PAPER-A: CONDENSED MATTER PHYSICS
(B.Sc. Semester-V)

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CONTENTS

- Crystal System
- SC, BCC, FCC, HCP

Crystal system

- Crystals are grouped into seven crystal systems, according to characteristic symmetry of their unit cell.
- The characteristic symmetry of a crystal is a combination of one or more rotations and inversions.

Auguste Bravais
(1811-1863)

Lattices

- In 1848, Auguste Bravais demonstrated that in a 3-dimensional system there are fourteen possible lattices
- A Bravais lattice is an infinite array of discrete points with identical environment
- seven crystal systems + four lattice centering types = 14 Bravais lattices
- Lattices are characterized by translation symmetry

Four lattice centering types

No.	Type	Description
1	Primitive	Lattice points on corners only. Symbol: P.
2	Face Centered	Lattice points on corners as well as centered on faces. Symbols: A (bc faces); B (ac faces); C (ab faces).
3	All-Face Centered	Lattice points on corners as well as in the centers of all faces. Symbol: F.
4	Body-Centered	Lattice points on corners as well as in the center of the unit cell body. Symbol: I.

The Seven Crystal Systems

The 230 space groups can be grouped into seven crystal systems

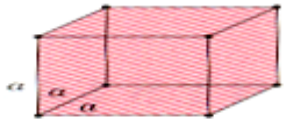
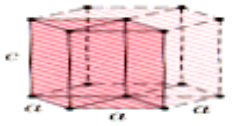
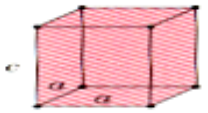
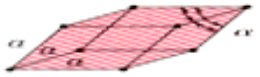
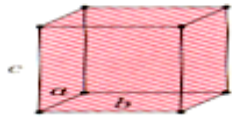
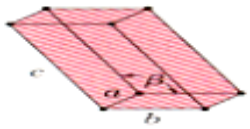
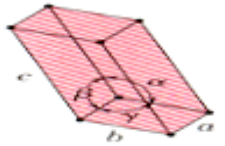
Table 2.1 The crystal systems

Crystal system	Minimum symmetry requirement	Conventional choice of axes	Constraints on interaxial angles and axial lengths
Triclinic	None	No constraints	None
Monoclinic	One 2-fold axis	***b*** parallel to 2-fold ***a*** and ***c*** perpendicular to 2-fold	α and $\gamma = 90°$
Orthorhombic	Three perpendicular 2-fold axes	***a***, ***b***, and ***c*** parallel to 2-fold axes	α, β, and γ all 90°
Trigonal*	One 3-fold axis	***c*** parallel to 3-fold ***a*** and ***b*** perpendicular to 3-fold	$\beta = 120°$, α and $\gamma = 90°$ ***a*** and ***b*** equal length
Tetragonal	One 4-fold aixs	***c*** parallel to 4-fold ***a*** and ***b*** perpendicular to 4-fold	α, β, and γ all 90° ***a*** and ***b*** equal length
Hexagonal	One 6-fold axis	***c*** parallel to 6-fold ***a*** and ***b*** perpendicular to 6-fold	$\beta = 120°$, α and $\gamma = 90°$ ***a*** and ***b*** equal length
Cubic	Four 3-fold axes	***a***, ***b***, and ***c*** related by 3-fold axis	α, β, and γ all 90° ***a***, ***b*** and ***c*** equal length

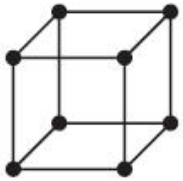
*A special case of the trigonal system, known as the rhombohedral system, is not discussed here.

CRYSTAL SYSTEM

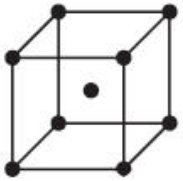
Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

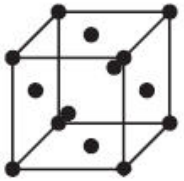
The 14 Crystal (Bravais) Lattices



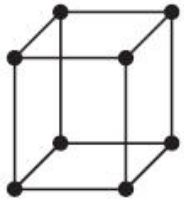
Simple cubic



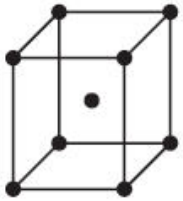
Body-centered cubic



Face-centered cubic

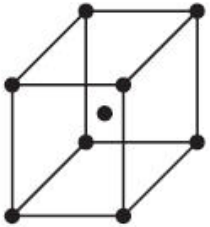


Simple tetragonal

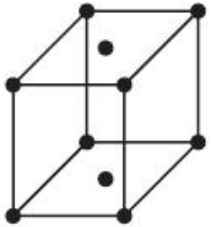


Body-centered tetragonal

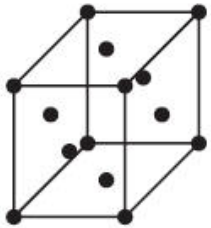
Simple orthorhombic



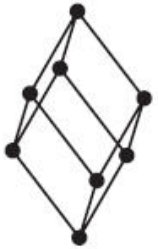
Body-centered orthorhombic



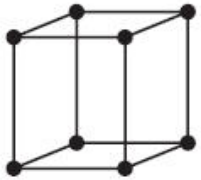
Base-centered orthorhombic



Face-centered orthorhombic

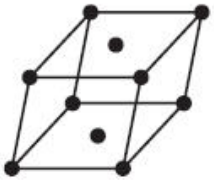


Rhombohedral

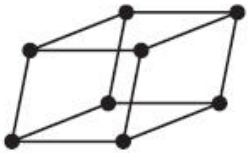


Hexagonal

Simple monoclinic



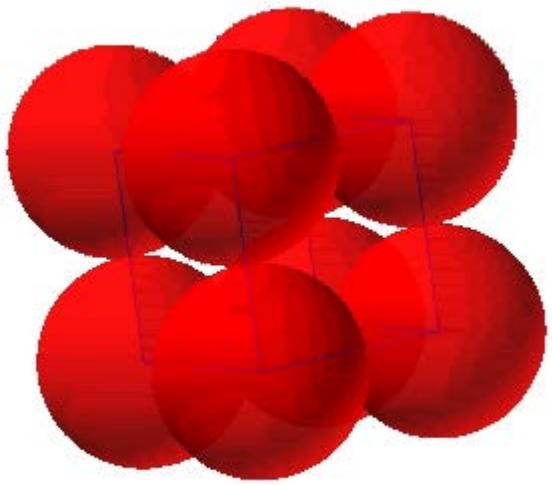
Base-centered monoclinic



Triclinic

Simple Cubic Structure (SC)

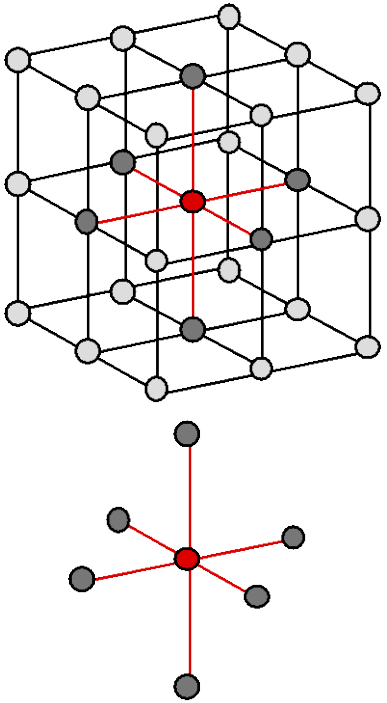
- Rare due to low packing density (only Po has this structure)
- Close-packed directions are cube edges.



Click once on image to start animation

(Courtesy P.M. Anderson)

- Coordination # = 6
  (# nearest neighbors)

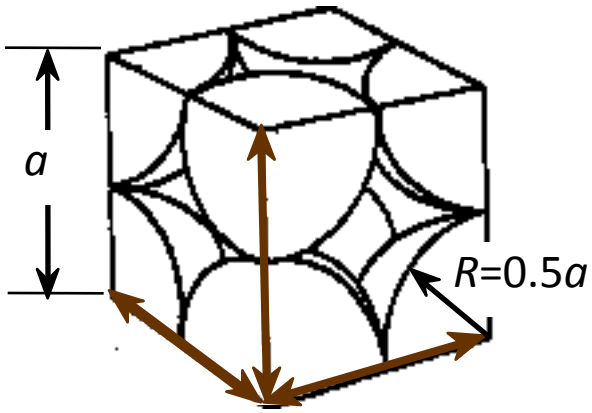


Atomic Packing Factor (APF):SC

$$APF = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains 8 x 1/8 =

1 atom/unit cell

Adapted from Fig. 3.24,
Callister & Rethwisch 8e.

$$APF = \frac{\text{atoms}}{\text{unit cell}} \times \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}}$$

$$APF = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

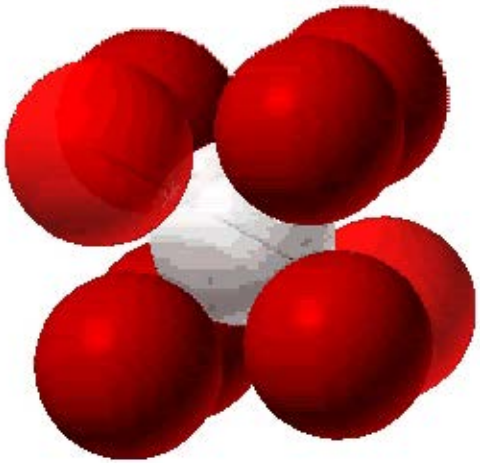
Body Centered Cubic Structure (BCC)

- Atoms touch each other along cube diagonals.

  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

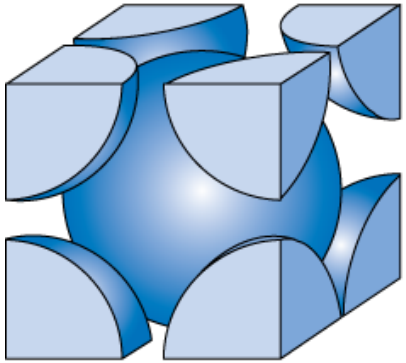
ex: Cr, W, Fe (α), Tantalum, Molybdenum

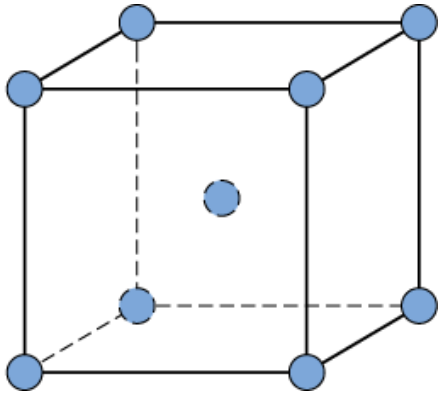
- Coordination # = 8



Click once on image to start animation

(Courtesy P.M. Anderson)



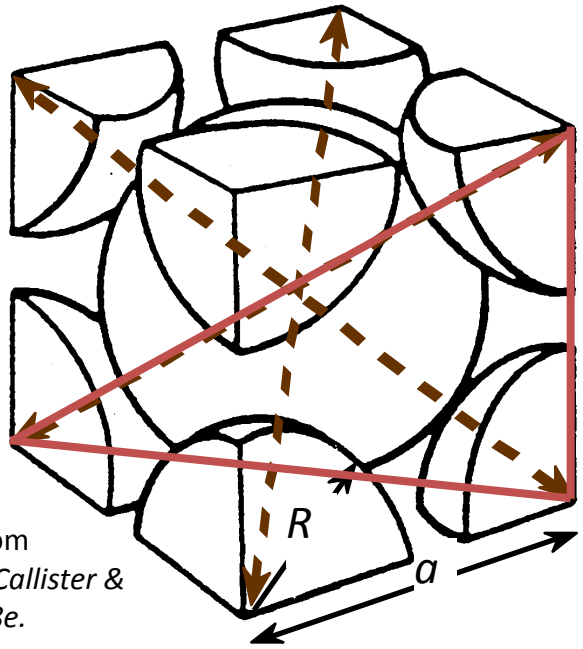


Adapted from Fig. 3.2, *Callister & Rethwisch 8e.*

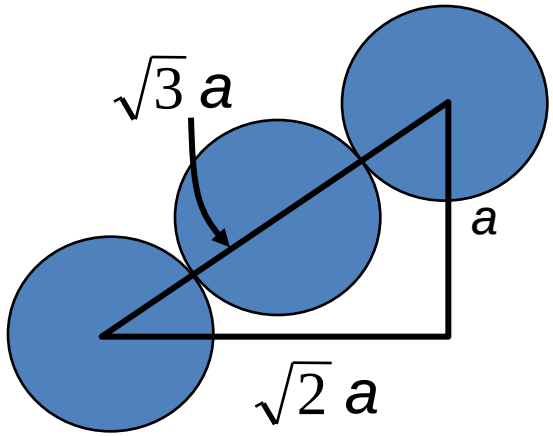
2 atoms/unit cell: 1 center + 8 corners x 1/8

Atomic Packing Factor: BCC

- APF for a body-centered cubic structure = 0.68



Adapted from Fig. 3.2(a), *Callister & Rethwisch 8e.*



Close-packed directions:

length = $4R = \sqrt{3}\,a$

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

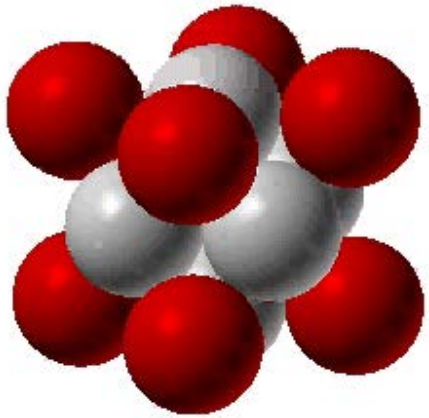
Face Centered Cubic Structure (FCC)

- Atoms touch each other along face diagonals.

  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

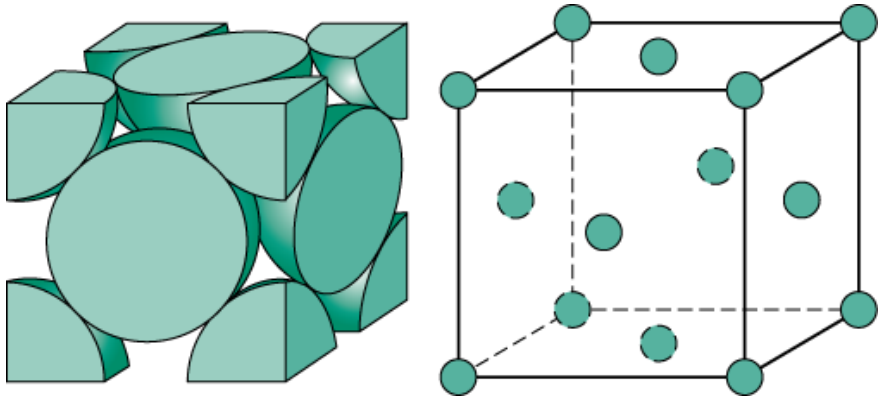
ex: Al, Cu, Au, Pb, Ni, Pt, Ag

- Coordination # = 12



Click once on image to start animation

(Courtesy P.M. Anderson)



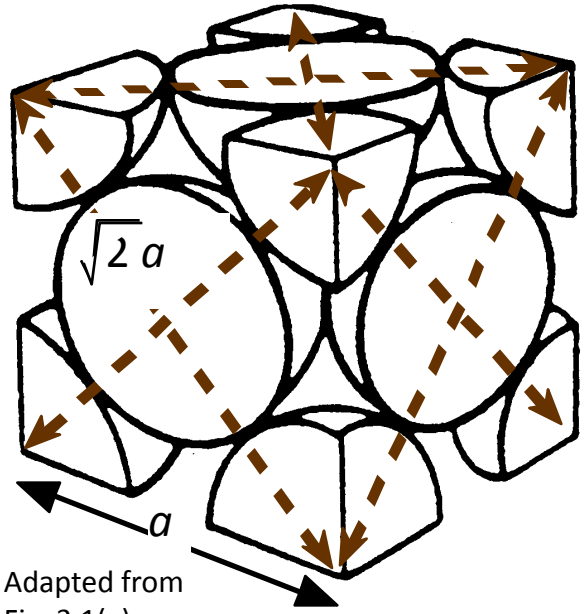
Adapted from Fig. 3.1, *Callister & Rethwisch 8e.*

4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74

maximum achievable APF



Adapted from Fig. 3.1(a), *Callister & Rethwisch 8e.*

Close-packed directions:

length = $4R$ = $\sqrt{2}\,a$

Unit cell contains:

6 x 1/2 + 8 x 1/8

= 4 atoms/unit cell

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

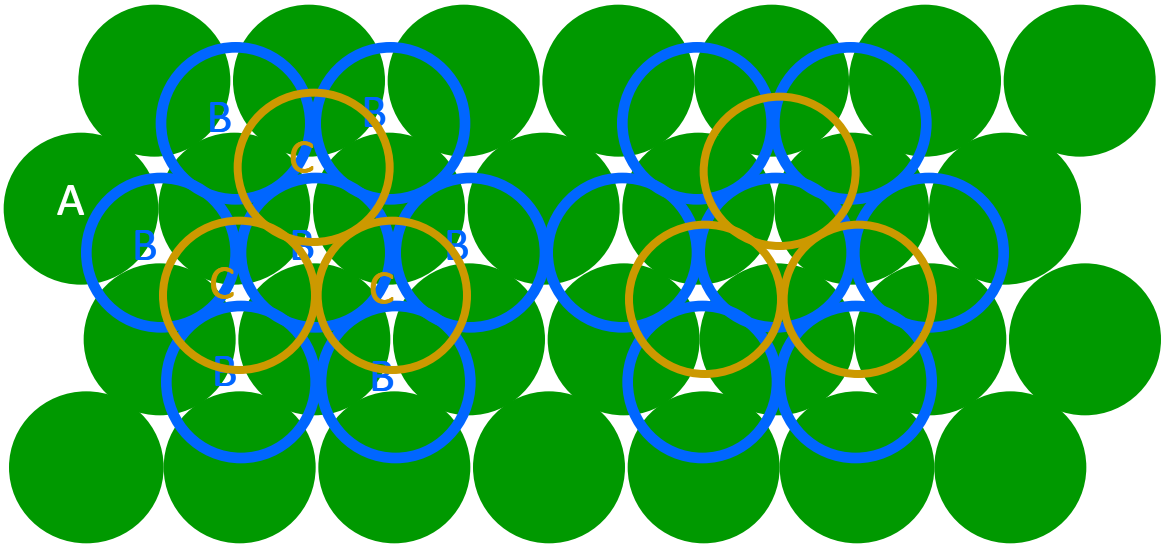
FCC Stacking Sequence

- ABCABC... Stacking Sequence
- 2D Projection

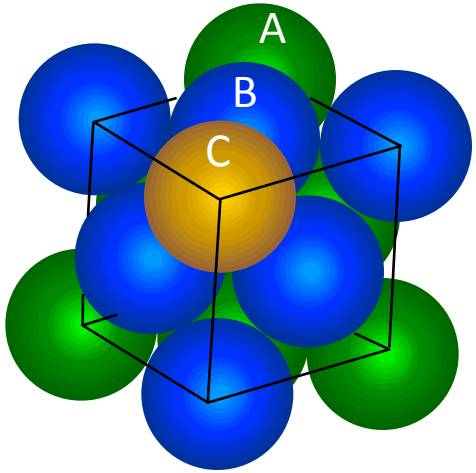
A sites

B sites

C sites

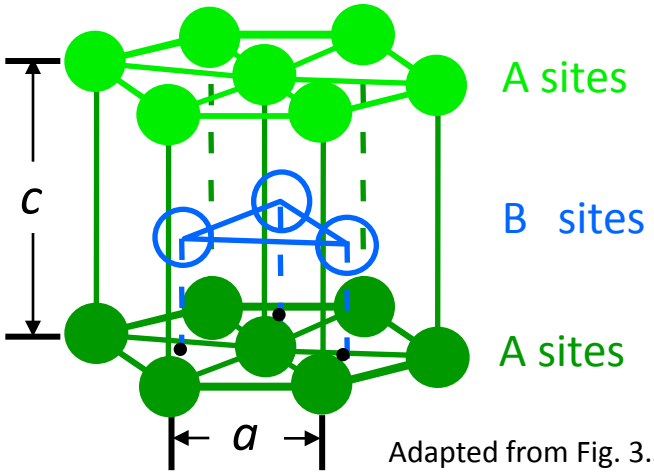


- FCC Unit Cell



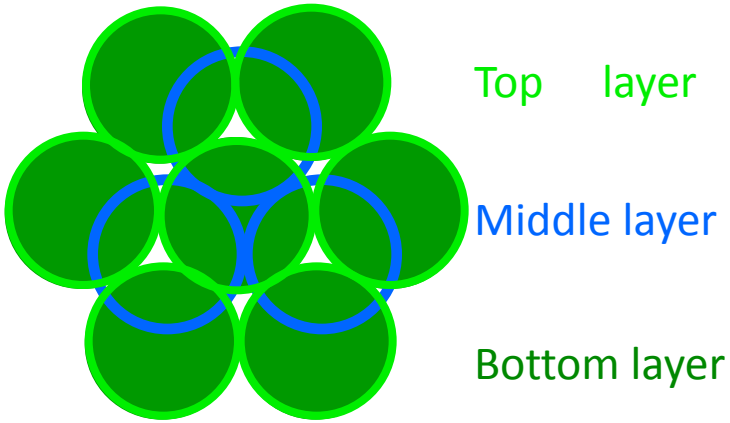
Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3(a), *Callister & Rethwisch 8e.*

- 2D Projection

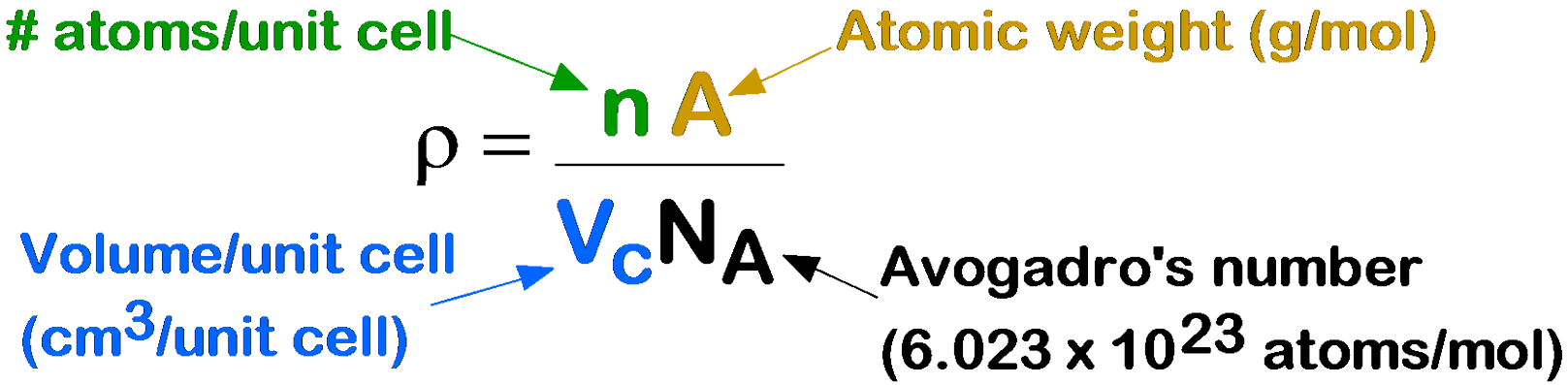


- Coordination # = 12
- APF = 0.74
- c/a = 1.633

6 atoms/unit cell

ex: Cd, Mg, Ti, Zn

THEORETICAL DENSITY, ρ



Example: Copper

Data from Table inside front cover of Callister (see next slide):

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius R = 0.128 nm (1 nm = 10^{-7}cm)

$V_C = a^3$; For FCC, $a = 4R/\sqrt{2}$; $V_C = 4.75 \times 10^{-23} cm^3$

Result: theoretical $\rho_{Cu} = 8.89$ g/cm^3

Compare to actual: $\rho_{Cu} = 8.94$ g/cm^3

REFERENCES

- Introduction To Solid State Physics- Kittle
- Elementary Solid state Physics- Omar
- Solid state Physics- S. O. Pillai

THANK YOU !