Co-ordinations number, Packing factor and Density

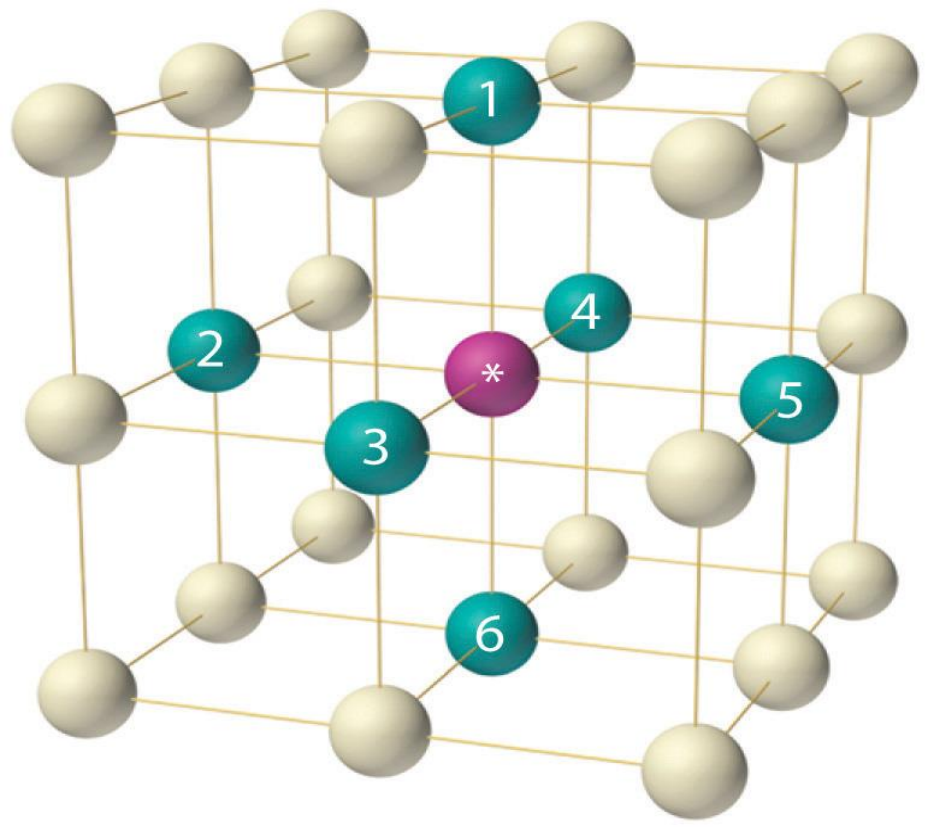
Dr. Mehnaz Sharmin
Department of Physics
Bangladesh University of Engineering and Technology
Dhaka-1000, Bangladesh

Co-ordination number

The points in a Bravais lattice that are closest to a given point are called its nearest neighbors. Because of the periodic nature of a Bravais lattice, each point has the same number of nearest neighbors. This number is thus a property of the lattice and is referred to as the coordination number of the lattice.

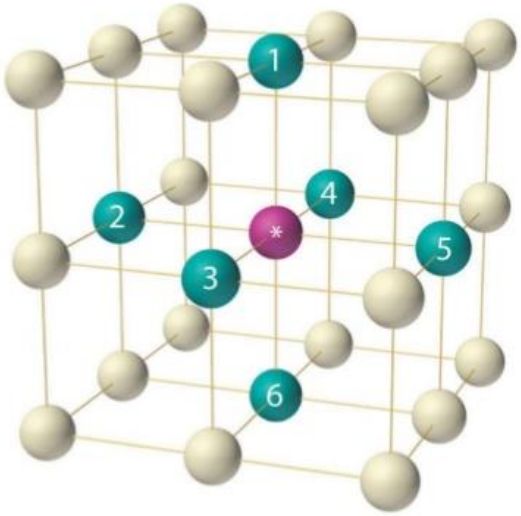
For an atom in the interior of a crystal lattice the number of atoms touching the given atom is the **bulk coordination number**; for an atom at a surface of a crystal, this is the **surface coordination number**.

Bulk coordination number> Surface coordination number



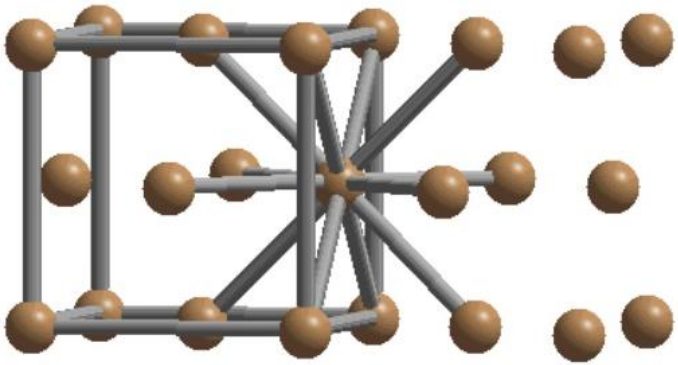
Co-ordination number of Simple Cubic Structure is 6

SC-coordination number



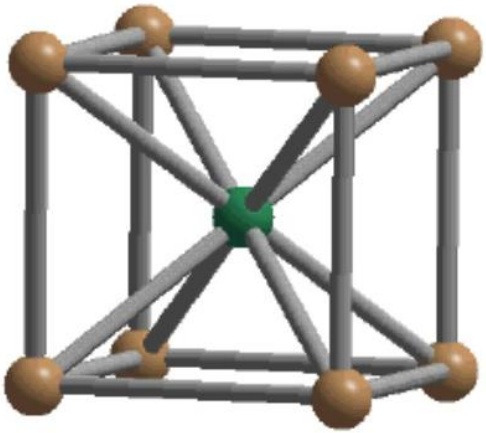
6

FCC-coordination number



4+4+4=12

BCC-coordination number



8

Characteristics of Cubic Crystals

Type of lattice	Simple cubic (SC)	Body centered cubic (BCC)	Face centered cubic (FCC)
Volume	a^3		
Lattice points per unit cell	1	2	4
Volume of the primitive cell	a^3	$a^3/2$	$a^3/4$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Coordination number	6	8	12
Nearest neighbor distance	a	$a\sqrt{3}/2$	$a/\sqrt{2}$
Number of 2^{nd} nearest neighbors	12	6	6
2^{nd} neighbor distance	$\sqrt{2}a$	a	a
Packing factor	$\pi/6=0.52$	$\sqrt{3}\pi/8=0.68$	$\sqrt{2}\pi/6=0.74$

Packing Factor

"In crystallography, atomic packing factor (APF) or packing fraction is the fraction of volume in a crystal structure that is occupied by atoms."

- It is dimensionless and always less than unity.
- For practical purposes, the APF of a crystal structure is determined by assuming that atoms are rigid spheres. The radius of the spheres is taken to be the maximal value such that the atoms do not overlap.
- For one-component crystals (those that contain only one type of atom), the APF is represented mathematically by,

$$\mathbf{APF} = \frac{\textbf{Volume occupied by the sphere in unit cell}}{\textbf{Volumeof the unit cell}} = \frac{\mathbf{N_{atoms} V_{atom}}}{\mathbf{V_{Unit\ cell}}}$$

Where, N_{atoms} = Number of atoms in the unit cell

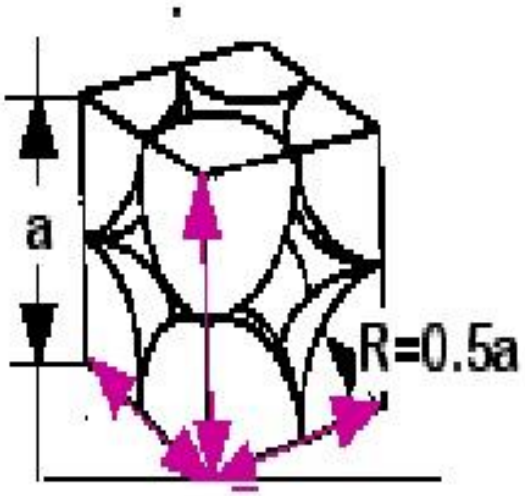
V_{atom} = volume of an atom

$V_{unit\ cell}$ = volume of the unit cell.

For Elements (one component structures) APF_{max} is about 0.74.

For multiple-component structures, the APF can exceed 0.74.

Atomic Packing Factor of SC

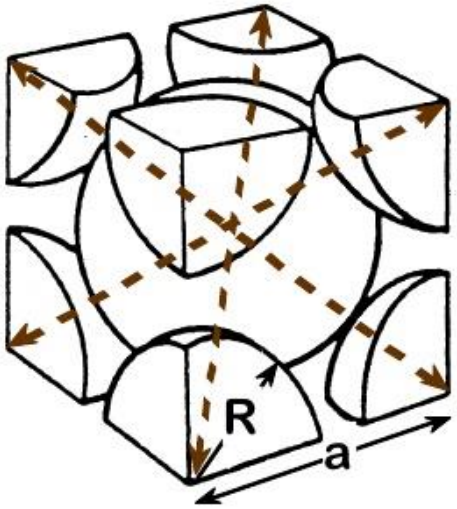


APF = 0.52 for simple cubic

$$APF = \frac{\text{atom}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3} = \frac{\pi}{6} = 0.52$$

contains 8 x 1/8 = 1atom/unit cell

ATOMIC PACKING FACTOR: BCC



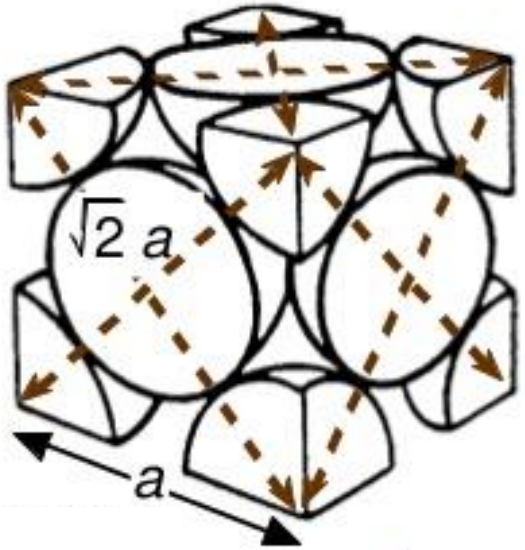
Close-packed directions:
length = 4R
$= \sqrt{3}\, a$

Unit cell contains:
1 + 8 x 1/8
= 2 atoms/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{2 \cdot \frac{4}{3}\pi (\sqrt{3}a/4)^3}{a^3} = \frac{\sqrt{3}\pi}{8} = 0.68$$

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74
  maximum achievable APF



Close-packed directions:
length = $4R = \sqrt{2}\,a$

Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} = \frac{4\left(\frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3\right)}{a^3 \cdot \frac{\text{volume}}{\text{unit cell}}} = \frac{\sqrt{2}\pi}{6} = 0.74$$

Density

Let us consider a cubic cell of lattice constant 'a' contains 'n' atoms per unit cell, then density of the crystal material is defined as,

$$\rho = \frac{\text{Mass of the unit cell}}{\text{Volume of the unit cell}} = \frac{\text{Mn}}{\text{NV}} = \frac{\text{Mn}}{\text{N}a^3} \text{ ; So, } a = \sqrt[3]{\frac{Mn}{N\rho}}$$

Where,

M = Atomic weight

N = Avogadro's number = 6.023×10^{23} mol^{-1} = 6.023×10^{26} $kmol^{-1}$

M/N = Mass of each atom or molecule

n = Number of lattice point per unit cell

V = Volume of the unit cell = a^3 (for cubic crystal), a = lattice constant

The number of lattice points can be determined if we know the volume, density and molecular weight of the constituent atom of the cell.

Exercise

1.Calculate the number of atoms per unit cell for an FCC lattice of copper (Cu) crystal. It is given that a = 3.6 Å, atomic weight of Cu = 63.6, density of Cu is 8960 kg/m^3 and N = 6.023×10^{26} kmole^{-1}.

Answer: 3.96≈ 4.

2. Aluminium has fcc structure. If the density of Al is 2.7 x 10^3 kg/m^3. Calculate the unit cell dimensions and the atomic diameter. (At wt. of al; = 26.98, Avogadro No. = 6.023 x10^{26} kmole^{-1}).

Answer: a = 4.05 *Å*, *atomic diameter,* D = 2.86 *Å*.

- Worked out problems in the book **"Solid State Physics" by M. A. Wahab**, Page no. 9, 10.

- Practice the problems in the exercise of the mentioned chapter.