Lattices:

Crystallography:

The study of the geometric form and other physical properties of crystalline solids by using X-rays, neutron beams and electron beams constitutes the science of crystallography.

Particularly X-rays play an important role in the development of crystallography. Solids can be classified as crystalline solids and amorphous solids. Crystalline solids or crystals, are those in which the atoms or molecules are arranged in a very regular and orderly fashion in a three dimensional pattern. Each atom or molecule is fixed at a definite part in space at a definite distance from and in a definite angular orientation to all others surrounding it. This is called internal spatial symmetry of atomic or molecular orientation and is an essential feature of crystals.

Further when a crystal breaks, the broken pieces are all having regular shape. The crystalline solids have directional properties and therefore they are called anisotropic substances.

Crystalline solids may be made up of metallic crystals or non-metallic crystals. Some of the metallic crystals are copper, silver, aluminium, tungsten and magnesium. Non-metallic crystals are crystalline carbon, crystallized polymers or plastics metallic crystals have wide use in Engineering owing to their favourable properties of strength, ductility, conductivity and reflection.

Amorphous solids have no regular structure and in which; the molecule is the basic structural solid- These solids have no directional properties and therefore they are called isotropic subtances. An amorphous structure does not generally possess elasticity but only plasticity (an exception to this statement is rubber). Most important amorphous materials are glasses, plastics and rubbers. The structure of the crystalline solids are mainly determined by X-ray diffraction methods, and neutron diffraction methods. Knowing the structural properties of a crystal one can determine its thermal, electrical, mechanical and optical properties.

Definitions in Crystallography:

Lattice points:

Lattice points denote the position of atoms or molecules in the crystals.

Space lattice:

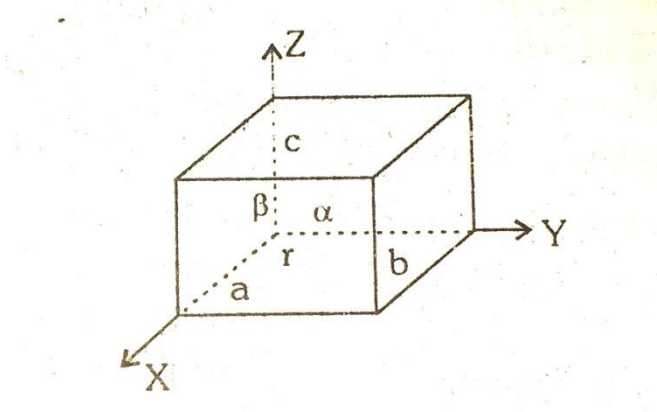
An infinite three dimensional array 'of points showing how atoms or molecules' are arranged in a crystal is known as space lattice. Thus the angular arrangement of the space positions of the atoms or molecules in a crystal is called space lattice or lattice array. In the lattice array, every point has surroundings or, environments identical to that of every other point in the array.

Unit Cell:

The unit cell is the smallest block or geometric figure from which the entire crystal is built up by repetition in three dimensions. It may be considered as the brick of a wall where the latter represents the crystal. We know that the shape of the wall will depend upon the shape of the brick similarly the shape of the crystal will depend upon the shape of the unit cell. It is also known as fundamental elementary pattern of a crystal because it is repeated again and again to form the lattice structure of a crystal. In general an unit cell may be defined as that volume of a solid from which the entire crystal can be

constructed by transitional repetition dimensions. Since the unit cell which reflection the structure of the crystall lattice, has all the structure properties of the given crystal lattice, it is not necessary [to study the whole crystal lattice to get the clear idea about the whole crystal lattice.

Lattice parameters of an unit cell:



The lines drawn parallel to the lines of intersection of any three faces of the unit cell which do not lie in the same plane are called crystallographic axes. An arbitary arrangement of crystallographic axes marked x, y and z defining an unit cell is shown in the above figure.

The angles b/w the three crystallographic axes are known as interfacial angles or interaxial angles.

Tire angle b/w the axes y and z = α

The angle b/w

the axes z and X = β

The angle b/w-the axes X and y = γ

Thus the above angles α, β and γ are the interfacial angles. The intercepts a, b and c define the dimensions of an unit cell and are known as its primitives or characteristic intercepts on the axes. These three quantities a, b and c are also called the fundamental translational vectors.

The primitives a, b and c and interfacial angles are the basic lattice parameters because they determine the form and actual; size of the unit cell and hence the space lattice. But if we do not know the actual values of primitives but only their ratio and the values of interaxial angles then we can only determine the form of the unit cell and not its actual size. The unit cell formed by the primitives a, b and c is called primitive cell. In a. primitive cell there is only one lattice point. If there are two more lattice points then it is not a primitive cell.

In the case of simple cubic crystal lattice, the primitive cell and unit cell are equal since it has only one lattice point in its unit cell. But most of the unit cells of various crystal lattices contain two or more lattice points and it is not necessary that the unit cell should be equal to the primitive ceil.

In a space lattice all lattice points may be included in a set of parallel and equally spaced planes known as lattice planes. These planes give the orientations of the possible faces of a crystal of the substance-in question.

In theory, there are 230 such space lattices or space groups divided into 32 crystal classes. These can be arranged in 7 crystal systems depending on the relative lengths and direction of the axes of symmetry.

In 1848, Bravais showed that fourteen classes of lattice were sufficient in three dimensions. According to Bravais there are 14 possible types of space lattices in the seven systems of crystals.

one	triclinic
two	monoclinic
four	orthorhombic

two	tetragonal
one	hexagonal
one	rhombohedral {
three	cubic

In fact, it has been proved mathematically that there are only fourteen independent ways of arranging points in three dimensional space such that each arrangement conforms to the definition of a space lattice, thus the above fourteen possible space-lattices of the seven crystal systems are called Bravais lattices.

The space lattices formed by unit cells are marked by the following symbol.

Primitive lattice – P

Body centred lattice – I

Face central lattice – F

Base centred lattice – C

Miller indices:

Miller indices are the set of three integers (h k l) which is used to designate the different crystal planes in the reciprocal lattice of the crystal.

The reciprocal lattice is an infinite periodic three dimensional array of points whose spacings are inversely proportional to the distances b/w the planes in the direct lattice. The concept of reciprocal lattice is adopted since it is easy to interpret the diffraction patterns obtained on the photographs. The use of Miller indices for rotation of the crystallographic planes is universal.

Symmetry elements of a crystalline solid:

The seven crystal systems are characterised by three symmetry elements:

i) The centre of symmetry

ii) The planes of symmetry

iii) the axes of symmetry

A symmetry operation is an operation performed on an object or pattern which brings it to a position which is absolutely indistinguishable from the old position. A symmetry element is an operator which performs the symmetry operation.

i) Centre of symmetry:

The point in a crystal such that any line passing through it meets the surface of the crystal at equal distances, in both directions is known as centre of symmetry or centre of inversion, i.e. the centre lies at equal distances from various symmetrical positions.

ii) Plane of symmetry:

An imaginary plane passing through a crystal such that portions on the two sides of the plane are exactly alike is known as a plane of symmetry. This is also known as bilateral symmetry.

iii) Axis of symmetry:

Axis of symmetry is a line passing through the crystal such that if the crystal is rotated above this line as axis, it will present the same appearance more than once during one complete revolution.

Crystal structure of important engineering materials:

Atomic radius 'r':

Atomic radius is defined as half the distance b/w the nearest neighbouring atoms in a crystal.

Co-ordination number:

It is the number of neatest equidistant neighbours that an atom has in an unit cell. Its

value depends upon the type of crystal structure. The co-ordination number is calculated by taking the nearest neighbouring atoms at a distance, 2r.

Density of packing:

It is the ratio of Volume occupied by atoms in an unit cell to the total volume of the unit cell. It is also called packing factor or packing fraction.

i.e. packing fraction, P.F = v/V

where v = Volume occupied by atoms in the unit cell &

V = total volume of the unit

Types of structures:

a) Simple Cubic (SC) structure packing fraction is

52%

b) Body. entered Cube (BGC) structure packing fraction = 68%

c) Face Centred Cubic (FCC) structure paction fraction = 0.74 or 74%

FCC has high packing fraction and most of the metals like Copper, Aluminium and Silver have this structure.

d) Hexagonal closed packed (HCP) structure density of packing is 0.74 or 74%

Other important structures are

a) Diamond cubic structure P.F = 34%

b) Zinc blende or sphalerite cubic structure.

c) Sodium chloride structure

d) Caesium chloride structure

Polymorphism &Allotropy:

A change in temperature or pressure, it not accompanist by melting or vaporization, may cause a solid to change its internal arrangement of atoms. The ability of a material to have more than one structure is called polymorphism.

If the change in structure is reversible, then the polymorphic change is known as Allotropy.