Crystal structure

Crystal of a material may be defined as a small body having a regular polyhedral form bounded by the smooth surfaces which are acquired under the action of its intermolecular forces.

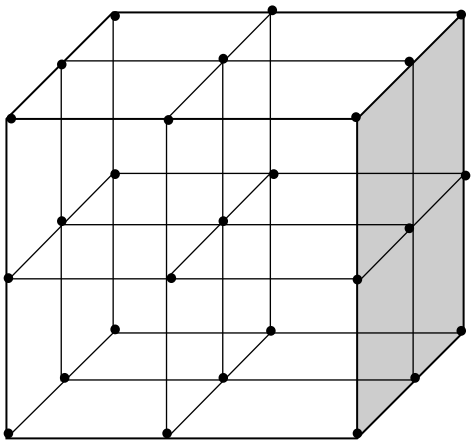
The regular arrangement of constituent particles repeating throughout the solid is known as crystal structure. The solid with crystal structure are known as crystalline solid. Crystalline solids are very important because most of the engineering materials have crystal structure. The reason is:

i) The force between constituent particles is maximum that is more balanced.
ii) The potential energy of the solid is minimum, so the structure is more balanced.

Space lattice or crystal lattice

The regular arrangement of points in the space in three dimension infinitely such that every points has identical surroundings.

The crystal structure can be best understood by using the space lattice. As the constituent particles are very small they can be compared with points. Space lattice can be produced by replacing every constituent particle by a point in the space. Finally an arrangement of points similar to arrangement of constituent particles is produced. A space lattice can be represented by a network of lines in three dimensions such that the space is divided into equal volume. The intersection of any two lines represents the position of the constituent particle. Mathematically a space lattice can be denoted by lattice vector.



Space Lattice

$\vec{l} = l_1\vec{a} + l_2\vec{b} + l_3\vec{c}$ Where l_1, l_2 & l_3 are integers and $\vec{a}, \vec{b}$ & $\vec{c}$ are translatory vector.

Unit cell: A smallest group of points which are assumed in a cell is known as unit cell.

To describe crystal structure it is not necessary to give the position of all the points but it is enough to give the position of smallest group of points. The smallest groups of points are known as unit cell. The properties of unit cell are same as the properties of whole crystal.

To explain the properties of unit cell two set of dimensions are used.

i) Length of each side a, b and c. These are known as primitives.

ii) Three interfacial angle α, β and γ.

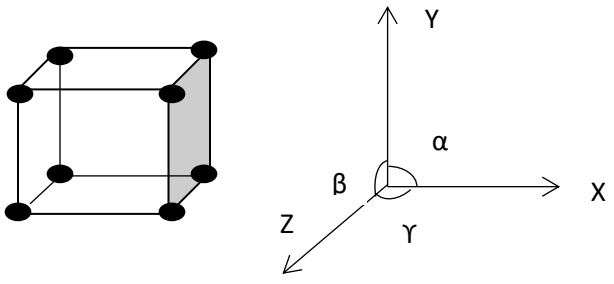
These two sets of dimensions are known as lattice parameters.

Primitive Cell: It is a simplest unit cell having points only in the corners.

OR

Primitive cell is the simplest type of unit cell which contains one lattice point per unit cell.

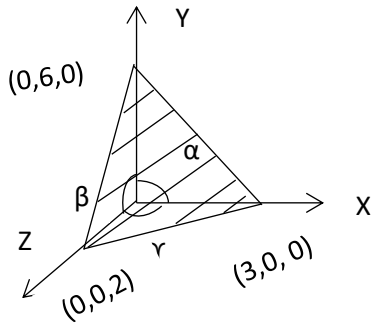
A simple cubic cell is an example of primitive cell. FCC & BCC are non-primitive cell.



Miller Indices: Miller suggested a method of notation of planes by small whole numbers. According to this method the notation of a plane depends upon the intercepts of the plane on the three crystallographic axes. However miller suggested it is more convenient to take reciprocal of the intercepts. By taking reciprocal an infinity intercept can be made as zero.

Miller indices do not indicate the exact position of the plane but they indicate the relative position of the plane from a selected origin. Miller indices are denoted by (h,k,l). A negative indices is denoted by a bar ($\bar{h}$) on the top.

		X-axis	Y-axis	Z-axis
i)	Intercept	2a	b	3c
ii)	Numerical Parameter	2	1	3
iii)	Reciprocal	1/2	1/1	1/3
iv)	Small whole Number	$\frac{3,6,2}{6}$		
v)	Miller Indices (3, 6, 2).			



Important features of Miller indices of crystal planes:

i) All the parallel planes have the same Miller indices.

ii) A plane parallel to one of the coordinate axis has an intercept of infinity.

iii) If the Miller indices of two planes have the same ratio then the planes are parallel to each other. For example (8 4 4) and (4 2 2) or (2 1 1).

Types of Crystal system: Depending on the geometry of unit cell the crystal systems are divided into seven groups.

i)	Cubic	$a = b = c$	$\alpha=\beta=\gamma=90^0$
ii)	Tetragonal	$a = b \neq c$	$\alpha=\beta=\gamma=90^0$
iii)	Orthorhombic	$a \neq b \neq c$	$\alpha=\beta=\gamma=90^0$
iv)	Monoclinic	$a \neq b \neq c$	$\alpha=\beta=90^0 \neq \gamma$
v)	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^0$
vi)	Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^0$
vii)	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^0, \gamma = 120^0$

Bravais Lattice: According to Bravais, there are fourteen possible types of space lattices in these seven crystal system.

i) Cubic
   a) Simple cubic
   b) Body Centered cubic
   c) Face Centered cubic

ii) Tetragonal
   a) Simple Tetragonal
   b) Body Centered Tetragonal

iii) Orthorhombic
   a) Simple Orthorhombic
   b) End Centered Orthorhombic
   c) Body Centered Orthorhombic
   d) Face Centered Orthorhombic

iv) Monoclinic
   a) Simple monoclinic
   b) End centered monoclinic

v) Triclinic

a) Simple Triclinic

vi) Rhombohedral

a) Simple Rhombohedral

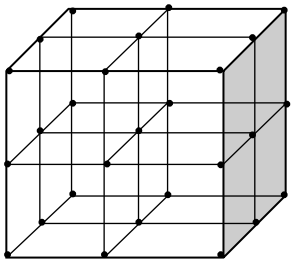
vii) Hexagonal

a) Simple Hexagonal

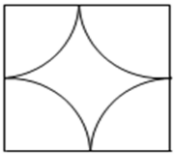
Simple Cubic

Co-ordinate Number: Number of atoms directly surrounding a given atom.

CN = 6



Atomic Radius (r)



a = 2r

$a = 2r$

$r = \frac{a}{2}$

Number of atoms = $\frac{1}{8}$ x 8 =1

Packing Density or Packing Fraction $= \frac{Volume \text{ of atoms in a unit cell (v)}}{Volume \text{ of unit cell (V)}}$

$v = \frac{4}{3}\pi r^3$

$v = \frac{4}{3}\pi\left(\frac{a}{2}\right)^3$

$v = \frac{\pi a^3}{6}$

$V = a^3$

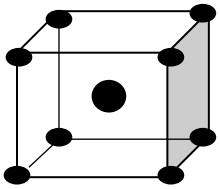
Packing density or Packing fraction = $= \frac{v}{V}$

$$= \frac{\pi}{6} = 0.52$$

Body Centered Cubic:

CN = 8

Atomic Radius



$(4r)^2 = a^2 + \left(a\sqrt{2}\right)^2$

$r = \frac{\sqrt{3}a}{4}$

Number of atoms $= \frac{1}{8}$ x 8+1=2

Packing density = 0.68

Face Centered Cubic

CN = 12

Number of atoms $= \frac{1}{8}$ x 8+$\frac{1}{2}$ x 6 = 4

Atomic Radius

$a^2 + a^2 = (4r)^2$

$$r = \frac{a}{2\sqrt{2}}$$

Packing Density = 0.74