The atomic packing factor [A.P.F]:

It can be defined as the ratio between the volume of the basic atoms of the unit cell (which represent the volume of all atoms in one unit cell) to the volume of the unit cell it self.
For cubic crystals,

A.P. F its depends on the riadus of atoms and characrtiziation of chemical bondings .

Atomic Packing Factor for Simple Cubic :-

no. of atoms = 1

volume of one atom = $\frac{4}{3}\pi r^3$

volume of unit cell (cubic) = a^3

when , (a = 2r)

Filling Factor = $\frac{1*\frac{4\pi r^3}{3}}{a^3}$

$$= \frac{\frac{4\pi r^3}{3}}{(2r)^3} = \frac{\frac{4\pi r^3}{3}}{8r^3} = \frac{\pi}{6} = 52\%$$

Atomic Filling Factor for BCC:-

no of atoms =2

volume of tow atoms =2* $\frac{4}{3}\pi r^3$

volume of unit cell (cubic) = a^3

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

Filling Factor = $\frac{2*\frac{4\pi r^3}{3}}{a^3}$

$$= \frac{\frac{8\pi r^3}{3}}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\frac{8\pi r^3}{3}}{\frac{64}{3\sqrt{3}}r^3} = \frac{\sqrt{3}\pi}{8} = 68\%$$

Atomic Filling Factor for FCC:-

no of atoms = 4

volume of four atoms = $4* \frac{4}{3}\pi r^3$

volume of unit cell (cubic) = a^3

when $r = \frac{a\sqrt{2}}{4} = \frac{a}{2\sqrt{2}}$

Filling Factor = $\frac{4*\frac{4\pi r^3}{3}}{a^3}$

$$= \frac{\frac{16\pi r^3}{3}}{(2\sqrt{2}r)^3} = \frac{\frac{16\pi r^3}{3}}{16\sqrt{2}\,r^3} = \frac{\sqrt{2}\pi}{6} = 74\%$$

Miller Indices:

• Miller Indices are used to refer to specific lattice planes of atoms.
• They are reciprocals of the fractional intercepts (with fractions cleared) that the plane makes with the crystallographic x,y and z axes of three nonparallel edges of the cubic unit cell.

Miller Indices – Procedure:

1. Choose a plane that does not pass through origin
2. Determine the x,y and z intercepts of the plane
3. Find the reciprocals of the intercepts
4. Fractions?
a. If Yes, Clear fractions by multiplying by an integer to determine smallest set of whole numbers, then go to b

b. If No, Place a „bar" over the Negative indices
5. Enclose in parenthesis (hkl) where h,k,l are miller indices of cubic crystal plane for x,y and z axes.

Note / if the one of axies value was negative then move the center of cubic to negative value direction .

Example 1

Draw the follwing plances in the cubic crystal ?

$(0\bar{1}0)$ −5 ، $(\bar{1}00)$ −4 ، (001) −3 ، (010) −2 ، (100) − 1

$(00\bar{1})$ −6 ،

Ans.

1 − (100)

$$x = \frac{1}{1} = 1$$

$$y = \frac{1}{0} = \infty$$

$$z = \frac{1}{0} = \infty$$

then miller indices are $(1\infty\infty)$

2- (010)

$$x = \frac{1}{0} = \infty$$

$$y = \frac{1}{1} = 1$$

$$z = \frac{1}{0} = \infty$$

then miller indices are $(\infty 1\infty)$

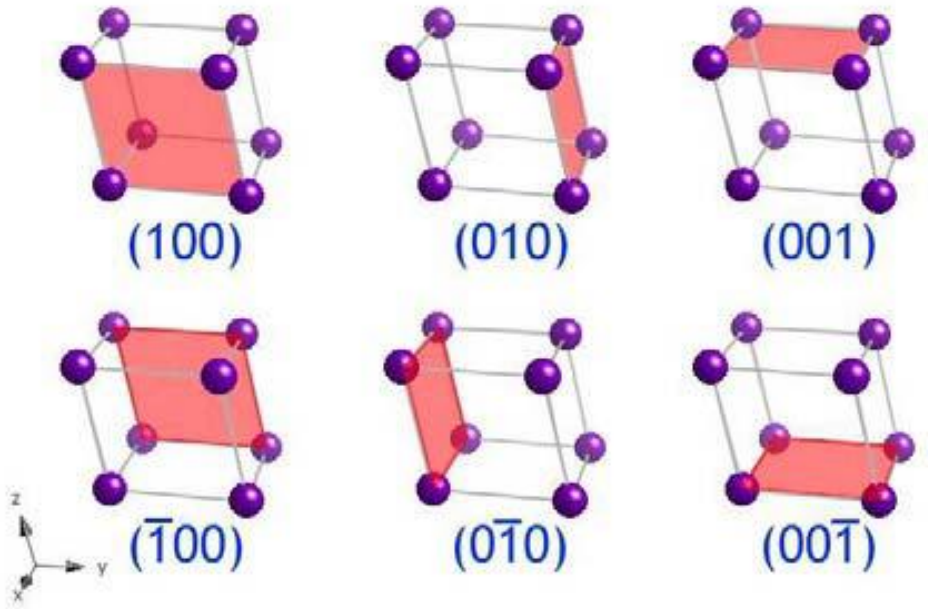
3- (001)

$$x = \frac{1}{0} = \infty$$

$$y = \frac{1}{0} = \infty$$

$$z = \frac{1}{1} = 1$$

then miller indices are$(\infty\ \infty 1)$



Example 2 :-

Draw the follwing plances in the cubic crystal ?

، $(1\bar{1}0)$ -5 ، $(10\bar{1})$ -4 ، (011) - 3 ، (110) - 2 ، (101) - 1
$(01\bar{1})$ -6

1-(101)

$$x = \frac{1}{1} = 1$$

$$y = \frac{1}{0} = \infty$$

$$z = \frac{1}{1} = 1$$

then miller indices are $(1\ \infty 1)$

2- (110)

$$x = \frac{1}{1} = 1$$

$$y = \frac{1}{1} = 1$$

$$z = \frac{1}{0} = \infty$$

then miller indices are$(1\ 1\infty)$

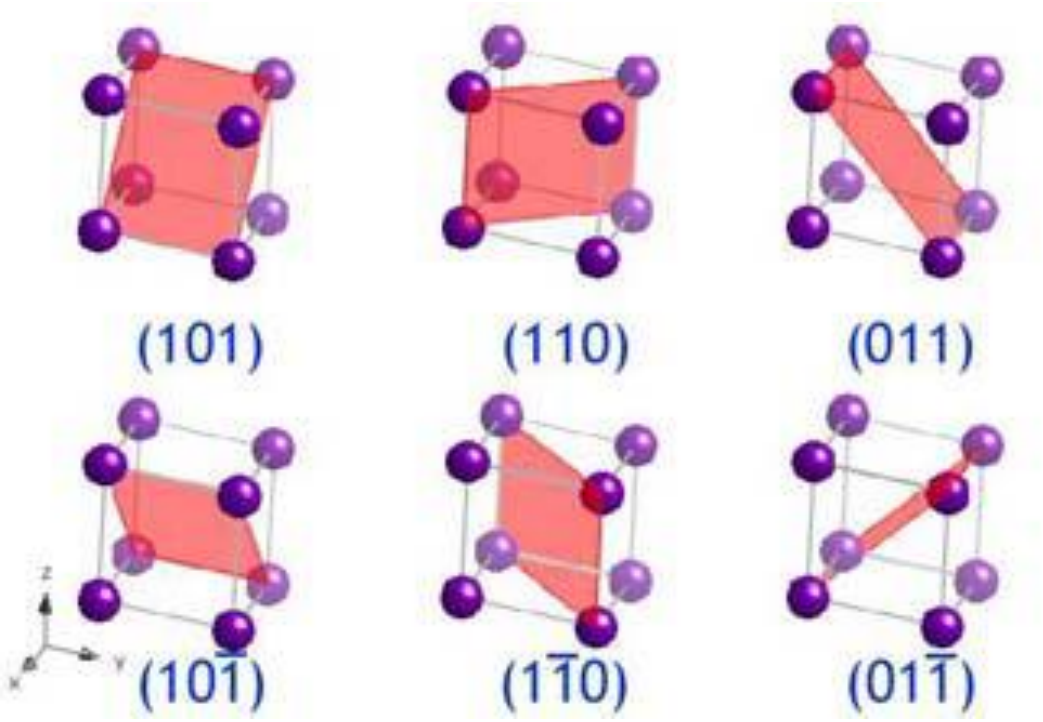
3- (011)

$$x = \frac{1}{0} = \infty$$

$$y = \frac{1}{1} = 1$$

$$z = \frac{1}{1} = 1$$

then miller indices are $(\infty 11)$



Interplaner Distance between paraalls plances

The space lattice consist from many crystall plances which separated by interplaner smallest distance
The distance can be calcalated by using x- ray diffraction , by using the law below :-

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Where d_{hkl} = interplanar spacing between parallel closest planes with Miller indices *h*, *k*, and *l*

a = lattice constant (edge of unit cube).

h, *k*, *l* = Miller indices of cubic planes being considered.

Angles between crystal planes :-

The crystal consist many from plance which contact with them in vairty angles , The angle between crystal planes can be calculated by using the following equation :-

$$\cos\theta = \frac{h1h2 + k1k2 + l1l2}{\sqrt{(h1^2 + k1^2 + l1^2)} * \sqrt{(h2^2 + k2^2 + l2^2)}}$$

Example :-

Find the angle between the plances $(1\bar{1}1)$ & (111)?

$$\cos\theta = \frac{h1h2 + k1k2 + l1l2}{\sqrt{(h1^2 + k1^2 + l1^2)} * \sqrt{(h2^2 + k2^2 + l2^2)}}$$

$$\cos\theta = \frac{1 + (-1) + 1}{\sqrt{1+1+1} * \sqrt{1+1+1}}$$

$\cos\theta = \frac{1}{3}$

$\cos\theta = 0.333$

$\cos^{-1} 0.333 = \theta$

$\theta = 70.32°$

Example 2

Find the interplaner distance for plane (220) , which have FCC Craystal and raidus of atom (1.414 A) ?

Solution:-

The crystal is FCC then

$$a = \frac{4r}{\sqrt{2}}$$

$$a = \frac{4(1.414)}{\sqrt{2}} = \frac{4(1.414)}{1.414} = 4\ A°$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{hkl} = \frac{4}{\sqrt{4 + 4 + 0}} = 1.414\ A°$$

Example: (H.W)
Copper has an FCC crystal structure and a unit cell with a lattice constant of 0.361 nm. What is its interplanar spacing d_{220}?