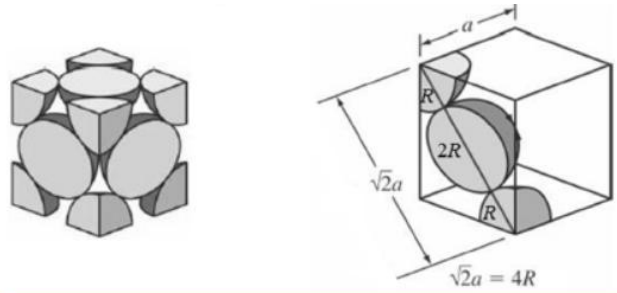
Atomic packing factor

Atomic packing factor (APF) or packing efficiency indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and volume of the unit cell.

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Atomic packing factor (FCC lattice)

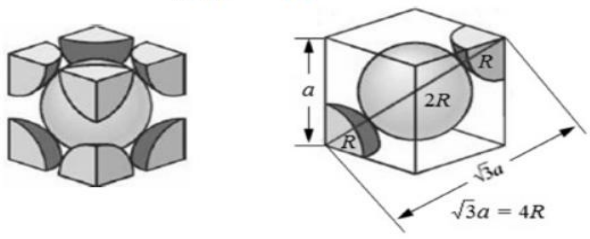
In the FCC unit cell effective number of atoms = 8 corner atoms x (1/8) (each atom is shared by 8 unit cells) + 6 face centered atoms x1/2 (each shared by two unit cells) = 4 atoms. Considering the atoms as hard spheres of radius *R*.
The relation between *R* and the FCC cell side *a* as shown in the figure below is $\sqrt{2}a = 4R$



$$APF(FCC) = \frac{4 \times \frac{4}{3}\pi R^3}{a^3} = \frac{16 \times 2\sqrt{2}\pi a^3}{3 \times 64 a^3} = 0.74$$

Atomic packing factor(BCC lattice)

For BCC crystals effective number of atoms per unit cell is 8 x 1/8 + 1 = 2 and the relation between R and a is $\sqrt{3}a = 4R$



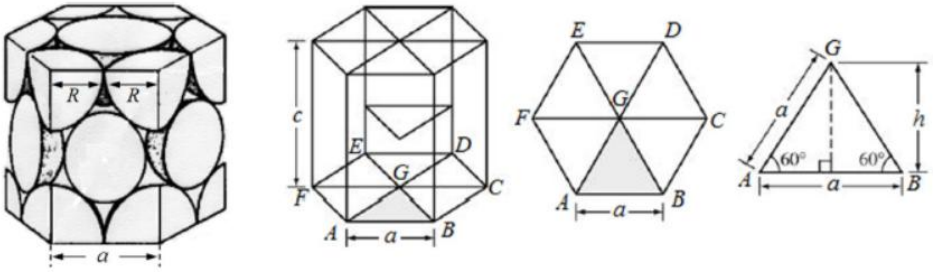
$$APF(BCC) = \frac{2 \times \frac{4}{3}\pi R^3}{a^3} = \frac{8 \times 3\sqrt{3}\pi a^3}{3 \times 64 a^3} = 0.68$$

Atomic packing factor(HCP lattice)

In the Hexagonal unit cell, number of atoms = 12 corner atoms x 1/6 (shared by six unit cells) + Two face atoms x 1/2 + 3 interior = 6.

$$2R = a$$

Unit cell volume = (6 x ½ x a x h) x c = (3 x a x a sin60°) x c
= $3a^2 c \sin 60°$

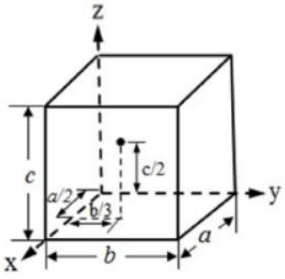


$$APF(HCP) = \frac{6 \times \frac{4}{3}\pi R^3}{3a^2 c \sin 60°} = \frac{8\pi a^3}{3 \times 8 \times 1.414 a^3} = 0.74$$

Point Coordinates

Position of any point in a unit cell is given by its coordinates or distances from the x, y and z axes in terms of the lattice vectors a, b and c.

Thus the point located at a/2 along x axis, b/3 along y axis and c/2 along z axis, as shown in the figure below, has the coordinates $\frac{1}{2}\frac{1}{3}\frac{1}{2}$



Miller Indices

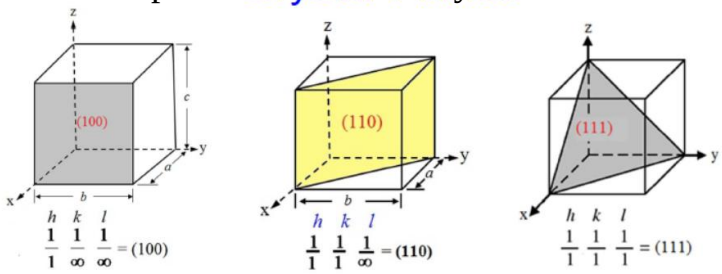
Planes in a crystal are described by notations called Miller indices

-Miller indices of a plane, indicated by h k l, are given by the reciprocal of the intercepts of the plane on the three axes.

-The plane, which intersects X axis at 1 (one lattice parameter) and is parallel to Y and Z axes, has Miller indices

h = 1/1 = 1, k = 1/∞ = 0, l = 1/∞ = 0. It is written as (hkl) = (100).

-Miller indices of some other planes in the cubic system are shown in the figures below



To find the Miller Indices of a plane, follow these steps:

1-Determine the intercepts of the plane along the crystal axes
2-Take the reciprocals
3-Clear fractions
4-Reduce to lowest terms and enclose in brackets ( )
Example: Intercepts on a, b, c : ¾, ½, ¼ (h k l) = (4/3, 2, 4) = (2 3 6)

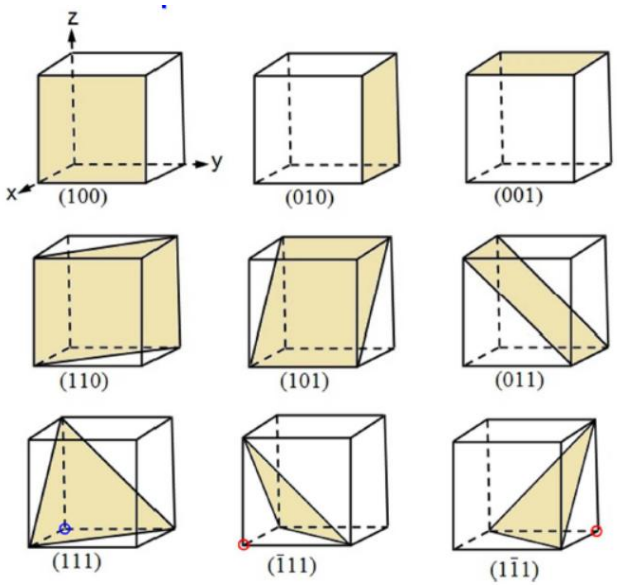
Crystal Planes

Planes can also have negative intercept e.g. 1, -1/2, 1 h k l = 1 -2 1. This is denoted as (1 $\bar{2}$ 1)

Family of planes {hkl}

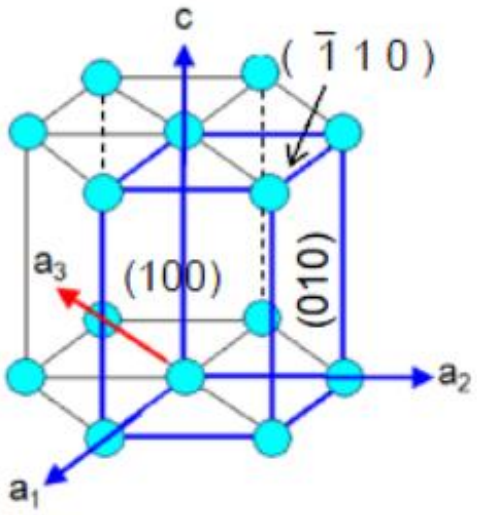
Planes having similar indices are equivalent, e.g. faces of the cube (100), (010) and (001). This is termed as a family of planes and denoted as {100} which includes all the (100) combinations including negative indices.
Some other equivalent planes are shown in the next slide.

Equivalent Planes



Note the shift of origin from blue to red circle for the negative indices
Planes in Hexagonal system
-In the cubic system all the faces of the cube are equivalent,
that is, they have similar indices.
In order to address this, a fourth axis (a3) which is opposite to the vector sum of a1 and a2 is used and a corresponding fourth index *i* is used along with *hkl*. Therefore the indices of a plane is given by *(hkil)* where *i = -(h+k)*. Sometime *i* is replaced with a dot and written as (h k . l)

-However, this is not the case in the hexagonal system. The six prism faces for example have indices (1 0 0), (0 1 0), ($\bar{1}$ 1 0), ($\bar{1}$ 0 0), (0$\bar{1}$ 0), (1$\bar{1}$ 0), which are not same.



The indices of six faces now become (1 0$\bar{1}$ 0), (0 1$\bar{1}$ 0), ($\bar{1}$ 1 0 0), ($\bar{1}$ 0 1 0), (0$\bar{1}$ 1 0), (1$\bar{1}$ 0 0) which are now equivalent and belong to the {1 0$\bar{1}$ 0 } family of planes.