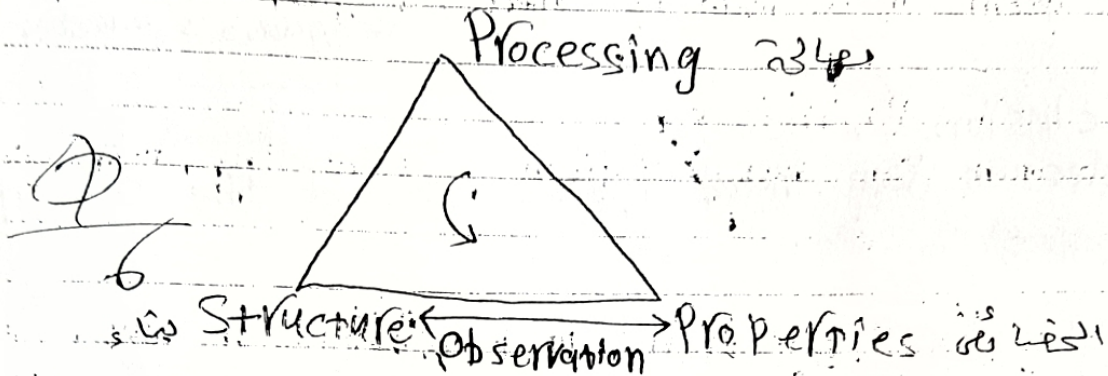


Applied By: Ahmad Jundi

(Material Science)

## Material Science & Engineering

Material Science is the Investigation of the Relationship among Processing, structure, properties & performance



Properties are the way the material response to the environment & external forces.

Mechanical Properties are response to mechanical forces

Atoms: nucleus (p + n) + e

Charged electrons (-), Protons (+)  $1.6 \times 10^{-19}$  Coulombs

Atomic Mass: mass of (p) + mass of (n)

Proton & Neutron have the same mass  $\Rightarrow 1.67 \times 10^{-27}$  Kg

e:  $9.11 \times 10^{-31}$  Kg

amu (Atomic Mass Unit): is often used to express atomic mass. 1 amu is defined as 1/12 of the atomic mass of the common isotopes of carbon.

atomic weight = weighted average of atomic masses

A.W Carbon = 12.011 amu

Mole is the amount of matter that has a mass in gram equal to the atomic mass in amu (A mole of carbon has a mass of 12 grams).

Number of atoms in a mole is called Avogadro's number =  $6.022 \times 10^{23}$

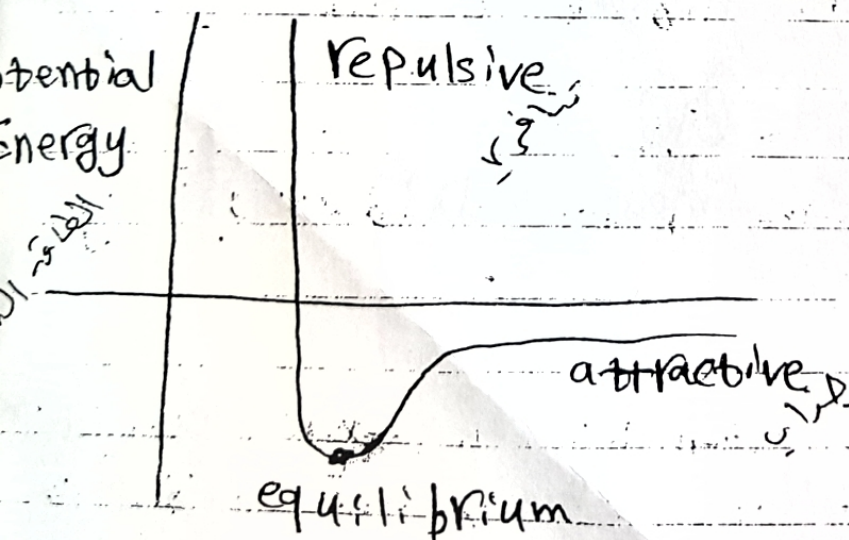
Pauli's exclusion principle

Only one electron can have a given set of the four quantum numbers.

Valence electrons: Electrons that occupy the outer most shell (they are responsible for bonding)

Electronegativity: a measure of how willing atoms are to accept electrons.

Bonding Energies & Forces:





Electron Volts: the energy lost/gained by an electron when it is taken through a potential difference of one volt.

$$E = q \times V$$

$$q = 1.6 \times 10^{-19} \text{ Coulombs}$$

$$V = 1 \text{ Volt}$$

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

## Types of Bonding:

- I Primary bonding:** electrons are transferred or shared.  
Strong (100-1000) (KJ/mol) or 1-10 eV/atom
- ① **Ionic:** Strong Coulomb interaction among negative atoms (have an extra  $e^-$  each) & positive atoms (lost an  $e^-$ ):  $\text{Na}^+ \text{Cl}^-$
- ② **Covalent:** electrons are shared between the molecules to saturate the valency ( $\text{H}_2$ )
- ③ **Metallic:** atoms are ionized, losing some electrons from the valency bond
- II Secondary bonding:** no  $e^-$  transferred or shared.  
Interaction of atomic/molecular dipoles  
Weak  $< 100 \text{ KJ/mol}$
- Ionic:**  
Mutual ionization occurs by electron transfer  
Ion: charged atom  
Anion:  $-$       Cation:  $+$
- Ions are attracted by strong Coulomb's interaction.  
nondirectional (Ions may be attracted to another in any direction)

### \* Covalent Bondings:

- Electrons are shared between molecules formation.
- Cooperative sharing of valence electrons can be described by orbital overlap.



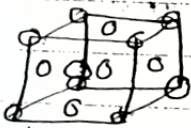
- Highly directional in the direction of greatest orbital overlap

### \* Metallic Bondings:

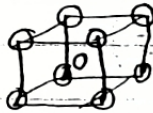
- Valence electrons are detached from atoms and spread in electron sea that glues the ions together.
- nondirectional

## Chapter 3:

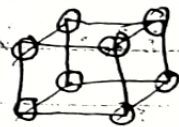
Lattice: is a collection of points which called lattice points



Face center



Body center



Simple Cubic

### \* Types of Solids:

1. Crystal material: atoms self-organize in a periodic array.
2. Single crystal: atoms are in a repeating or periodic array over the entire extent of the material.
3. Polycrystalline material: comprised of many small crystals of grains.



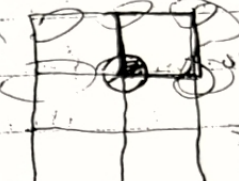
# \*Crystal Structure:

Consider the following:

- ① atoms as being hard spheres with well-defined radii.
- ② The shortest distance between two like atoms is one diameter.

Unit cell (uc): is the smallest structural unit or building block that can describe the crystal structure. (Repetition of the unit cell generates the entire crystal).

ال وحدة وحدة بنسبة 1/4 من الزاوية 2D  
 ال وحدة = 1/8 = 3D



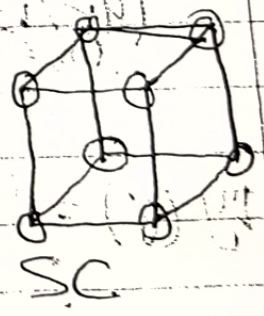
\* For each unit cell in 2D there is only 1/4 of an atom at each corner.

\* At each corner in 2D we will always draw full ~~circle~~ circle represent atom.

\* it is understood that only the fraction of the atom that is contained inside the UC contributes to the total of atoms 1/4 atom

Lattice Parameter: describes the size & shape of the UC

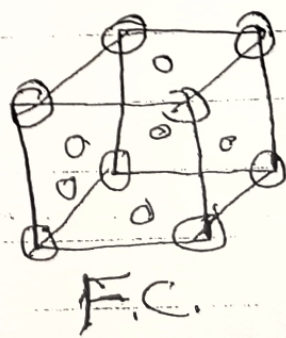
$$\left( \frac{\text{Lattice Point}}{\text{corner}} \right) \left( \frac{\text{corners}}{\text{cell}} \right) = \frac{\text{Lattice Point}}{\text{Cell}}$$



$$\frac{1}{8} \times \frac{8}{1} = 1$$

$$\frac{1}{8} \times 8 + 6 \times \frac{1}{2} = 4$$

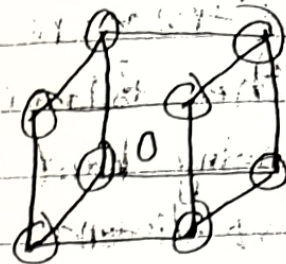
عدد الذرات من الزاوية  
من اصة كل وجه



$$\frac{1}{8} \times 8 + (1) \times (1) = 2$$

Lattice Point

نقطة الشبكة  
مع الشبكة الخاصة



B.C.

الذرات في وحدة بنكريبي هي عدد الذرات في الواقع التي يتبع في الشبكة

\* Hexagonal Close - Packed (HCP):

\* HCP is one more common structure of metallic crystal.

\* Six atoms form regular hexagon surrounding one atom in center. Another plane is situated half way up unit cell (c-axis).

\* Packing Factor =  $\frac{\text{number of atoms/cell} \times \text{Volume of each atom}}{\text{Volume of unit cell}}$

P.F. is the fraction of space occupied by an atom.

P.F. FCC:

Lattice Point

$$P.F. = \frac{(4) \left( \frac{4}{3} \right) \pi r^3}{\left( \frac{4r}{\sqrt{2}} \right)^3} = 0.74$$

P.F. FCC

$$\text{Density } (\rho) = \frac{(\text{atom/cell}) (\text{atomic mass})}{(\text{Volume of u.c.}) (N_{\text{Avogadro}})}$$



Ex: Calculate the atomic radius in cm for the following  
 a) BCC metal units  $a_0 = 0.3294 \text{ nm}$  and one atom per lattice point  
 b) FCC metal units  $a_0 = 4.0862 \text{ \AA}$

a)  $r = \frac{\sqrt{3} a_0}{4} = 0.1428 \text{ nm} = 1.428 \times 10^{-8} \text{ cm}$

b)  $r = \frac{\sqrt{2} a_0}{4} = 1.4447 \text{ \AA} = 1.4447 \times 10^{-8} \text{ cm}$

Ex: Determine the crystal structures for the following:

- a) a metal with  $a_0 = 4.9489 \text{ \AA}$ ,  $r = 1.75 \text{ \AA}$   
 b) " " " "  $a_0 = 0.42906 \text{ nm}$ ,  $r = 0.1859 \text{ nm}$   
 c) by ratio between  $a$  &  $r \Rightarrow$  fcc  
 d) BCC

Ex:  $\rho$  for an element which has the BCC structure is  $0.855 \text{ g/cm}^3$ ,  $A.W = 39.09 \text{ g/mol}$ . Calculate  
 1) lattice parameter.  
 2)  $r$ .

$$0.855 = \frac{(2)(39.09)}{(a_0)^3 (6.023 \times 10^{23})}$$

$$a_0 = 5.3335 \times 10^{-8} \text{ cm}$$

$$r = 2.3103 \times 10^{-8} \text{ cm}$$

Ex: a metal having a cubic structure  $\rho = 2.6 \text{ g/cm}^3$ ,  $A.W = 87.323$   
 $a = 1.0849 \text{ \AA}$ . Determine crystal structure

$$x = 4$$

FCC

Coordinate # is the # of atoms touching a particular atom.

\* A metal has a hexagonal structure with  $a_0 = 0.4546 \text{ nm}$  and  $c_0 = 1.186 \text{ nm}$ ,  $\rho = 9.808 \text{ g/cm}^3$ ,  $A.W = 268.98 \text{ g/mol}$ . Determine:

- ① the Volume of U.C.
- ② How many atoms are in each U.C.

$$V_{\text{hex}} = a_0^2 c_0 \cos 30^\circ = 0.21226 \text{ nm}^3 = 2.1226 \times 10^{-22} \text{ cm}^3$$

$$\rho = \frac{\text{atoms} (A.W)}{\text{Volume} (\text{cm}^3)} \Rightarrow \text{atoms} = \rho / (\text{cm}^3)$$

Ex: A metal has an orthorhombic structure with  $a_0 = 0.1218 \text{ nm}$ ,  $b_0 = 0.45186 \text{ nm}$  and  $c_0 = 0.7657 \text{ nm}$ ,  $V = 0.1218 \text{ nm}^3$ ,  $\rho = 5.904 \text{ g/cm}^3$ ,  $A.W = 69.72 \text{ g/mol}$ .

Determine:

- ① # of atoms in each U.C.
- ② P.F

$$V_{\text{orthorhombic}} = a_0 b_0 c_0 = 1.560 \times 10^{-22} \text{ cm}^3$$

$$\rho \Rightarrow \# \text{atoms} = 8$$

$$\text{P.F} = \frac{(\# \text{atom/cell}) (A.W)}{(\text{Volume}) (\rho)} = \frac{(8) (69.72)}{(1.560 \times 10^{-22}) (5.904 \text{ g/cm}^3)}$$

$$\text{P.F} = \frac{(\# \text{atom/cell}) \text{ Volume of each mass}}{\text{Volume of unit cell}} = \frac{8 \left( \frac{4\pi}{3} \right) (0.1218 \text{ nm}^3)}{0.1560 \text{ nm}^3}$$



Ex: Above  $882^\circ\text{C}$ , a metal has a BCC structure with  $a_0 = 0.332\text{ nm}$ . Below this temperature, the metal has a H.C.P structure with  $a = 0.2978\text{ nm}$  &  $c = 0.4735\text{ nm}$ . Determine the Percent Volume change when BCC metal transforms to HCP. Is this contraction or expansion?

HCP more ductile than BCC

$$V_{\text{BCC}} = 0.63859\text{ nm}^3 = a_0^3$$

$$V_{\text{H.C.P}} = 0.03637\text{ nm}^3$$

$$\Delta V = V_2 - V_1$$

$$= V_{\text{H.C.P}} - V_{\text{BCC}}$$

ان الب يغير تفرس

$$\text{Contraction} = (-)$$

$$\Delta V = \frac{V_{\text{BCC}} - V_{\text{HCP}}}{V_{\text{BCC}}} \times 100\% = -0.62 \Rightarrow \text{Contraction}$$

Ex:  $\alpha$ -metal has a Cubic structure with  $a_0 = 0.8931\text{ nm}$  &  $\rho = 7.47\text{ g/cm}^3$ . B-metal has different cubic structure with  $a_0 = 0.6326\text{ nm}$ ,  $\rho = 7.26\text{ g/cm}^3$ ,  $A_w = 54.938\text{ g/mol}$ ,  $r = 0.112\text{ nm}$ . Determine the % Volume change from  $\alpha$  metal to B metal.

$$1) 7.47 = \frac{(x)(54.938)}{(0.8931 \times 10^{-7}\text{ cm})^3 (6.023 \times 10^{23})} \Rightarrow x = 58 \text{ atom/cell}$$

$$2) x = 20$$

$$\Delta V = \left( \frac{58}{20} \right) \frac{\text{Volume B} - \text{Volume } \alpha}{\text{Volume } \alpha}$$

Correction factor

$$= \frac{58}{20}$$

$$= +3.05\% \text{ (Expansion)}$$

A typical paper exp weighs  $0.54\text{ g}$  and consists of BCC Iron.

Calculate

(a) # of u.c

(b)

$$a_0 = 2.866 \times 10^{-8}\text{ cm}$$

$$\rho = 7.87\text{ g/cm}^3$$

# of atoms

$$1) \# \text{ of atoms} = \frac{W}{P \times V} = 3.185 \times 10^{21} \text{ cell}$$

$$2) 6.33 \times 10^{21} \text{ atoms}$$



$$\text{Planar (P)} = \frac{\# \text{ atoms per face}}{\text{area of face}}$$

$$\text{Planar P.F.} = \frac{\text{area of atoms surface}}{\text{area of face}} = \frac{\pi r^2}{a^2}$$

Repeat distance; the distance between Lattice points along the direction.

\* FCC [110]  
If we start 0,0,0 Location, the <sup>next</sup> lattice point is at the center (1/2, 1/2, 0).  
the distance between lattice points is an half of the diagonal  
 $\frac{1}{2} \sqrt{2} a_0$

### Interstitial Sites

In all crystal structures, there are small holes between the usual atoms into which smaller atom may placed.

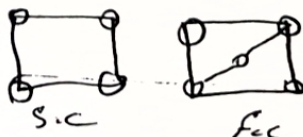
### \* Polymorphism and Allotropy

\* Some materials may exist in more than one crystal structure.  
\* If the material is an element solid, it is called allotropy.  
an example of allotropy is carbon which can exist as diamond, graphite.

### Anisotropy

properties are different in different directions

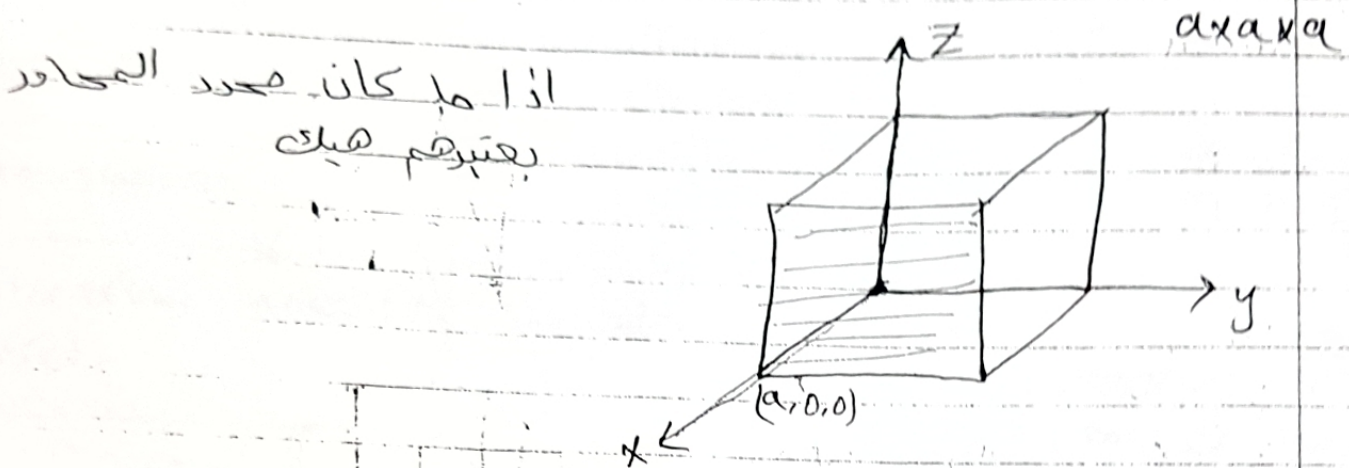
Different directions in a crystal have a different packing.  
for example, atoms along the edges of FCC u.c. are more separated along the face diagonal. this causes Anisotropy in the properties.





## # Miller Indices:

The orientation of a surface or crystal plane may be defined by considering how plane intersects the major crystallographic axes of the solid.



### Steps:

- 1 Identify the intercepts on  $x, y, z$ .

Intercepts  
( $a, \infty, \infty$ )

- 2 ~~Specify~~ Specify the intercepts in fractional coordinate point ( $x, y, z$ ),  $\frac{1}{a} \times b \times c$

Fractional Co. ( $x/a, y/b, z/c$ )

( $a/a, \infty/a, \infty/a$ )

1,  $\infty, \infty$

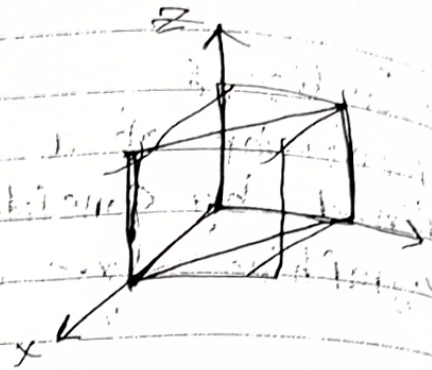
- 3 Take the reciprocal of the fractional intercepts coordinates.

( $1, 0, 0$ )

Inter:  $a, a, \infty$  to know crystal graphic

F.c.c:  $1, 1, \infty$  U.Bentamtion

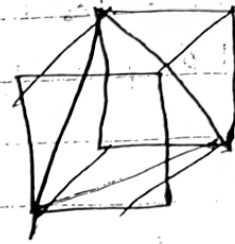
M.I:  $(1, 1, 0)$



Inter:  $a, a, a$

F.c.c:  $1, 1, 1$

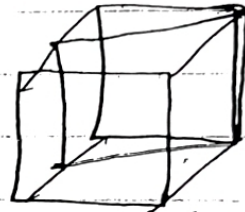
M.I:  $1, 1, 1$



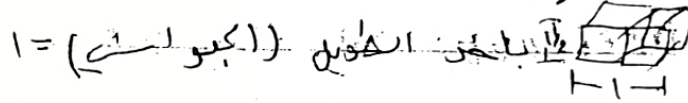
Inter:  $\frac{1}{2}a, a, \infty$

F.c.c:  $\frac{1}{2}, 1, \infty$

M.I:  $2, 1, 0$  لحال  $x$  احسان الافي 2



بالطاني مافه  
1/2



كان عني

## \* Bragg's Law

$$n\lambda = 2d \sin \theta$$

\* this law explains why the faces of crystals appear to reflect x-ray beam at certain angle ( $\theta$ ). where:  
 $d$  is the distance between atoms layers in a crystal.  
 $\lambda$  is the wave length of the x-ray beam.  
 $n$  is an integer

XRD: X-Ray Diffraction.



## \* Crystal Structure of Ionic materials:

Ionic material must have crystal structures that ensure electrical neutrality, yet <sup>Permit</sup> Ions from the different sizes to be packed efficiently.

① Ionic Radii: the crystal structures of ionically bonded compound, is described by placing the anion of the normal lattice point cell and the cation located at one or more of the interstitial site.

② Electrical neutrality: the overall material have to be electrically neutral.

Allotropy: the ability of the element to exist more than one crystal structure depending on Temp. & pressure.

Polymorphisms Compound have more than one crystal structure.

## Chapter 4

\* Crystals are like people it is the defects in them which tend to make them interesting Colin Humphrey.

\* Defect in Solids (0D) Point defects.

- Vacancies
- Interstitial,
- Impurities.

1 - D  $\circ$  edge screw edge + screw

2 - D  $\square$  Surface defect (1D + 2D)

3 - D  $\square$  Volume defects