Crystal Structure:

- Lattice translation vector:

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

Where, n_1, n_2 and n_3 are arbitrary constants and a, b, c are lattice parameters.

- Symmetry operations:

Four major types of symmetry operations-

(i) Translation operation (Translational symmetry)

(ii) Rotation operation (Rotational symmetry)

- 1- fold, 2- fold, 3-fold, 4-fold, 6-fold rotational symmetry operations are possible.
- 5- fold rotational symmetry operation is not possible.

(iii) Inversion operation (Inversion symmetry)

(iv) Reflection symmetry (Mirror symmetry)

- Bravais Lattices:
  - There are 4 two dimensional crystal systems and 5 Bravais lattices in 2 Dimension.

(a) Oblique lattice ------ $a \neq b, \gamma \neq 90^0$

(b) Square lattice ------- $a = b, \gamma = 90^0$

(c) Hexagonal lattice ------ $a = b, \gamma = 120^0$

(d) Rectangular lattice ------- (i) Rectangular Primitive ($a \neq b, \gamma = 90^0$)

(ii) Rectangular centred ($a \neq b, \gamma = 90^0$)

  - There are 7 three dimensional lattice systems and 14 Bravais lattices in 3 dimension.

(i) Cubic lattice ------- $a = b = c, \alpha = \beta = \gamma = 90^0$

- Simple Cubic
- Body centred cubic
- Face centred cubic

(ii)Tetragonal ---------- $a = b \neq c, \alpha = \beta = \gamma = 90^0$ — Simple, Body centred

(iii) Orthorhombic -------- $a \neq b \neq c, \alpha = \beta = \gamma = 90^0$ — Simple, Body centred, Face centred, End centred

(iv) Rhombohedral or trigonal ---------- $a = b = c, \alpha = \beta = \gamma \neq 90^0$ ------- Simple

(v) Hexagonal ---------- $a = b \neq c, \alpha = \beta = 90^0, \gamma = 120^0$ ---------- Simple

(vi) Monoclinic --------- $a \neq b \neq c, \alpha = \gamma = 90^0 \neq \beta$ — Simple, End centred

(vii) Triclinic ---------- $a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^0$ ---------- Simple

- The number of atoms per unit cell:

  For simple cubic ------- 01

  For bcc ---------- 02

  For fcc ------- 04

- Atomic radius of:

  Simple cubic structure, $r = \frac{a}{2}$

  Body centred cubic structure, $r = \frac{\sqrt{3}}{4}a$

  Face centred cubic structure, $r = \frac{a}{2\sqrt{2}}$

  Where, a is the lattice constant.

- Packing fraction: It is defined as the ratio of the volume occupied by the atoms present in a unit cell to the total volume of the unit cell.
- Packing fraction of:

  Simple cubic = 52%

  Body centred cubic = 68%

  Face centred cubic = 74%

- Rules for finding Miller Indices
  - ✓ Find the intercepts of the plane on the crystallographic axes
  - ✓ Take reciprocals of these intercepts
  - ✓ Simplify to remove fraction

- Find the Miller Indices of a plane having intercepts $3a, 3b, 2c$
  - ➢ Intercepts: 3, 3, 2
  - ➢ Reciprocals: $\frac{1}{3}, \frac{1}{3}, \frac{1}{2}$
  - ➢ Simplification: 2, 2, 3

    The Miller Indices (223)

- Interplaner spacing of a set of parallel planes with Miller Indices (hkl)

$$d = \frac{1}{\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{\frac{1}{2}}}$$

For a cubic crystal $a = b = c$

$$\therefore d = \frac{a}{(h^2 + k^2 + l^2)^{\frac{1}{2}}}$$

- Find the interplaner spacing between the (221) planes of a cubic lattice of length 450 pm.
  - ➢ Here, h = 2, k = 2, l = 1 and $a = 450\ pm = 450 \times 10^{-12} m$

$$\therefore\ d = \frac{450 \times 10^{-12}}{(2^2 + 2^2 + 1^2)^{\frac{1}{2}}} = \frac{450 \times 10^{-12}}{3} = 150\ pm$$

- Angle between two planes with Miller indices ($h_1\ k_1\ l_1$) and ($h_2\ k_2\ l_2$)

$$cos\theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{({h_1}^2 + {k_1}^2 + {l_1}^2)}\sqrt{({h_2}^2 + {k_2}^2 + {l_2}^2)}}$$

- In a cubic unit cell, find the angle between the normal to the planes (111) and (121).
  - The normals to the planes (111) and (121) are directions [111] and [121]. Let θ be the angle between the normals.

$$cos\theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{({h_1}^2 + {k_1}^2 + {l_1}^2)}\sqrt{({h_2}^2 + {k_2}^2 + {l_2}^2)}}$$

$$= \frac{1 \times 1 + 1 \times 2 + 1 \times 1}{\sqrt{(1^2 + 1^2 + 1^2)}\sqrt{(1^2 + 2^2 + 1^2)}} = 0.9428$$

$$\theta = \cos^{-1}(0.9428)$$

- Relation between lattice constant and density

$$\rho = \frac{nM}{Na^3}$$

$$where, n = no.\ of\ atoms\ per\ unit\ cell$$

M= Atomic weight, N= Avogadro's number, a= lattice constant, ρ= density.

- The lattice constant of iron (in bcc) is 2.86 Å. What is the density of iron, taking the atomic weight of iron as 55.85 amu.
  - Given, $a = 2.86Å = 2.86 \times 10^{-8}$cm

    For bcc, n= 2, M=55.86 amu = 55.86 g/mol, N= 6.023×10^{23}

$$\therefore \rho = \frac{nM}{Na^3} = \frac{2 \times 55.85}{6.023 \times 10^{23} \times (2.86 \times 10^{-8})^3} = 7.93\frac{g}{cc}$$

- X- rays are used to determine the structure of solids and for the study of X-ray spectroscopy. X- rays have the same order of wavelength as the atomic diameter or interplaner spacing. Thus a crystal acts as a three dimensional grating for X-rays.

- Bragg's law: $2dsin\theta = n\lambda$, Where,

  $d = interplaner\ spacing, \lambda = wavelength\ of\ X-rays, \theta = Angle\ of\ incidence$

- The spacing between successive planes in NaCl is 2.82Å. X- rays incident on the surface of the crystal is found to give rise to 1st order Bragg's reflection at glancing angle of 8.8^0, calculate the wavelength of x-rays. (Given, sin 8.8^0=0.152)
  - Given, d = 2.82Å= 2.82×10^{-10}m, n= 1, $\theta = 8.8^0$, $sin8.8^0 = 0.152$

$$\therefore 2dsin\theta = n\,\lambda$$

$$=> 2 \times 2.82 \times 10^{-10} \times 0.152 = 1 \times \lambda$$

$$\lambda = 8.5 \times 10^{-9} m$$

- Reciprocal lattice vector, $G = ha^* + kb^* + lc^*$

  Where, $a^* = 2\pi\frac{b\times c}{a.(b\times c)}$, $b^* = 2\pi\frac{c\times a}{a.(b\times c)}$, $c^* = 2\pi\frac{a\times b}{a.(b\times c)}$,

- Bragg's law in reciprocal lattice, $2\vec{k}.\vec{G} + G^2 = 0$
- Reciprocal lattice:

For simple cubic, $a^* = \frac{2\pi}{a}\hat{\imath}$, $b^* = \frac{2\pi}{a}\hat{\jmath}$, $c^* = \frac{2\pi}{a}\hat{k}$

For bcc, $a^* = \frac{2\pi}{a}(\hat{\imath} + \hat{\jmath})$, $b^* = \frac{2\pi}{a}(\hat{\jmath} + \hat{k})$, $c^* = \frac{2\pi}{a}(\hat{k} + \hat{\imath})$

For fcc, $a^* = \frac{2\pi}{a}(\hat{\imath} + \hat{\jmath} - \hat{k})$, $b^* = \frac{2\pi}{a}(-\hat{\imath} + \hat{\jmath} + \hat{k})$, $c^* = \frac{2\pi}{a}(\hat{\imath} - \hat{\jmath} + \hat{k})$

- Simple cubic lattice is self reciprocal whereas, bcc and fcc lattices are reciprocal to each other.

- Atomic scattering factor, $f = \frac{amplitude\ of\ radiation\ scattered\ from\ an\ atom}{amplitude\ of\ radiation\ scattered\ from\ an\ electron}$

- Geometrical structure factor,

$$F = \frac{amplitude\ of\ radiation\ scattered\ by\ the\ entire\ unit\ cell}{amplitude\ of\ radiation\ scattered\ by\ a\ point\ electron\ at\ the\ origin}$$

- Brillouine zone: It is the locus of all those k-values in the reciprocal lattice which are Bragg reflected.