



(5) Packing fraction or Density of packing (F) \Rightarrow
The fraction of total vol. of the unit cell occupied by atoms is called packing fraction. It may also be defined as the ratio of vol. occupied by the atoms in unit cell to the total vol. of the unit cell.

$$\text{Packing fraction (F)} = \frac{\text{Vol. occupied by the atoms in unit cell}}{\text{Total vol. of the unit cell}}$$

$$F = \frac{V}{V}$$

* Packing efficiency or % of packing = $P.F \times 100$
(% of total space occupied by the particles in unit cell)
 $= \frac{V}{V} \times 100$

* The fraction of vacant space can be calculated from the % packing fraction

Ex (1) In SC unit cell \Rightarrow

$$V = z \times \text{vol. of one atom} = 1 \times \frac{4}{3} \pi r^3 = \frac{4}{3} \pi \left(\frac{a}{2}\right)^3$$

$$V = a^3$$

$$P.F = \frac{V}{V} = \frac{\frac{4}{3} \pi \left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = \frac{3.14}{6} = 0.5236$$

$$\begin{aligned} \text{\% of Packing fraction (or packing efficiency)} &= 100 \times P.F \\ &= 100 \times 0.5236 \\ &= 52.36 \end{aligned}$$

$$\text{\% of vacant space} = 100 - \text{\% of P.F} = 100 - 52.36 = 47.64$$

$$\text{fraction of vacant space} = 0.4764$$

i.e., about 52% of the SC unit cell occupied by the atoms and $\approx 48\%$ is empty or vacant.

II In fcc unit cell $\rightarrow z = 4$

$$U = z \times \frac{4}{8} \pi r^3 = 4 \times \frac{4}{8} \pi \left(\frac{\sqrt{3}a}{4}\right)^3 = \frac{16\pi a^3}{6} = \frac{\pi a^3}{3\sqrt{3}}$$

$$V = a^3$$

$$P.F = \frac{U}{V} = \frac{\pi a^3}{3\sqrt{3} a^3} = \frac{\pi}{3\sqrt{3}} = \frac{3.14}{3 \times 1.732} = 0.7406$$

$$\% \text{ of P.F} = 100 \times P.F = 100 \times 0.7406 = 74.06 \approx 74$$

$$\% \text{ of vacant space} = 100 - 74.06 = 25.94 \approx 26$$

$$\text{Fraction of vacant space in unit cell} = 1 - P.F = 1 - 0.7406 = 0.2594$$

i.e. $\approx 74\%$ of the unit cell is occupied by the atoms and $\approx 26\%$ empty.

III In BCC unit cell $\rightarrow z = 2$

$$U = z \times \frac{4}{8} \pi r^3 = 2 \times \frac{4}{8} \pi \left(\frac{\sqrt{3}a}{4}\right)^3 = \frac{\sqrt{3}}{8} \pi a^3$$

$$V = a^3$$

$$P.F = \frac{U}{V} = \frac{\frac{\sqrt{3}}{8} \pi a^3}{a^3} = \frac{\sqrt{3} \pi}{8} = \frac{1.732 \times 3.14}{8} = 0.6802$$

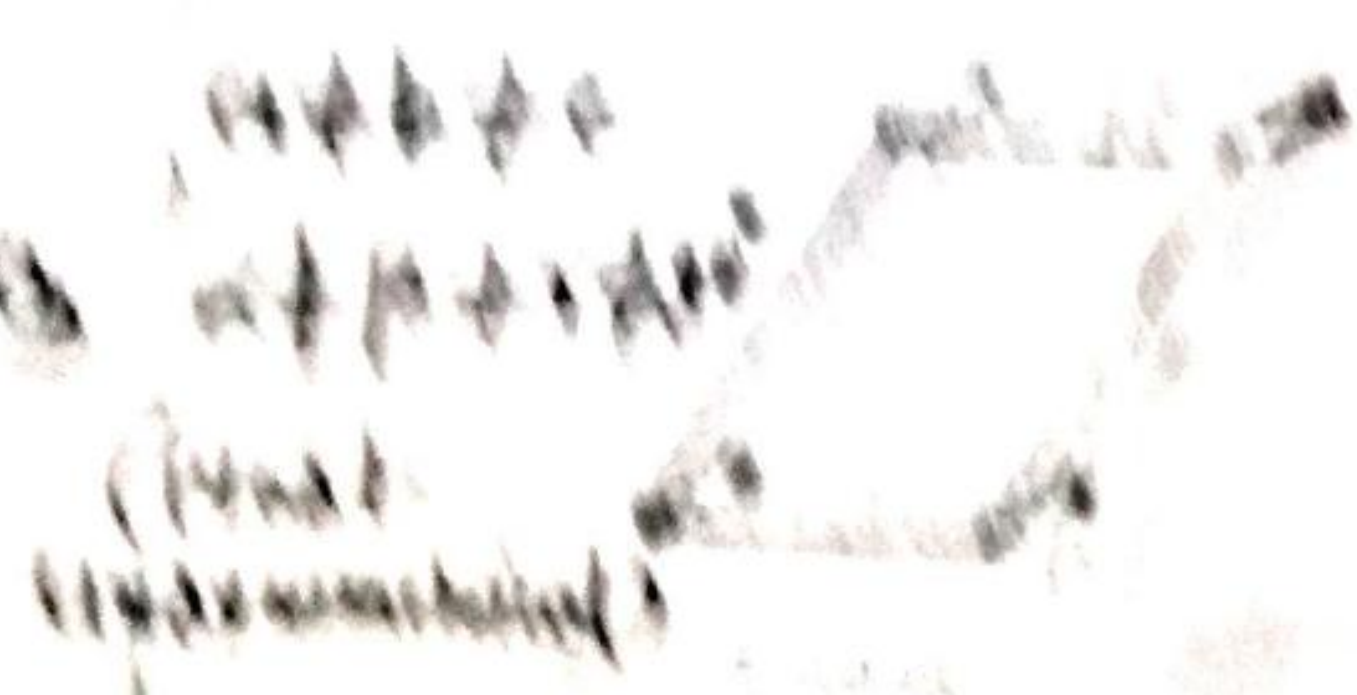
$$\% \text{ of P.F} = 100 \times 0.6802 = 68.02$$

$$\% \text{ of vacant space} = 100 - 68.02 = 31.98$$

$$\text{Fraction of vacant space} = 1 - 0.6802 = 0.3198$$

i.e. in BCC unit cell $\approx 68\%$ space occupied by the atoms and $\approx 32\%$ is empty.

1. $a \neq b \neq c$
 $\alpha \neq \beta \neq \gamma$
 2. $a \neq b = c$
 $\alpha \neq \beta = \gamma$
 3. $a = b \neq c$
 $\alpha = \beta \neq \gamma$
 4. $a = b = c$
 $\alpha = \beta = \gamma$



The 14 Bravais lattices
 (Trigonal, Hexagonal, Rhombohedral)
 etc.

$a = b \neq c$
 $\alpha = \beta = \gamma \neq 90^\circ$
 $\gamma = 120^\circ$

$a = b = c$
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$
 Quartz, NaN_3