Engineering Materials MECH 390

Tutorial 1

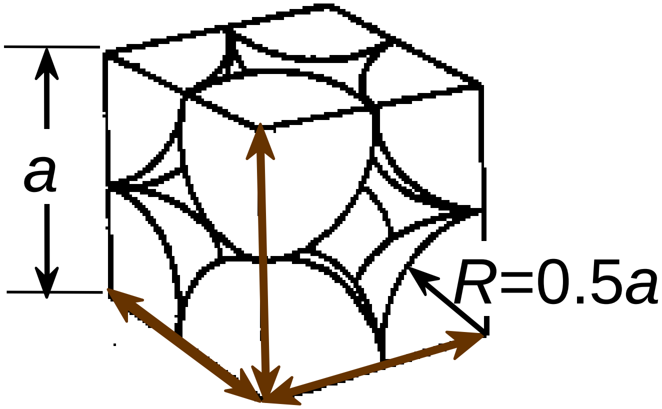
Chapter 3

The Structure of Crystalline Solids

Atomic Packing Factor (APF)

$$\text{APF} = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}} \qquad \frac{\mathbf{V_s}}{\mathbf{V_c}}$$

*assume hard spheres



close-packed directions

contains 8 x 1/8 =

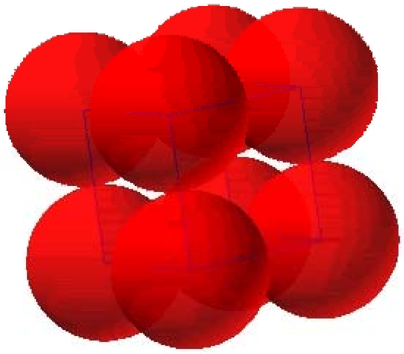
1 atom/unit cell

Adapted from Fig. 3.23, *Callister 7e.*

$$\frac{\text{atoms}}{\text{unit cell}} \qquad \frac{\text{volume}}{\text{atom}}$$

$$\text{APF} = \frac{1 \quad \frac{4}{3}\pi\,(0.5a)^3}{a^3} = 0.52$$

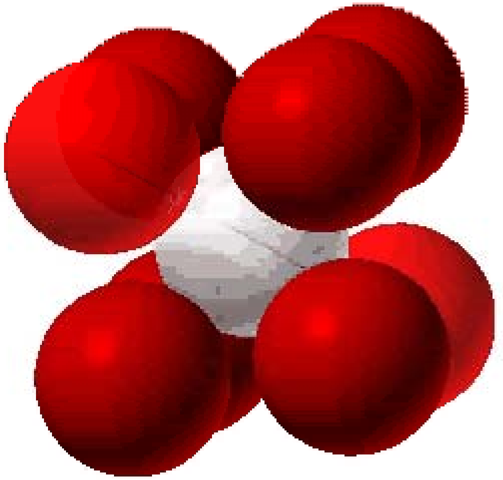
$$\frac{\text{volume}}{\text{unit cell}}$$



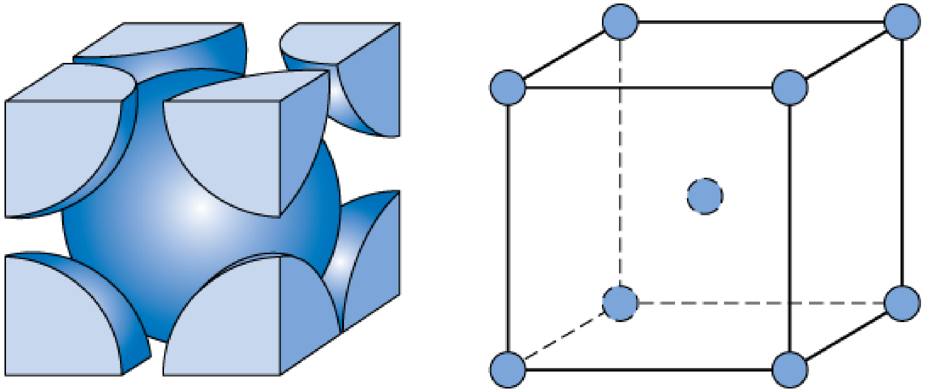
Body Centered Cubic Structure (BCC)

- Atoms touch each other along cube diagonals.

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



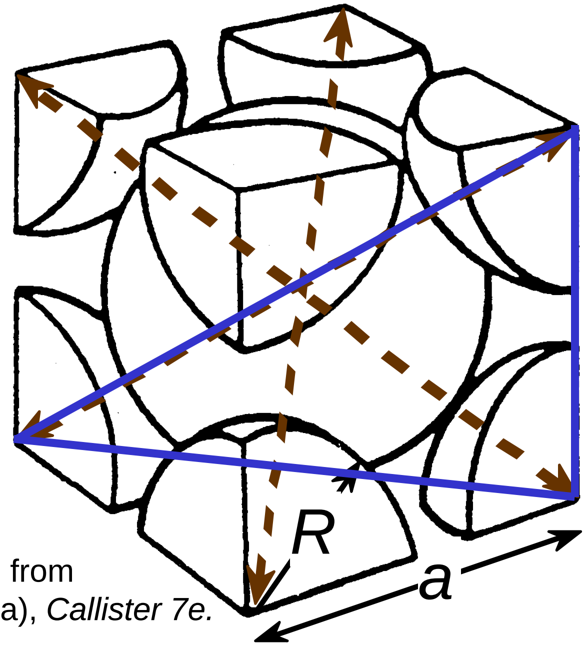
(Courtesy P.M. Anderson)



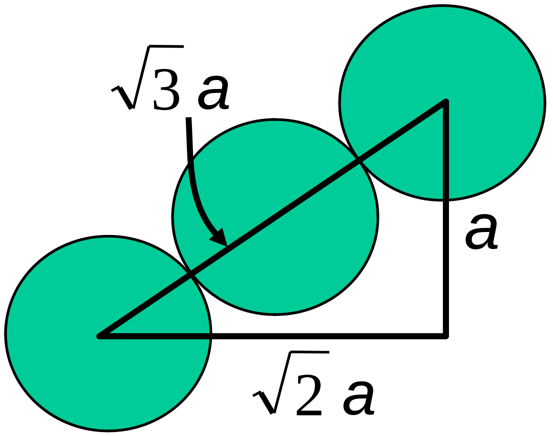
Adapted from Fig. 3.2, *Callister 7e.*

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

Atomic Packing Factor: BCC



Adapted from
Fig. 3.2(a), *Callister 7e.*



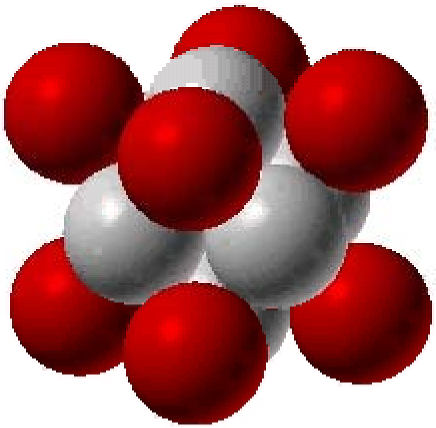
Close-packed directions:
length = $4R = \sqrt{3}\,a$

$$\mathrm{APF} = \frac{\overbrace{2}^{\frac{\text{atoms}}{\text{unit cell}}}\;\overbrace{\frac{4}{3}\pi(\sqrt{3}a/4)^3}^{\frac{\text{volume}}{\text{atom}}}}{\underbrace{a^3}_{\frac{\text{volume}}{\text{unit cell}}}} = 0.68$$

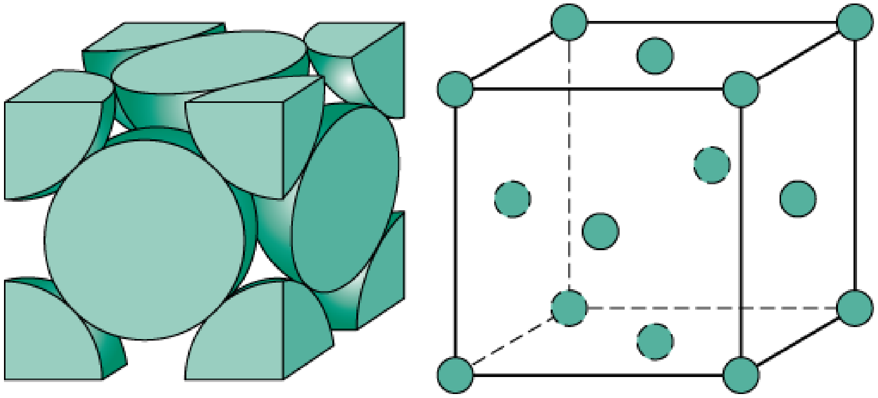
Face Centered Cubic Structure (FCC)

- Atoms touch each other along face diagonals.

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



(Courtesy P.M. Anderson)

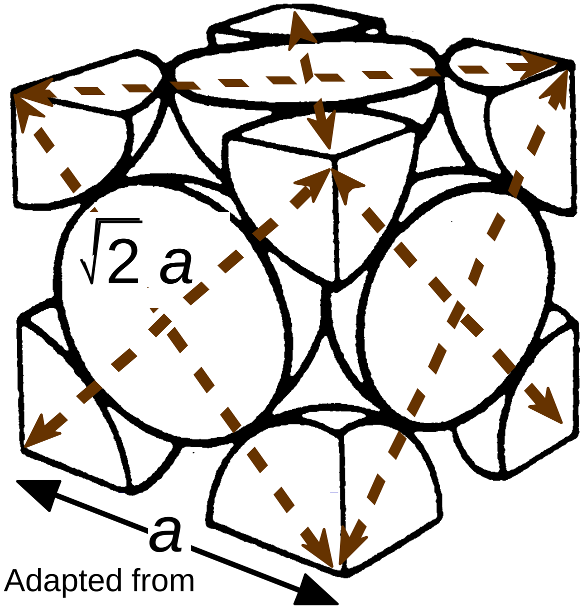


Adapted from Fig. 3.1, *Callister 7e.*

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

Atomic Packing Factor: FCC

maximum achievable APF



Adapted from
Fig. 3.1(a),
Callister 7e.

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

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

$\frac{\text{atoms}}{\text{unit cell}}$ $\frac{\text{volume}}{\text{atom}}$

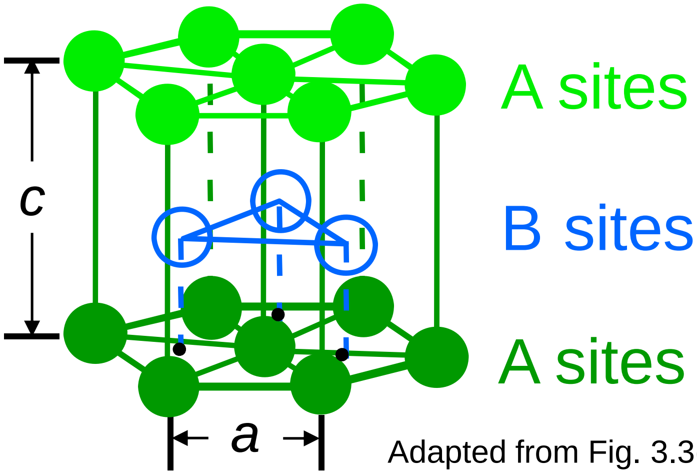
$$\text{APF} = \frac{4 \;\; \frac{4}{3}\pi\,(\sqrt{2}a/4)^3}{a^3}$$

= 0.74

$\frac{\text{volume}}{\text{unit cell}}$

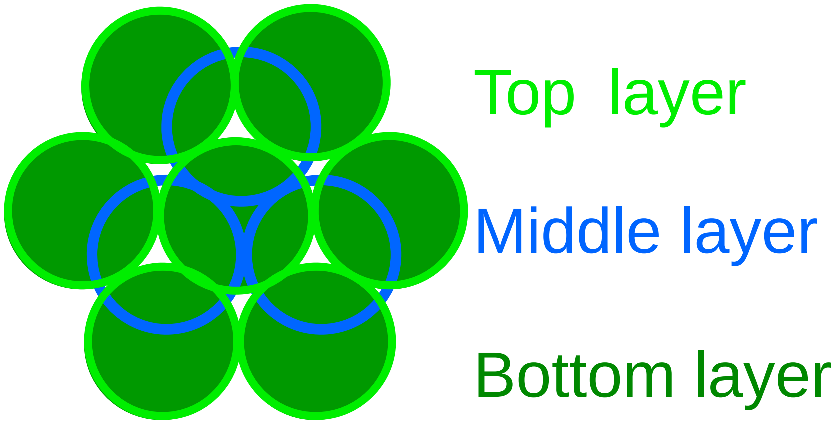
Hexagonal Close-Packed Structure (HCP)

- 3D Projection



Adapted from Fig. 3.3(a), *Callister 7e.*

- 2D Projection



6 atoms/unit cell

- APF = 0.74

ex: Cd, Mg, Ti, Zn

- c/a = 1.633

Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

$$\rho = \frac{n\,A}{V_C N_A}$$

ρ =density g/cm^3

where n = number of atoms/unit cell

A = atomic weight (g/mol)

V_C = Volume of unit cell = a^3 for cubic (cm^3)

N_A = Avogadro's number

= 6.023×10^{23} atoms/mol

P3.8:Calculate the radius of an iridium atom, given that Ir has FCC crystal structure, a density of 22.4 g/cm^{3,} and atomic weight of 192.2g/mol ?

ρ =22.4 g/cm^3 A=192.2 g/mol

N_A = Avogadro's number = 6.023 x 10^{23} atoms/mol

FCC, **n** = 4 atoms/unit cell, and $\mathbf{V_C} = 16R^3\sqrt{2}$

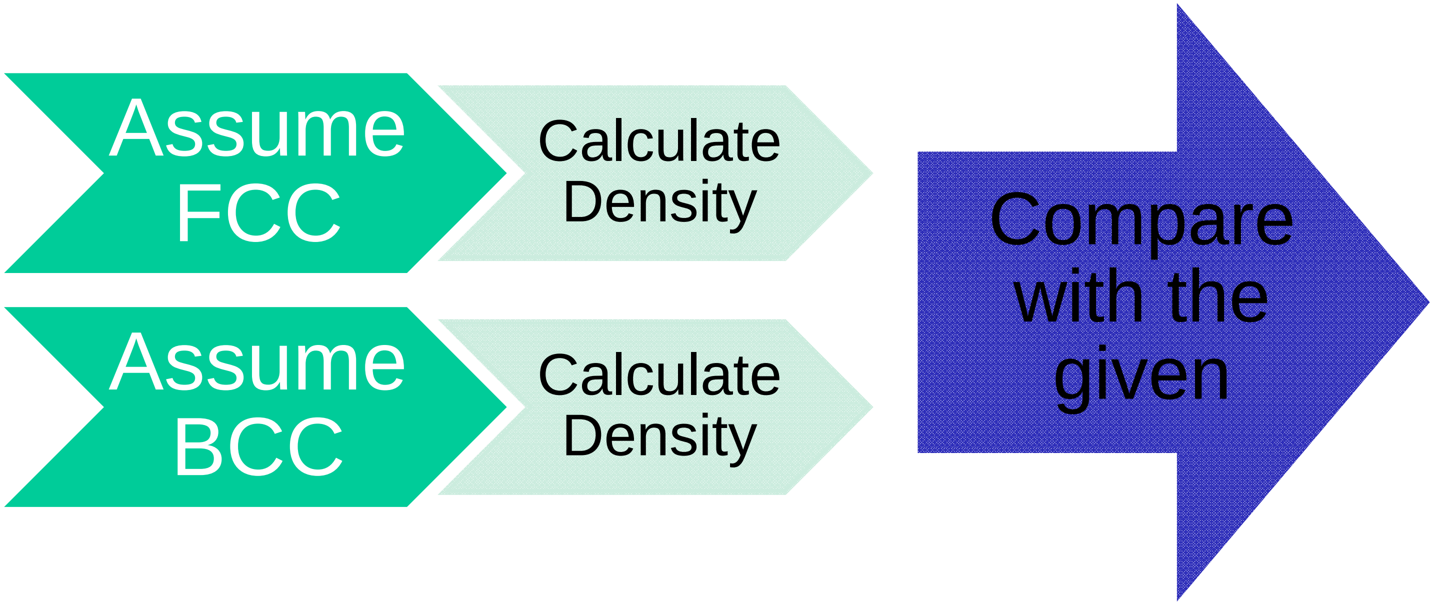
Density $$\rho = \frac{nA_{Ir}}{V_C N_A}$$

$$R = \left(\frac{nA_{Ir}}{16\rho N_A\sqrt{2}}\right)^{1/3} = \left[\frac{(4\text{ atoms/unit cell})(192.2\text{ g/mol})}{(\sqrt{2})(16)(22.4\text{ g/cm}^3)(6.023\times10^{23}\text{ atoms/mol})}\right]^{1/3}$$

$$= 1.36\times10^{-8}\text{ cm} = 0.136\text{ nm}$$

What would be the APF for this case?

P#2:Niobium has an atomic radius of 0.1430nm and a density of 8.57 g/cm^3 .Determine whether it has FCC or BCC crystal ?



Assume FCC

Calculate Density

Assume BCC

Calculate Density

Compare with the given

R=0.1430nm

ρ =8.57 g/cm^3

A=92.91 g/mol

N_A = Avogadro’s number = 6.023 x 10^{23} atoms/mol

For FCC, $n = 4$, and $a = 2R\sqrt{2}$

$$\rho = \frac{nA_{\mathrm{Nb}}}{a^3 N_{\mathrm{A}}} = \frac{nA_{\mathrm{Nb}}}{(2R\sqrt{2})^3 N_{\mathrm{A}}}$$

$$= \frac{(4\ \text{atoms/unit cell})(92.91\ \text{g/mol})}{\left\{\left[(2)(1.43 \times 10^{-8}\ \text{cm})(\sqrt{2})\right]^3 /(\text{unit cell})\right\}(6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 9.33\ \text{g/cm}^3$$

For BCC, $n = 2$, and $a = \frac{4R}{\sqrt{3}}$

$$\rho = \frac{nA_{\mathrm{Nb}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_{\mathrm{A}}}$$

$$\rho = \frac{(2\ \text{atoms/unit cell})(92.91\ \text{g/mol})}{\left\{\left[\frac{(4)(1.43\ \times\ 10^{-8}\ \text{cm})}{\sqrt{3}}\right]^3 /(\text{unit cell})\right\}(6.023 \times 10^{23}\ \text{atoms}/\text{mol})}$$

$$= 8.57\ \text{g/cm}^3$$

Therefore, Nb has a ??? crystal structure.

Chapter 4
Imperfections in Solids

Equilibrium No. of Vacancies

- Equilibrium concentration varies with temperature!

No. of vacancies/cm^3

Activation energy

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

Total no. of atoms

Temperature in K

Boltzmann's constant(depends on Q_V unit

(1.38 x 10^{-23} J/atom-K)

(8.62 x 10^{-5} eV/atom-K)

$$N = \frac{N_A \cdot \rho}{A}$$

Avogadro's number = 6.023 x 10^{23} atoms/mol

density g/cm^3

atomic weight (g/mol)

Specification of composition

1- weight percent

$$C_1 = \frac{m_1}{m_1 + m_2} \text{x}\, 100$$

m_1 = weight or mass of component 1

2- atom percent

$$C_1^{'} = \frac{n_{m1}}{n_{m1} + n_{m2}} \text{x}\, 100$$

n_{m1} = number of moles of component 1

$$n_{m1} = \frac{m_1'}{A_1} \qquad \left.\begin{array}{l}\text{mass in gram}\\ \text{atomic weight}\end{array}\right\} \text{For material 1}$$

4-2:Calculate the number of vacancies per cubic meter in gold at 900 Cº .The energy for vacancy formation is 0.98 eV/atom. Furthermore, the density and atomic weight for Au are 18.63g/cm^3 (at 900 Cº) and 196.9g/mol, respectively.

T(K)=900+273=1173K

$$N_v = N\exp\left(-\frac{Q_v}{kT}\right) \qquad \text{and } N= \frac{N_A \rho_{Au}}{A_{Au}}$$

$$= \frac{N_A \rho_{Au}}{A_{Au}} \exp\left(-\frac{Q_v}{kT}\right)$$

$$= \frac{(6.023 \times 10^{23}\,\text{atoms/mol})(18.63\ \text{g/cm}^3)}{196.9\ \text{g/mol}} \exp\left[-\frac{0.98\ \text{eV/atom}}{(8.62 \times 10^{-5}\ \text{eV/atom}-\text{K})(1173\ \text{K})}\right]$$

$$= 3.52 \text{ x } 10^{18}\ \text{cm}^{-3} = 3.52 \text{ x } 10^{24}\ \text{m}^{-3}$$

What would be the equation of Q_V if every thing is known?

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

4-10:What is the composition, in atom percent, of an alloy that contains 33g copper and 47g zinc ?

The number of moles of Cu is:

$$n_{m_{Cu}} = \frac{m'_{Cu}}{A_{Cu}} = \frac{33 \text{ g}}{63.55 \text{ g/mol}} = 0.519 \text{ mol}$$

Likewise, for Zn

$$n_{m_{Zn}} = \frac{47 \text{ g}}{65.39 \text{ g/mol}} = 0.719 \text{ mol}$$

$$C'_{Cu} = \frac{n_{m_{Cu}}}{n_{m_{Cu}} + n_{m_{Zn}}} \times 100 = \frac{0.519 \text{ mol}}{0.519 \text{ mol} + 0.719 \text{ mol}} \times 100 = 41.9 \text{ at\%}$$

$$C'_{Zn} = \frac{0.719 \text{ mol}}{0.519 \text{ mol} + 0.719 \text{ mol}} \times 100 = 58.1 \text{ at\%}$$

Thank you for your attention