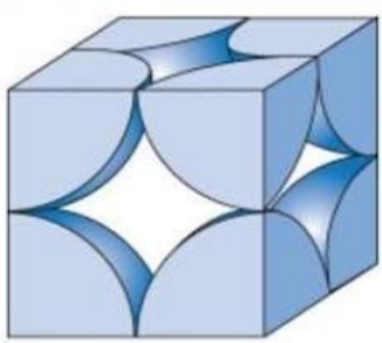
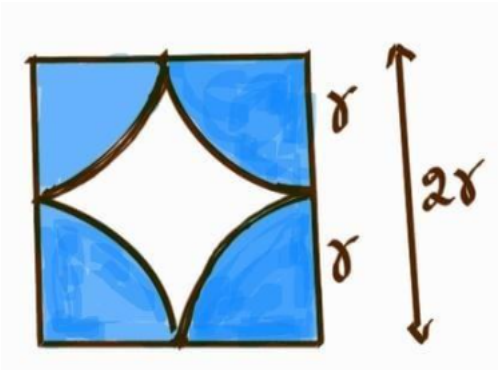
PACKING FACTOR(PF) OR ATOMIC PACKING FACTOR(APF)

- **Definition**: In crystallography, Packing Factor is defined as the fraction of volume (space) occupied by atoms in a unit cell.
- It is dimensionless and always less than unity (1).
- For practical purposes, the PF of a crystal structure is determined by assuming that atoms are rigid spheres.
- Its mathematical representation is, **PF=** V_{atoms} /$V_{unit\ cell}$ = n × v/V
- **Where:** n→ no. of atoms in a unit cell
  V → volume of atom in a unit cell
  V→volume of unit cell
  V_{atoms}→ volume of atoms in a unit cell= n.4/3. πr^3
  $V_{unit\ cell}$→ volume of unit cell = a^3 (since a = b = c)
- **Therefore, PF = n.4/3. πr^3 / a^3**
- **Where:** r → radius of atom
  a → nearest neighbouring distance (or) lattice constant.

1. PF OF SIMPLE CUBIC CRYSTAL (SC CRYSTAL)

- In a simple cubic structure, atoms in a unit cell are arranged only at the 8 corners of the cube, and each atom is surrounded by 6 nearest-neighboring atoms. Hence, the coordination number is 6
- In this structure, each corner atom is shared by 8-unit cells. Hence, the contribution of each corner atom is 1/8 of an atom
- Therefore, total no. of atoms per unit cell, n = 8 X 1/8 = 1
- So, the effective number of lattice points in an SC crystal is 1, thus SC is a primitive cell.
- **Volume of atoms in a unit cell:** V_{atoms} = n. 4/3. Πr^3 = 1. 4/3. Πr^3 = 4/3. Πr^3 .....(1)
- In this structure, atoms touch each other **along the edges**.





- **From the figure:** nearest neighbouring distance (lattice constant), a = 2r
- **Volume of unit cell:** $V_{unit\ cell} = a^3 = (2r)^3 = 8r^3$ .....(2)
- **Now, PF** = $V_{atoms} / V_{unit\ cell}$

  $= 4/3.\ \Pi r^3 / 8r^3$

  $= \Pi/6$

  $= 3.14/6$

- **PF = 0.5233 = 0.52**

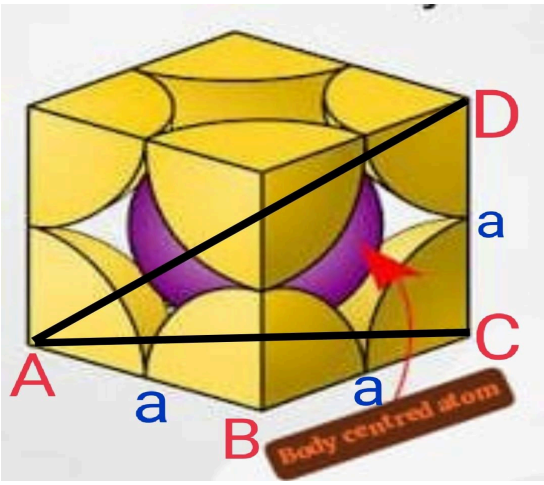
  or

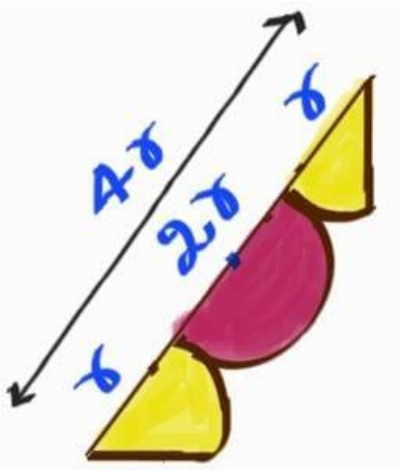
  PF = 52% ……(3)
- Hence, SC structure is loosely packed.
- Only one element, Polonium (Po) at a certain temperature exhibits this structure.

2. PF OF BODY CENTERED CUBIC (BCC) STRUCTURE

- In a BCC structure, atoms in a unit cell are arranged at each of the eight corners and one atom in the center of the cube.
- As the body centered atom is entirely within the unit cell and it is not shared by surrounding unit cells.
- **Number of atoms in a unit cell:** n=1/8 x 8+1 = 1+1 = 2
- **Volume of atoms in a unit cell:** $V_{atoms} = n.\ 4/3.\ \Pi r^3 = 2.\ 4/3.\ \Pi r^3 = 8/3.\ \Pi r^3$ .....(1)

- In this structure, the corner atoms do not touch each other, but each corner atom touches the body-centered atom **along the body diagonal**. Therefore, the coordination number for the BCC structure is 8.





- **From the figure:**

$$AC^2 = AB^2 + BC^2 = a^2 + a^2 = 2a^2$$

- $\mathbf{AC^2 = 2a^2}$
- **And** $AD^2 = AC^2 + CD^2 = 2a^2 + a^2 = 3a^2$

$$(4r)^2 = 3a^2$$

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

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

- $\mathbf{a = 4r/\sqrt{3}}$
- **Volume of unit cell:** $V_{unit\ cell} = a^3 = (4r/\sqrt{3})^3 = 64r^3/3\sqrt{3}$ …….(2)
- **Now, PF =** $V_{atoms} / V_{unit\ cell}$

$$= 8/3.\ \Pi r^3 / 64r^3/3\sqrt{3}$$

$$=(8\Pi r^3/3) \times (3\sqrt{3}/ 64r^3)$$

$$= \sqrt{3}\ \Pi/8$$

$$= 1.732 \times 3.14/8$$

- **PF = 0.679 = 0.68**

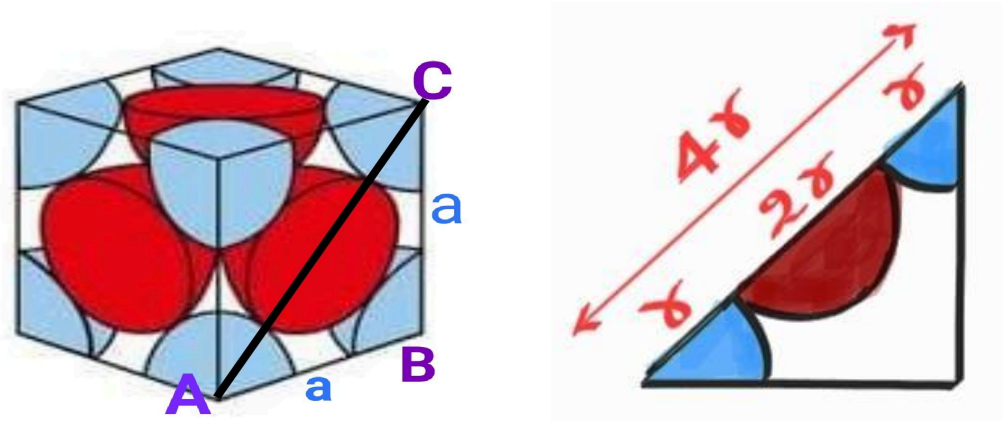
  Or

  PF = 68% ……(3)

- Therefore, the BCC structure is closely packed.
- The elements that exhibit BCC structure are: Li, Na, K, Cs, Fe, W, V.

3. P F OF FACE CENTERED CUBIC(FCC) STRUCTURE

- In a face-centered cubic (FCC) structure, each unit cell contains 8 atoms at the corners and 6 atoms at the center of each of its six faces.
- Each corner atom is shared by 8 surrounding unit cells, while each face-centered atom is shared by 2 surrounding unit cells.
- **No. of atoms in an FCC unit cell:** n = 8 X 1/8+ 6 X 1/2 = 1 + 3 => n= 4
- **Volume of atoms in a unit cell:** V_{atoms} = n. 4/3. Πr^3 = 4. 4/3. Πr^3 = 16/3. Πr^3 **…….(1)**
- In this structure, corner atoms touch each other **along the face diagonal**. A face atom is in contact with four atoms at the corners of the face it's centered on. Additionally, this atom also touches four atoms in the layer directly above it and four atoms in the layer directly below it.Therefore, coordinate number of FCC is 12.



- **From the figure:** $AC^2 = AB^2 + BC^2 = a^2 + a^2 = 2a^2$

$$AC^2 = 2a^2$$

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

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

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

- **Volume of unit cell:** $V = a^3 = (4r/\sqrt{2})^3 = 64r^3/2\sqrt{2}$ ……..(2)
- **Now, PF =** $V_{atoms} / V_{unit\ cell}$

$$= 16/3.\ \Pi r^3 / 64r^3/2\sqrt{2}$$

$$=(16\Pi r^3/3) \times (2\sqrt{2}/ 64r^3)$$

$$= \Pi/8 /3\sqrt{2}$$

$$= 3.14/ (3 \times 1.414)$$

- **PF = 0.74**

Or

PF = 74% ……..(3)

- Therefore, the FCC structure is the most closely packed.
- The elements that exhibit FCC structure are Al, Au, Ag, Cu, Pb, Ni, Ca, Pt, and etc.