Crystal structure of Metallic Solids

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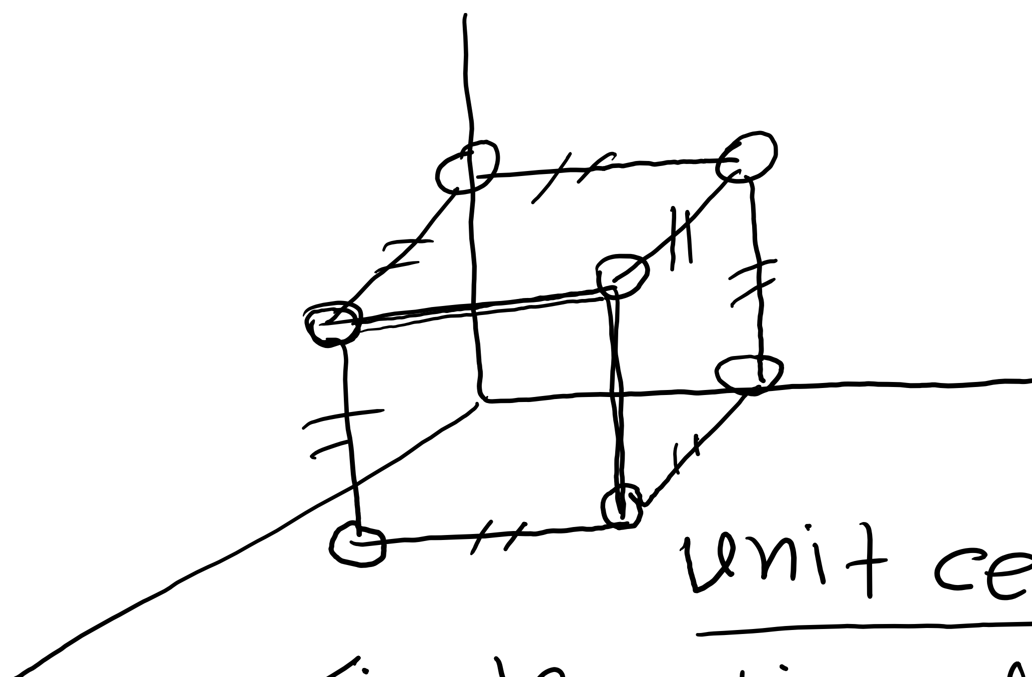
Prepared By: By Professor Dr. Akm Rahman

In this Lecture we will cover structure of crystalline solids. The lecture includes mathematical demonstrations of unit cell, Types of Crystal, unit cell volume, Atomic packing factor, density, crystallographic point, directions, planes.

Crystal structure- A structure where atoms and molecules are orderly oriented. In the crystalline materials molecules have a meaningful order, which is viewed as a repetitive structure.

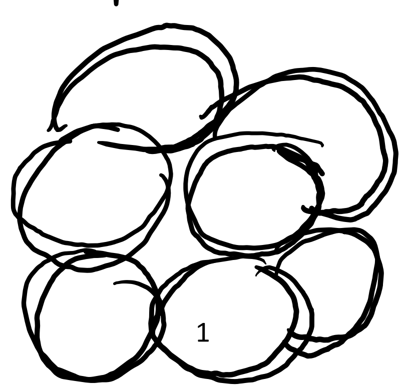
Unit Cell→ Unit cell is a repetitive 3-D unit that represents the crystalline structure of the material.

Assume a 3D- network of a unit cell below-



unit cell

Simple cubic cell



There are some factors behind crystal formation. Those factors determine the types of crystal. Factors are as follows-

1. Atomic radius
2. Inter atomic energy
3. Electronegativity of the atoms in the molecules (For example : Na and Cl; Ni and Cu)

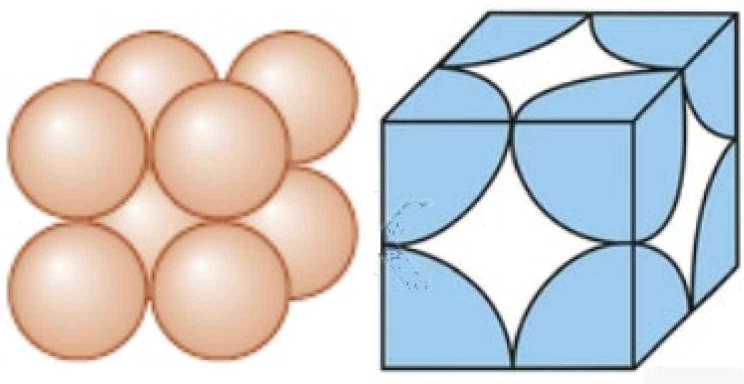


Fig: Unit Cell Structure of Simple- Cubic cell

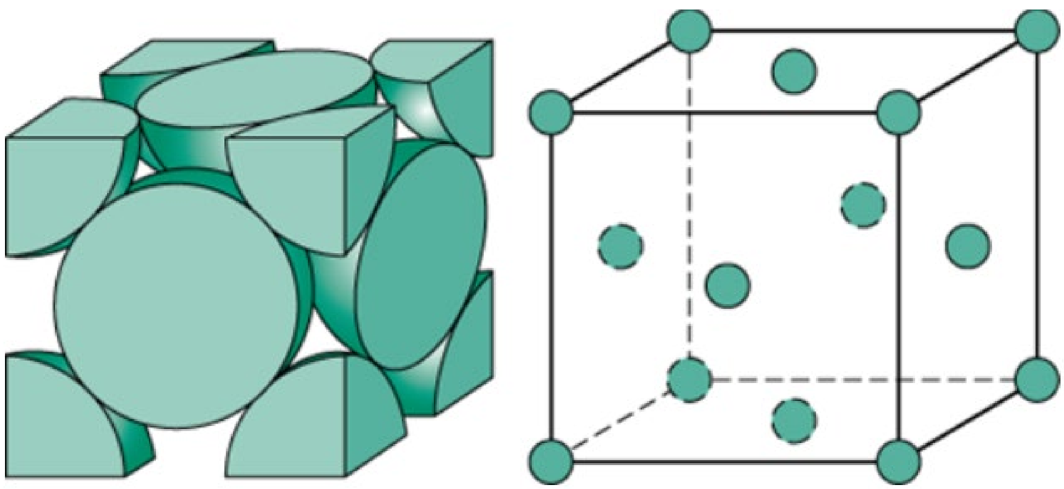


Fig: Unit Cell structure of Face-Centered Cubic

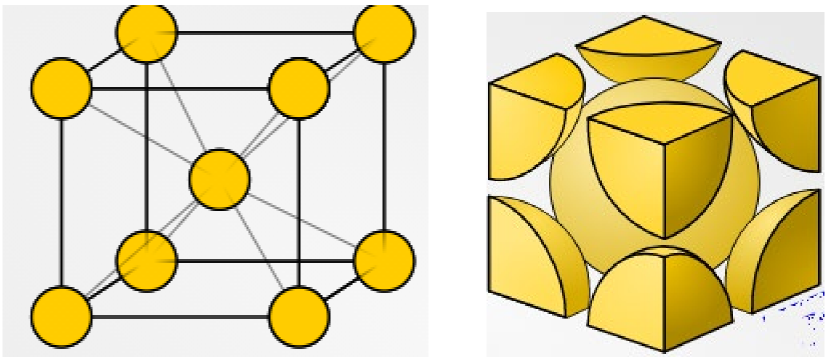


Fig: Unit Cell structure of Body-Centered Cubic

Calculation of No. of Atoms and Atomic Packing Factor

To calculate Number of atoms in unit cell the following equation is considered-

$$N = N_i + \frac{N_f}{2} + \frac{N_C}{8}$$

For FCC crystal structure, N=0+6/2+8/8=4

Now, how can we determine the packing factor of a unit cell?

APF= Atomic Packing Factor

APF= $\frac{VOlume\ of\ Atoms\ in\ unit\ Cell}{Total\ Unit\ Cell\ Volume}$

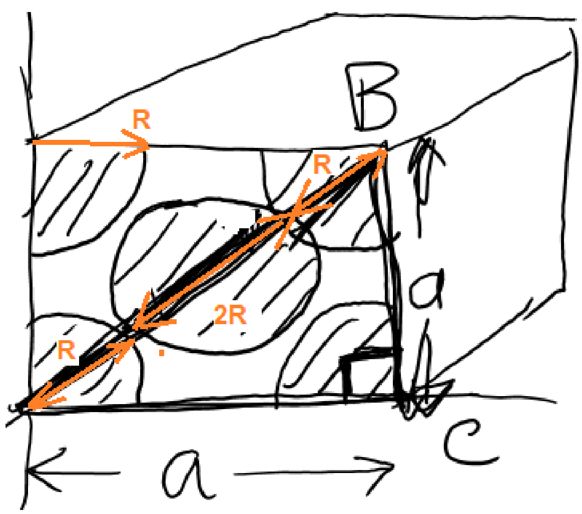
If we consider F.C.C crystal, to find the APF, we need to first find the relationship between

a= Lattice Parameter

R= Atomic Radius

Then Volume of a single atom

Therefore, APF=N*Volume of an Atom/a^3



Assumptions: Several Assumptions are needed to make in line with the calculations-

1. Atoms are spherical
2. Atoms are hard such as hard balls

By Applying the rule of right-angle triangle-

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

$$4R^2 = a^2 + a^2$$

$$16R^2 = 2a^2$$

$$a=2\sqrt{2}R$$

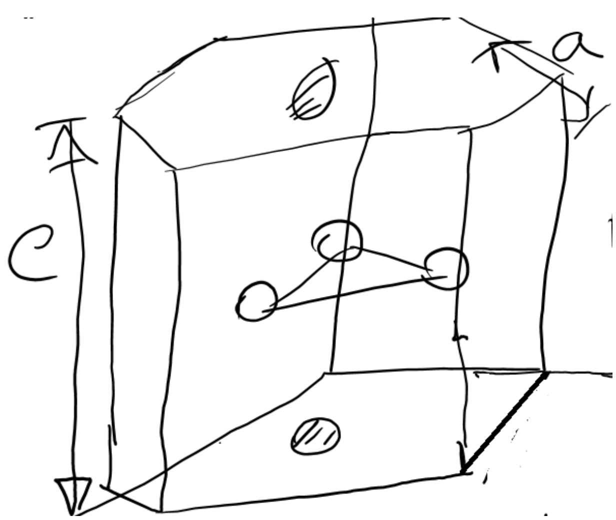
Volume of spherical atoms $V=\frac{4}{3}\pi R^3$

Therefore, $APF=\frac{4*(\frac{4}{3}\pi R^3)}{(2\sqrt{2}R)^3}=0.74$

In other words, APF%=74%

This means that the atomic packing in FCC crystal structure is 74% within the maximum possible packing limit.

Can you show APF of HCP crystal structure?

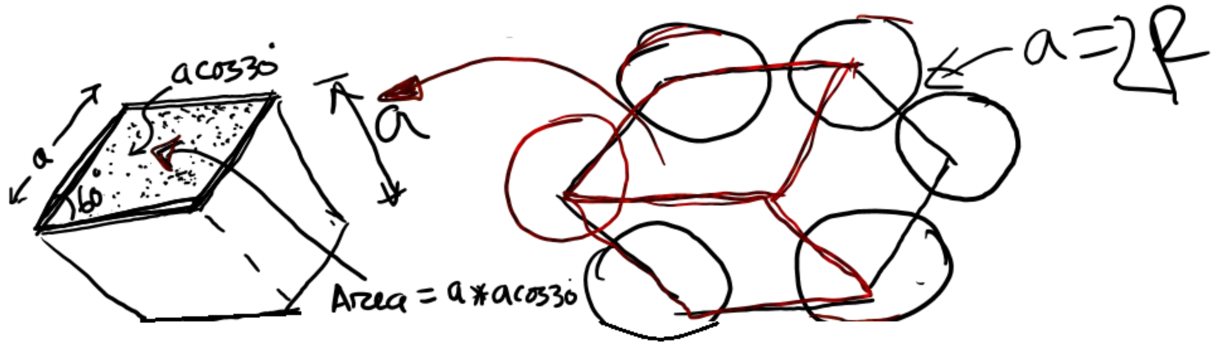


In HCP crystal, Interior Atom, Ni=3

Face Atom Nf=2

N= Ni+ Nf/2+Nc/6= 3+1+2=6

Now lets find unit cell volume-



Hexagonal base area= $3.a^2$.cos 30°

Now find unit cell volume= Hexagonal Base Area *c=$3.a^2$.c.cos 30°

Also, we see that a=2R

If the ratio of c/a=1.633, APF of HCP can be determined as 0.746.

Theoretical Density:

Theoretical density is a measure of density of a metal based on the atomic packing in a Crystal structure.

Theorical density can be calculated using the following equation-

$$\rho = \frac{n.A}{V_c.N_A}$$

Where, n= No of atoms in a unit cell

N_A= Avogadro's Number, atoms/mol

V_c= Volume of the unit cell, cm^3

A=Atomic number, gm/mol

Table 3.1 Atomic Radii and Crystal Structures for 16 Metals

Metal	Crystal Structure[a]	Atomic Radius[b] (nm)	Metal	Crystal Structure	Atomic Radius (nm)
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

[a] FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.

[b] A nanometer (nm) equals 10^{-9} m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.

Example:

Find Density of Cu

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

$$= \frac{4\ Atoms \times 63.5\ g/mol}{16\sqrt{2} \times (1.28 \times 10^{-8})\ cm^3 \times 6.023 \times 10^{23} atms/mol}$$

$= 8.89$ gm/cm^3

Given:

NA=6.023×10^{23} atoms/mol

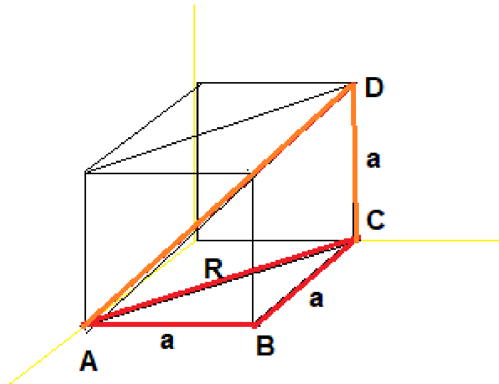
Vc=a^3= $(2\sqrt{2}R)^3$=$16\sqrt{2}R^3$=

=$16\sqrt{2}(0.128\text{nm})^3$

=

Similarly, you can find the density of BCC Iron

For BCC Iron,



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

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

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

$$16R^2 = 3a^2$$

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

$Vc=a^3=(4R/\sqrt{3})^3=64R^3/3\sqrt{3}=64(0.1241)^3/3\sqrt{3}$

$=0.023\ nm^3$

Therefore,

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

$$= \frac{2\ Atoms \times 56\ g/mol}{0.023x10\ E{-24}\ x\ 6.023 \times 10^{23} atms/mol}$$

$=8.08\ gm/cm^3$