SNS COLLEGE OF ENGINEERING

Coimbatore-641 107

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Affiliated to Anna University, Chennai

DEPARTMENT OF PHYSICS

COURSE NAME :19PY101-ENGINEERING PHYSICS

I YEAR / I SEMESTER

UNIT 4 – CRYSTAL PHYSICS

TOPIC 4 – COORDINATION NUMBER AND PACKING FACTOR FOR SC & BCC

1. How do you find the coordination number of a unit cell?
2. How do you calculate packing factor?

Important parameters in crystal structure

1.Number of atoms per unit cell (N)

The total number of atoms shared by a unit cell is known as number of atoms per unit cell. This can be determined if the arrangement of atoms inside the unit cell is known.

2. Atomic radius (AR)

Atomic radius is defined as half of the distance between any two nearest neighbor atoms which have direct contact with each other.

3. Co-ordination Number (CN)

- Every atom in a crystal structure is surrounded by other atoms.
- The term coordination number is defined as the number of nearest neighbours directly surrounded by an atom.
- When the coordination number is large the structure is closely packed.

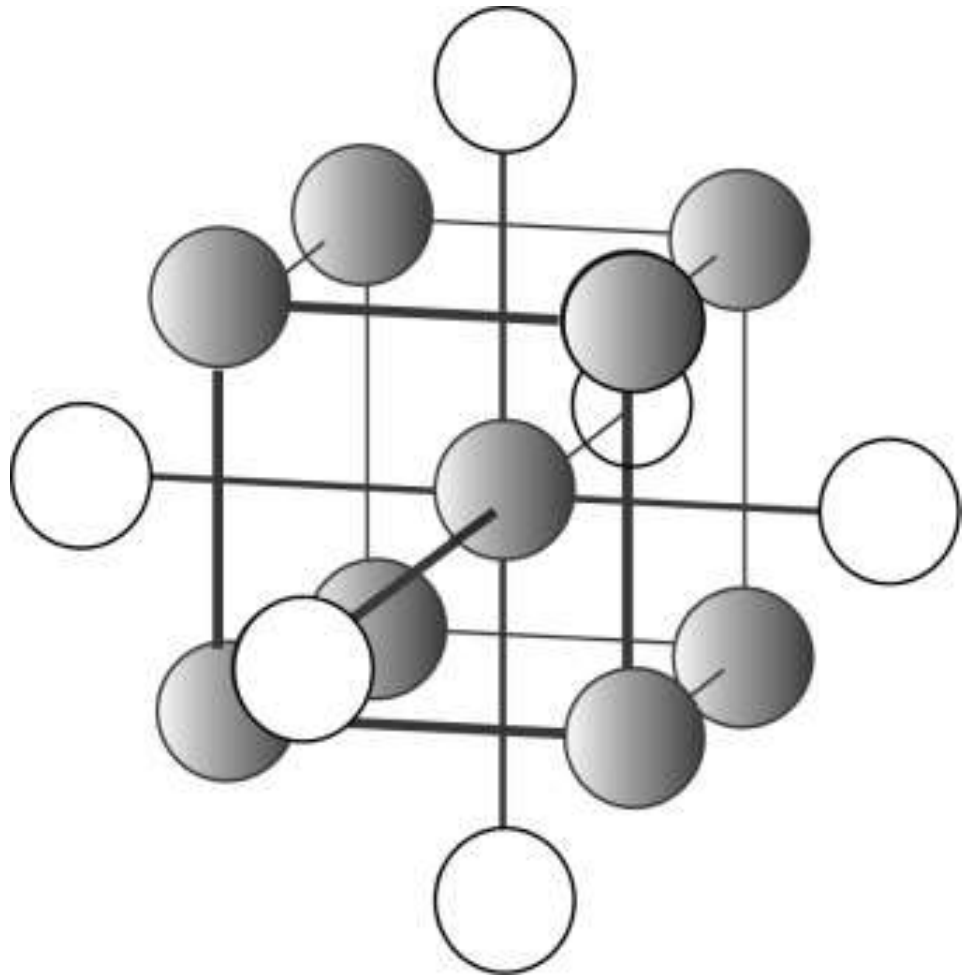
4. **Packing density (or) Atomic packing factor (APF).**

It is defined as the ratio of volume of all the atoms in the unit cell to the volume of the unit cell.

1. Coordination Number For simple cubic structure:

- The simple cubic structure shares 8 atoms, one in each corner,
- Each atom in the corner is shared by 8 adjacent unit cells.
- Hence $1/8^{th}$ part of an atom is present in every corner of the cube.
- There are eight corners.

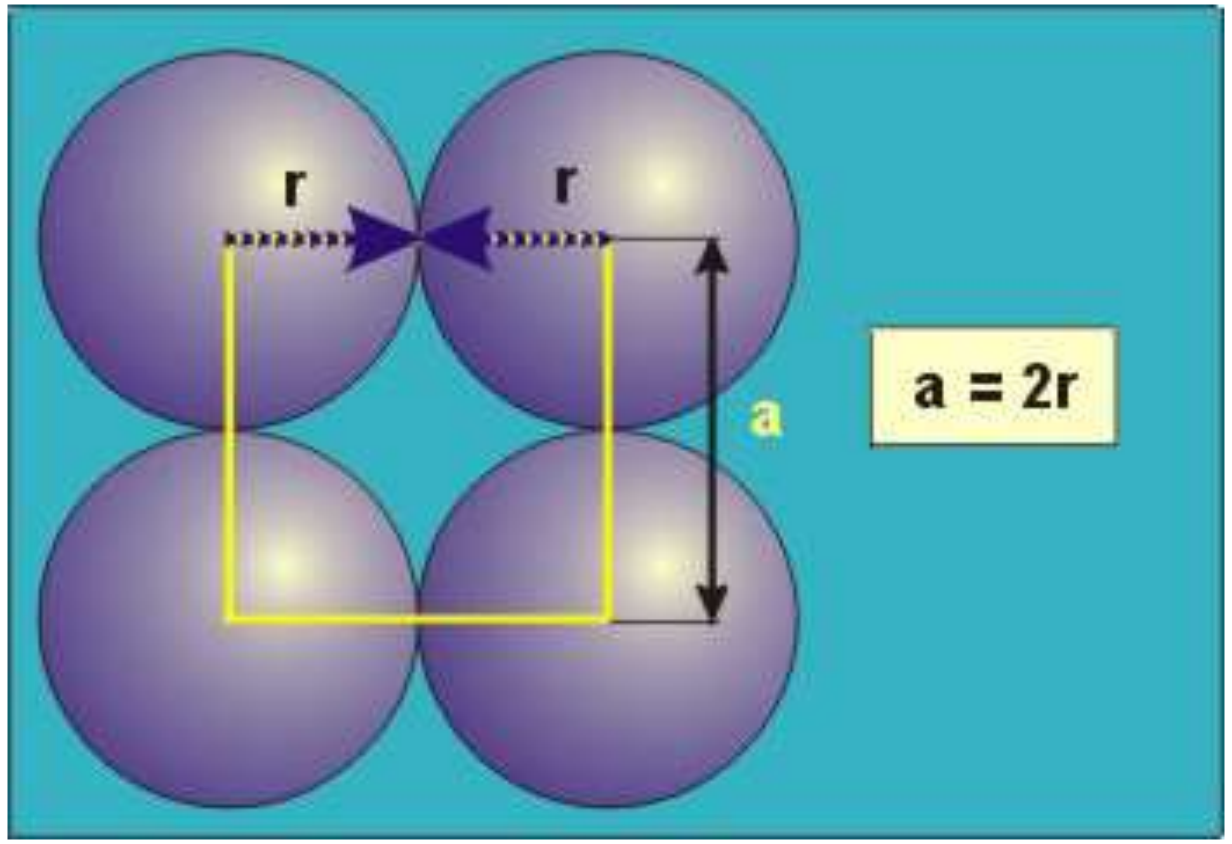
Therefore Total no of atoms in a unit cell =1/8*8=1 atom.



2. Atomic Radius For simple cubic structure:

Each corner atom touches each other along the edges of the cube. If ‘r’ is the atomic radius and ‘a’ is the side of the cube,

$$r = a/2$$

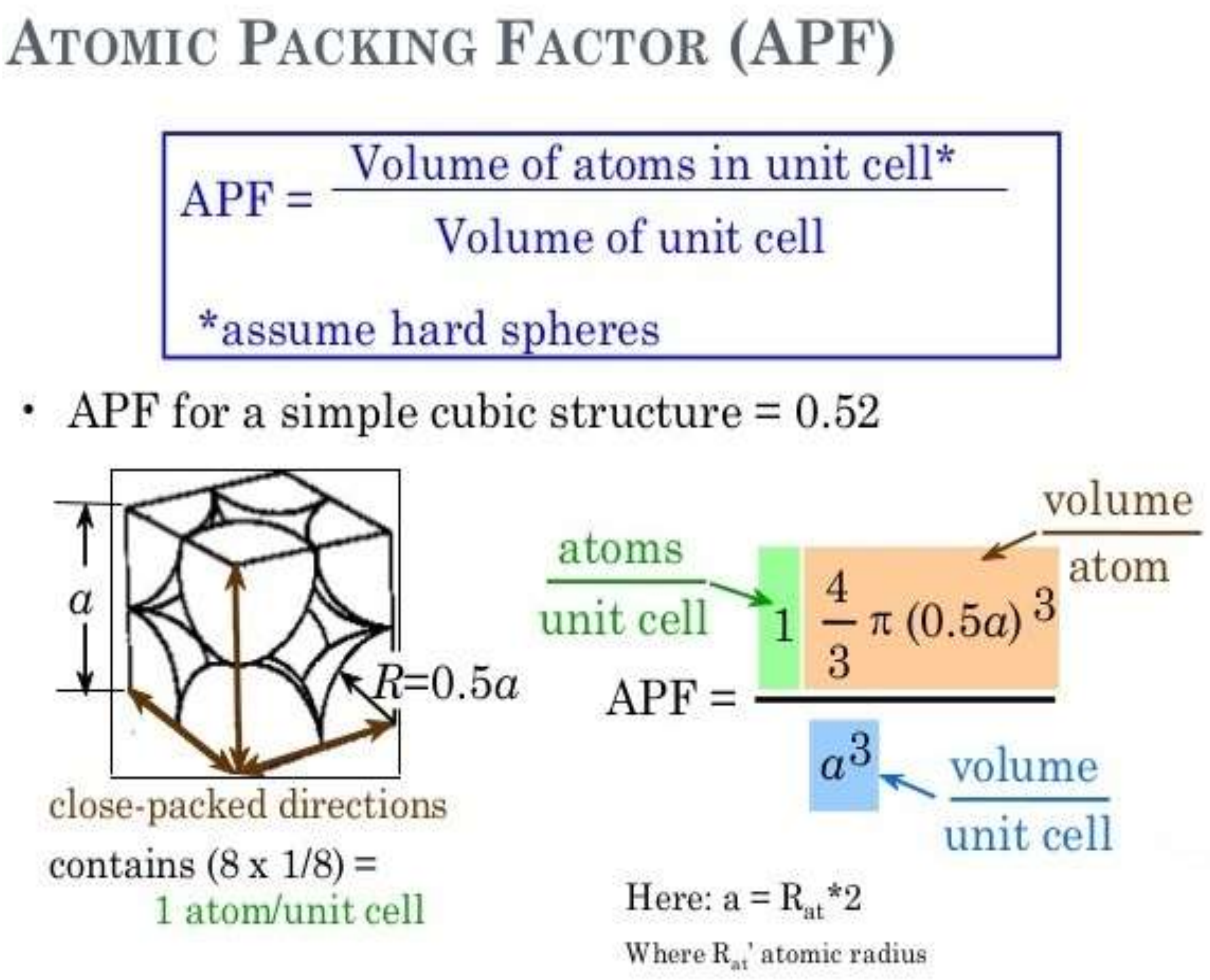


ATOMIC PACKING FACTOR : SC

This means that 52% of the space in the unit cell is occupied and the remaining 48% is unoccupied.

Therefore, the stability of the crystal forming simple cubic structure is less.

Example: **Polonium**



For body centered cubic structure:

Here there are two types of atom 1. Corner atom and 2. Body center atom

There are 8 corner atoms one at each corner of unit cell and one atom at body centre of unit cell.

Number of corner atoms per unit cell = 1/8*8=1

Number of body centered atom per unit cell

Total number of atoms per unit cell in BCC = Total number of corner atoms + Total number of Body centered atoms

$= 1 + 1 = 2$

ASSESSMENT

- How will be change the atomic packing factor?
- Difference between SCC and BCC?

BCC structure the unit cell has 8 atoms at the corners of the cube and 1 atom at the centre of the cube.

The corner atoms do not touch each other, but each corner atom touches the central atom.

If ‘r’ is the atomic radius and ‘a’ is the side of the cube,

In triangle Δ ADC,

$$AD^2 = AC^2 + DC^2$$

$$= AB^2 + BA^2 + DC^2 \quad \text{(from } \Delta ABC\text{)}$$

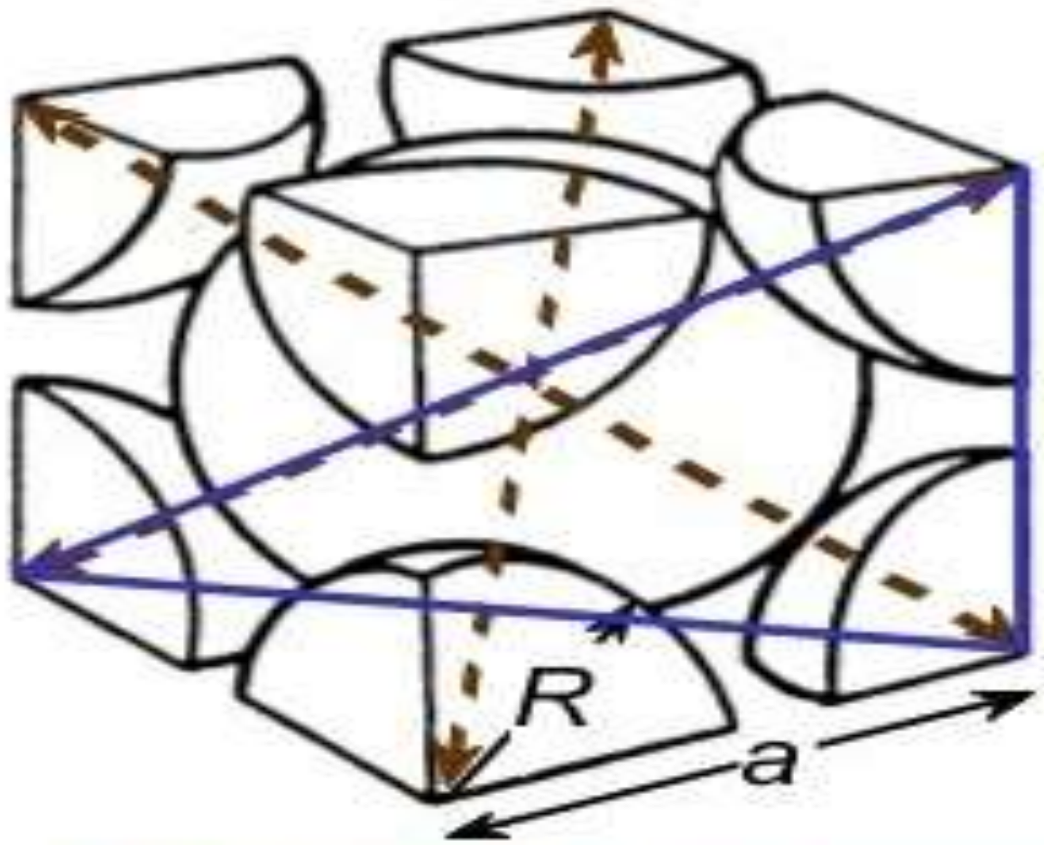
$$(4r)^2 = a^2 + a^2 + a^2$$

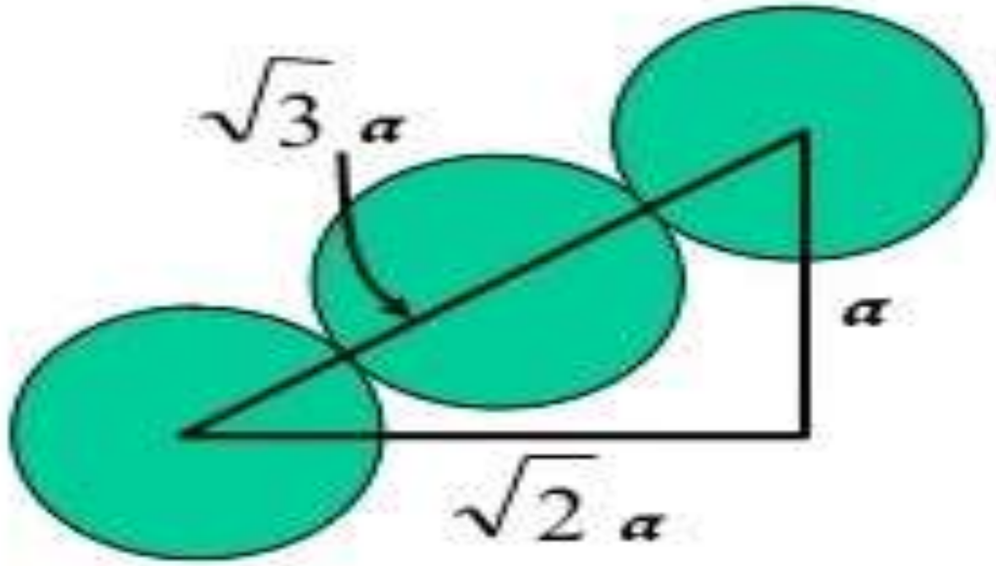
$$16r^2 = 3a^2 \quad ; \quad r^2 = 3a^2/16$$

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

Atomic Packing Factor: BCC

- APF for a body-centered cubic structure = 0.68





Close-packed directions:
length = $4R = \sqrt{3}\,a$

$$\text{APF} = \frac{2 \cdot \frac{4}{3}\pi\left(\sqrt{3}a/4\right)^3}{a^3}$$

- 2 ← $\frac{\text{No. atoms}}{\text{unit cell}}$
- $\frac{4}{3}\pi(\sqrt{3}a/4)^3$ ← $\frac{\text{volume}}{\text{atom}}$
- a^3 ← $\frac{\text{volume}}{\text{unit cell}}$

References

- https://images.app.goo.gl/TewweVUHmpEe7dit5
- https://images.app.goo.gl/Ks8SUv3CNjkaE2VZ6
- https://images.app.goo.gl/Jsxr4FwCDBRafQRFA

Thank You