$. Hence the number of atoms per unit cell for face centred cubic structure = 1+3 = 4

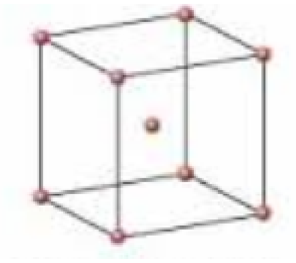
Packing fraction = Volume of atoms in the unit cell / Volume of unit cell

The packing fraction in this case is $f = \frac{4.\frac{4}{3}\pi r^3}{a^3} = 0.74$

Thus the packing fraction of fcc structure is 74%. It means that only 74% of the unit cell is packed with atoms and remaining 26% is vacant and hence this structure is closely packed. Copper, Aluminium are fcc structure.

Body-Centered Cubic (bcc) Structure

Many elements possess structures which are not close packed in the above sense; they have loosely packed instead. One of these is the body centered cubic structure, the unit cell (conventional) of which is sketched in fig. We observe that in addition to the atoms at the eight corners, there is also an atom at the body center of this cubic cell; hence the name body-centered cubic (bcc). Now, since corner atom is shared among eight cells which touch there and the body centered atom belongs exclusively to the cell under consideration. So the contribution of each corner atom to a particular unit cell is only $\frac{1}{8}$. As there are eight corner atoms in a unit cell the contribution of number of corner atoms per unit cell is $\frac{1}{8}x8 = 1$. In body centered cubic structure there is a body centered atom meant of each unit cell. Hence the number of atoms per unit cell for body centered cubic structure = 1+1=2



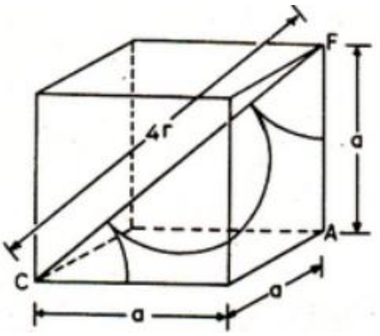


Figure: a) body centered structure b) Atomic radius of bcc structure

Each atom in the structure has only 8 nearest neighbours i.e. the coordination number of the structure is 8 and the structure is thus loosely packed. The looseness of the structure can be envisioned easily. Assuming the atoms as the hard spheres, their radius in a close packing is determined by the condition i.e. r = $\frac{1}{4}\sqrt{3a}$. Here 4r is the length of body diagonal. Thus

packing fraction $f = \frac{2.\frac{4}{3}\pi r^3}{a^3} = 0.68$

Thus the packing fraction of bcc structure is 68%. It means that only 68% of the unit cell is packed with atoms and remaining 32% is vacant and hence this structure is closely packed. The alkali and many of the alkaline-earth metals crystallize the bcc structure.

Sodium chloride (NaCl) structure

NaCl is an ionic crystal. In the NaCl lattice Na and Cl ions are situated side by side. It consists of 2 fcc sublattices. One of the Cl ion having its origin at (0,0,0) and the other of Na ions having origin at $(\frac{a}{2},0,0)$. Each ions in NaCl lattice has 6 nearest neighbour ion at a distance $\frac{a}{2}$. That is the coordination number is 6. Each unit cell is NaCl has 4 Na ions and 4 Cl ions. Thus there are 4 molecules in each unit cell. The unit cell of NaCl cubic structure is shown in the figure.

This structure, thus, may also be considered as composed of the two types of ions arranged alternately at the lattice points of a simple cubic lattice. In crystal each ion is surrounded by six nearest neighbours of the opposite kind (co-ordination number =6) and twelve nearest neighbours of the same kind as the reference ion.

To find the number of Na+ and Cl- ions per unit cell :

We have 2 types of Na+ ions . They are midpoint Na+ ions and Body centered Na+ ions. Each Na+ ions situated at the midpoint of the axial length is shared by 4 unit cells.

We have 12 mid points Na+ ions. Number of midpoint Na+ ions per unit cell= $\frac{1}{4}x12 = 3$

Each body centered Na+ ions is shared by the particular unit cell alone.

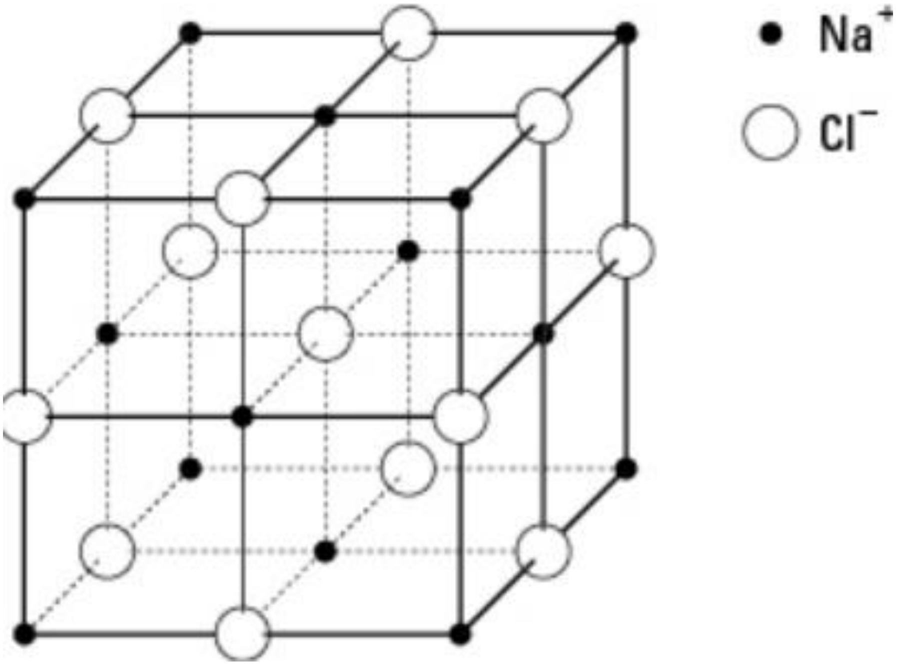


Figure : Sodium Chloride Crystal structure

Therefore number of body centered Na+ ions per unit cell =1

Therefore total number of Na+ per unit cell = 3+1=4

We have 2 types of Cl - ions. They are corner Cl- ions and face centered Cl- ions.

Each corner is shared by 8 unit cell= $\frac{1}{8} x 8 = 1$

Each face centered Chlorine ions shared by two unit cell , we have a fcc ions.

Number of face centered Cl ions per unit cell = $\frac{1}{2} x 6 = 3$

Total number of chlorine ions per unit cell = 1+3=4

thus there are 4 Na+ ions and 4 Cl- ions in the NaCl unit cell.

That is 4 NaCl molecules per unit cell

Cesium Chloride (CsCl) Structure

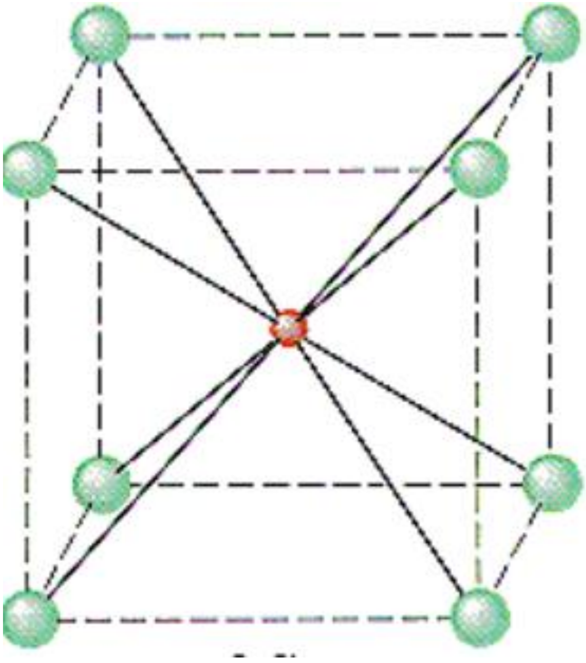


Figure : Cesium Chloride Crystal structure

The space lattice of CsCl is simple cubic. Cs+ and Cl^- have approximately same size. CsCl crystal consists of two inter penetrating simple cubic lattice. The cesium chloride structure is shown in figure. This structure may be considered as resulting from the combination of two simple cubic sub lattices, one of Cs ions and the other of CI ions, disposed such that a corner of one sub lattice is the body center of the other. The space lattice is therefore actually simple cubic with a basis of one Cs ion at (0, 0, 0) and one CI ion at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ is separated by one-half of the body diagonal of the unit cube. There is only one molecule per unit cell. Each ion at the centre of a cube of ions of the opposite kind.

One sub lattice is occupied by Cs^+ and the other by Cl^- ion, hence each Cs^+ ion has

8 nearest Cl^-

That is the coordination number of this structure = 8. The Cl^- ions are situated at all the eight corners to form a simple cubic arrangement. Cs^+ ion occupies cubic size. Number of Cs^+ ions and Cl^- ions per unit cell is 1.

Unit II: Dielectric Properties:

Local Field – Clausius - Mossotti Relation – Polarizability - Electronic Polarizability – Ionic Polarizability – Orientational Polarizability – Dielectric Constant – Frequency Dependence Of Dielectric Constant - Measurement Of Dielectric Constant – Ferro Electricity – Hysteresis – Piezoelectricity-Superconductivity:

Local field (or) Internal field

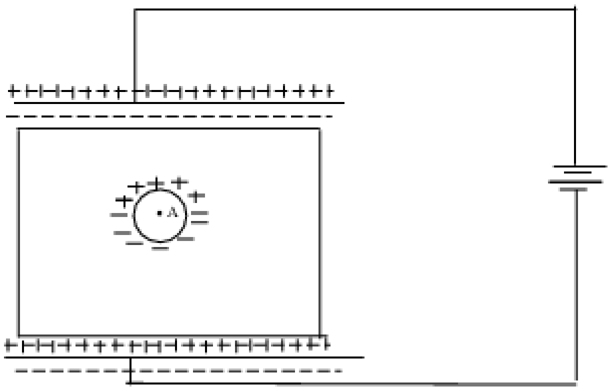


Figure : Local field

When a dielectric is placed between the plates of a parallel plate capacitor and let there be an imaginary spherical cavity around the atom inside the dielectric. The electric field experienced by the atom is called as internal field.

Glass, mica and paraffin paper are examples of dielectric material. Dielectric materials are insulators in which electric charge does not flow. There are no free electrons *to* move in the material. The electric field acting at an atom in a dielectric material is known as the local field or internal field $E_{1,}$ which is different has applied external field E.

Let a dielectric be placed between the plates of a parallel plate capacitor. To evaluate the local field it is necessary to calculate the total field acting on an atom A. Imagine a spherical cavity surrounded by the atom A inside the dielectric material. It is assumed that the radius of the spherical cavity is sufficiently larger than the radius of the atom.

The internal field at the atom A is made up of the four components E_1,E_2,E_3,E_4.

E_1 is the field intensity at A due to the charge on the plates.

From the field theory $E_1 = D/\varepsilon_0$ but $D = P + \varepsilon_0 E$

where D is the displacement vector

$$E_1 = (P + \varepsilon_0 E)/\varepsilon_0 = P/\varepsilon_0 + E$$

$$\text{ie. } E_1 = E + P/\varepsilon_0$$

E_2 is the field intensity at A due to the charge induced on the two sides of the dielectric material.

$$E_2 = -P/\varepsilon_0$$

E_3 is the field intensity at A due to the other atoms in the imaginary cavity. Because of the symmetry $E_3 = 0$

E_4 is the field intensity at A produced by the polarization charges on the cavity surface.

$$E = P/3\varepsilon_0$$

Therefore the total internal field $E_i = E_1 + E_2 + E_3 + E_4$.

$$E_i = E + P/\varepsilon_0 + -P/\varepsilon_0 + 0 + P/3\varepsilon_0$$

$$E_i = E + P/3\varepsilon_0$$

Derivation of the Clausius – Mossotti relation

The Clausius-Mosotti equation is applicable only to dielectric materials like germanium, silicon and carbon which have cubic structure. In these materials, there are no ions and no permanent dipoles and so the ionic polarization and orientation are zero. That is

$$\alpha_i = \alpha_0 = 0$$

The total polarization vector $P = N \alpha_e E_i$ ----------------- (1)

Where N is the number of molecules per unit volume. α_e is the electronic polarizability and E_i the internal field.

But, $E_i = E + P/3\varepsilon_0$ ------------------ (2)

where ε_0 is the permittivity of free space .

Substituting equation (2) in (1)

$P = N \alpha_e (E + P/ 3\varepsilon_0)$

$= N \alpha_e E + N \alpha_e P/ 3\varepsilon_0$

$P - N \alpha_e P/ 3\varepsilon_0 = N \alpha_e E$

$P (1 - N \alpha_e / 3\varepsilon_0) = N \alpha_e E$

$P = N \alpha_e E / (1 - N \alpha_e / 3\varepsilon_0)$ ----------------------------------- (3)

We know that , Electric field density $D = \varepsilon_0 E + P$ -------------- (4)

Therefore $P = D - \varepsilon_0 E$

$P/E = (D - \varepsilon_0 E)/E$

$P/E = D/E - \varepsilon_0$

$P/E = \varepsilon - \varepsilon_0$ (where $\varepsilon = D/E$)

$= \varepsilon_0 \varepsilon_r - \varepsilon_0$ (where $\varepsilon = \varepsilon_0 \varepsilon_r$)

$= \varepsilon_0 (\varepsilon_r - 1)$

From this $P = \varepsilon_0 (\varepsilon_r - 1) E$ --------(5)

From equations (3) and (5)

$\varepsilon_0 (\varepsilon_r - 1) E = N \alpha_e E / (1 - N \alpha_e / 3\varepsilon_0)$

$\varepsilon_0 (\varepsilon_r - 1) = N \alpha_e / (1 - N \alpha_e / 3\varepsilon_0)$

$(1 - N \alpha_e / 3\varepsilon_0) = N \alpha_e / [\varepsilon_0 (\varepsilon_r - 1)]$

$1 = N \alpha_e / 3\varepsilon_0 [1+3/(\varepsilon_r - 1)]$

$3\varepsilon_0 / N \alpha_e = [\varepsilon_r - 1+3] / [\varepsilon_r - 1]$

$[\varepsilon_r - 1] / [\varepsilon_r + 2] = N \alpha_e / 3\varepsilon_0$ ------------------------ (6)

This equation is known as Clausius -Mossotti equation. By knowing the value of ε_r, we can determine the value of eletronic polarizability, α_e of the material.

$$\frac{[\varepsilon r - 1]}{[\varepsilon r + 2]} = \frac{N\alpha_e}{3\varepsilon_0}$$

Polarizability

The polarizability is the relative tendency of a charge distribution, like the electron cloud of an atom or molecule, and consequently of any material body, to have its charges displaced by any external electric field.

When a dielectric material is placed in an external electric field $\mathbf{E}_0$ the positive and negative charges are displaced from their equilibrium positions by very small distances throughout the volume of the dielectric. This phenomenon is called polarization. This results the formation of a large number of dipoles each having same dipole moment in the direction of the field. The material is said to be polarized with a Polarization **P**.

The polarization **P** is defined as the dipole moment per unit volume, averaged over the volume of a cell.

The effect of polarization is to reduce the magnitude of the external field $\mathbf{E}_0$. Thus the magnitude of the resultant field is less than the applied field, *i.e.*, $E < E_0$.

We may write $\mathbf{E} = \mathbf{E_0} + \mathbf{E_1}$

The field $\mathbf{E}_1$ is called the depolarization field, for within the body it tends to oppose the applied field $\mathbf{E}_0$. For ordinary electric fields, the polarization **P** is proportional to the macroscopic field **E**. It is expressed as $\mathbf{P} = \varepsilon_0 \chi_e \mathbf{E}$

Here, χ_e is the electric susceptibility.

The electric displacement vector **D** for an isotropic or cubic medium is defined as

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E} = \varepsilon_0 \mathbf{E} + \mathbf{P}$$

Here, ε_r, is the relative permittivity or dielectric constant of the dielectric. ε_r is related to the electric susceptibility as $\varepsilon_r = 1 + \chi_e$

The physical quantities of primary interest are the field vectors **E** and **D**, the polarization **P**, together with the electric susceptibility χ_e and dielectric constant ε_r.

$$D = \varepsilon_0 E+P$$

Polarization

When a dielectric material is subjected to an electric field the positive charges of the material are displaced in the direction of the field while the negative charges are displaced in the opposite direction. This displacement produces local dipoles throughout the material. Thus the process of producing dipoles by an application of the electric field in a material is called polarization in the material. The different types of polarization are

i) Electronic polarization

ii) Ionic polarization

iii) Orientational polarization

iv) Space Charge polarization

i) Electronic polarization

Consider a dielectric material. Let Ze is the charge of nucleus and electrons cloud of charge -Ze is distributed in a space of radius R. The charge density ρ is given by

$$\rho = \frac{Charge}{Volume}$$

$$\rho = \frac{-ze^2}{4/3\pi R^3} \qquad \text{-------------------------} \ (1)$$

When an external electric field of intensity E is applied , the nucleus and electron experienced a Lorentz force -Ze E. Due to this force the nucleus and electron cloud are pulled out . But a Coulomb force is developed between them, which attracts the nucleus and electron cloud. At equilibrium the two forces are equal and opposite .

Lorentz force = Ze E

Coulomb's force= $\frac{q_1 q_2}{4\pi\varepsilon_0 x^3}$ ------------------------ (2)

Where x is the distance between nucleus and the electron cloud.

Here q_1 = Ze

q_2 = volume x charge density = $4/3\pi x^3$. ρ

using equation (1) $q_2 = 4/3\pi x^3 . \frac{-ze^2}{4/3\pi R^3}$

$$q_2 = \frac{-zex^3}{R^3}$$

Substituting the value of q_1 and q_2 (2) we get the

$$\text{Coulomb's force} = \frac{-z^2e^2x}{4\pi\varepsilon_0 R^3}$$

At equilibrium Lorentz force is equal to Coulomb' force

$$-ZeE = \frac{-z^2e^2x}{4\pi\varepsilon_0 R^3}$$

Therefore $E = \frac{zex}{4\pi\varepsilon_0 R^3}$

$$x = \frac{4\pi\varepsilon_0 R^3 E}{Ze}$$

Now the induced dipole moment $\mu_e = Zex = Ze = \frac{4\pi\varepsilon_0 R^3 E}{Ze}$

$\mu_e = 4\pi\varepsilon_0 R^3 E$

$\mu_e = \alpha_e E$

$\alpha_e = 4\pi\varepsilon_0 R^3$

Which is the electronic polarizability. It is independent of temperature. Electronic polarization occurs in all materials. The atoms undergo electric strain when they are placed in an electric field. Then there is a displacement of a positively charged nucleus and the negatively charged electrons of the atom in opposite directions. When we apply the field the electrons around the nucleus shifts towards the positive end of the field.

ii) Ionic polarization

The ionic polarizability is due to the shift of positive and negative ions in opposite direction, when an ionic solid is placed in an electric field.

Ionic polarization is also independent of temperature. The ionic polarizability (α_1) is inversely proportional to the square of the natural frequency of the ionic molecule and to its reduce mass.

Suppose an electric field is applied in the positive x-direction of an ionic solid. Then the positive ions move to the right by a distance x_1 and the negative ions move to the left by a distance x_2. The resultant dipole moment per unit cell due to ionic displacement is given by.

$\mu = e(x_1 + x_2)$ ---------------------- (1)

If $\beta 1$ and β_2 are the restoring force constants of cation and anion and F is the force acting on the ions due to the applied electric field

Then, $F = \beta 1 \; x_1 = \beta_2 \, x_2$

$$x_1 = \frac{F}{\beta_1} \text{ and } x_2 = \frac{F}{\beta_2}$$

If ω_0 is the angular frequency of the molecule then $\beta 1 = m\omega_0^2$

and $\beta_2 = m\omega_0^2$, the above equation can be rewritten as

$$x_1 = \frac{eE}{m\omega_0^2} \quad \text{and} \quad x_2 = \frac{eE}{M\omega_0^2}$$

Where M is the mass of positive ion, m is the mass of negative ion and ω_0 is the angular frequency of the molecules in which the ions are present.

$$x_1+x_2 = \frac{eE}{\omega_0^2}\left(\frac{l}{m}+\frac{l}{M}\right)$$

$$\mu = e(x_1 + x_2) = \frac{e^2E}{\omega_0^2}\left(\frac{l}{m}+\frac{l}{M}\right)$$

$$\alpha_i = \frac{\mu}{E} = \frac{e^2}{\omega_0^2}\left(\frac{l}{m}+\frac{l}{M}\right)$$

Thus the ionic polarizability is inversely proportional to the square of the natural frequency of the ionic molecule and to its reduced mass.

iii) Orientational polarization

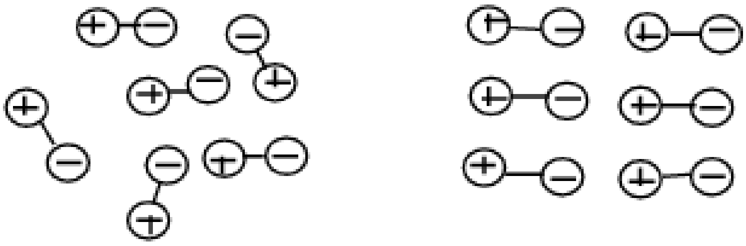


Figure: Orientational Polarization

Orientational polarization occurs mainly in liquids, which contain permanent dipoles. These are called non-polar molecules. But in molecules positive and negative charges do not coincide so that the molecules carry dipole moment even in the absence of external electric field.

These are called polar molecules. When an external electric field is applied on such molecules they tend to align themselves in the direction of applied field. This is called as Orientational polarization. The orientation polarization is inversely proportional to the absolute temperature of the material. Orientational polarizability α_0 can be shown to be equal to $\mu^2/3kT$.

Thus the orientation polarizability is inversely proportional to the temperature.

iv) Space charge polarization

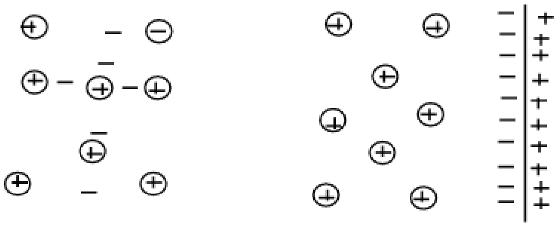


Figure : Space charge polarization

Space charge polarization occurs due to accumulation of charges at the electrodes or at the interfaces of multiphase dielectrics. This is possible when one of the phases present has much higher resistivity than the other. Space charge polarization is the slowest process as it involves the diffusion of ions over several interatomic distances. This kind of polarization is found in ferrites, semiconductors and also in composite insulators when they are heated to higher temperature.

The total polarizability

The total polarizability of the material can be written as $\alpha = \alpha_e + \alpha_i + \alpha_s + \alpha_o$

Compared to all other polarizabilities space charge polarizability is very small and so it is omitted in the calculation of total polarizability

$$= 4\pi\varepsilon_0 R^2 + \frac{e^2}{\omega_0^2}\left(\frac{l}{m} + \frac{l}{M}\right) + \frac{\mu^2}{3kT}$$

This equation is known as Langavin- Debye equation .

Dielectric Constant

Dielectric materials are insulators. A dielectric is a material in which all the electrons are tightly bound to the nuclei of an atom. Thus there are no free electrons to carry current. Hence the electrical conductivity of a dielectric is very low. The conductivity of the ideal dielectric is zero. Glass, plastic, mica ,oil are examples of dielectrics.

The molecules of dielectrics are classified as nonpolar and polar.

A non polar molecule is one in which the centre of gravity of the positive charges (protons) coincides with the centre of gravity of the negative charges (electrons). The nonpolar molecules have symmetrical structure and zero electric dipole moment. Examples are H_2,N_2,O_2,CO_2, benzene etc.

A polar molecules is one in which the centre of gravity of the positive charges is separated from the centre of gravity of the negative charges by infinite distance. The polar molecule is thus an electric dipole and has an intrinsic permanent dipole moment. Examples are H_2O, HCl, CO, N_2O, NH_3 etc.

The dielectric characteristics of a material are determined by the dielectric constant or relative permittivity ε_r of that material . It is the ratio between the permittivity of the medium and the permittivity of free space.

The electric displacement vector for an isotropic or cubic medium can be defined as

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E} = \varepsilon_0 \mathbf{E} + \mathbf{P} \qquad \mathbf{......1}$$

Here, ε_r is called the relative permittivity or dielectric constant of the dielectric.

$$\varepsilon r = \frac{\varepsilon_0 E + P}{\varepsilon_0 E} = 1 + \chi_e$$

The susceptibility is related to the dielectric constant by

$$\chi_e = \frac{P}{\varepsilon_0 E} - 1$$

Frequency dependence of total polarizability

When an electric field is applied on a dielectric material, polarization process occurs as a function of time.

$P(t) = P_0 [1- e^{-t/tr}]$ where P_0 is the maximum polarization and t_r is the relaxation time. It is the time taken for a polarization process to reach 0.63 of the maximum value.

Electronic polarization is extremely rapid and is complete immediately the voltage is applied. Even when the frequency of the applied voltage is very high in the optical range 10^5 Hertz, electronic polarization occurs during every cycle of the applied voltage. So the electronic polarization is sometimes called as optical polarization.

Ionic polarization is slower than electronic polarization as the displacement involved here is for the much heavier ions as compared to the electron cloud in the electronic polarization. The frequency with which ions can be displaced over a small interatomic distance will be of the order of lattice vibration frequency 10^3 Hertz. The ionic polarization occurs at the frequency of the applied voltage in the infrared range

Orientational polarization is slower than ionic polarization. Orientaional polarization occurs when the frequency of the applied voltage is in the audio range 10^4 Hertz.

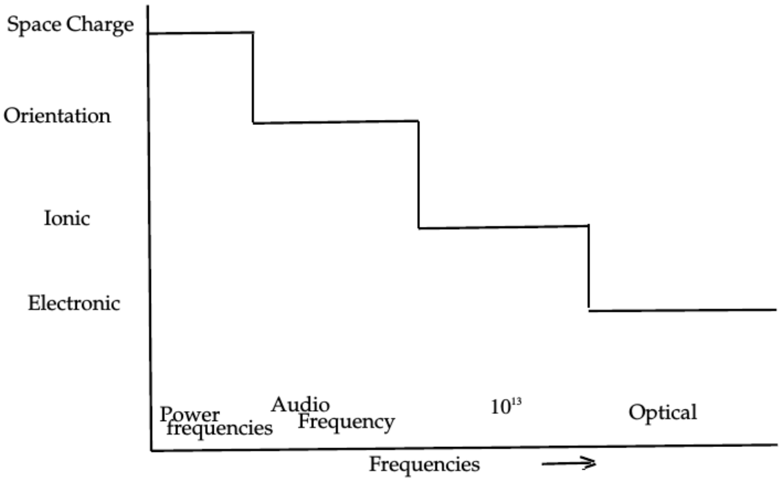


Figure: Frequency dependence of Polarizability

Space charge polarization is the slowest process as it involves the diffusion ions over several interatomic distances. Space charge polarization occurs at power frequencies 50 hertz.

Determination of dielectric constant

To measure the dielectric constant we use a high voltage bridge called Schering bridge. The bridge consist of four arms as shown in the diagram.

The first arm consists of a resistance r_1 connected in series with the capacitor C_1, the second arm has non inductive variable resistance R_3, the third arm has a variable capacitance C_4 and resistance R_4 connected in parallel and the fourth arm is connected with a standard capacitor C_2, N is the ac null detector and S is the high frequency oscillator.

Principle: First without the dielectric slab we measure the capacity of the capacitor in arm 1 as C1. Then we introduce the dielectric slab in between the plates of the capacitor C1 and measure the capacity as C_1' . The Dielectric constant $\varepsilon_r = \frac{C_1^1}{C_1}$

Experiment Theory: Without the dielectric slab inside C_1 balance the bridge by adjusting R_3 and C_4 . Under null deflection condition we have $\frac{P}{Q} = \frac{R}{S}$

P= resistance in arm 1 = $\frac{1}{j\omega C_1}$

Q= resistance in arm 2 = $\frac{1}{j\omega C_2} + r1$

R= Resistance in arm 3 = R_3

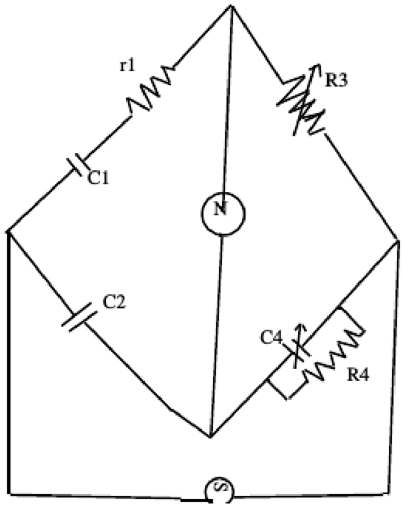


Figure: Schering bridge

S= Resistance in arm 4 = $\dfrac{\dfrac{1}{j\omega C_4} R_4}{\dfrac{1}{j\omega C_4} + R_4}$

Since $\dfrac{l}{Z_4} = \dfrac{1}{1/j\omega C_4} + \dfrac{1}{R_4}$

$$Z_4 = j\omega C_4 + \frac{1}{R_4}$$

The first part of the experiment should be carried out without inserting dielectric material inside the capacitor C_1 and the balance should be obtained by adjusting C_4 and R_3, When the current flowing through the detector becomes zero, then

$$\frac{P}{Q} = \frac{R}{S}$$

$$\frac{r_1 + \dfrac{1}{j\omega C_1}}{j\omega C_2} = \frac{R_3}{\dfrac{R_4}{1 + j\omega R_4 C_4}}$$

Equating real and imaginary parts we get

$r_1 = \dfrac{C_4 R_3}{C_2}$ and $C_1 = \dfrac{R_4}{R_3} . C_2$

Since R_4 and C_2 are fixed, the dial of R_3 is calibrated to read the capacitance directly.

The second part of the experiment is carried out, by inserting the dielectric specimen between the plates of capacitor C_1. Once again the bridge is balanced. Now the dial reading in R_3 will directly give the value of the new capacitance C_1'

The dielectric constant of the specimen $\dfrac{C_1'}{C_1} = \varepsilon_r$

The dielectric constant value at different frequencies can be determined by varying the frequency of the oscillator.

Ferroelectricity

The ferroelectric effect is an electrical phenomenon where by certain materials exhibit a spontaneous dipole moment even in the absence of an applied field. The dielectric materials which exhibit electric polarization in the absence of an applied electric field are known as ferroelectric materials.

Examples of ferroelectric substances are Rochelle salt and Barium titanate. In the absence of any field , ferromagnetic crystals has an electric dipole moment ie. permanent polarization. This means that in ferroelectric state the centre of positive charge of the crystal does not coincides with the negative charge.

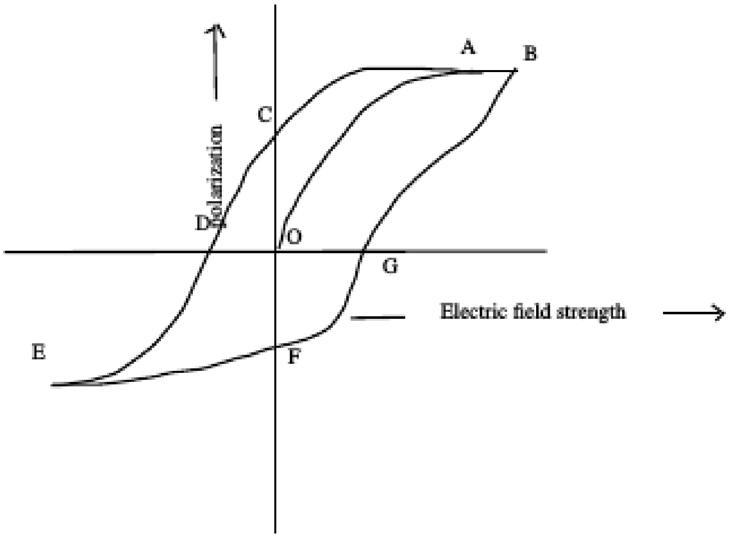
Under the action of electric field, the displacement of centers of positive and negative charge occurs. The polarization associated with the displacement creates in the internal field. The internal field both increases and stabilizes the polarization. So a part of polarization exists even if the field is removed.

The dielectric constants of these materials are very large compared to ordinary dielectric materials. For dielectric materials the polarization is a linear function of applied electric field but for ferroelectric materials polarization is non linear function of applied field.

In ferroelectric material the polarization can be changed and even reversed by an external electric field and becomes non polarized. If the non polarized ferroelectric crystal is heated above a critical temperature it becomes stable and this temperature is called as Curie temperature. The crystal undergoes a phase transition from the polarized phase (ferroelectric phase) into unpolarized phase (paraelectric phase)

Hysteris Loop

If a ferroelectric material is subjected to an applied electric field from zero, the polarization increases rapidly as shown in the curve OA. If the electric field strength further increased, the rate of polarization increases until saturation is reached as shown by the curve AB in the figure. If the electric field strength is reversed to zero, the polarization decreases along the curve BAD and does not become zero. The value of the polarization represented by OC, which present in the material even when the external electric field is zero is known as remnant polarization. In order to make the polarization zero, a certain value of the electric field strength is to be applied in the negative direction known as Coercive field . The electric field strength is further increased in a negative direction so that the reverse polarization increases rapidly until the saturation is reached E. If the electric field strength is again reversed to make it positive, polarization will follow the curve EFGB as shown in the figure. In the figure ABCDEFGB is called as Hysteresis loop.



When the temperature increases the height of the loop decreases slightly but width decreases considerably until it becomes a straight line. The temperature at which the loop reduces to straight line is known as Curie temperature. Above this temperature polarization of the ferroelectric material vanishes

Piezoelectric effect

When a dielectric crystal is subjected to a mechanical pressure, electricity is produced. This phenomenon is called piezoelectric effect and the electricity produced is known as piezoelectricity. According to inverse piezo electric effect when a voltage is applied, the material become strained. Conversely, an applied electric field can cause a piezoelectric material to change dimensions.

Piezoelectricity is the ability of certain crystals to generate voltage in response to applied mechanical stress. This property is used to convert mechanical energy into electrical energy and vice-versa(transducer). The word piezoelectric is derived from the Greek piezein which means to squeeze or press. The piezoelectric effect is reversible that the piezoelectric crystal can change shape by a small amount when subjected to an externally applied voltage.

In a piezoelectric crystal the positive and negative electrical charges are separated, but symmetrically distributed so that the crystal overall is electrically neutral. When a mechanical stress is applied, this symmetry is disturbed and charge asymmetry generates voltage across the material. For example a 10^{-2} m cube of quartz with 2 kN of corresponding applied force on it, can produce a voltage of 12,500 V.

In a piezoelectric crystal, the polarization 'P' is related to mechanical stress 'T' or conversely the electric stress 'E' is related to the mechanical strain 'S'. Thus we can define a piezoelectric coefficient 'd' relating polarization to stress and strain to field by the equation.

$$d = \left(\frac{\partial P}{\partial T}\right)_E = \left(\frac{\partial S}{\partial E}\right)_T$$

Where the suffix 'E' indicates that the field is held constant and the suffix T indicates that the mechanical stress is held constant. In other words the piezoelectric coefficient is given by the rate of change of polarization with mechanical stress at constant field or the rate of change of mechanical strain with field at constant electric stress. The units of 'd' are Coulomb per newton or meter per volt.

Superconductivity

In certain substances when the temperature is reduced below a particular value the resistivity of the substance becomes zero. And hence the conductivity becomes infinity. This property is called as superconductivity and such substances are called as superconductors.

Superconductivity was first observed in1911 by the Dutch physicist HK Onnes in the course of his experiments on the electrical conductivities of metals at low temperatures. He observed that as purified mercury is cooled, its resistivity vanished abruptly at 4.2 K. Above this temperature the resistivity is small, but finite, while the resistivity below this point is so small that it is essentially zero. The temperature at which the transition takes place is called the critical temperature (T_C). The temperature (T_C) which marks the transition of a normal conductor to the superconducting state is defined as the transition temperature. Above the critical temperature (T_C) the substance is in the familiar normal state, but below (T_C) it enters an entirely different superconducting state. The superconducting state is marked by a sudden fall of the electrical resistivity of the material to nearly zero, which it is cooled to a sufficiently low temperature.

Unit III : Statistical Mechanics

Statistical Mechanics- probability- principle of equal a priori probability -microstate and macro state- thermodynamic probability -constrains on a system -static and dynamic systems -most probable state (equilibrium state) -concept of a cell in a compartment -ensemble and average properties Degrees of freedom -position space -momentum space- phase space- the mu- space and gamma space

Statistical Basis

The classical statistics successfully explained the phenomenon like temperature, pressure, energy etc., This is applicable to the identical, distinguishable particles of any spin. The molecules of a gas are particles of this kind. But failed to explain other observed phenomenon like black body radiation, specific heat at low temperature etc. For this, new approach was introduced by Bose, Einstein, Fermi and Dirac. The Planck's quantum concept of discrete exchange of energy between systems was used. The new statistics was subdivided into two categories (i) Bose-Einstein statistics and (ii) Fermi-Dirac statistics.

Bose-Einstein statistics: This is applicable to the identical, indistinguishable particles of zero or integral spin. These particles are called *bosons.* The examples of bosons are helium atoms at low temperature and the photons.

Fermi-Dirac statistics: This is applicable to the identical, indistinguishable particles of half-integral spin. These particles obey Pauli Exclusion Principle and are called *fermions.* The examples of fermions are electrons, protons, neutrons etc.

Probability

The probability of an event may be defined as the ratio of the number of cases in which the event occurs to the total number of cases.

Thus, the probability of an event = Number of cases in which the event occurs / number of cases

Suppose an event can happen in a ways and fails to happen in b ways, then the probability of happening the event= $\frac{b}{a+b}$ and the probability of failing the event= $\frac{b}{a+b}$. Here *(a+b)* represents the total number of equally likely possible ways. It should be noted that the sum of these two probabilities is always 1, since the event must either occur or fail.

Thus, the probability of a 'sure' event is assumed to be equal to 1 and of an impossible event to be equal to zero. Thus, the probability of a random event lies between 0 and 1, *i.e.*,

$$0 \le P \le 1$$

This is further explained by the following experiments:

4. **Throwing a coin:** Suppose we toss a coin. Either the 'head' can come upward or the 'tail' *i.e.* an event can occur in a total number of two equally likely ways. The number of ways in which the 'head' can come up is only *one.* Therefore, the probability that the 'head' may come up is $\frac{1}{2}$. Similarly, the probability that the 'tail' may come up is also $\frac{1}{2}$.

5. **Throwing a dice:** A dice is a homogeneous, regular and balanced cube with six faces marked number of dots from 1 to 6 engraved on them. It is supposed that the die is symmetrical and cannot fall of its edges. When the die is thrown it falls one of its faces upwards *i.e.,* yields one of the six results and no other. All outcomes are equally likely in a single throw of dice. Out of six possible results only one is favorable for the appearance of six spots. In other words, the probability of any one face (say with a number 3) to come up is 1/6. The set of all possible outcomes can be written as

S (1, 2, 3, 4, 5, 6). The probability of the dice coming up with an even number is 3/6 as there are only three even numbers on the dice 2, 4, and 6.

$$\text{Therefore, } P \text{ (even)} = \frac{3}{6} = \frac{1}{2}$$

Likewise, the probability of the dice coming up with odd number is $\frac{3}{6} or \frac{1}{2}$

The probability of the dice coming up with any number less than 6 is given by

$$P\text{ (a number less than 6)} = \frac{5}{6}$$

as there are five numbers 1, 2, 3, 4, 5 which are less than 6.

Zero probability: If we want to know the probability of the dice coming up with a face marked with a number 7. The die has only six faces marked serially from 1 to 6. There is no face marked as 7. Therefore, probability of appearing a number 7 is zero, *i.e.,*

$$\text{Therefore, } P\text{ (number 7)} = \frac{0}{6} = 0$$

In other words, impossible event is always zero.

Probability one: The probability of appearing any number less than 7 is one. This is because all the six faces of the die are marked from 1 to 6, *i.e.,* the numbers less than 7.

$$P\text{ (number} < 7) = \frac{6}{6} = 1$$

Total probability: If a is the number of cases in which the event occurs and b the number of cases in which the event fails, then

$$\text{Probability of occurrence of the event} = \frac{a}{a+b}$$

$$\text{and Probability of failing the event} = \frac{b}{a+b}$$

The sum *i.e.,* the total probability is always one, since the event may either occur or fail.

Principle of Equal a Priori Probability

Suppose we toss a coin it is clear in mind that the coin will fail either with its ‘head’ up or ‘tail’ up. Similarly if a six face cubical dice is thrown, it is sure that the dice will fall with one of its six faces upward. In the same way, if we have an open box divided into two equal sized compartments X and Y, and a small particle is thrown from a large distance in such a way that it must fall in either of the two compartments, then the probability of the particle to fall in the compartment marked X is equal to the probability that it may fall into the compartment marked Y. again there is an equal probability.

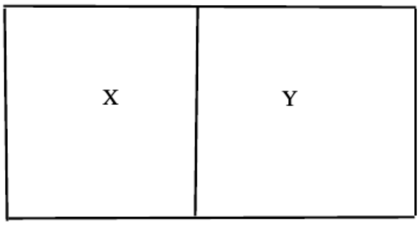


Figure: equal sized compartments

This probability of assuming equal probability for events which are equally likely to occur is known as the principle of equal a priori probability.

A priori means something which exists in our mind prior to and independently of the observations we are going to make.

This principle of equal a priori probability will not hold good, if in the above example, the two compartments are of unequal size.

The postulate of equal a priori probability is the fundamental basis of statistical mechanics. The basis for this postulate is provided by the ergodic hypothesis. According to the principle of conservation of density in phase space, the density of a group of phase points remains constant along their trajectories in a phase space. If at any time, the phase points are distributed uniformly in phase space, the phase point move in such a way that their density is uniform at all times. So the representative points move in the space in the same fashion as an incompressible fluid. For other spaces the density will range from region to region while there will be no change in phase space. This means, there is no crowding together of phase points in any particular region of phase space. The property of no crowding of phase points in any particular region of phase space bounded by a moving surface and containing a definite number of phase points does not change with time. The property of no crowding of phase points in any particular region of phase space and the constancy of volume element in phase-space with time indicates the validity of postulate of equal a priori probability.

Macrostate and Microstate

Macrostate: Consider 4 distinguishable particles and we wish to distribute them into two similar compartments in an open box. Let the particles be *a*, *b*, *c* and *d*. When any particle thrown into the box, it must fall into one of the two compartments. Since the compartments are alike, the particles have the same a priori probability of going into either of them and will be ½. The possible ways in which 4 particles can be distributed in two compartments are shown in table.

Thus, there are 5 different distributions (0,4),(1,3),(2,2),(3,1), and (4,0). each compartment wise distribution of a system of particles is known as a macrostate. A system of n particles distributed in a similar compartment, the various macrostates are (0,n),(1,n-1),(2,n-2),….(n-1,n). Therefore the total number of macrostates for n particles is (n+1).

Microstate: Since the particles are distinguishable, the number of different possible arrangements in each compartment is as shown below.

Macrostate	Possible arrangements		Number of microstates (W)
	Compartment1	Compartment 2	
0,4	0	abcd	1
1,3	a b c d	bcd cda dab abc	4
2,2	ab ac	cd bd	

	ad bc bd cd	bc ad ac ab	6
3,1	bcd cda dab ab	a b c d	4
4,0	abcd	0	1

Each distinct arrangement is known as microstate of the system. The distribution (0,4) has only one arrangement, distribution (3,1) has 4 distinct arrangement , distribution (2,2) has 6, distribution (3,1) has 4 and (4,0) has only one. Thus a given macrostate may consists of a number of microstates. In the above example of 4 particles, the total number of microstates is $16=2^{4.}$ In general for a system of n particles, total number of microstates is $2^{n.}$ Thus a given macrostate corresponds to many microstates and it is very natural to assume that at any time the system is equally likely to be in any of these microstates.

Thermodynamic Probability

The number of microstates corresponding to any given macrostate is called its thermodynamic probability. In other words, the thermodynamic probability of a particular macrostate is defined as the number of microstates corresponding to that macrostate. In general, this is a very large number and is represented by W.

The number of microstates corresponding to a given macrostate is equal to the number of meaningful arrangements or permutations of various particles in the macrostate excluding those permutations which are meaningless i.e. merely interchange the order of particles in a particular compartment (or cell). For the case of n particles and two compartments (or cells), if r is the number of particles in the compartment No. 1 and the remaining (n-r) are in compartment No. 2 then

No. of meaningful arrangements $= \dfrac{n!}{r!\left(n-r\right)!} = {}^{n}c_{r}$

Therefore the number of microstates in a macrostate (r, n – r) or thermodynamic probability.

$$W_{(r,n-r)} = \frac{n!}{r!(n-r)!} = {}^{n}c_{r} \qquad \ldots\ldots\ldots\ldots(1)$$

Applying this to a system of 4 distinguishable particles, for a macrostate (1,3), r = 1,

(n – r) = 3 and n = 4 the number of microstates.

$$W_{(1,3)} = \frac{4!}{1!3!} = 4$$

Similarly, for a macrostate (2,2), r = 2, (n – r) = 2 and n = 4 the thermodynamic probability i.e. no. of microstates will be

$$W_{(2,2)} = \frac{4!}{2!2!} = 6$$

The probability (or) occurrence of a macrostate us defined as the ratio of the number of microstates (i.e. thermodynamic probability W) in it to the total number of possible microstates of the system,

Thus , $$P_{macro} = \frac{\text{No. of micro states in the macro state}}{\text{Total no. of micro states of the system}} \qquad \text{----(2)}$$

The total number of ways of arranging n distinguishable particles in c numbered compartments = C^{n}

If there are only 2 compartments or cells, then the total no. of microstates of the system = 2^{n}. For 4 Particles system, total no. of microstates will be 2^{n}= 16.

we get. $P_{macro} = \dfrac{W}{C^{n}} = \dfrac{W}{2^{n}}$

Substituting W from eqn(1)

$$P_{(r,n-r)} = \frac{n!}{r!\,(n-r)!}\,x\,\frac{1}{2^n} = \frac{1}{2^n}\,{}^{n}c_r$$

This gives the probability of macrostate (r, n-r)

Constraints on a System

A set of conditions or restrictions that must be obeyed by a system are known as constraints.

Let us take an example of the distribution of 3 particles in two compartments; the system must obey the constraint that total number of particles in the two compartments must be 3. In general, if there are N particles to be distributed in two compartments and there are n_1 particles in compartment no. 1 and n_2 particles in compartment no. 2, then we must have

$$n_1 + n_1 = N$$

This relation is known as equation of constraint on the system.

A typical set of constraints is

$$\Sigma E = constant = N$$

$$\Sigma E_i n_i = constant = E$$

Where n_i is the number of particles (or molecules) in the *i*th compartment (or *i*th cell), E_i is the energy of each particle (or molecule) in the i th compartment (or i th cell).

Accessible states

Accessible states are the states consistent with the given constraints of the system.

Suppose we wish to distribute 3 particles in two compartments, The system has four macro and 8 microstates when particles are distinguishable and only four microstates when they are indistinguishable. If we put the constraint that no compartment should remain empty, then the macrostate (3, 0) and (0, 3) cannot exist. The system will then have only two macrostates (2, 1) and (1, 2) with their corresponding microstates. Thus, there will be only two macrostates and six microstates, when the particles are distinguishable, and only two microstates when they are indistinguishable.

Macrostate	Microstates			
	Particles distinguishable		*Particles indistinguishable*	
	Description	*Number*	*Description*	*Number*
3 ,0	*(abc, 0)*	1	*(aaa, 0)*	1
2, 1	*(ab, c) (bc, a), (ca, b)*	3	*(aa, a)*	1
1, 2	*(c, ab), (a, bc), b, ac)*	3	*(A, aa)*	1
0, 3	*0, abc)*	1	*(0, aaa)*	1

Suppose again we put the constraint that the particles are indistinguishable, then we shall have four macrostates (3,0), (2,1), (1,2) and (0,3) but each macrostate will have only one microstate as shown in . The total number of microstates will also be four.

Thus, the constraints decrease the number of macro as well as microstates of the system.

Accessible macrostates: The macrostates which are allowed under a constraint are called accessible macrostates.

For example, in distributing 3 particles in 2 compartments under the constraint that no compartment will remain empty, the only accessible macrostates are (2,1) and (1,2).

Inaccessible macrostates: The macrostates which are not allowed under a constraint are called inaccessible macrostates.

In the above example, the macrostates (3,0) and 0,3) are inaccessible macrostates.

Static and Dynamic Systems

Static System: A system is said to be static of the constituent particles of the system remain at rest in a particular microstate.

In static system, the particles do not change their relative positions in the compartment in which they are located. They do not move from one compartment to even the neighboring compartment. In other words, the static systems do not change of their own due to internal forces or the internal conditions. However, the change in possible due to external forces or causes.

Whenever the change in static system takes place due to external causes or forces, the system from one macrostate to another macrostate. The system now stays in the macrostate ever after the external cause of force is withdrawn.

Example: A system of tossed coin is an example of static system. After every toss, the coins remain permanently latched in the last state.

Dynamic system: A system is said to be dynamic if the constituent particles of the system can move so that the system goes from one microstate to another.

The particles of the dynamic system change their relative positions within the compartment in which they are. They also go from one compartment to another. Thus, both the micro as well as macrostates of the system change with time. Dynamic systems can change of their own due to internal causes or forces. They can also undergo changes due to external causes or forces affecting.

Example: Any gas is an example of dynamic system. The molecules of gas are always in constant, random motion, continuously colliding with one another, following Brownian motion. During this, they change their position, momentum and energy continuously.

If the dynamic system is disturbed by some external causes or forces and then left to itself the system tends to approach the macrostate with maximum thermodynamic probability and remains there or stays very close to the most probable macrostate.

Most probable state (Equilibrium state)

The most probable state of a system is that macrostate which has the maximum probability of occurrence. In the case of N particles distributed in two compartments, the probability of occurrence of the most probable state is given by

$$P_{max} = \frac{{}^{N}C_{N/2}}{2^{N}}$$

In a Static system, the particles remain latched i.e. at rest when put in a compartment or placed in a cell.

But in dynamic system, the particles are in a constant state of motion and are not stationary. Suppose, such molecules are enclosed in a vessel having two compartments, using a permeable partition. Due to collisions, the number of molecules in the two compartments go on changing and the system moves from one macrostate to another very large number of times per second. This number is generally of the order of millions of billions. Some macrostates are more probable than the other depending upon frequency of the microstate. When the number of particles, in a dynamic system is very large, the system exists practically all the time in the most probable macrostate. This is because the probabilities of macrostates fall extremely rapidly, even for a very small deviation from the most probable state. This most probable state is known as the equilibrium state of the system. A dynamic system always tends to go from a state of lower probability towards the state of maximum probability i.e., the equilibrium state. Even it is disturbed by some external causes of force, again it quickly comes back to its equilibrium state.

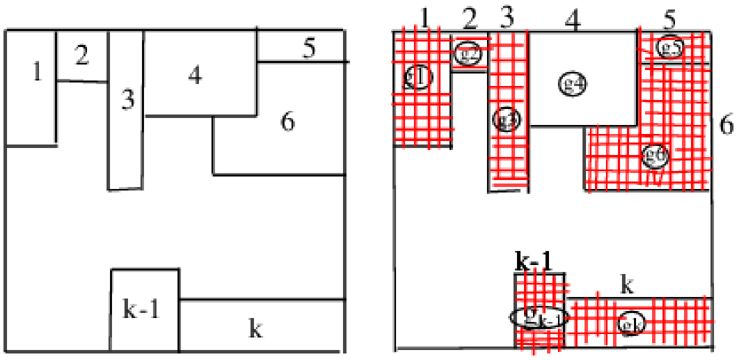
Concept of a cell in a compartment

In practice, if we wish to distribute n distinguishable particles in k compartments which are of unequal size, we find that the a priori probability of a particle going into a particular compartment is not the same. Large probability in a bigger compartment. This is because of unequal size of the compartment. This difficulty is overcome by introducing the concept of a cell.

Each compartment is divided into a very large number of sub-compartments, called as cells, in such a way that each cell is of same size. Therefore, all the cells have the same a priori probability. The size of the cell is very very small and hence the number of cells in each compartment is exceedingly large. For a given size of the cell, the number of cells in each compartment is fixed.

Distribution of particles

The concept of a cell is well understood by considering the distribution of particles in different compartments marked as 1, 2, 3, ... *i..., k-1, k* of unequal size. We wish to distribute n distinguishable particles in these k compartments. As the compartments are of unequal size, a priori probability of a particle going into particular compartment is not the same. To overcome this difficulty, we introduce a concept of a cell. For this purpose we divide each compartment, from compartment I to k, into cells of equal sizes, so that compartment 1 contains g_1 cells, compartment 2 contains g_2 cells, compartment 3 contains g_3 cells and so on, the i^{th} compartment containing g_i cells and lastly k^{th} compartment has g_k cells.



(a) (b)

Figure: Distribution of particles in different size compartments

As the compartments are of unequal size as shown in the figure the number of cells in each compartment will be different. The total number of cells, each of same size = $g_1 + g_2 + \dots\dots + g_i + \dots\dots\dots g_k = G$ Hence

(ι) Since all the cells are of same size, there is an equal a priori probability i.e. a particle in a given compartment can go into any cell within the compartment with equal probability.

(ιι) Moreover, since the size of the compartment is big, the number of cells in any compartment are exceedingly large.

Ensemble and Average Properties

The usual meaning of ensemble is the whole or all the parts taken together. In statistical mechanics an ensemble is a collection of identical systems with all accessible microstates represented in it. Consider a system of 4 particles in two similar compartments. The system, under constraint $\Sigma n_i = 4$, has 16 different microstates. We can draw all the sixteen microstates as 15 identical systems. Consider just one system, which at time t = 0 has a particular microstate, say (*ab*, *cd*). Then due to interactions among the particles, the system will pass through all the accessible microstates as time passes. In a short time, we may find that same microstates repeat more frequently than the other. But if we observe for long enough time, then we should expect all the microstates are repeated with equal frequency. In the present case of 15 accessible states, suppose we make 48 observations in all, then we expect that each microstate should appear just 3 times. But in practice, some microstates may occur even 7 times and some microstates may not occur at all in these 48 observations. On the other hand, if we make 48 x 10^{20} observations in all, then the observed frequency of each of the 16 microstates would not be different from 3 x 10^{20} by more than (say) 1 part in 10^{12} or so.

An ensemble for a system of 4 particles in two equal compartments

We may either make these 48 x 10^{20} times observations on a single particle system or at a single time on a collection of 48 x 10^{20} identical systems. The conclusion would be the same. Here we take into consideration the postulate of equal a priori probabilities. It is a fundamental postulate of statistical mechanics and it says that a system can exist in each of the accessible microstates with equal probability. In other words, no preference is to be given to any one or more microscopic states over others.

The probability of particular macrostate is given by the number of microstates falling under it divided by the total number of accessible microstates. Let a macrostate be designated by suffix *j* and let W_j represent the frequency with which it occurs in the ensemble is given by

$$P_j = \frac{W_j}{\Sigma W_j}$$

If any property *x* has value x_j in the j^{th} macrostate then the average value of this property over the ensemble, denoted by x or < x >, is given by

$$X = \langle x \rangle = \Sigma_j x_j \; p_j = \frac{\Sigma xj W_j}{\Sigma W_j}$$

It may be noted that we have no means of knowing how the system really passes through the various macrostates, much less about the further details of the microstates.

Degrees of Freedom

From the statistical point of view, a monatomic gas constitutes the simplest system. The energy expression for a system involved f co-ordinates of position and f co-ordinates of momentum. We then say that a system comprising one molecule has f degrees of freedom. If there are of N molecules in the system, the energy expression for the system of N molecules has Nf co-ordinates of position and Nf co-ordinates of momentum. Thus, the system has Nf degree of freedom.

Position Space

Consider a system consisting of N particles distributed in a given volume V. If the system is Static all particles will remain fixed at various points in space. To completely specify the position of any particle in the three dimensional space, we must know the values of its three Cartesian coordinates x, y and z which are mutually perpendicular to each other. As there are N particles, a knowledge of 3 N co-ordinates gives complete information about such a static system.

The three-dimensional space in which the location of a particle is completely given by the three position coordinates, is known as position space.

A small element in position space is denoted by volume element dV and is expressed as

$$dv = dx\, dy\, dz$$

Momentum Space

If the system is dynamic, its particles move about with various velocities and hence posses moments. A complete specification of such a system cannot be described in terms of position co-ordinates only. For a dynamic system, we must specify the three components of momentum* with the help of three velocity components v_x v_y and v_2 in addition to the three position coordinates x, y and z.

If m is the mass of the particle moving with a velocity v, its momentum $p = mv$.

The three components of momentum are

$$p_x = mv_{x,} \;;\; p_y = mv_y \;;\; p_z = mv_z$$

Just as the position of particle is completely given by the three position co-ordinates x, y and z in three dimensional position space, the momentum of the particle is completely specified by the three mutually perpendicular momentum coordinates p_x p_y and p_z three-dimensional space known as momentum space and the small volume element in momentum space is given d_{px} d_{py} d_{pz}.

Phase Space`

A combination of position space and momentum space is known as phase space. This, phase space has 6 dimensions, i.e. three position coordinates and three momentum coordinates, all mutually perpendicular to each other. The position of a particle in phase space is specified by a point with six coordinates x, y, z, px’ py’ pz’ Complete information about any particle in a dynamic system can be obtained from a knowledge of these six coordinates which completely determine its position as well as moments.

A small element in phase space is denoted by dt and is given by

$$d_t = (dx\ dy\ dz)\ (dp_x\ dp_y\ dp_z)$$

The mu-space

Let us limit ourselves to a system comprising of 1 molecule. Moreover, consider it to be mono-atomic as the simplest system. The state of the gas in completely known if the position and momentum of each atom of the gas is specified. The position of an atom can be specified in terms of its rectangular coordinates x, y and z. This is position space. The momentum of an atom is completely known if its rectangular momentum components p_x , p_y and p_z are specified. This is called momentum space. These six quantities x, y, z, p_x , p_y , p_z for each atom is known, the state of the gas can be determined. The space covered by the infinite set of these six coordinates is called the phase space for a single monatomic molecule.

Since the energy of a molecule is given by $(p_x^2 + p_y^2 + p_z^2)$ /2m which is equal to $p^2/2m$, the momentums space representation also gives representation of energy of the state.

Such a six-dimensional space for a single particle is called molecular phase space or mu-space or μ-space. Since 6-dimensional diagram can not be drawn, phase space is purely a mathematical concept.

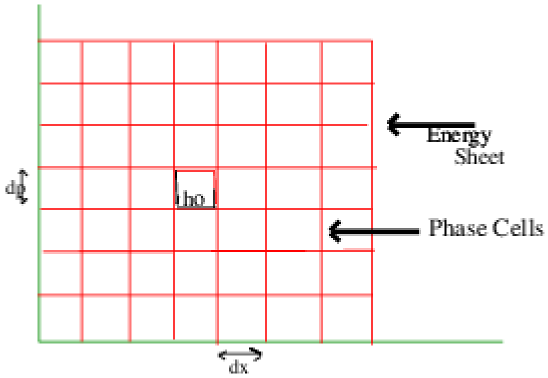


Figure : Phase cells

Suppose that position or momentum of one of the molecules is changed slightly. The phase point of this molecule will undergo a displacement in the phase space; and the microscopic state of the gas will be modified. To explain further, let us consider that the mu phase space is divided into two-dimensional energy sheet, having position coordinate as x-axis and momentum coordinate as p_x-axis. Let us subdivide the range of variables x and p_x into arbitrary small discrete intervals called as phase cells of arbitrary size.

Gamma Space

If we deal with a system of N molecules, there are two methods. One is to have the 6-dimensional (3 position + 3 momentum) phase space representation, and we take N points to represent the positions and moments of the N molecules at a given instant. This is called μ – space or mu-space representation.

The other alternative method is space representation. It is a 6N-dimensional phase space representation in which a single point represents a state of entire N- particle system and is referred as the representative point. This is in contrast to the μ-space. Which refers to only one particle, ie. one point for one particle. The space representation is mathematically more difficult to handle. But it has one great advantage. If an ensemble is to be represented, this 6N-dimensional representation alone is applicable. Different points will then represent the corresponding all microstates of another macrostate. The space is considered to be a conceptual Euclidean space having $2fN$ rectangular axes.

In general case of , f degrees of freedom per molecules we shall have:

1) position space f dimensional

2) momentum space	f dimensional
3) Mu space	$2f$ dimensional
4) gamma space	$2fN$ dimensional

UNIT IV: Nuclear Physics and Radiation Physics

Nuclear Physics: Nuclear constituents, size, mass, spin and charge - binding energy - binding energy curve - nuclear fission - chain reaction – nuclear reactor

Radiation Physics: radioactive disintegration – half-life period - radiation hazards

Nuclear constituents

The atomic nucleus was discovered in 1911 by Rutherford. Rutherford's α- particle scattering experiments showed that the atom consists of a very small nucleus surround by orbiting electrons. All atomic nuclei are made up of elementary particles called protons and neutrons. A proton has a positive charge of the same magnitude as that of an electron. A neutron is electrically neutral. The proton and the neutron are considered to be two different charge states of the same particle which is commonly called as nucleon. A species of nucleus known as a nuclide, is represented schematically by $_ZX^A$ where Z, the atomic number, indicates the number of protons, A the mass number, indicates the total number of protons plus neutrons an X is the chemical symbol of the species.

$$N = \text{Number of neutrons} = A-Z.$$

As an example, the chlorine nucleus $_{17}Cl^{35}$ has Z=17 protons, A= 35 nucleons and

$$N = 35-17=18 \text{ neutrons.}$$

Classification of nuclei:

Isotopes are nuclei with the same atomic number Z but different mass numbers A. The nuclei $_{14}Si^{18}$, $_{14}Si^{29}$, $_{14}Si^{30}$ and $_{14}Si^{32}$ are all isotopes of silicon. The isotopes of an element all contains the same number of protons but have different number of neutrons. Since the nuclear charge is responsible for the characteristic properties of an atom, all the isotopes of an element have an identical chemical behavior and differ physically only in mass.

Isobars are nuclei with the same mass number A, but different atomic number. The nuclei $_8O^{16}$, $_7N^{16}$ are examples of isobars. The isobars are the atoms of different elements and have different physical and chemical properties.

Isotones are nuclei with an equal number of neutrons . Some isotones are ${}_6C^{14}$, ${}_7N^{15}$ and ${}_8O^{16}$.

There are atoms which have the same Z and same A, but differ from one another in their nuclear energy states and exhibit difference in their internal structure. Such nuclei are called isomeric nuclei or isomers.

Nuclei having the same mass number A, but with proton and neutron number interchanged (ie., the number of proton in one is equal to the number of neutrons in the other) ae called mirror nuclei.

Examples. ${}_4Be^7$ (Z=4 and N=3) and ${}_4Li^7$ (Z=3 and N=4)

General properties of nucleus

Nuclear size: Rutherford's work on the scattering of α particles showed that the mean radius of an atomic nucleus is of the order of 10^{-14} to 10^{-15} m while that of the atom is about 10^{-10} m. Thus the nucleus is about 10000 times smaller in radius than the atom.

The empirical formula for the nuclear radius is

$$R= r_0A^{1/3}$$

Where A is the mass number and $r_0 = 1.3\times10^{-15}$ m = 1.3 fermi. Nuclei are so small that the Fermi (fm) is an appropriate unit of length. 1 fm = 10^{-15} m. From this formula we find that the radius of the ${}_6C^{12}$ nucleus is $R = (1.3)(12)^{1/3}$= 3 fm. Similarly, the radius of the ${}_7Ag^{107}$ nucleus is 6.2 fm and that of the ${}_{92}U^{238}$ nucleus is 8.1fm.

Nuclear mass: We know that the nucleus consists of protons and neutrons. Then the mass of the nucleus should be assumed nuclear mass=$Zm_p + Nm_n$.

Where m_p and m_n are the respective proton and neutron masses and n is the neutron number. Nuclear masses are experimentally measured accurately by mass spectrometers.

Nuclear density: The nuclear density ρ_N can be calculated from

$$\rho_N= \frac{nuclear\ mass}{nuclear\ volume}$$

Nuclear mass = A m_N, where A = mass number and m_N = mass of the nucleon = 1.67×10^{-27} kg.

Nuclear volume = $\frac{4}{3}\pi R^3 = \frac{4}{3}\pi (r_0 A^{1/3})^3 = \frac{4}{3}\pi r_0^3 A$

$\rho_N = 1.816 \times 10^{17}$ kg m^{-3}.

Note the high value of the density of the nucleus. This shows that the nuclear matter is in an extremely compressed state. Certain stars (the white dwarf) are composed of atoms whose electron cells have collapsed owing to enormous pressure, and the densities of such stars approach that of pure nuclear matter.

Nuclear charge: The charge of the nucleus is only due to the protons contained in it, since the neutrons have zero charge . Each proton has a positive charge of 1.6×10^{-19} C. The nuclear charge is Ze where Z is the atomic number of the nucleus.

Nuclear magnetic dipole moments: We know that the spinning electron has an associated magnetic dipole moment of 1 Bohr magneton. i.e., $\mu_e = \frac{(eh/2\pi)}{2m_e}$. Proton has a positive elementary charge and due its spin, it should have a magnetic dipole moment. According to Dirac's theory, where $\mu_N = \frac{eh/2\pi}{2m_p}$ where m_p is the proton mass. μ_N is the nuclear magneton and is the unit of magnetic moment. μ_N has a value of 5.050 x 10^{-27} J/T. Since $m_p = 1836\ m_e$, the nuclear magneton is only 1/1836 of a Bohr magneton. For nucleons, however, measurements give $\mu_p = 2.7925$ and $\mu_n = -1.912\ \mu_N$.

Electric quadrupole moment: In addition to its magnetic moment, a nucleus may have an electric quadrupole moment. An electric dipole moment is zero for atoms and nuclei in stationary states. This is a consequence of the symmetry of nuclei about the centre of mass. However, this symmetry does not need to be spherical; there is nothing precluding the nucleus from assuming the shape of an ellipsoid of rotation, for instance. Indeed most nuclei do assume approximately such shape and the deviation from spherical symmetry is expressed by a quantity called the electric quadrupole moment.

Binding energy

An atomic nucleus consists of particles such as protons and neutron. The nuclear mass is found to be less than the combined masses of the particles contained in it. The energy equivalent of the missing mass of the nucleus is called the binding energy of the nucleus . The missing mass is known as the mass defect.

The theoretical explanation for the mass defect is based on Einstein's equation $E=mc^2$. When the Z protons and N neutrons combine to make a nucleus, some of the mass (Δm) disappears because it is converted into an amount of energy $\Delta E= (\Delta m)\ c^2$. This energy is called the binding energy (BE) of the nucleus. If he B.E. is large, the nucleus is stable. A nucleus having the least possible energy, equal to the B.E., is said to be in the ground state. If the nucleus has an energy $E > E_{min}$, it is said to be in the excited state. The case $E = 0$ corresponds to dissociation of the nucleus into its constituent nucleons.

$(\Delta m) = \{(Zm_p + Nm_n) - M\}$

Where M is the experimentally determined mass of a nuclide having Z protons and N neutrons,

$BE= (\Delta m)\ c^2$

$BE = \{(Zm_p + Nm_n) - M\}\ c^2$. Joule

If the mass defect is found in a.m.u then the binding energy BE= (Δm) x 931 MeV

since 1 a.m.u = 931 MeV

If BE > 0, the nucleus is stable and energy must be supplied from outside to disrupt it into its constituents. If BE < 0, the nucleus is unstable and it will disintegrate by itself. To disrupt a stable nucleus into its constituents protons and neutrons, the minimum energy required is the binding energy. The magnitude of the B.E. of a nucleus determines its stability against disintegration. The binding energy of deuteron is 2.2MeV. It breaks into proton and neutron when a gamma particle of energy 2.2MeV interacted with the deuteron.

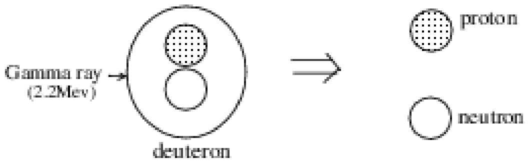


Figure: deuteron breaks into proton and netron with energy2.2MeV

Binding energy curve

The binding energy per nucleon is found by dividing the total binding energy BE by the number of nucleons contained in it. The quantity B/A is called the average binding energy ratio.

$$B.E.\,per\ nucleon = \frac{total\ B.E.\,of\ a\ nucleus}{the\ number\ of\ nucleons\ it\ contains}$$

The binding energy per nucleon is plotted as a function of mass number A. the curve shows some fluxuations at low mass number region and then increases gradually until it reaches a maximum of 8.79 MeV. The curve then drops slowly to about 7.6 MeV at the highest mass numbers. Evidently nuclei of intermediate mass are the most stable, since the greatest amount of energy must to be supplied to liberate each of their nucleons. This fact suggest that a large amount of energy will be liberated if heavier nuclei can somehow be split into lighter ones or if light nuclei can somehow be joined to form heavier ones. The former process is known as nuclear fission and the later as nuclear fusion. Both the processes indeed occur under proper circumstances and do evolve energy as predicted.

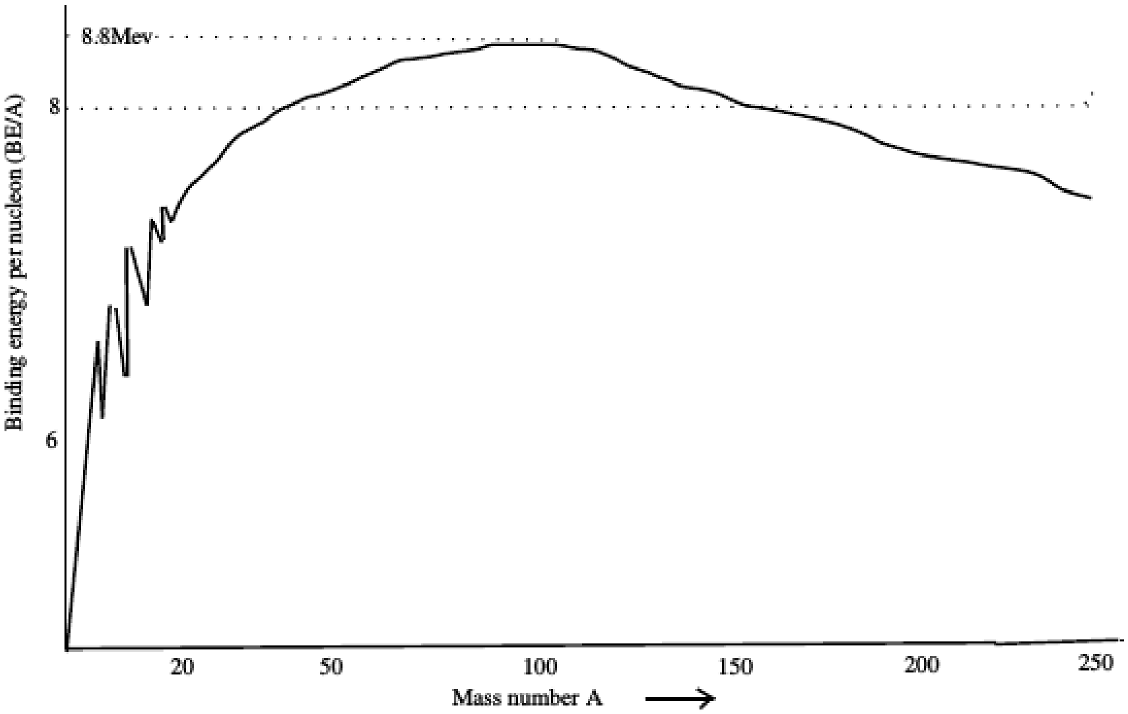


Figure: Average Binding energy curve

Significance of the binding energy curve

The curve gives important results

1. The binding energy curve enables us to understand the nature of the force hold the nucleons together in the nucleus. When the value of B/A is small, we say that the nucleus is loosely bound. On the other hand when the value of B/A is large, the nucleus is tightly bound.

2. It also gives an insight into nuclear fission in the nucleus.

3. To understand about alpha decay that happens with heavy elements.

Nuclear fission

The process of breaking up of the nucleus of a heavy atom into two, more or less equal fragments with the release of large amount of energy is known as fission.

When uranium is bombarded with neutrons, a uranium nucleus captures a slow neutron, forming an unstable compound nucleus. The compound nucleus split into nearly two equal parts. Some neutrons are also released in this process.

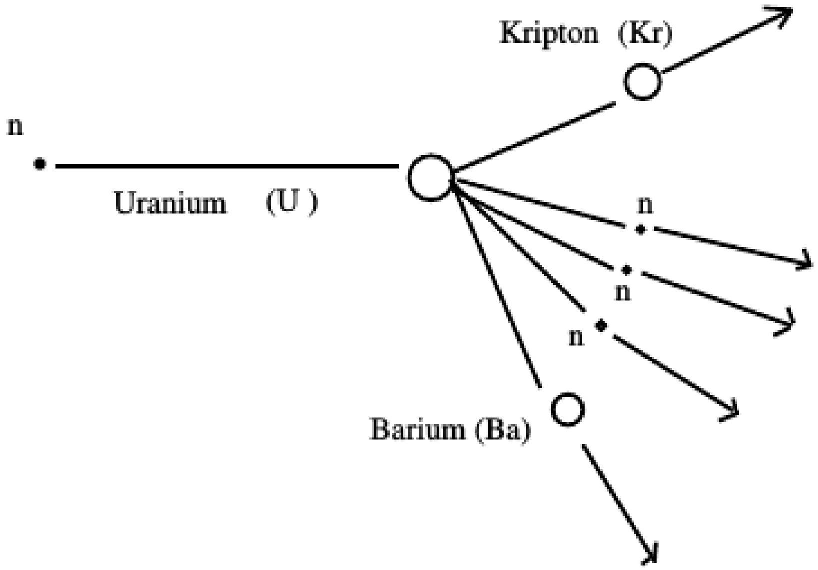


Figure: Fission reaction

The schematic equation for the fission process is

$$_{92}U^{235} + {}_{0}n^{1} \rightarrow {}_{92}U^{236*} + X + Y + \text{neutrons.} \qquad (1)$$

$_{92}U^{236*}$ is a highly unstable isotope of uranium, and X and Y are the fission fragments. The fragments are not uniquely determined, because there are various combinations of fragments possible and a number of neutrons are given off. Typical fission reactions are

$$_{92}U^{235} + {}_{0}n^{1} \rightarrow {}_{92}U^{236*} \rightarrow {}_{56}Ba^{141} + {}_{36}Kr^{92} + 3{}_{0}n^{1} + Q \qquad (2)$$

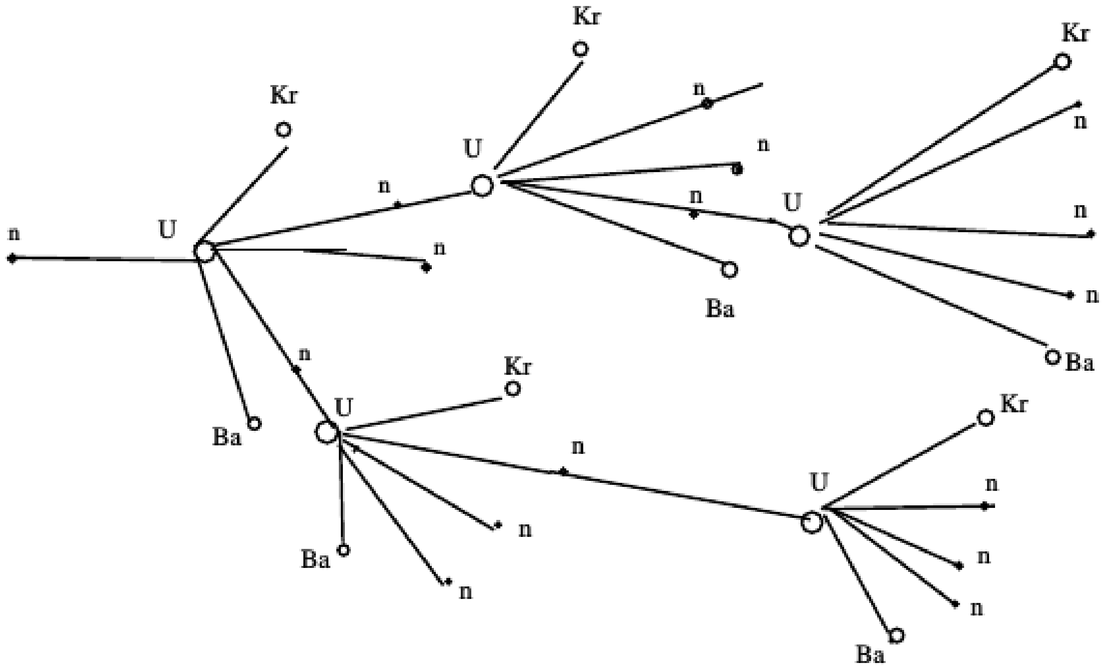
$$_{92}U^{235} + {}_{0}n^{1} \rightarrow {}_{92}U^{236*} \rightarrow {}_{54}Xe^{140} + {}_{38}Sr^{94} + 2{}_{0}n^{1} + Q \qquad (3)$$

Where Q is the energy released in the reaction.

According to equation (2) $_{92}U^{235}$ is bombarded by slow moving neuron, the nucleus becomes unstable ($_{92}U^{236*}$) and splits into $_{56}Ba^{141}$ and $_{36}Kr^{92}$ releasing 3 neutrons and energy Q. According to equation (3) the number of 2 neutrons are released. So in each fission average of 2.5 neutrons are released.

Chain reaction:

A chain reaction is a self-propagating process in which number of neutrons goes on multiplying rapidly almost in geometrical progression during fission till whole of fissile material is disintegrated.



suppose a single neutron causing fission in a uranium nucleus produces 3 prompt neutrons. The three neutrons in turn may cause fission in three uranium nuclei producing nine neutrons. These 9 neutron in turn to cause fission in nine uranium nuclei producing 27 neutrons. And so on. The number of neutrons produced in n such generations is 3^n neutrons . The ratio of secondary neutrons produced to the original neutrons is called the multiplication factor (k).

Consider 1 kg of ${}_{92}U^{235}$ which contains $6.023 \times 10^{26}/ 235$ or about 25×10^{23} atoms. Each fission will release on the average 2.5 neutrons. The velocity of the neutron among the uranium atoms is such that a fission capture of thermal neutron by the ${}_{92}U^{235}$ nuclei takes place in about 10^{-8} s each of this fission, in turn, release 2.5 neutrons. Let us assume that all these neutrons are available for inducing further fission reactions. Let n be the number of stages of fission captures required to disrupt the entire mass of 1 kg of ${}_{92}U^{235}$. Then

$(2.5)^n = 25\times10^{23}$ or n = 60.

The time required for 60 fissions to take place = 60×10^{-8}s = 0.6 μs

Since each fission releases about 200 MeV of energy, this means that a total of $200 \times 25 \times 10^{23} = 5 \times 10^{26}$ MeV of energy is released in 0.6 μs.

The release of this tremendous amount of energy in such a short time interval leads to a violent explosion. This results in powerful air blasts and high temperature of the order of 10^7 K or more, besides intense radioactivity. The self-propagating process describes here is called a chain reaction.

Two types of chain reaction are possible. In one, the chain reaction is first accelerated so that the neutrons are built up to a certain level an there after the number of fission producing neutrons is kept constant. This is controlled chain reaction. Such a controlled chain reaction is used in nuclear reactor. In the other type of chain reaction, the number of neutrons is allowed to multiply indefinitely and the entire energy is released all at once. This type of reaction takes place in atom bombs.

Multiplication factor (K):

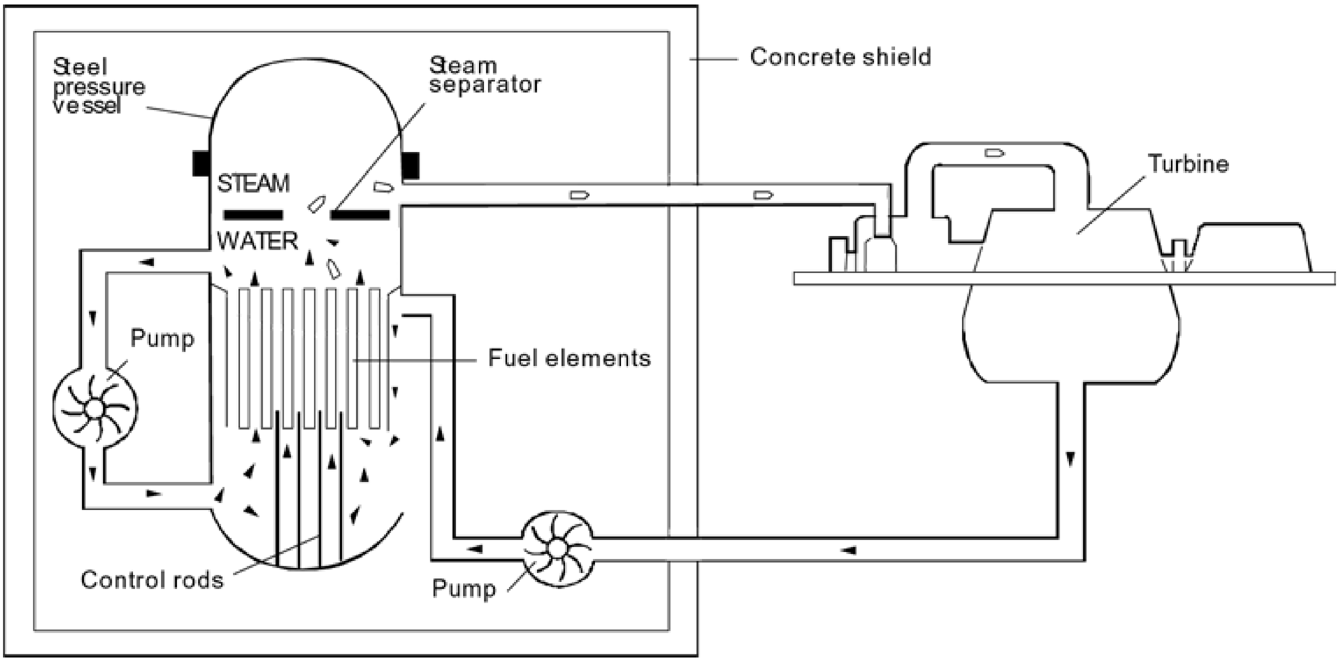
The ratio of secondary neutrons produced to the original neutrons is called the multiplication factor. It is defined as

$$K = \frac{\text{number of neutrons of one generation}}{\text{number of neutrons of the preceding generation}}$$

The fission chain reaction will be “critical” or steady when $k = 1$, it will be building up or “supercritical” when $k>1$ and it will be dying down o “subcritical” when $k<1$.

Nuclear reactors

The atom bomb is due to an uncontrolled chain reaction. A very large amount of energy is liberated within an extremely small interval of time. Hence it is not possible to direct this energy for any useful purpose. But, in a nuclear reactor, the chain reaction is brought about under controlled conditions. If the chain reaction is put under control, after some time a steady state is established. Under a steady state, the rate of energy production also attains a constant level. Such a device in which energy is released at a given rate is known as a nuclear reactor.



Nuclear reactors consists of five main elements:

1. The fissionable material called the fuel,
2. Moderator,
3. Neuron reflector,
4. Cooling system and
5. The safety and control systems.

(1) The fissionable substance: During the fission of U^{235} a large amount of energy is released. The commonly used fissionable materials ae the uranium isotopes U^{233}, U^{238}, the thorium isotopes Th^{232}, and the plutonium isotopes Pu^{239}, Pu^{240} and Pu^{241}.

(2) Moderator: The function of the moderator is to slow down the highly energetic neutrons produce in the process of fission of U^{235} to thermal energies. Heavy water (D_2O), graphite, beryllium, etc., are used as a moderators. Ideally, moderators have low atomic weight and low absorption cross section for neutrons

(3) Neutron reflector: By the use of reflector on the surface of reactors, leakage of neutrons can be very much reduced and the neutron flux in the interior can be increased. Materials of high scattering cross section and low absorption cross section are good reflectors.

(4) Cooling system: The cooling system removes the heat evolved in the reactor core. This heat is evolved from the K.E. from the fission fragments when they are slowed down in the fissionable substance and moderator. The coolant or heat transfer agent (water steam, He, CO_2, air and certain molten metals and alloys) is pumped though the reactor core. Then, through a heat exchanger, the coolant transfers heat to the secondary thermal system of the reactor.

(5) Control and safety system: The control systems enable the chain reaction to be controlled and prevent it from spontaneously running away. This is accomplished by pushing control rods into the reactor core. These rods are of a material (boron or cadmium) having a large neutron absorption cross section. These rods absorb the neutrons and hence cut down the reactivity. By pushing in the rods, the operation of the reactor can be made to die down, by pulling them put to build up. The safety systems protect the space surrounding the reactor against intensive neutron flux and gamma rays existing in the reactor core. This is achieved by surrounding the reactor with massive walls of concrete and lead which would absorb neutrons and gamma rays.

Uses of nuclear reactor:

1. Nuclear power: Nuclear reactors are used in the production of electric energy.

2. Production of radio isotopes: Nuclear reactors are useful in producing a large number of radio isotopes. To produce radio isotopes, a suitable compound is drawn into the center of the reactor core where the flux of neutrons may well be more than 10^{16}/m^2/sec. sodium 24 is manufactured in this way.

$$_{11}Na^{23} + {}_0n^1 \rightarrow {}_{11}Na^{24*}$$

3. Scientific research: Reactors produce a number of radioactive materials needed for research purposes. The reactors provide a huge source of neurons. Using these neutrons, several useful radioisotopes have been artificially produced and several nuclear reactions have been studied. Effects of neutron in biological tissues is also studied. Radiation damage is also studied.

Natural radioactivity

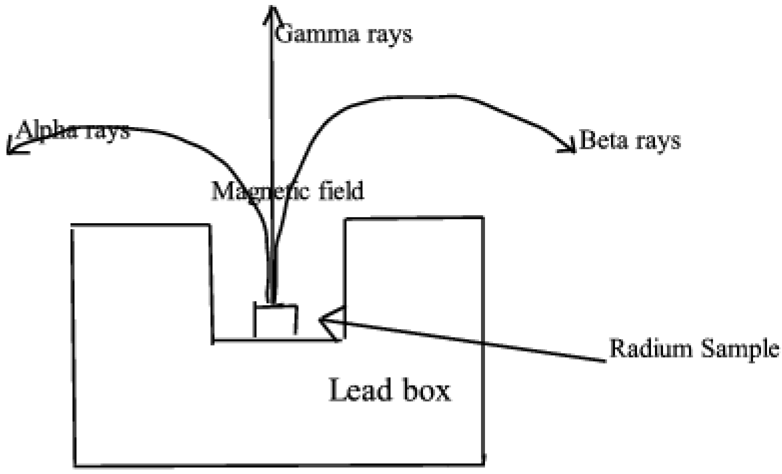


Figure : Radiation from the Radium source

When a sample of radium element is kept in a box, it is found that radiations come out of the sample. When a magnetic field is applied perpendicular to the direction of the radiation it is found that three kinds of radiations are emitting. These radiations are named as Alpha(α) ,Beta(β) and Gamma(γ) rays. When they are subjected to electric field ,these α rays are deflected to the one direction, indicating that they are positively charged. The β rays are deflected to the right and hence they are negatively charged. The γ rays are not affected by magnetic field hence they are uncharged. Alpha rays are Helium nucleus (${}_{2}^{4}He$), composed of two protons and two neutrons. In other words we can say that alpha particle is a doubly ionized helium nucleus. Beta rays are electrons coming out from the nucleus. When a neutron converts into proton a beta particle is emitted. ${}_{19}^{40}K \rightarrow {}_{-1}^{0}e + {}_{20}^{40}Ca$. The gamma rays are high energy electromagnetic radiations consisting of photons. An excited state nucleus comes to the ground state by emitting a gamma ray.

Radioactive disintegration

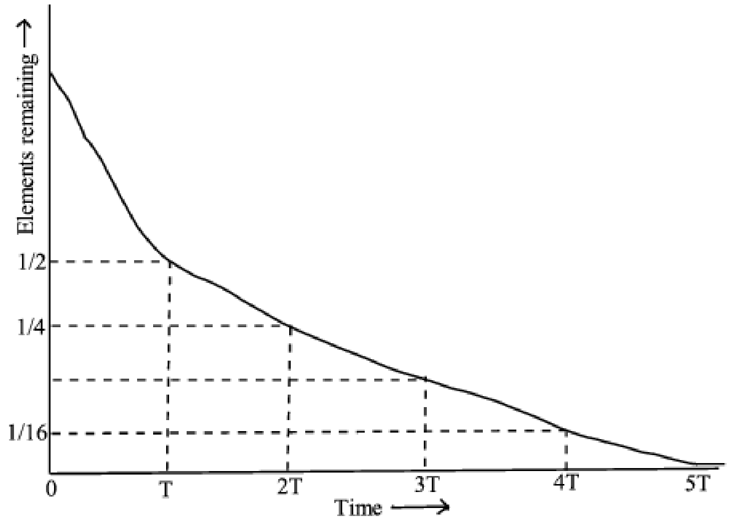


Figure : Exponential decay of radioactivity

Let N be the number of atoms present in a particular radioelement at a given instant t. Then, the rate of decrease $-\frac{dN}{dt}$ is proportional to N.

$$-\frac{dN}{dt} = \lambda N \qquad \ldots\ldots\ldots(1)$$

Here λ is a constant known as the disintegration constant or decay constant of the radioactive element. It is defined as the ratio of the amount of the substance which disintegrates in unit time to the amount of substance present.

Eqn (1) can be written as $\frac{dN}{N} = -\lambda dt$ t.

Integrating, $\log_e N = -\lambda t + C$ ………..(2)

Let the number of radioactive atoms initially present be $N_{0.}$

Then, when t = 0, $N = N_{0,}$

$$\log_e N_0 = C.$$

Substituting for C in eqn (2), we get, $\log N = -\lambda t + \log N_0$

or $\log_e \frac{N}{N0} = -\lambda t$

or $N = N_0 e^{-\lambda t}$ ………….(3)

This equation shows that the number of atoms of a given radioactive substance decreases exponentially with time.

Definition of half-life period:

The half-life period of the radioactive substance is defined the time required for one half of the radioactive substance to disintegrate ($T_{1/2}$) .

Value of half-life period: we know the relation $N = N_0 e^{-\lambda t}$

If $T_{1/2}$ be the half-life period, then at

$T = T_{1/2},\ N = N_0/2$

$\therefore N_0/2 = \log_e 2$ or $e^{\lambda T}{}_{1/2} = 2$

Or $\lambda T_{1/2} = \text{loge}2$ or $T_{1/2} = \frac{\log e\, 2}{\lambda}$

$$T_{1/2} = \frac{\log e\, 2}{\lambda} = \frac{0.6931}{\lambda} .$$

Radiation hazards

When an atom bomb explodes, very powerful neutron beams, alpha rays, beta rays, and gamma rays are emitted. These nuclear radiations hit on living objects and humans to produce tremendous heat causing destruction and life loss. Likewise radiations from nuclear power reactor affect the workers and the surroundings. Lab technicians working in x-ray lab are also affected, depending on the dosage they receive.

Radiation causes ionization in the molecule of living cells. The ionization results in removal of electrons from the atoms, thus forming ions. The ions react with other atoms in the cells causing damage. When the dose of radiation received is a few, the cells recover and damage rapidly. Also, the human body can replace the damaged cells. Under heavy dosage, cells divide permanently to produce abnormal cells and they become dangerous. This is the origin of the high risk of cancer, as a result of radiation exposure.

Human body is made up of many organs and each organ is made up of specialized cells. Ionizing radiations such as x-rays, beta rays, alpha rays and neutron beam can cause damage to cells ending with blindness, impotency, liver damage and even cancer. For example, if a gamma radiation passes through a cell, the water molecules near the DNA might be ionized and the ions might react with the DNA, causing it to break.

All cells are not equally sensitive to radiation. In general, cells that divide rapidly and / or those that are non- specialized cells show the effects of radiation at even low dosage levels than the cells that are less rapidly dividing and more specialized. Examples of more sensitive cells are these which produce blood. This system, called hematopoietic system, is the most sensitive biological indicator of radiation exposure.

Unit V : Relativity and Quantum Mechanics

Relativity: Frames of references - postulates of special theory of relativity - Lorentz transformation equations - Wave mechanics: matter waves - de Broglie wavelength - properties of wave functions - Quantum mechanics: postulates of quantum mechanics - Schrödinger equation - time dependent form

Frame of reference

A frame of reference is a coordinate system, by which the position of a particle at a particular time could be specified and hence its motion could be analyzed. The essential requirement of a frame of reference is that it should be rigid.

An object is in motion, when its position is changing with time to an observer. Motion is a relative concept since it must be referred to a particular frame of reference in which the observer is situated. Different observers may use different frames of reference. For example, most of the observations made on the earth are as in the frame of reference attached to it. In atomic physics, the motion of electron is determined as in the frame located at the nucleus. Since different observers may use different frames of reference, it is important to know how observations made by different observers are related. Such relations are made possible by means of transformation equations.

An inertial frame is defined as the frame of reference in which the Newton's first law (law of inertia) is obeyed. An object, subject to no net external force, moves with a constant velocity when observed in an inertial frame. A frame of reference having constant relative velocity with respect to an inertial frame is also an inertial frame. Thus inertial frames are unaccelerated frames. The special theory of relativity deals with motions, referred to inertial frames only. The earth can be taken as an example of inertial frame.

Postulates of the special theory of relativity

There are two laws of special theory of relativity. They are ,

1. The laws of physics have the same mathematical form in all inertial frames.
2. The velocity of light in vacuum (free space) is constant and it is independent of the velocity of the source and the observer.

Lorentz transformation Equations

Lorentz derived a set of transformation equations for coordinates of an event, making use of the postulates of the special theory of relativity. i.e; velocity of light is assumed to be a constant, independent of the relative motion between the frames of reference

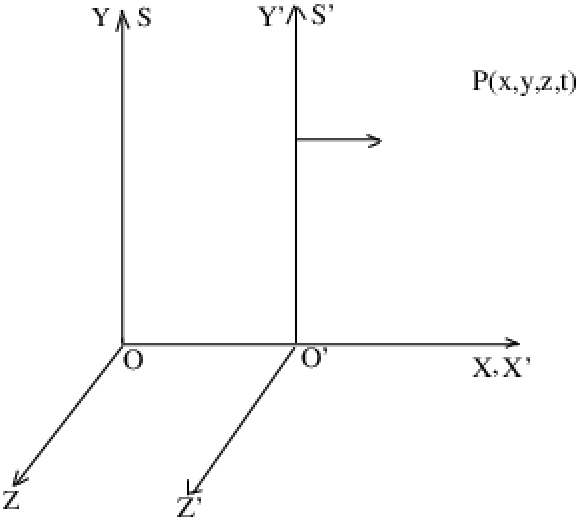


Figure: Two inertial frames of reference

Let S and S' be two inertial frames, in which the S' frame moves with velocity *v* along the positive X- direction with respect to the frame S. Let O and O' be two observers at the origin of each coordinate frame.

Let the coordinates of an event *P* in the *S* frame be (x, y, z, t) and those in the S' frame be (x^1, y^1, z^1, t^1). Let the origins coincide at t=t'=0. Let a source of light be located at O and that a flash of light is emitted at $t=t^1=0$. The flash spreads out as a spherical wave with centre at the origin in S frame. According to the postulates of the theory of relativity, the flash spreads out as spherical wave in S' frame also, with origin at O'. If the velocity of light be c, the equation to the wave front in S is

$x^2+y^2+z^2=c^2t^2$ …… …….. ……… (1)

And in the frame S' it will be given by

$x^{1\,2}+y^{1\,2}+z^{1\,2}=c^2t^{1\,2}$ ……..……..……… (2)

To find the relation connecting x’ and x,y’ and y,z’ and z;t’ and t, we assume that the transformation as linear.

$x^1=k\,(x-vt)$

$y^1= y$

$z^1=z$

and $t^1 = At + Bx$ ……………..…… (3)

where A, and B and k are constants to be determined. Putting the values of x^1, y^1, z^1 and t^1 in equation (2).

$k^2\,(x-vt)^{\,2} + y^2 + z^2 = c^2\,(At + Bx)^2$

$k^2\,(x^2- 2xvt+v^2t^2) + y^2 + z^2 = c^2\,(A^2t^2 + 2ABxt + B^2x^2)$

$(k^2- B^2c^2)\,x^2 + y^2 + z^2 = (A^2c^2-k^2v^2)\,t^2 + 2\,(ABc^2 + k^2v)\,xt$

Comparing this with equation (1) $x^2+y^2+z^2 = c^2t^2$,

We find $(k^2-B^2c^2) = 1$ ……….……… (4)

$(A^2c^2 – k^2v^2) = c^2$ …………… (5)

$ABc^2 + k^2v = 0$ …………..… (6)

From equation (4), $k^2-B^2c^2=1$

$$B^2=\frac{k^2-1}{c^2}$$

$$B = \sqrt{\frac{k^2-1}{c^2}} \qquad \text{………………….. (7)}$$

From equation (5), $A^2c^2-k^2v^2=c^2$

$A^2\,c^2=c^2 + K^2v^2$

$$A^2=\frac{c^2+k^2v^2}{c^2}$$

$$A = \sqrt{\frac{c^2 + k^2v^2}{c^2}} \qquad \ldots\ldots \qquad \ldots.. \ \ldots\ldots \qquad (8)$$

Putting these values in eqn. (6)

$ABc^2 + k^2v=0$

$$\left(\sqrt{\frac{k^2-1}{c^2}}\right) \quad \left(\sqrt{\frac{c^2+k^2v^2}{c^2}}\ c^2\right) + k^2v = 0$$

$$\left[\ \sqrt{k^2-1}\ \right] \quad \sqrt{c^2+k^2v^2} \quad = \quad (-\ k^2v)$$

Squaring, $(k^2 - 1)\ (c^2 + k^2v^2) = k^4v^2$

$k^2c^2 + k^4v^2 - c^2 - k^2v^2 = k^4v^2$

$k^2c^2 - k^2v^2 - c^2 = 0$

$k^2\ (c^2 - v^2) = c^2$

$$k^2 = \frac{c^2}{c^2 - k^2v^2}$$

$$k = \sqrt{\frac{c^2}{c^2-v^2}} \quad = \quad \frac{1}{\sqrt{1-v^2/c^2}} \qquad \ldots\ldots \qquad \ldots.. \ \ldots\ldots \qquad (9)$$

Putting this in equation (8), $A = \sqrt{\dfrac{c^2+k^2v^2}{c^2}}$

$$A = \sqrt{1+\frac{k^2.v^2}{c^2}} \quad But \quad \frac{k^2}{c^2} = \frac{1}{c^2-v^2}$$

$$= \sqrt{\frac{c^2 - v^2 + v^2}{c^2 - v^2}}$$

$$A = \sqrt{\frac{c^2}{c^2 - v^2}} \quad = \frac{1}{\sqrt{1 - v^2/c^2}} \qquad \ldots\ldots \quad \ldots.. \ \ldots\ldots \qquad (10)$$

From (9) and (10). We find that $A=k$, Putting $A=k$ in equation (6)

$$ABc^2 + k^2v = 0$$

$$kBc^2 + k^2v = 0$$

$$k\,(Bc^2 + kv) = 0$$

$$Bc^2 + kv = 0$$

$$B = \frac{-kv}{c^2}$$

Thus, the constants are

$$\mathrm{A} = \mathrm{k} = \frac{1}{\sqrt{1 - v^2/c^2}}\ ;\ B = \frac{-kv}{c^2}$$

Substituting these values in equation (3),

$$x^1 = \frac{x - vt}{\sqrt{1 - v^2/c^2}} \qquad \ldots\ldots \quad \ldots.. \ \ldots\ldots \qquad (11)$$

$$y^1 = y \qquad \ldots\ldots \quad \ldots.. \ \ldots\ldots \qquad (12)$$

$$x^1 = x \qquad \ldots\ldots \quad \ldots.. \ \ldots\ldots \qquad (13)$$

and $t^1 = \frac{1}{\sqrt{1 - v^2/c^2}} + (\frac{-kv}{c^2})x$

$$t^1 = \frac{1}{\sqrt{1 - v^2/c^2}} - \frac{vx/c^2}{\sqrt{1 - v^2/c^2}}$$

$$t^1 = \frac{t - vx/c^2}{\sqrt{1 - v^2/c^2}} \qquad \ldots\ldots \quad \ldots.. \ \ldots\ldots \qquad (14)$$

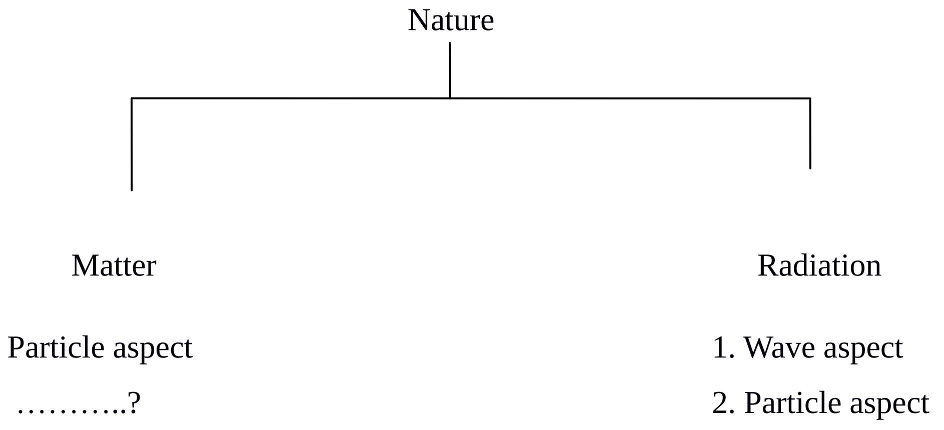
The set of equations (11) through (14) are known as Lorentz transformation. Equations for space and time coordinates. Thus, knowing x, y, z and t for an event in S frame, the corresponding coordinates $x^{1,}$ y^{1}, z^{1} and t^{1} in S^{1} frame can be calculated using the above transformation equations.

Wave Mechanics

Matter has particle aspects. The particle aspects of matter are mass, momentum, volume, density etc. Similarly radiation (heat, light etc) has wave aspect The wave aspect of radiation are wavelength, amplitude, frequency etc. The matter and radiation are the two forms in which nature exhibits itself.

A part from the wave aspect, radiation is found to have the particle aspect also. This has been proved experimentally by the X-ray scattering known as Compton scattering and the photoelectric effect. i.e; radiation is found to have dual (double) properties.

1. Since Nature loves symmetry, the counter part of radiation namely matter must also have dual properties. i.e; matter must have particle aspect as well as wave aspect.



2. Moreover there is close similarity between the laws of mechanics (physics of particles) and

optics (physics of radiation).

Hence matter and radiation must have similarity of behavior also. If one of these has both wave aspect and particle aspect, the other also must exhibit dual behaviour.

3. Radiation phenomena like interference and diffraction are described by integer rules. Electrons revolve around the nucleus in various orbits defined by integers. This suggests that electron has an intrinsic property which makes it behave like a wave.

4. Einstein's mass energy relation $E = mc^2$ shows the equivalence of mass and radiation. Hence, as radiation (energy) has dual behaviour, matter also must have particle aspect as well as the wave aspect, though only one aspect is exhibited at a time.

Based on the above arguments, Louis de Broglie proposed the theory of matter waves. According to de Broglie's theory, every particle, set into motion, is associated with a wave known as the matter wave, which advances along with the particle. The matter wave is set up as the result of the disturbance produced in the matter field surrounding the particle due to particle's motion. The matter wave is not electromagnetic in nature.

The wave length 'λ' of matter wave depends on the momentum of the particle. If m is the mass and v is the velocity of the particle, the wavelength $\lambda = \frac{h}{mv}$ where h is the Planck's constant.

A material particle is associated with a matter field in the same way as photon is associated with an electromagnetic field.

Expression for de Broglie wavelength

Consider a radiation of frequency v. The radiation consists of a stream of photons, each of energy $E = hv$, where h is the Planck's constant. This is according to Planck's quantum theory.

Let each photon behave as a particle and let m be the equivalent mass of a photon. According to the special theory of relativity, the energy of each such photon is given by $E = mc^2$, where c is the velocity of the photon (velocity of light). Hence

$$mc^2 = hv$$

$$mc = \frac{hv}{c}$$

Now let us consider the wave aspect of the radiation. i.e. radiation spreads out as a wave. From the equation for wave motion, we have the velocity of light c = $\nu\lambda$, where λ is the wavelength of the radiation.

Hence, $\frac{\nu}{c} = \frac{1}{\lambda}$. Putting this in equation (1), we have

$$mc = \frac{h}{\lambda}$$

The wavelength $\lambda = \frac{h}{mc}$

i.e,: $\lambda = \frac{Planck's\ constant}{momentum}$

De Broglie argued that the same formula for the wavelength λ could be applied to any particle of mass *m* moving with a velocity *v*. Then the wavelength of the matter wave associated with the particle becomes

$$\lambda = \frac{h}{mv}$$

This wavelength is called the de Broglie wavelength of the matter-waves. The wavelength λ is in inversely proportional to the mass and velocity of the particle.

Wave function and its physical significance

After the advent of the theory of matter waves, an advanced branch of physics known as Quantum Mechanics had been, developed in 1926 by Erwin Schrodinger. This new mathematical tool enables us to describe the motion of particles in the atomic scale fairly well. Problems involving nuclei, atoms, molecules and compounds can be understood and solved easily with the help of Quantum Mechanics.

Apart from wavelength, wave amplitude is an important property of waves. As far as the matter wave is concerned, its amplitude is a variable of the wave motion.

When a particle is in motion, it exhibits wave - like property. But we know that the position of a particle (of known momentum p) cannot be precisely located. Rather, it may extend up to a region (Δx) in space (due to uncertainty principle). This makes us think that the wave form representing a particle in motion is a wave - packet, whose amplitude $\psi(x)$ is varying from point to point within the region and practically zero outside the region as shown in Figure. It can be proved that

The velocity of wave packet = particle velocity v

i.e., when the particle moves with velocity v, the wave packet (represented by dotted line) also moves along with the particle with velocity v. Since the particle's position may be anywhere in a region, its matter wave is not a single wave of wavelength λ and $\lambda + d\lambda$. The resulting combination is a wave packet. Thus, in wave mechanics, the particle's motion is characterized by the wave packet's motion and interaction between particles can be described in terms of interaction between the wave packets of these particles.

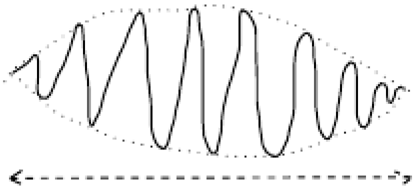


Figure : wave packet

The amplitude of the wave packet, representing the particle's motion is called the wave function of the particle. The wave function ψ is not directly related to any measurable quantity. The wave function, as such, has no physical significance since it is not physically observable. In the most general form, the wave-function ψ can be expressed as a complex quantity (that is, a function containing imaginary quantity $i = \sqrt{-1}$) such as

$\psi = A + i B$, Its modulus is $|\psi| = \sqrt{A^2 + B^2}$

Its value is twofold. i.e., (i) it has a real part (ii), it has an imaginary part. Here A is the real part and B is the imaginary part of ψ

A complex wave function can carry more information (due to its amplitude and phase) about the physical properties of a particle. The complex conjugate = A - iB, Taking the product of ψ and ψ^*,

$\psi\psi^* = (A+iB)(A-iB) = A^2 + B^2 = |\psi^2|$ is real quantity. Since the product ($\psi\psi^*$) is a positive real quantity, it is an observable physical quantity. According to Max Born, the quantity, ($\psi\psi^*$) represents the intensity of the matter wave and gives us a measure of the probability of finding the particle in a given region of space, in which ψ is known.

Properties of wave function

1) The wave function is a state function i.e., it corresponds to a given coordinate x in one dimension or (x,y,z) in three dimensions, at a given instant of time t and it is a single valued function. Moreover, the wave function is continuous everywhere (even across boundaries).

2) Let ψ (x) be the wave function (Probability amplitude) of a particle in a given state. Then, by Born's interpretation of ψ(x), the probability that the particle may be found at x is given by

$$p = |\psi\ (x)|^2$$

or $P = \psi^*\ (x)\ \psi\ (x)$

The probability that the particle may be found in a region of space dx is given by

$$P = \psi^*\ (x)\ \psi\ (x)\ x \text{ range.}$$

$$P = \psi^*\ (x)\ \psi\ (x)\ dx$$

in three dimensional space, the probability that the particle may be found within a volume element of dV = *dx dy dz* is given by

$$P = \psi^*\ (x,y,x)\ \psi\ (x,y,z)\ dx\ dy\ dz.$$

The total probability that the particle is anywhere within a given bound space is

$$P = \int \psi^*\ \psi\ dV.$$

The integral is volume integral. If the boundary extends upto infinity, the limits of integration are from 0 to infinity. When we say that a particle exists in the universe (somewhere in space), the total probability given above must be equal to unity.

i.e., P = 1 (maximum value)

$$\int \psi^*\ \psi\ dx\ = 1.$$

The wave function that satisfies the above condition is known as normalized wave function and the above condition is normalization condition. Any physically acceptable wave function (that is obtained as a solution in any probable) is valid if it satisfies the normalization condition.

3) The wave function and its derivatives are continuous, finite and single valued. Such a wave function is called well behaved wave function. Also $\psi(x)$ tends to zero as x shoots to infinity.

Postulates of Quantum mechanics

Quantum mechanics is a mathematical tool that enables accurate description of motion of matter on atomic scale. It is based on the following postulates.

1) Every physically measurable quantity that relates to the motion of a particle can be represented by a linear operator.

Dynamical variable	Operator
Position (x)	x and y
Momentum *(p)*	$-i\hbar\frac{\partial}{\partial x} or - i\hbar\nabla$
angular momentum *(L= r x p)*	$-i\hbar(rx\nabla)$
Kinetic energy *(T = p^2 / 2m)*	$\frac{h^2}{2m}\frac{\partial^2}{\partial x^2} or \frac{h^2}{2m}\nabla^2$
total energy *[H = p^2/2m+V(r)]*	$\frac{h^2}{2m}\nabla^2 + V$
Energy *(E)*	$i\hbar\frac{\partial}{\partial t}$

Displacement, velocity, momentum, angular momentum, torque, kinetic energy, total energy etc are some examples of physical quantity, relating to the motion of particle. Each of these dynamical variables can be represented by a linear operator. An operator is indicated by a cap on the top.

An operator operating on one function transforms it into another.

An operator Âis said to be linear if $\hat{A}(\psi_1+\psi_2) = \hat{A}\psi_1 + \hat{A}\psi_2$ and $(\hat{A}\psi)$

$= a(\hat{A}\psi)$

2) When an operator on a wave function corresponding to a given state it yields back the wave function along with the eigen value for that operator.

For example, when $y = e^{3x}$, $\frac{d^2y}{dx^2} = 9e^{3x} = 9y$

In this equation $\frac{d^2}{dx^2}$ is a differential operator. It operates on the function $y = e^3x$. As a result of the operation, the eigen value 9 is obtained. Eigen value means 'characteristic' value corresponding to the given state.

In general an operator H operating on the function u_1 will give the eigen value E_1 as $Hu_1=E_1u_1$

$Hu_2 = E_2u_2$ and so on. Similarly for another state function u_2.

One or other of the eigen value (such as E_1, E_2 ...) is the only possible result of the measurement of the quantity represented by the operator (such as H).

3) When a given system is in a state defined by the function ψ_m the mean of the measurable values of a physical quantity represented by an operator Â is given by

$$\langle A \rangle = \int \psi^* \hat{A} \, \psi \, dx$$

$\langle A \rangle$ is known as the expectation value of the quantity A. Care should be taken to see that the ψ used here is normalized wave function.

4) A single wave function is regarded as a superposition of wave functions corresponding to physically distinguishable eigen states. A given wave function ψ can be expressed as a linear combination of different state functions u_1, u_2, u_3, ... etc as

$$\psi = a_1 u_1 + a_2u_2 + a_3u_3 + \ldots.$$

Where a_1, a_2, a_3... are complex constants, u_1, u_2, u_3 are the state (wave) functions

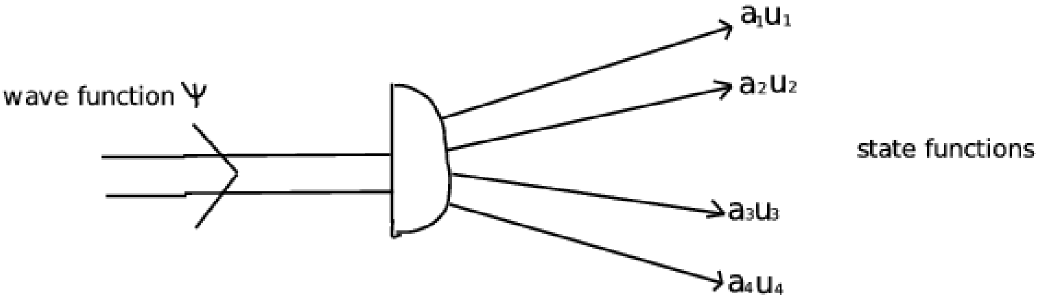


Figure: State function

Schrodinger's wave equation: Time dependent form

When a stretched string is plucked, a wave travels along the string. The displacement of the string is perpendicular to the direction of the wave. If the wave propagates along the X direction, the displacement is along the Y direction. The equation to the wave propagation is given by $\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}$

Where is the velocity of the wave. The general solution of this differential equation is

$Y = Ae^{\,i(kx-wt)}$ ………………(1)

Where k is the propagation constant (k=2 π/λ), and ω is the angular frequency, $\omega = 2\pi v$, Here λ and v are wavelength and frequency respectively. A is the amplitude of the wave. $i = \sqrt{-1}$.

When a particle is set into motion, it can be represented by the matter wave of wave function ψ. The above equation (1) can be used to represent the matter wave and in that case, the amplitude y is replaced by wave function ψ

$\Psi = Ae^{\,i(kx-wt)}$ ………………(2)

The momentum p of the particle can be expressed in terms of k as

$P=hk$ (k is propagation constant)

$k = \frac{p}{h}$

Similarly, the energy (E) of the particle can be expressed in terms of ω as

$E = h\,\omega$ *(ω is angular frequency)*

$$\omega = \frac{E}{h}$$

Putting the values of K and ω in equation (2)

$$\psi = A \exp \quad i \quad \frac{px}{h} - \frac{Et}{h}$$

$$\psi = A \exp \quad \frac{i}{h}\left(px - Et\right) \qquad \text{……….3}$$

Differentiation ψ with respect to x twice,

$$\frac{\partial \Psi}{\partial x} = A \exp\left(\frac{i}{h}\left(px - Et\right)\right) \left(\frac{ip}{h}\right)$$

$$\frac{\partial \Psi}{\partial x} = \left(\frac{ip}{h}\psi\right)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = (\frac{ip}{h})^2 \psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{-p2}{h2}\psi \quad .$$

$$p^2 \ \psi = -h^2 . \ \frac{\partial^2 \Psi}{\partial x^2} \qquad \text{………..4}$$

Differentiating ψ in equation (3) with respect to t,

$$\Psi = A \exp\left(\frac{i}{h}\left(px - Et\right)\right)$$

$$\frac{\partial \Psi}{\partial t} = A \exp \left(\frac{i}{h}\left(px - Et\right)\right) \left(\frac{iE}{h}\right)$$

$$\frac{\partial \Psi}{\partial t} = -\left(\frac{iE}{h}\right) \psi$$

$$E \ \psi = \frac{-h}{i} \quad \frac{\partial \Psi}{\partial t} \qquad \text{………..5}$$

When the particle moves at ordinary speed, the total energy E of the particle is the sum of its kinetic energy and potential energy.

Kinetic energy = $\frac{p2}{2\text{m}}$ and Potential energy is V.

The total energy $E = \frac{p2}{2\text{m}} + V$

Multiplying both sides by the wave function ψ

$$E\psi = \left(\frac{p2}{2\text{m}} + V\right)\psi$$

$$E\,\Psi = \frac{p2\Psi}{2\text{m}} + V\,\psi$$

Substituting the value of E ψ and p^2 ψ from equation (5) and (4),

$$\frac{-h}{i}\ \frac{\partial\Psi}{\partial t} = \frac{-h^2}{2\text{m}}\ \frac{\partial^2\Psi}{\partial x^2} + V\ \psi. \text{ Since, } i^2 = -1,\ \frac{-h^2}{i} = i\,h$$

$$i\,h\ \frac{\partial\Psi}{\partial t} = \frac{-h^2}{2\text{m}}\ \frac{\partial^2\Psi}{\partial x^2} + V\ \psi.$$

In three dimensions, the above equation becomes.

$$i\,h\ \frac{\partial\Psi}{\partial t} = \frac{-h^2}{2\text{m}}\ \nabla^2\,\psi + V\,\psi.$$

This is Schrodinger’s wave equation in the time-dependent from.

The Schrodinger equation for any particle can be set up, once the potential energy of the particle V is known. The equation can be solved for ψ and from this, any required physical property of the particle can be computed using the rules of quantum mechanics.