

Atomic radius

It is supposed that all the atoms in a crystal have the same size and are touching each other. Thus the atomic radius is the distance between the centers of two neighbouring atoms

In the case of simple cube, if r is the atomic radius and lattice parameter is a , then,

$$a = 2r$$

$$r = a/2$$

In the case of body centered cube, the atoms touch each other along the diagonal of the cube and we have

$$(4r)^2 = (\sqrt{2}a)^2 + a^2$$
$$r = \frac{\sqrt{3}}{4}a$$

In case of a face-centered cube the atoms are in contact along the diagonal of the faces

$$(4r)^2 = 2a^2$$
$$r = \frac{a}{2\sqrt{2}}$$

Atomic packing fraction

Also known as relative packing density is defined as the ratio of the volume of the atoms occupying the unit cell to the volume of the unit cell relating to the structure of the crystal.

In simple cubic structure the number of atoms per unit cell is one. The atomic radius is given by half of the lattice parameter.

$$\therefore \text{Volume occupied by the atom in the unit cell} = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi \left(\frac{a}{2}\right)^3$$

$$\text{Volume of the unit cell} = a^3$$

$$\therefore \text{Packing fraction } (f) = \frac{\frac{4}{3}\pi \left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = 52\%$$

Similarly, Packing fraction in *bcc* and *fcc* are 68% and 74% respectively.