 **1.1 INTRODUCTION**

There are four common states of matter (or phases) in the universe, solid, liquid, gas, and plasma. The state of matter affects a substance's properties, such as density, viscosity (how well it flows), malleability (how easy it is to bend), and conductivity. Changes between states of matter are often reversible.

**Solids**

In a solid, the positions of atoms are fixed relative to each other over a long time. That is due to the "friction" or cohesion between molecules. This cohesion is provided by various bonds. Only solids can be pushed on by a force without changing shape, which means that they can be resistant to change in shape. Solids also tend to be strong enough to hold their own shape in a container. Solids are generally denser than liquids. Solid becoming a gas is called sublimation.

**Liquids**

In a liquid, molecules are attracted to each other strongly enough to keep them in contact, but not strongly enough to hold a particular structure. The molecules can continually move with respect to each other. This means that liquids can flow smoothly, but not as smoothly as gases. Liquids will tend to take the shape of a container that they are in. Liquids are generally less dense than solids, but denser than gases.

**Gases**

In a gas, the chemical bonds are not strong enough to hold atoms or molecules together, and from this a gas is a collection of independent, unbonded molecules which interact mainly by collision. Gases tend to take the shape of their container, and are less dense than both solids and liquids. Gases have weaker forces of attraction than solids and liquids. Gas becoming a solid directly is called deposition.

**Plasma**

Plasma are gases that have so much energy that electrons of an atom cannot stay in orbit around one nucleus. The atomic ions and free electrons mix around like a hot soup.

Because the positive and negative charged particles are not stuck together, plasma is a good conductor. For example, air is not good at conducting electricity. However, in a bolt of lightning, the atoms in air get so much energy that they no longer can hold on to their electrons, and become a plasma for a brief time. Then an current is able to flow through the plasma, making the lightning.

Plasma is the most common state of matter in the universe. Both stars and the interstellar are mostly made of plasma.

                  Figure 1.1 transformation between different matter[1]

**1.2 CRYSTALLOGRAPHY**

**Crystallography**, branch of science that deals with discerning the arrangement and bonding of atoms in crystalline solids and with the geometric structure of crystal lattices. Modern crystallography is largely based on the analysis of the diffraction of X-rays by atoms acting as optical gratings. Using X-ray crystallography, chemists are able to determine the internal structures and bonding arrangements of minerals and molecules, including the structures of large complex molecules, such as proteins and DNA.

**Types of solids**

A crystal or **crystalline solid** is a solid material whose constituents are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions. For e.g. metals

an **amorphous** or non-crystalline solid is a solid that lacks the long-range order that is characteristic of a crystal for e.g. Glass-Ceramics.

                Figure 1.2 Arrangement of atoms in crystalline and amorphous[2]

**1.3 PROPERTIES OF CRYSTALLINE AND AMORPHOUS SOLIDS**

**Nature:**

Crystalline Solids – True Solids

Amorphous Solids – Pseudo – Solids or super-cooled liquids

**Geometry**:

Crystalline Solids – Particles are arranged in a repeating pattern. They have a regular and ordered arrangement resulting in a definite shape.

Amorphous Solids – Particles are arranged randomly. They do not have an ordered arrangement resulting in irregular shapes.

**Melting** Points

Crystalline Solids – They have a sharp melting points.

Amorphous Solids – They do not have sharp melting points. The solid tends to soften gradually over a temperature range.

**Isotopism**:

Crystalline Solids – Anisotropic in nature. i.e., the magnitude of physical properties (such as refractive index, electrical conductivity, thermal conductivity etc.) is different along with different directions of the crystal.

Amorphous Solids – Isotropic in nature. i.e., the magnitude of the physical properties is the same along with all directions of the solid.

Cleavage Property

**Crystalline Solids** – When cutting with a sharp edge, the two new halves will have smooth surfaces.

Amorphous Solids – When cutting with a sharp edge, the two resulting halves will have irregular surfaces.

**Rigidity**:

Crystalline Solids – They are rigid solids and applying mild forces will not distort its shape.

Amorphous Solids – They are not rigid, so mild effects may change the shape.

**Heat of Fusion:** (The change in enthalpy when a substance is heated to change its state from solid to liquid.)

Crystalline Solids – They have definite heat of fusion.

Amorphous Solids – They do not have definite heat of fusion

**1.4 SPACE LATTICE**

Crystals have a structure made up of a regular arrangement of their atoms (or particles). When such an arrangement of atoms is represented in a three-dimensional structure, this is a crystal lattice. So a lattice is an array of points in a particular order which describes the arrangement of particles of a crystalline solid.

**Properties**

·        Each point on the lattice represents one particle of the crystal, this is a lattice point.

·        This particular particle may be an atom, a molecule or even ions

·        These lattice points of a crystal are joined together by straight lines.

·        By joining of these points, we get the geometry (or shape) of the crystal

**Basis**

The crystal structure is formed by associating every lattice point with an assembly of atoms or molecules or ions, which are identical in composition, arrangement and orientation, is called as the basis.

                   Figure 1.3 Space lattice and basis forming crystal structure[3]

**1.5 Unit cell**

The space that is spanned by the translation vectors is called the unit cell. The unit cell constants define the length of the translation vectors and the angles between them. In a crystal, the unit cell contains the fundamental atomic structure that is repeated.

                               Figure 1.4 Unit cell and lattice points[4]

**Primitive and Non-primitive unit cell**

Primitive unit cell

A primitive cell is a unit cell that contains exactly one lattice point. It is the smallest possible cell. If there is a lattice point at the edge of a cell and thus shared with another cell, it is only counted half. Accordingly, a point located on the corner of a cube is shared by 8 cubes.

                 Figure 1.5 Unit cell atoms at corners only[5]

Non-primitive unit cell

Non-primitive cells are of three kinds:

* end-centered: an extra lattice point is centered in each of two opposing faces of the cell
* face-centered: an extra lattice point is centered in every face of the cell
* body-centered: an extra lattice point is centered in the exact middle of the cell
* They have larger volume than primitive unit cell.

#### ****Body centred cubic unit cell****. (BCC)

Figure 1.6 Arrangement of atoms in BCC[6]

In a body centred cubic unit cell, each corner is occupied by an identical particle and in addition to that one atom occupies the body centre. Those atoms which occupy the corners do not touch each other, however they all touch the one that occupies the body centre. Hence, each atom is surrounded by eight nearest neighbours and coordination number is 8. An atom present at the body centre belongs to only to a particular unit cell i.e. unshared by another unit cell.

Figure 1.7 no. of atoms in BCC

#### ****Face centred cubic unit cell****.(FCC)

Figure 1.8 Arrangements of atoms in FCC[6]

In a face centred cubic unit cell, identical atoms lie at each corner as well as in the centre of each face. Those atoms in the corners touch those in the faces but not each other. The atoms in the face centre is being shared by two-unit cells, each atom in the face centres makes (1/2) contribution to the unit cell.

Figure 1.9 no of atoms in FCC

Drawing the crystal lattice on paper is not an easy task. The constituents in a unit cell touch each other and form a three-dimensional network. This can be simplified by drawing crystal structure with the help of small circles (spheres) corresponding constituent particles and connecting neighbouring particles using a straight line as shown in the figure.

**End Face-Centred Cubic Lattice**:

In each end centred unit cell, there are 8 atoms at the eight corners of the cube, and one atom each is present at the centre of any two opposite faces.

                   Figure 1.10 Arrangements of atoms in End centred unit cell[4]

No of atoms present per unit cell = (8 x 1/8 ) + (2 x 1/2) = 2

**1.6 LATTICE PARAMETERS**

The lattice constant, or lattice parameter, refers to the physical dimension of unit cells in a crystal lattice

6 parameters

Length of axis along x, y, z axis written as a, b, c

Angle between y and z axis is α

Angle between x and z axis is β

Angle between x and y axis is γ

                                      Figure 1.11 Lattice parameters[7]

**1.7 CRYSTAL SYSTEMS**

Crystal system is a method of classifying crystalline substances on the basis of their unit cell. There are seven unique crystal systems. The simplest and most symmetric, the cubic (or isometric) system, has the symmetry of a cube. The other six systems, in order of decreasing symmetry, are hexagonal, tetragonal, trigonal (also known as rhombohedral), orthorhombic, monoclinic and triclinic.

Bravais lattice is a set of points constructed by translating a single point in discrete steps by a set of basis vectors. In 1848, the French physicist and crystallographer Auguste Bravais (1811-1863) established that in three-dimensional space only fourteen different lattices may be constructed. All crystalline materials recognised till now fit in one of these arrangements.

#### ****Cubic crystal system****

Crystallographic axes

Figure 1.12 3-D Model [8]

Cubic (or isometric) crystal system is also known as the isometric system. Cubic crystal system characterizes itself by its three equivalent crystallographic axes perpendicular to each other.

a = b = c

α = β = γ = 90°

Figure 1.13 Bravais lattices [8]

Bravais lattices

Figure 1.14 Bravais lattices of cubic system[8]

#### ****Hexagonal crystal system****

Crystallographic axes

Figure 1.15 3-D Model[8]

Hexagonal crystal system is based on four crystallographic axes. Three of the axes (denoted by a1, a2, and a3) are of the same length and lie in the hexagonal (basal) plane at 120° to one another (between the positive ends). A fourth axis (c), longer or shorter than other three, is perpendicular to this plane. Therefore, it is sufficient to give the a and c lattice parameters for the description of the hexagonal lattice.

Figure 1.16 Unit Cell [8]

The unit cell parameters are:

a = b ≠ c

α = β = 90° γ = 120°

Figure 1.17 Bravais lattice[8]

Figure 1.18 primitive (hP)[8]

#### ****Trigonal crystal system****

Crystallographic axes

Figure 1.19 3-D model[8]

The trigonal crystal system is described by three primitive vectors of equal length that make equal angles (≠90°) with one another. The trigonal unit cell is like a cube that has been stretched along on body diagonal.

a = b = c

α = β = γ ≠ 90°

Figure 1.20 Bravais lattices[8]

Figure 1.21 Bravais lattices[8]

An alternative cell is sometimes used to describe the rhombohedral lattice. The cell is of the same shape as the conventional hexagonal unit cell with two interior points equally spaced along a diagonal. In practice, the hexagonal description is more commonly used because it is easier to deal with coordinate system with two 90° angles.

a = b ≠ c

α = γ = 90° β = 120°

Figure 1.22 R-centred hexagonal lattice (hR) [8]

This figure shows the rhombohedral-centred hexagonal cell and its relationship to the primitive rhombohedral cell

Figure 1.23 R-centred hexagonal lattice (hR)[8]

#### ****Tetragonal crystal system****

Crystallographic axes

Figure 1.24 3D model[8]

Minerals of the tetragonal crystal system are referred to three mutually perpendicular axes. The two horizontal axes are of equal length, while the vertical axis is of different length and may be either shorter or longer than the other two.

a = b ≠ c

α = β = γ = 90°

Figure 1.25 Bravais lattices and primitive (tP) [8]

Figure 1.26 Body-centred (tI)[8]

#### ****Orthorhombic crystal system****

Crystallographic axes

Figure 1.27 3D model [8]

Minerals of the orthorhombic (or rhombic) crystal system are referred to three mutually perpendicular axes, each of which is of a different length than the others.

a ≠ b ≠ c

α = β = γ = 90°

Figure 1.28 Bravais lattices [8]

Figure 1.29 Bravais lattices[8]

Figure 1.30 Bravais lattices [8]

**Monoclinic crystal system**

Crystallographic axes

Figure 1.31 3-D model [8]

Minerals of the monoclinic crystal system are referred to three unequal axes. Two of these axes (a and c) are inclined toward each other at an oblique angle; these are usually depicted vertically. The third axis (b) is perpendicular to the other two and is called the ortho axis. The two vertical axes therefore do not intersect one another at right angles, although both are perpendicular to the horizontal axis.

a ≠ b ≠ c

α = γ = 90° ≠ β

Figure 1.32 Bravais lattices[8]

Figure 1.33 Bravais lattices[8]

#### ****Triclinic crystal system****

Crystallographic axes

Figure 1.34 3D model [8]

Minerals of the triclinic crystal system are referred to three unequal axes, all of which intersect at oblique angles. The triclinic system is sometimes called the anorthic system because there are no angles that are orthogonal.

a ≠ b ≠ c

α ≠ β ≠ γ ≠ 90°

Figure 1.35 Bravais lattice [8]

**1.8      SUMMARY**

* Crystallography is a field of science that deals with arrangements of atoms.
* There are three types of matter of state.
* Crystalline materials are those have periodic arrangements of atoms.
* Space lattice and basis form complete crystal.
* Unit cell is smallest repeating unit in crystals.
* There are 6 parameters of one-unit cell.
* There are 7 crystal systems and 14 Bravais lattice.

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