PH5P5
MATERIALS SCIENCE

CRYSTAL STRUCTURE AND DEFECTS

III B.Sc. PHYSICS
V SEMESTER

Dr. Marimuthu Sundarrajan
Assistant Professor of Physics
SCSVMV Deemed University

Crystalline and Amorphous solids

The materials can be classified in broad scope as

Crystalline materials

In crystalline solids the atoms are arranged in a periodic manner and the atomic arrangement is found to be uniform through out the material. There are single and polycrystalline materials. In polycrystalline materials, each of the constituent crystal has uniform atomic arrangement with in its boundary.

Examples; Quartz, Calcite, Sugar, Mica, Diamonds, table salt etc.

Non-crystalline materials or Amorphous solids

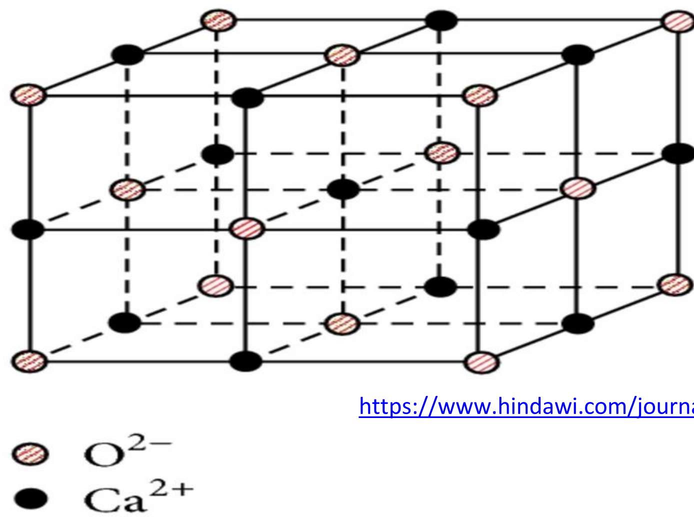
In amorphous solids , the atoms are arranged in a random manner and there is no periodic atomic arrangement in any part of the material

Examples; Plastics, Glass, Rubber, Metallic Glass, Polymers, Gel etc.

https://www.askiitians.com/iit-jee-solid-state/amorphous-and-crystalline-solids/

CRYSTAL STRUCTURE

A crystal structure refers to a structure in which atoms or molecules arranged in a uniform manner. The regular geometry of arrangement of atoms starts from a fundamental unit and this unit is called unit cell. When this unit cell geometry is repeated in three dimension, it results in a crystal structure and hence a crystal

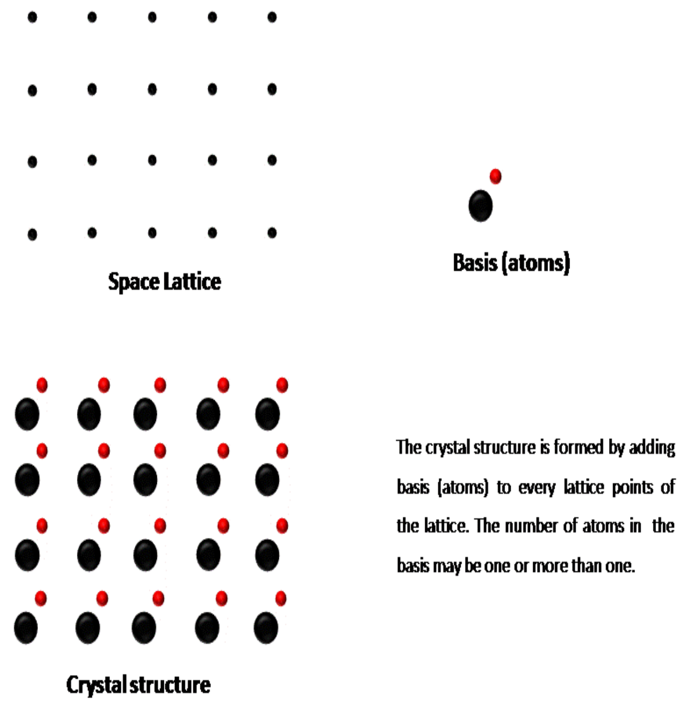


https://www.hindawi.com/journals/amse/2013/673786/fig4/

LATTICE AND BASIS

A lattice is a two dimensional plane which consists of periodic arrangement of points where atoms or group of atoms can be observed in a crystal

A basis is an atom or group of atoms that may be present in the lattice point of a crystal.

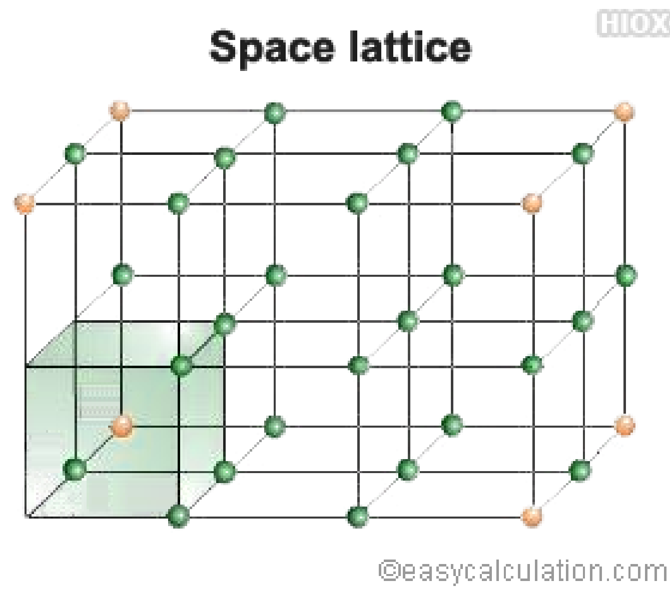


http://dionne.stanford.edu/MatSci202_2011/Lecture7_ppt.pdf

SPACE LATTICE

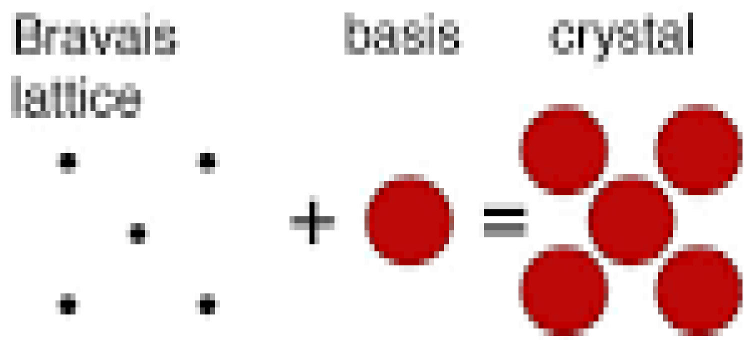
Space lattice

It is a three dimensional arrangement of lattice points in a space where atoms or group of atoms are arranged



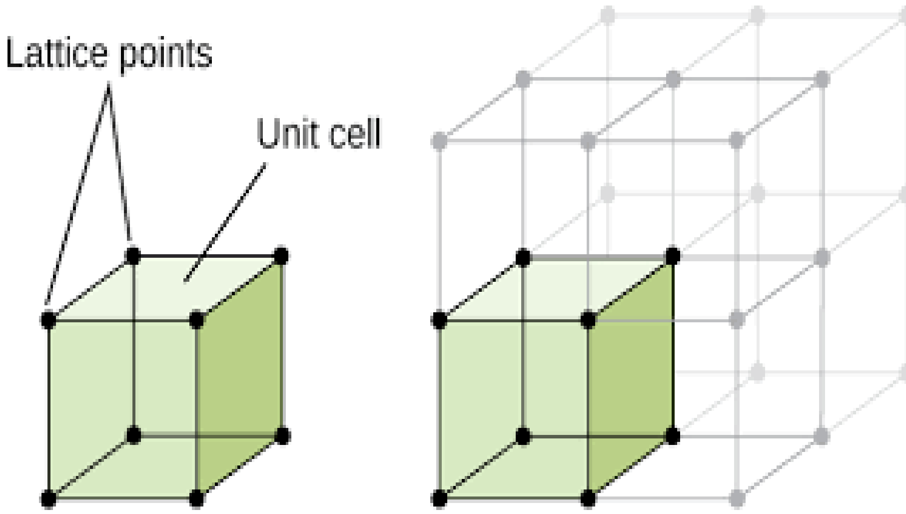
CRYSTAL =LATTICE + BASIS

Crystal structure is obtained when atoms or group of atoms (basis) occupy the space lattice points.



UNIT CELL
FUNDAMENTAL UNIT OF CRYSTAL

Unit cell is the fundamental unit of crystal lattice. When unit cell is repeated in a three dimensional way, it results in space lattice and hence crystal structure

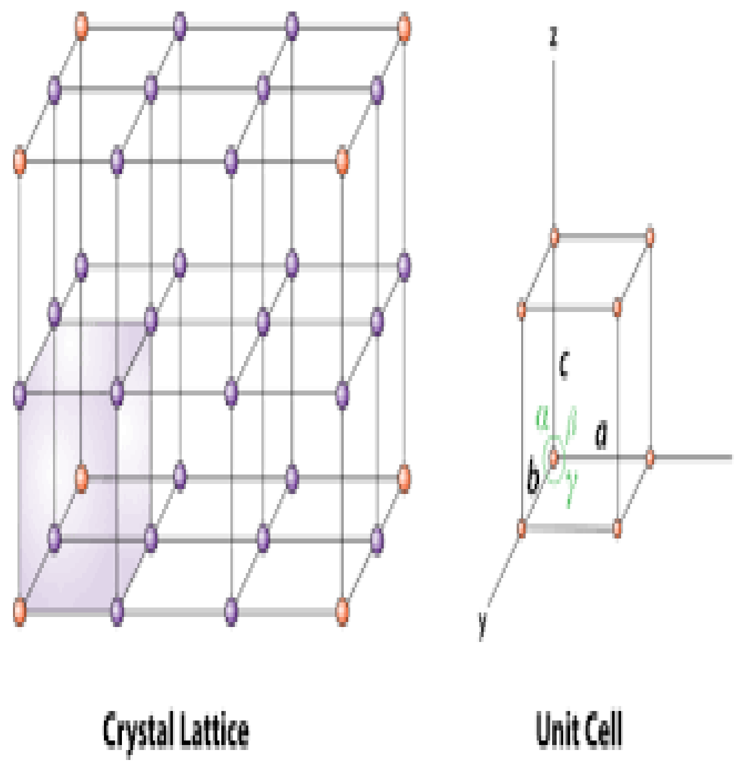


LATTICE PARAMETERS OF UNIT CELL

Lattice parameters define the dimension of unit cell in terms of axial lengths in x,y and z axes and angles between the planes through the x,y and z axes.

The **axial lengths** are called **lattice constants and angles** are called as **interfacial angles. Both lattice constants and angles are called lattice parameters.**

lattice constants, referred to as **a, b, and c and three interfacial angles as α, β and γ**



Credit: CK12 Foundation - Christopher Auyeung; License: CC BY-NC 3.0.

LATTICE CONSTANTS AND INTERFACIAL ANGLES

Crystallographic axes:

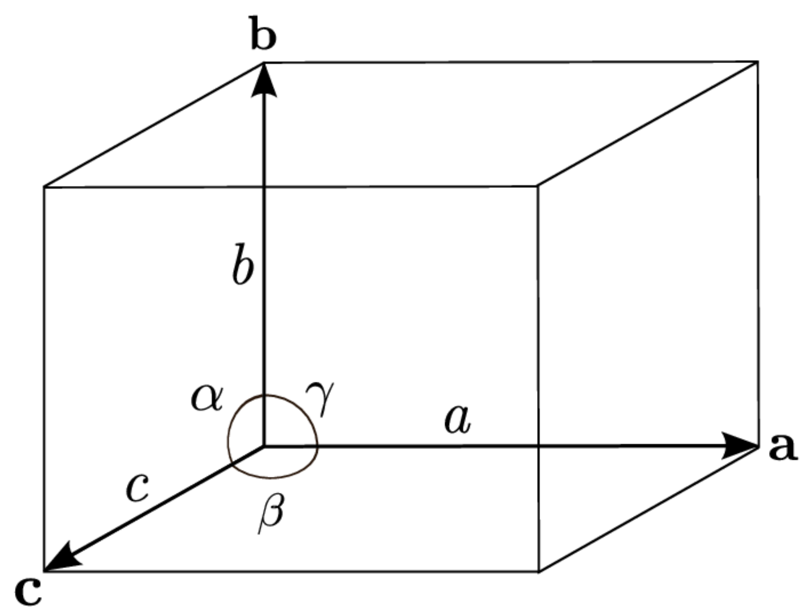
ox, oy, oz

Interfacial angles:

α, β, γ

Lattice constant:

a, b, c



Source : http://www.brainkart.com/article/Types-of-Cubic-System_2865/

EXAMPLES OF CRYSTALS

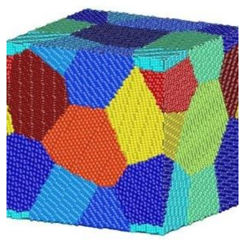
Large crystals

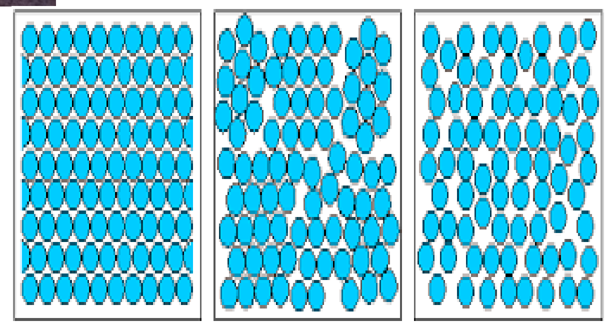
Diamonds and table salt.

Polycrystals

Polycrystal are made up of tiny induvidual crystals with boundaries.

M*etals, rocks, ceramics, and ice.*





Source :http://dmishin.blogspot.com/2014/08/crystal-growing-table-salt-sodium.html

CRYSTAL SYSTEMS & BRAVAIS LATTICES

The structure of crystals are broadly classified in to seven systems based on lattice parameters. The following are seven crystal systems

Cubic

triclinic

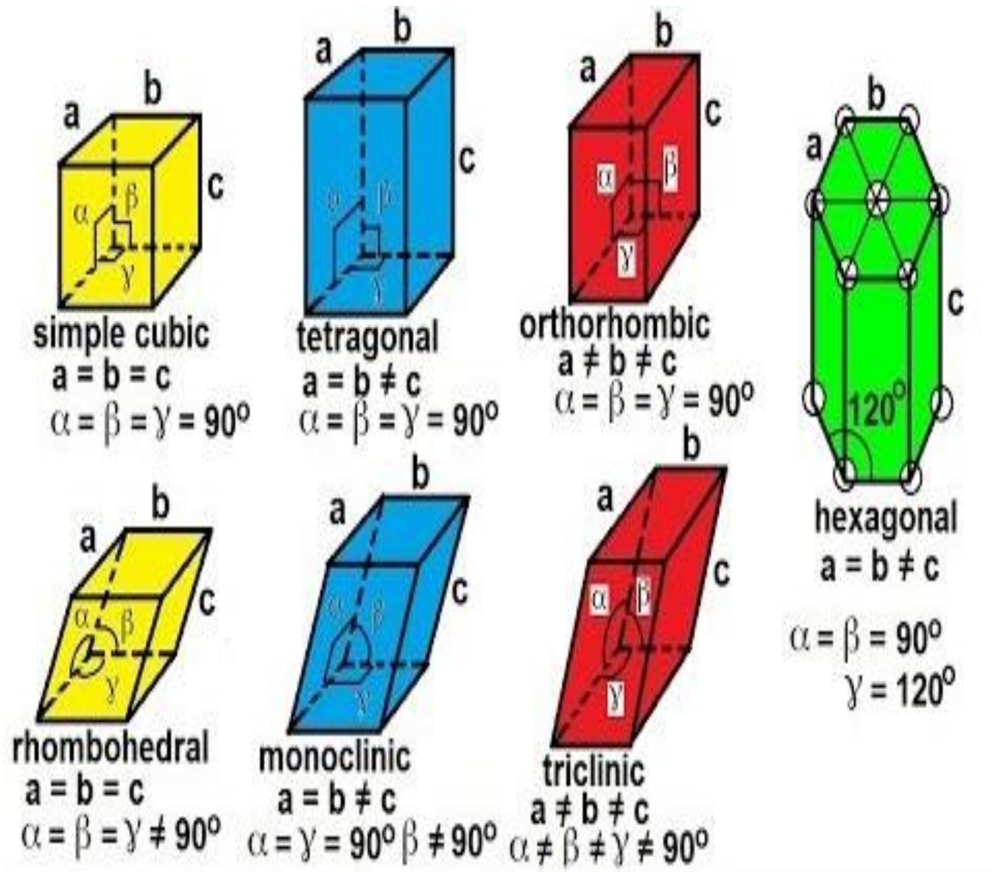
monoclinic

orthorhombic

tetragonal

trigonal

& hexagonal system



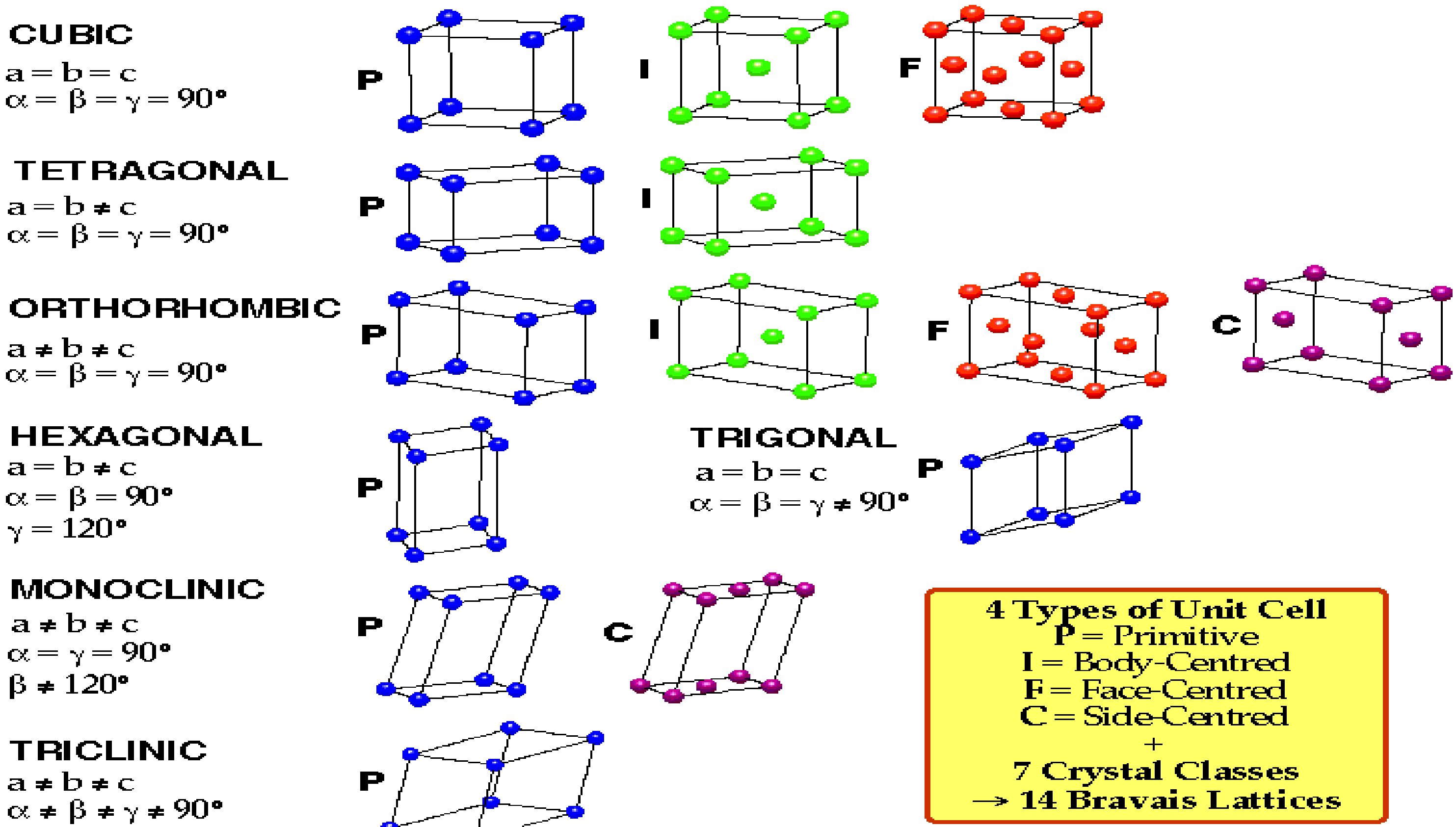
http://ocw.utm.my/pluginfile.php/1055/mod_resource/content/0/SSP2412%20PDF/3.%20Crystal%20Structure%20%20Defects.pdf

BRAVAIS LATTICES

In 7 crystal systems, Bravais Lattices refers to the **14 different 3-dimensional configurations** into which **atoms are** arranged in crystals with various lattice parameters.

The **smallest group** of symmetrically aligned **atoms** which can be repeated in an array to make up the entire crystal is called a **unit cell**

7 CRYSTAL SYSTEMS AND 14 BRAVAIS LATTICES

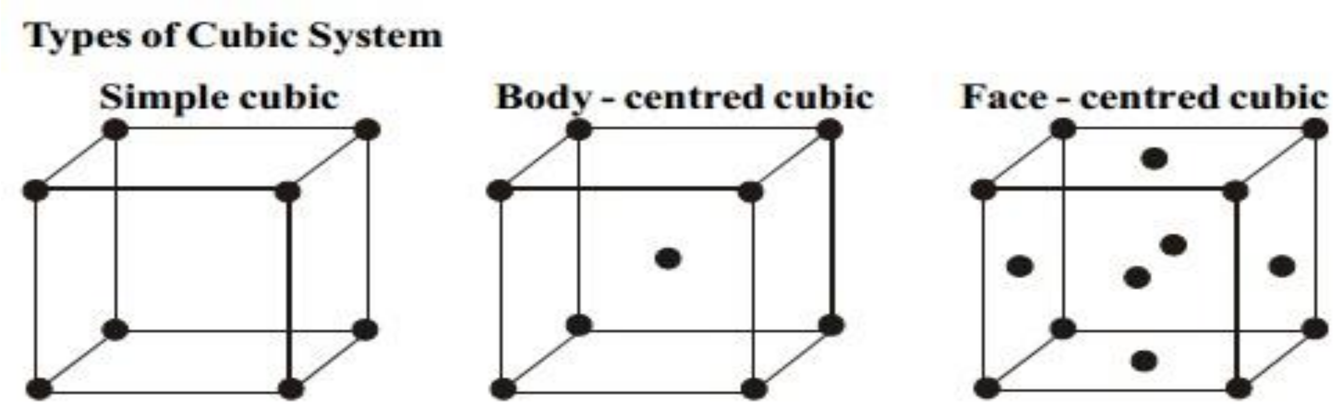


http://home.iitk.ac.in/~sangals/crystosim/crystaltut.html

CUBIC SYSTEM

Assignment of Atoms / unit cell

Simple Cubic



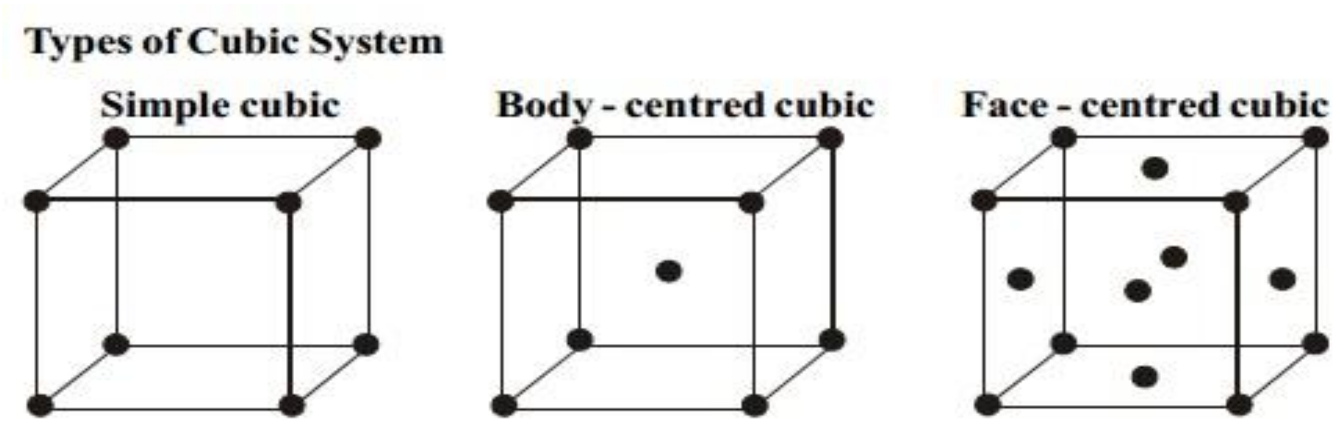
http://www.brainkart.com/article/Types-of-Cubic-System_2865/

- **Atoms are present at the corners only**
- **Each atom at the corner is shared equally by eight other unit cells**
- **Hence the contribution of each atom to the unit cell is 1/8.**

CUBIC SYSTEM

Assignment of Atoms/ unit cell

Body Centered Cubic lattice (BCC)

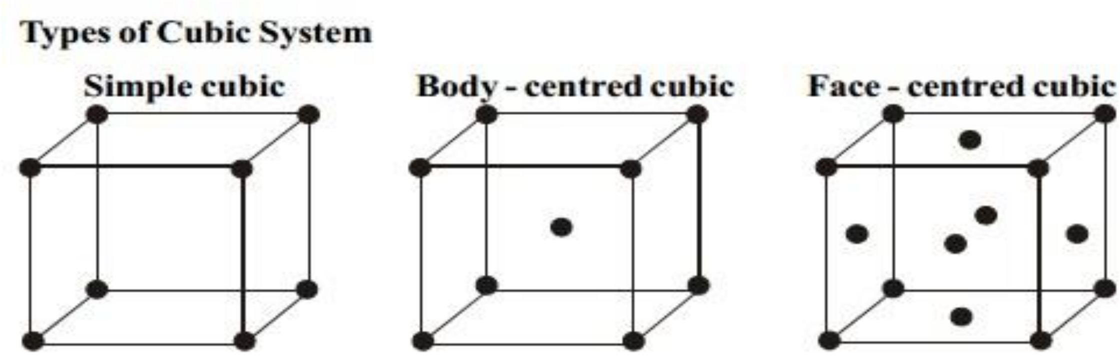


- **Atoms are present at the corners**
- **The contribution of corner atom to the unit cell is 1/8.**
- **One full atom at the centre of the unit cell**

CUBIC SYSTEM

Assignment of Atoms/ unit cell

Face Centered Cubic lattice (FCC)



- **Atoms are present at the corners**
- **The contribution of corner atom to the unit cell is 1/8.**
- **One face centred atom at the centre of all six faces**
- **The contribution face atoms to the unit cell is ½**

PRPOPERTIES OF UNIT CELL

Atoms per Unit cell

- This represents the content of atoms in unit cell

Atomic Radius

- It is the distance between the centers of two neighbouring atoms in contact

Coordination number

- It is the number of nearest equidistant neighbouring atoms to a given atom in a lattice

Atomic Packing factor (APF)

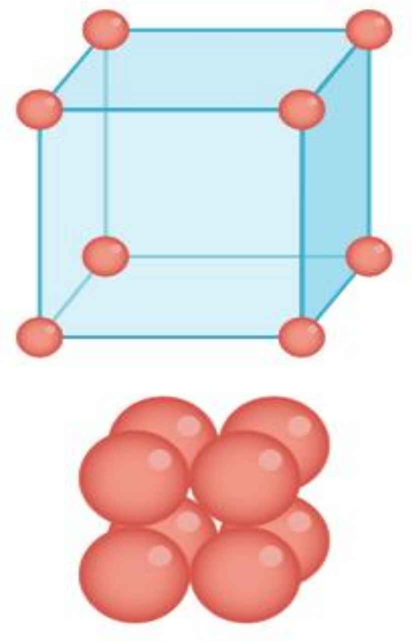
- It is the ratio of volume of atoms in a unit cell to the volume of unit cell

APF = Volume of atoms in unit cell / Volume of unit cell

SIMPLE CUBIC LATTICE (SC)

Number of Atoms / Unit cell

- Only corner atoms
- 8 corner atoms (1 per corner)
- Share of each corner atom = 1/8 of its volume
- Total no. of atoms **= 8 x 1/8 = 1 atom**



Simple cubic

https://www.coursehero.com/textbook-solutions/

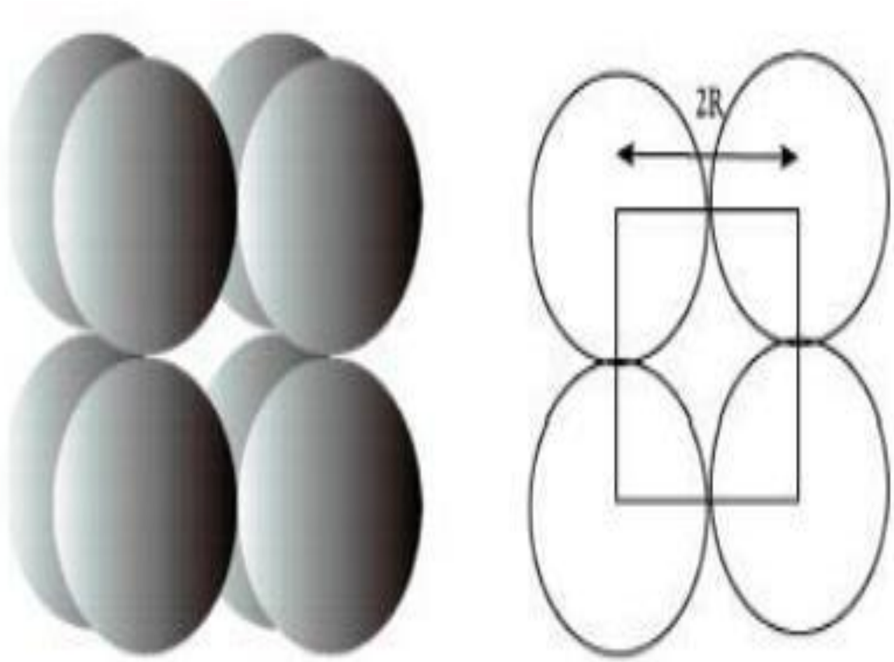
SIMPLE CUBIC LATTICE (SC)

Atomic radius

From figure

$$a = 2R$$

$$R = a/2$$



Source : https://www.slideshare.net/rpclemson/module2-71196024

SIMPLE CUBIC LATTICE (SC)

Coordination number

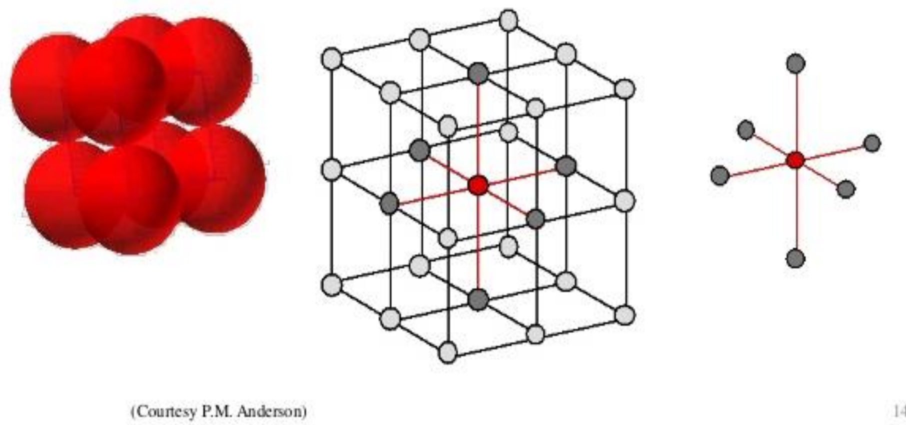
The corner atom

- has 4 atoms in its own plane
- 1 atom in lower plane
- 1 atom in upper plane
- All these are nearest neighbours

Therefore

the coordination number

4+1+1 = **6**



https://www.slideshare.net/rpclemson/module2-71196024

SIMPLE CUBIC LATTICE (SC)

Atomic Packing Factor

APF = Volume of atoms in unit cell / Volume of unit cell

no. of atoms $= 1$

volume of one atom $= \frac{4}{3}\pi r^3$

volume of unit cell (cubic) $= a^3$

when , $(a = 2r)$

$$\text{Filling Factor} = \frac{1 * \frac{4\pi r^3}{3}}{a^3}$$

$$= \frac{\frac{4\pi r^3}{3}}{(2r)^3} = \frac{\frac{4\pi r^3}{3}}{8r^3} = \frac{\pi}{6} = 52\%$$

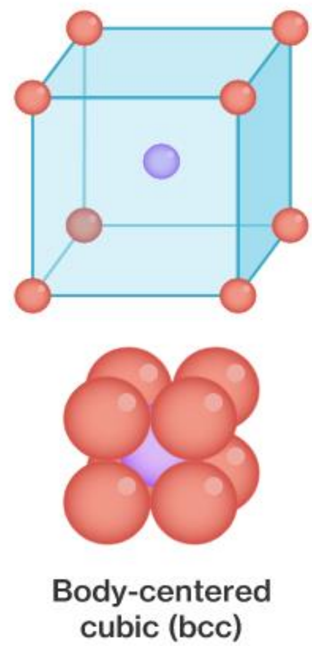
Source :http://www.uobabylon.edu.iq/eprints/publication_1_2901_199.pdf

BODY CENTRED CUBIC LATTICE (BCC)

Number of atoms/ unit cell

- 8 corner atom.
- 1 full body centered atom.
- Share of corner atom 8 x 1/8 =1
- Share of body centered atom =1
- Total no. of atoms per unit cell

1 + 1 = 2



https://www.coursehero.com/textbook-solutions/

BODY CENTRED CUBIC LATTICE (BCC)

Coordination number

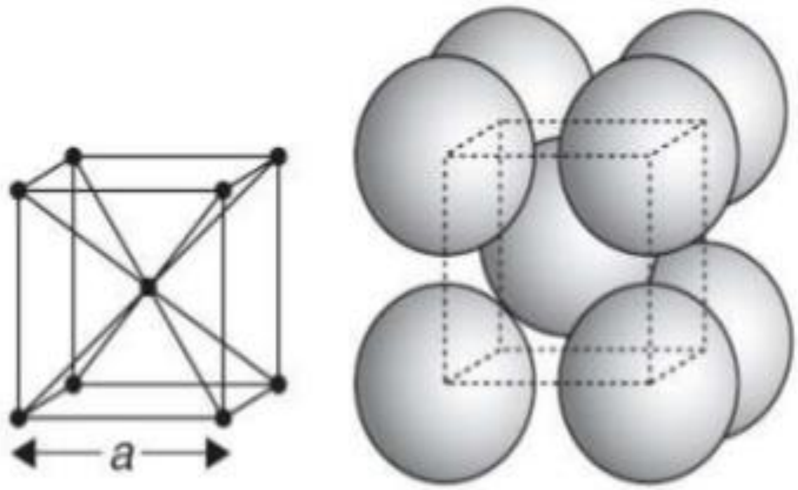
The body centered atom

- **has 4 atoms in upper plane**
- **4 atoms in lower plane**
- **All these are nearest neighbours**

Therefore

the coordination number

4+4 = 8

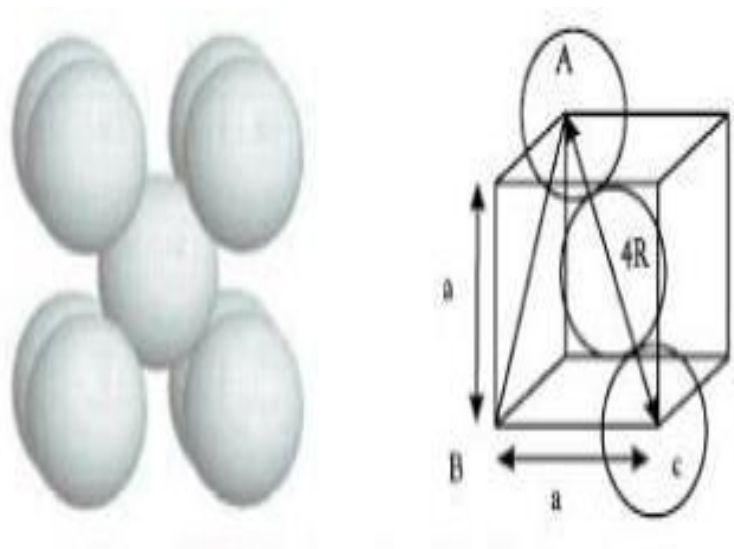


Source : https://www.slideshare.net/rpclemson/module2-71196024

BODY CENTRED CUBIC LATTICE (BCC)

Atomic radius

From figure



https://www.slideserve.com/mildred/unit-vii-crystal-structure

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

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

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

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

BODY CENTRED CUBIC LATTICE (BCC)

Atomic Packing Factor

APF = Volume of atoms in unit cell / Volume of unit cell

no of atoms =2

volume of tow atoms =2* $\frac{4}{3}\pi r^3$

volume of unit cell (cubic) = a^3

when $r = \frac{a\sqrt{3}}{4}$

Filling Factor = $\frac{2*\frac{4\pi r^3}{3}}{a^3}$

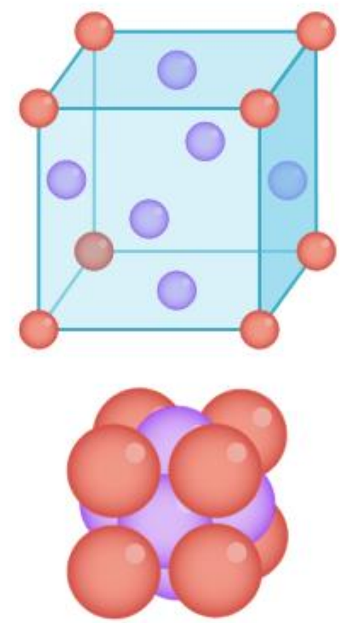
$$= \frac{\frac{8\pi r^3}{3}}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\frac{8\pi r^3}{3}}{\frac{64}{3\sqrt{3}}r^3} = \frac{\sqrt{3}\pi}{8} = 68\%$$

Source : http://www.uobabylon.edu.iq/eprints/publication_1_2901_199.pdf

FACE CENTRED CUBIC LATTICE(FCC)

Number of atoms

- 8 corner atom.
- 6 face centered atoms.
- Share of corner atom
  8x 1/8=1
- Share of each face centered atom = 1/2
- Total no. of atoms
  per unit cell = 1 + 6x(1/2)
  1+3 = 4



Face-centered cubic (fcc)

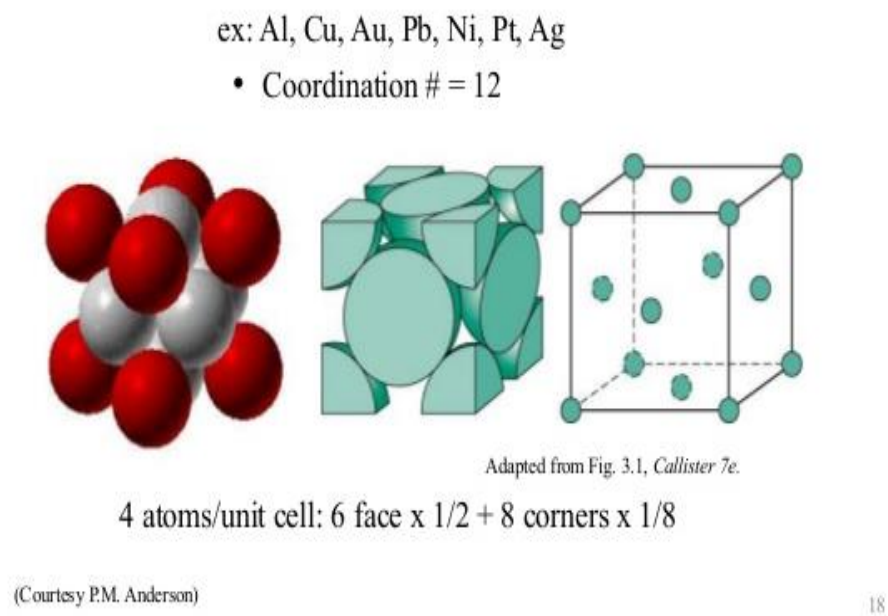
https://www.coursehero.com/textbook-solutions/

FACE CENTRED CUBIC LATTICE(FCC)

Coordination number

The face centered atom has

- 4 corner atoms in its own plane
- 4 face centred atoms in upper plane
- 4 face centred atoms in lower plane



Therefore

the coordination number

4+4 +4= **12**

Source : https://www.slideshare.net/rpclemson/module2-71196024

FACE CENTRED CUBIC LATTICE(FCC)

Atomic radius

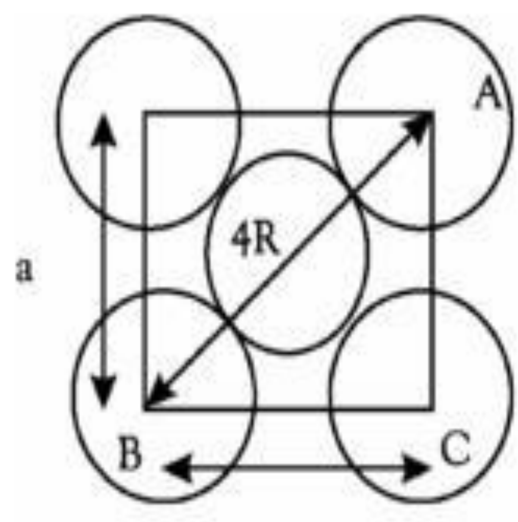
From figure

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

$16R^2 = 2a^2$

$R^2 = 2/16\ a^2$

$R = \sqrt{2}/4\ a = a/2 \sqrt{2}\ a$



Source :http://www.uobabylon.edu.iq/eprints/publication_1_2901_199.pdf

FACE CENTRED CUBIC LATTICE (FCC)

Atomic Packing Factor

APF = Volume of atoms in unit cell / Volume of unit cell

no of atoms $= 4$

volume of four atoms $= 4 * \frac{4}{3} \pi r^3$

volume of unit cell (cubic) $=$ a^3

when $r = \frac{a\sqrt{2}}{4} = \frac{a}{2\sqrt{2}}$

Filling Factor $= \frac{4 * \frac{4\pi r^3}{3}}{a^3}$

$$= \frac{\frac{16\pi r^3}{3}}{(2\sqrt{2}r)^3} = \frac{\frac{16\pi r^3}{3}}{16\sqrt{2}\, r^3} = \frac{\sqrt{2}\pi}{6} = 74\%$$

Source :http://www.uobabylon.edu.iq/eprints/publication_1_2901_199.pdf

HEXAGONAL CLOSE PACKED STRUCTURE

Ex: cobalt, cadmium, zinc, beryllium, magnesium, titanium and zirconium.

HCP structure consist of three layers

- ✓**In top and bottom layers,**

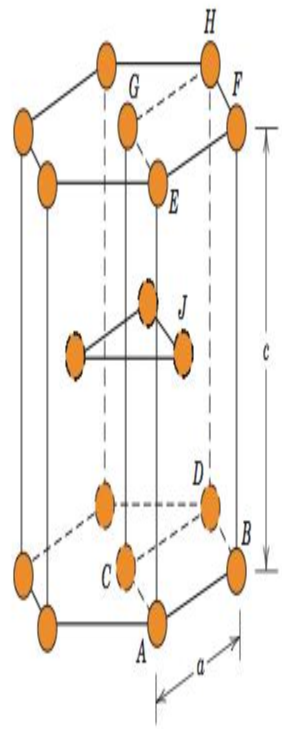
  six atoms at the corners of each hexagon and one atom at the centre of hexagon.

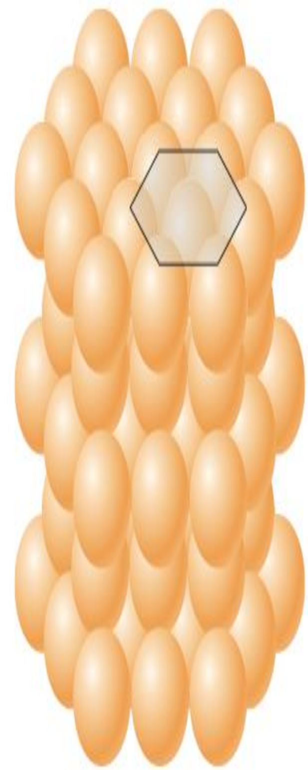
- ✓**In the middle layer**

  three atoms.

- ✓**The distance between atoms in hexagonal plane is "a"**

- ✓**The distance between central atoms of top and bottom hexagonal planes is "c"**





Credit: Callister & Rethwisch 5e

HEXAGONAL CLOSE PACKED STRUCTURE(HCP)

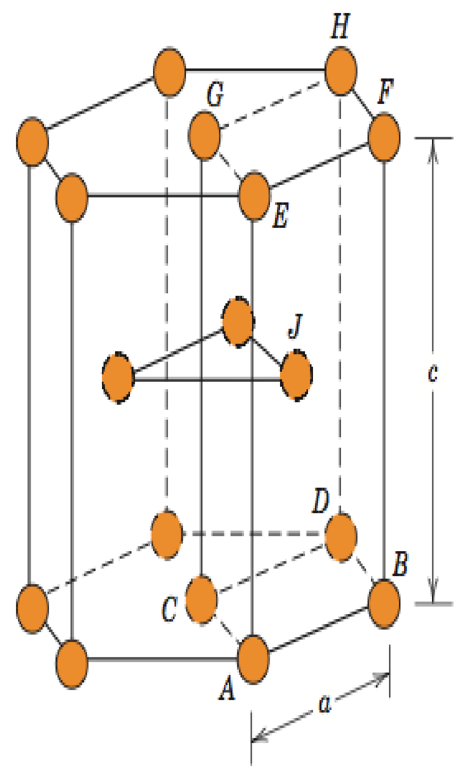
Number of atoms

- ✓ 12 corner atom.
- ✓ 2 face centered atoms.
- ✓ 3 central atoms
- ✓ Share of corner atom is 1/6

  (upper hexagonal plane 1/3 & lower hexagonal plane 1/3)
- ✓ Share of each face centered atom is 1/2
- ✓ Three full atoms at the centre
- ✓ Total no. of atoms

  per unit cell

  12x (1/6) + 2X(1/2) + 3 = **6**



Credit: Callister & Rethwisch 5e

HEXAGONAL CLOSE PACKED STRUCTURE(HCP)

Coordination number

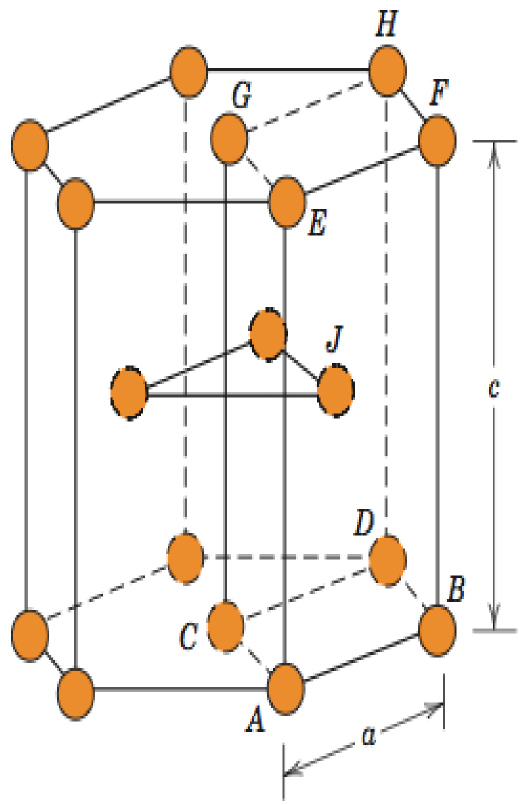
The face centered atom at the centre of hexagon has

- 6 corner atoms in its own plane
- 3 nearer central atoms in upper plane
- 3 nearer central atoms in lower plane

Therefore

Coordination number

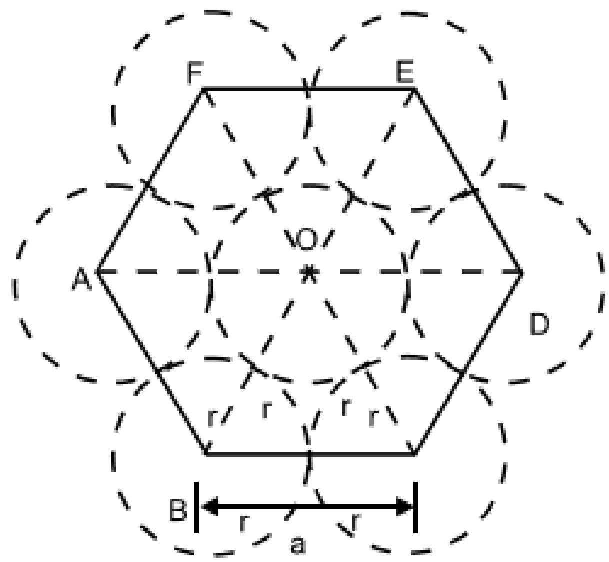
6+3 +3= **12**



HEXAGONAL CLOSE PACKED STRUCTURE(HCP)

Atomic radius

In HCP structure, the corner atoms in the hexagonal plane touch each other and all corner atoms touch the face centered atom.



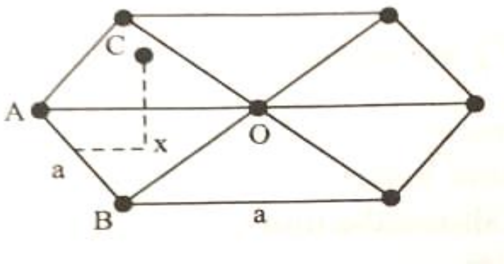
Therefore atomic radius

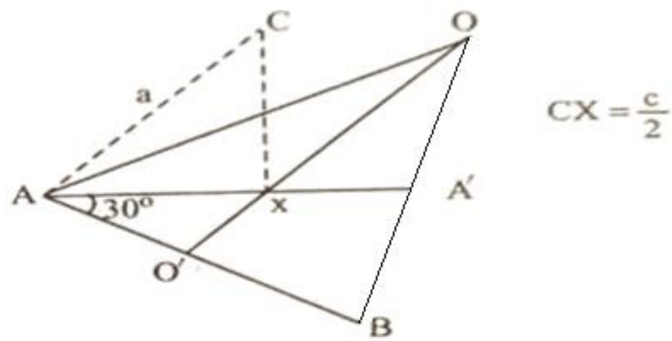
$a = 2r$

$r = a/3$

HEXAGONAL CLOSE PACKED STRUCTURE(HCP)

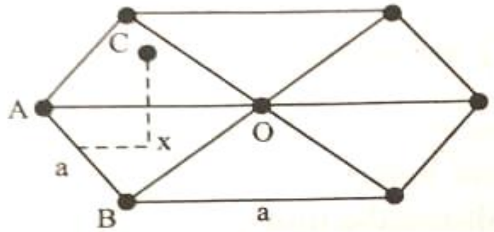
CALCULATION OF c/a RATIO

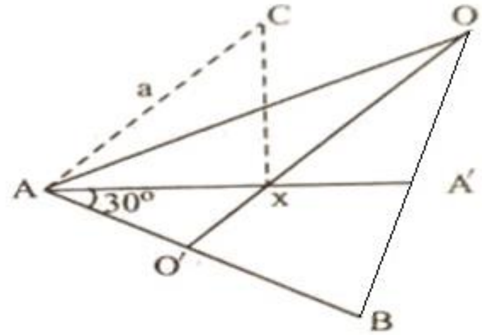




- Consider the figures a and b shown above.
- Each top and bottom hexagonal layers of hcp structure consist of 6 corner and 1 central atom.
- The middle layer consists of three full atoms. Consider one such atom
- Let C be the atom situated at the central plane of hcp structure

CALCULATION OF c/a RATIO (HCP)





$CX = \frac{c}{2}$

$$\angle A'AB = 30^\circ$$

$$\cos 30^\circ = \frac{AA'}{AB}$$

$$\text{Therefore } AA' = AB\cos 30 = a\frac{\sqrt{3}}{2}$$

$$\text{But } AX = \frac{2}{3}AA' = \frac{2}{3}a\frac{\sqrt{3}}{2}$$

$$= \frac{a}{\sqrt{3}}$$

In triangle AXC,

$$AC^2 = AX^2 + CX^2$$

$$\text{Hence } CX^2 = AC^2 - AX^2$$

$$= a^2 - \frac{a^2}{3} = \frac{2}{3}a^2$$

CALCULATION OF c/a RATIO (HCP)

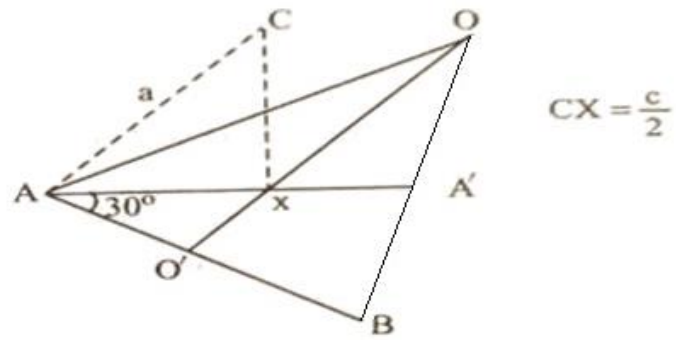
But $CX = \frac{c}{2}$

Therefore $\frac{c^2}{4} = \frac{2}{3}a^2$

or $\left(\frac{c}{a}\right)^2 = \frac{8}{3}$

or $\frac{c}{a} = \sqrt{\frac{8}{3}}$

$= 1.633$

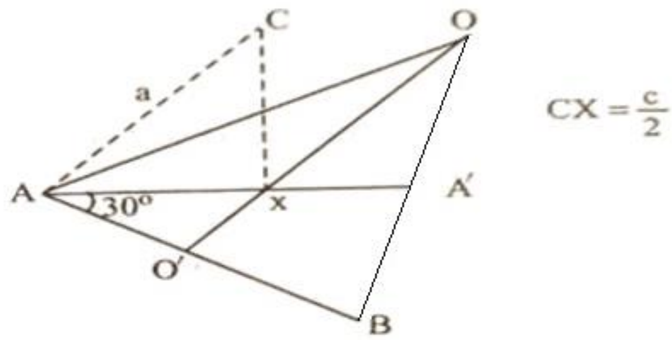


CALCULATION OF PACKING FACTOR (HCP)

Area of the base = 6 × area of the triangle ABO

$$= 6 \times \frac{1}{2} \times AB \times OO'$$

$$= 3 \times a \times \frac{\sqrt{3}}{2} a = \frac{3\sqrt{3}}{2} a^2$$



Volume of unit cell V = area of the base × height

$$= \frac{3\sqrt{3}}{2} a^2 c$$

$$\text{Packing factor} = \frac{v}{V} = \frac{6 \times \frac{4}{3}\pi r^3}{\frac{3\sqrt{3}}{2} a^2 c} = \frac{16\pi r^3}{3\sqrt{3}\, a^2 c}$$

CALCULATION OF PACKING FACTOR (HCP)

Substituting for $\frac{c}{a}$,

$$\text{Packing factor} = \frac{2\pi}{3\sqrt{3}}\sqrt{\frac{3}{8}}$$

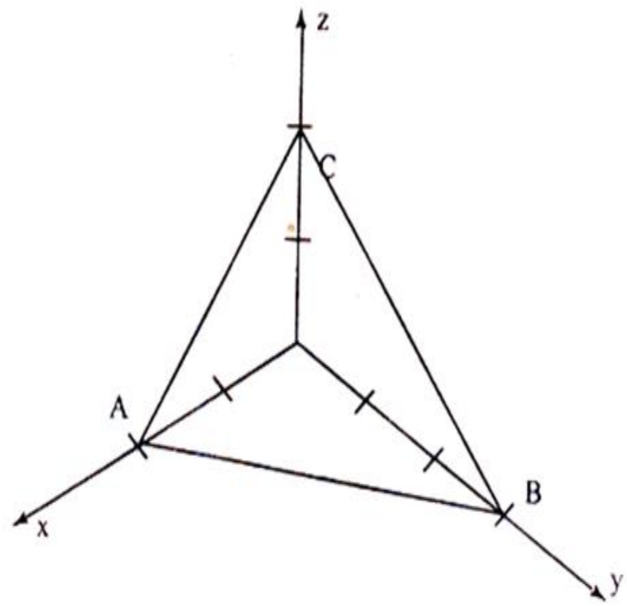
$$= \frac{\pi}{3\sqrt{2}} = 0.74$$

$$= 74\%$$

Since the packing density is 74%, the hcp structure is a closely packed structure. Since FCC also has same packing density, both HCP and FCC are called as closely packing structures

MILLER INDICES OF CRYSTAL PLANES

- Miller indices designate the directions of various planes in crystal structure.
- Miller Indices are set of three numbers enclosed in a parenthesis.
- In the figure the plane intercepts at x,y and z axes are 2,3 and 2 respectively.
- The orientation of this plane is represented by the Miller indices (3 2 3)



http://www.chemohollic.com/2016/08/all-bout-miller-indices.html

STEPS TO FIND MILLER INDICES

- ✓ Find the intercepts of the plane on three axes in terms of lattice constants

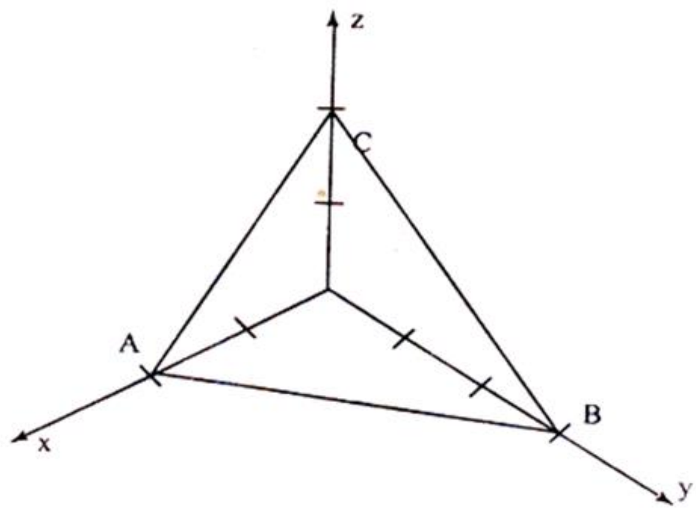
  2a, 3b, 2c
- ✓ Take the coefficients of intercepts

  2, 3, 2
- ✓ Take the ratio of reciprocals

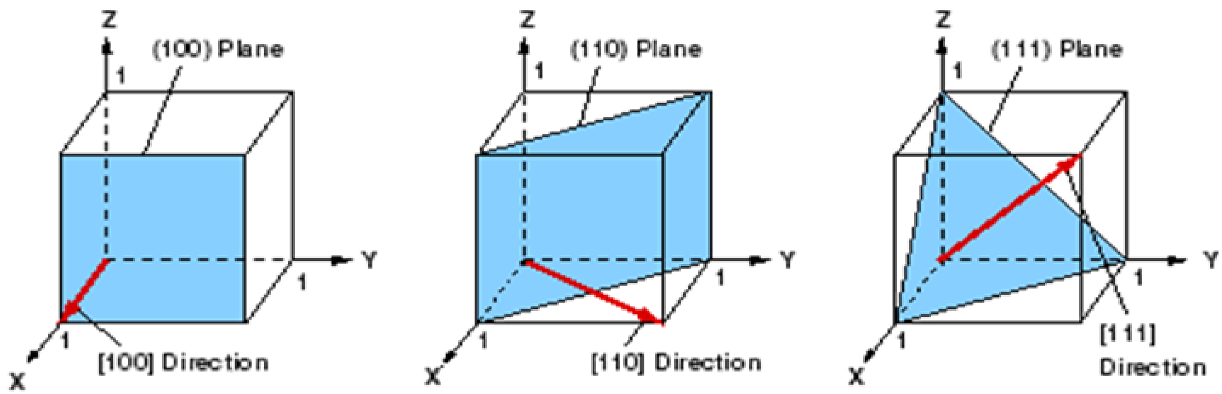
  1 / 2 : 1/3, 1 /2
- ✓ Convert these reciprocals in to whole number by multiplying with LCM

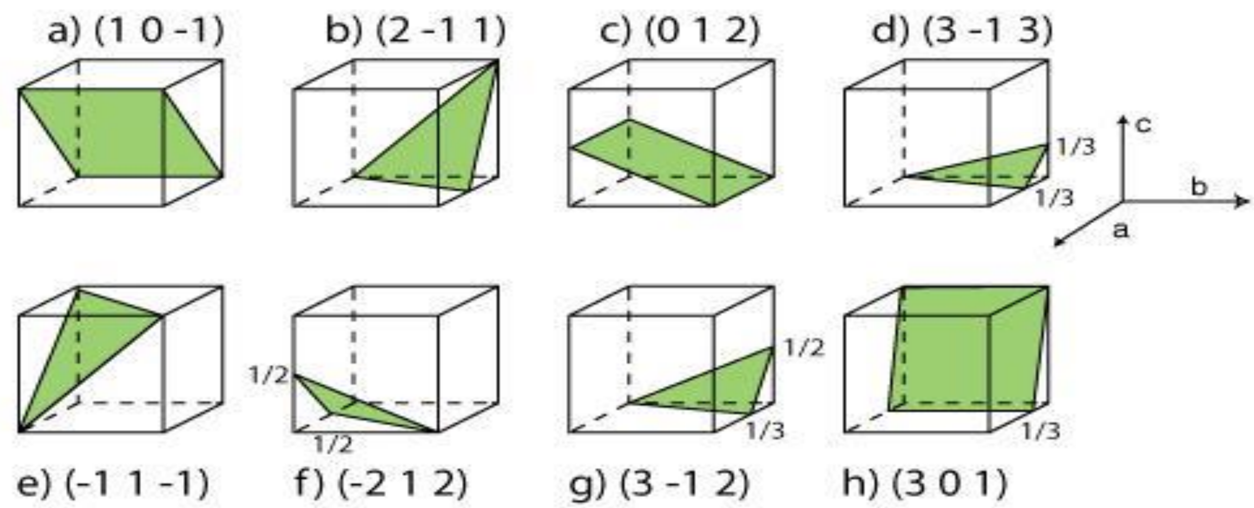
  3 2 3
- ✓ Enclose in parenthesis

  (3 2 3)
- ✓ **The Miller indices of the given plane is (3 2 3)**



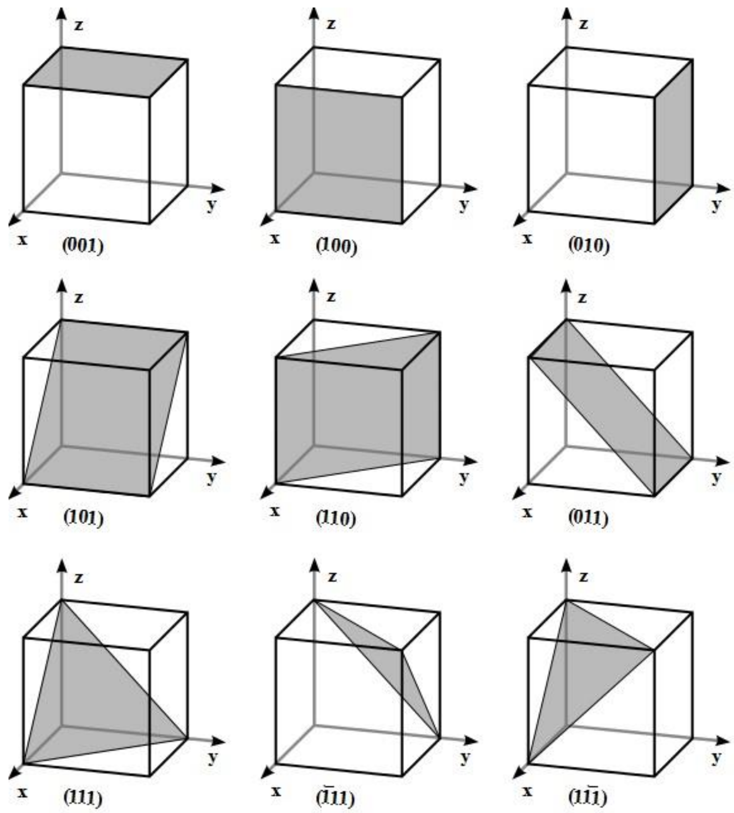
MILLER INDICES OF VARIOUS PLANES





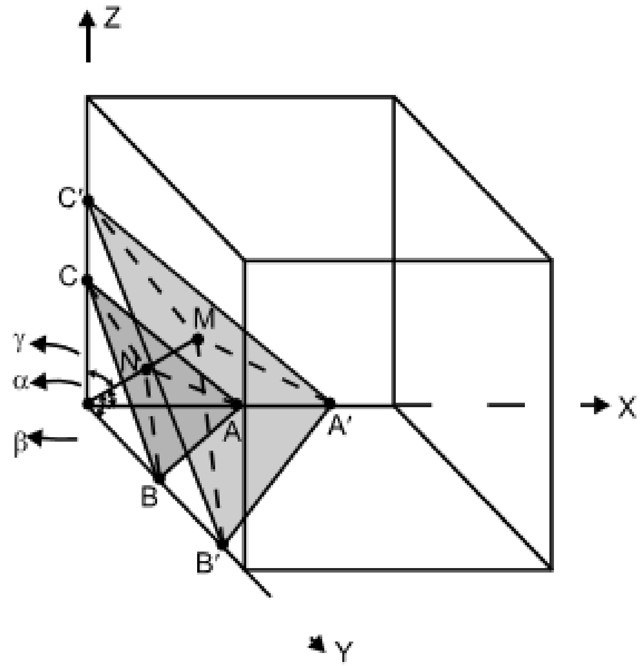
http://www.chemohollic.com/2016/08/all-bout-miller-indices.html

MILLER INDICES OF VARIOUS PLANES



http://www.chemoholic.com/2016/08/all-bout-miller-indices.html

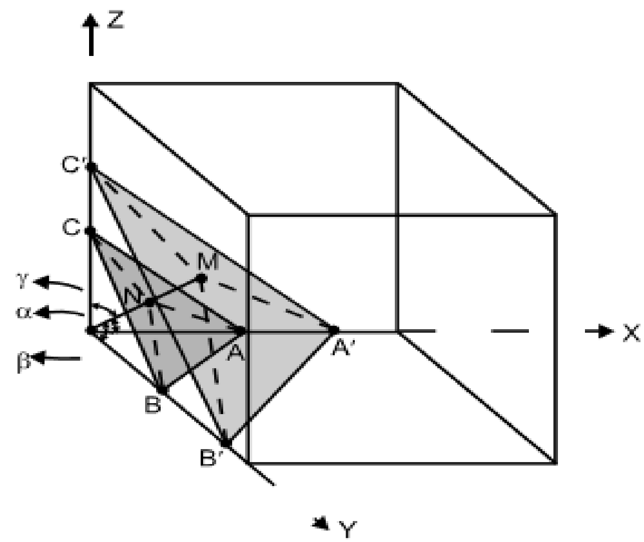
INTERPLANAR DISTANCE



Consider a cubic crystal it consists of number of unit cells. Consider a plane ABC whose miller indices are (hkl). Consider another one plane $A'B'C'$ whose

INTERPLANAR DISTANCE

miller indices are same as the miller indices of plane $ABC(hkl)$. The plane ABC makes OA, OB and OC as intercepts on the crystallographic axes OX, OY and OZ respectively whose values are equal to 'a'. In addition, the plane $A'B'C$ makes OA', OB' and OC' as intercepts on the crystallographic axes OX, OY and OZ respectively whose values are equal to '$2a$'. Draw a perpendicular $ON = d_1$ and $OM = d_2$ from the origin of the cube 'O' to the plane ABC and $A'B'C'$ respectively. The distance between the two plane is 'd' it is called inter planar distance. Let the normal ON and OM makes an angle α, β and γ with respect to the crystallographic axes OX, OY and OZ respectively.



From figure

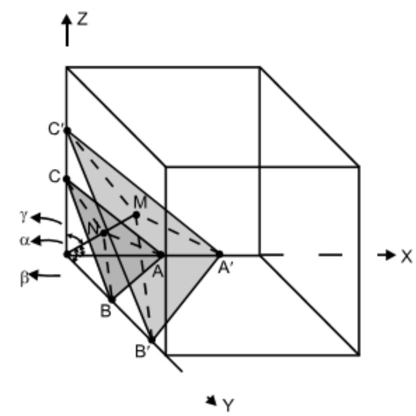
$$\angle NOX = \angle MOX = \alpha$$
$$\angle NOY = \angle MOY = \beta$$
$$\angle NOZ = \angle MOZ = \gamma$$
$$ON = d_1$$
$$OM = d_2$$
$$NM = d_2 - d_1 = d$$

INTERPLANAR DISTANCE

(i) To find the distance d_1

The reciprocal of miller indices (hkl) gives intercept values of the plane ABC on the crystallographic axes OX, OY and OZ. i.e., $OA = \frac{a}{h}; OB = \frac{a}{k}$ and $OC = \frac{a}{l}$ In right angled $\bigsqcup ONA$,

$$\cos\alpha = \frac{ON}{OA} = \frac{d_1}{\left(\frac{a}{h}\right)} = \frac{d_1 h}{a} \quad \therefore \quad \cos^2\alpha = \left(\frac{d_1 h}{a}\right)^2 \quad \text{or} \quad \cos^2\alpha = \frac{d_1^2 h^2}{a^2}$$



In right angled $\bigsqcup ONB$,

$$\cos\beta = \frac{ON}{OB} = \frac{d_1}{\left(\frac{a}{k}\right)} = \frac{d_1 k}{a} \quad \cos^2\beta = \left(\frac{d_1 k}{a}\right)^2 \quad \therefore \quad \cos^2\beta = \frac{d_1^2 k^2}{a^2}$$

In right angled $\bigsqcup ONC$,

$$\cos\gamma = \frac{ON}{OC} = \frac{d_1}{\left(\frac{a}{l}\right)} = \frac{d_1 l}{a} \quad \cos^2\gamma = \left(\frac{d_1 l}{a}\right)^2 \quad \therefore \quad \cos^2\gamma = \frac{d_1^2 l^2}{a^2}$$

INTERPLANAR DISTANCE

From the law of direction cosines,

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

$$\frac{d_1^2 h^2}{a^2} + \frac{d_1^2 k^2}{a^2} + \frac{d_1^2 l^2}{a^2} = 1$$

$$\frac{d_1^2}{a^2} h^2 + k^2 + l^2 = 1$$

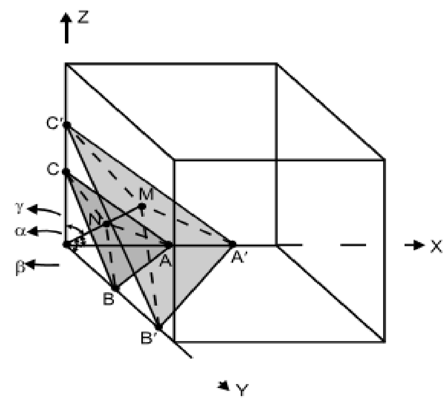
$$\therefore \quad d_1^2 = \frac{a^2}{(h^2 + k^2 + l^2)}$$

INTERPLANAR DISTANCE

(ii) **To find the distance d_2**

The reciprocal of miller indices (hkl) also gives intercept values of the plane $A'B'C'$ on the crystallographic axes OX, OY and OZ. i.e., In right angled $\sqcup OMA'$,

$$\cos\alpha = \frac{OM}{OA^1} = \frac{d_2}{\left(\frac{2a}{h}\right)} = \frac{d_2 h}{2a} \quad \cos^2\alpha = \left(\frac{d_2 h}{2a}\right)^2 \quad \therefore \quad \cos^2\alpha = \frac{d_2^2 h^2}{4a^2}$$



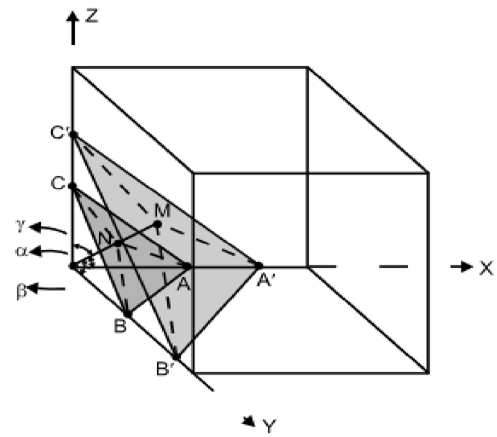
In right angled $\sqcup OMB'$,

$$\cos\beta = \frac{OM}{OB'} = \frac{d_2}{\left(\frac{2a}{k}\right)} = \frac{d_2 k}{2a} \quad \cos^2\beta = \left(\frac{d_2 k}{2a}\right)^2 \quad \therefore \cos^2\beta = \frac{d_2^2 k^2}{4a^2}$$

In right angled $\sqcup OMC'$

$$\cos\gamma = \frac{OM}{OC'} = \frac{d_2}{\left(\frac{2a}{l}\right)} = \frac{d_2 l}{2a} \quad \cos^2\gamma = \left(\frac{d_2 l}{2a}\right)^2 \quad \therefore \cos^2\gamma = \frac{d_2^2 l^2}{4a^2}$$

INTERPLANAR DISTANCE



From the law of direction cosines,

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

$$\frac{d_2^2 h^2}{4a^2} + \frac{d_2^2 k^2}{4a^2} + \frac{d_2^2 l^2}{4a^2} = 1$$

$$\frac{d_2^2}{4a^2}(h^2 + k^2 + l^2) = 1$$

$$\therefore \quad d_2^2 = \frac{4a^2}{(h^2 + k^2 + l^2)}$$

$$\boxed{d_2 = \frac{2a}{\sqrt{h^2 + k^2 + l^2}} \text{ or } \frac{2a}{(h^2 + k^2 + l^2)^{\frac{1}{2}}}}$$

From the equation (20) and (21)

Inter planar distance $d = d_2 - d_1$

$$d = \frac{2a}{\sqrt{h^2 + k^2 + l^2}} - \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\boxed{d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \text{ or } \frac{a}{(h^2 + k^2 + l^2)^{\frac{1}{2}}}}$$

What are the important features of Miller indices?

1. When a plane is parallel to any one of the three crystallographic axes, its intercepts on that axes is infinity (∞). Hence its miller index for that axis is Zero (0).
2. When the intercepts of a plane on any axis is negative a bar is put on the corresponding miller index.
3. All equally spaced parallel planes have the same index number (hkl).
4. Miller indices do not define a particular plane, it define a set of parallel planes.
5. It is only the ratio of the indices. i.e., the plane (211) and (422) are the same.
6. A plane passing through the origin is defined in terms of a parallel plane having non-zero intercepts.

X Ray Diffraction (XRD)

Useful for the findings on;

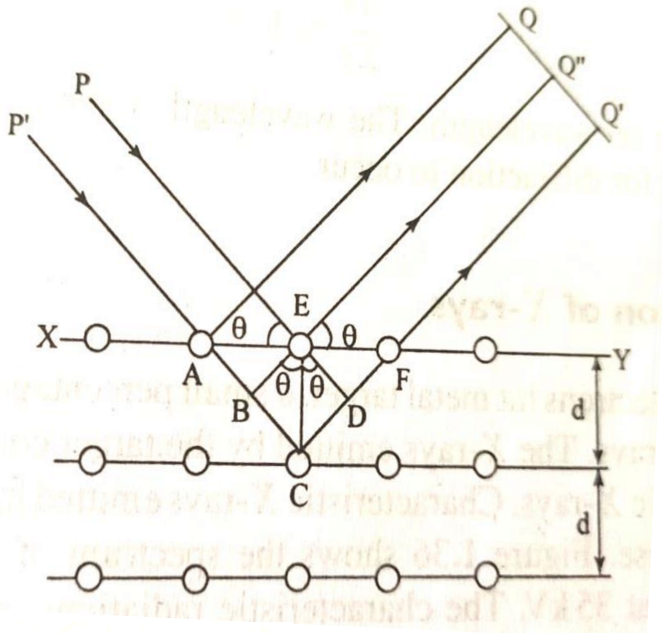
- Crystal structure of materials
- Orientation of single crystal grain
- Size and shape of small crystalline regions in polycrystalline materials
- Average spacing between layers of atoms

X Ray Diffraction

- Diffraction will occur when the size of the obstacle is of the order of wavelength of the incident radiation.
- **The evaluation of material structure is obtained from diffraction of incident radiation over the material atoms.**
- In material structure atoms are the obstacles and they diffract the incident radiation when the radiation wavelength is of the order of size of atoms.
- **In the case of X-rays this condition is met and hence X-ray diffraction is used to analyse material (crystal) structure.**
- The arrangement of atoms in the cleavage planes of a space lattice act as three dimensional grating and hence diffraction occurs.

Bragg's law

- **W.L Bragg discovered the reflection of X-rays in the cleavage plans of the crystal, when X-rays incident at some glancing angle, known as Bragg's angle.**
- The condition for the constructive interference between the reflected X-rays was given by the Bragg's law.



$$2d \sin\theta = \lambda \qquad (\because \quad n = 1)$$

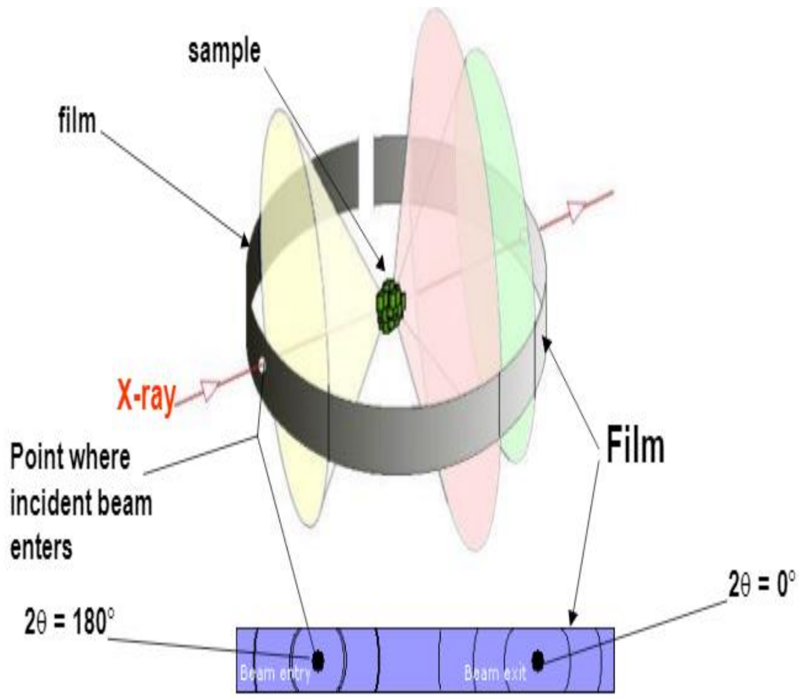
Powder X Ray Diffraction

This method is suitable to powder crystalline material or finely grained polycrystalline material

Also called as Debye-Scherrer method

Used in the findings;

- **Lattice parameters of crystals of known structure**
- **Identification of elements**



https://docplayer.net/11027738-X-ray-diffraction-xrd.html

Debye-Scherrer Method

Powder X Ray Diffraction

✓Powder specimen is taken in a small capillary tube

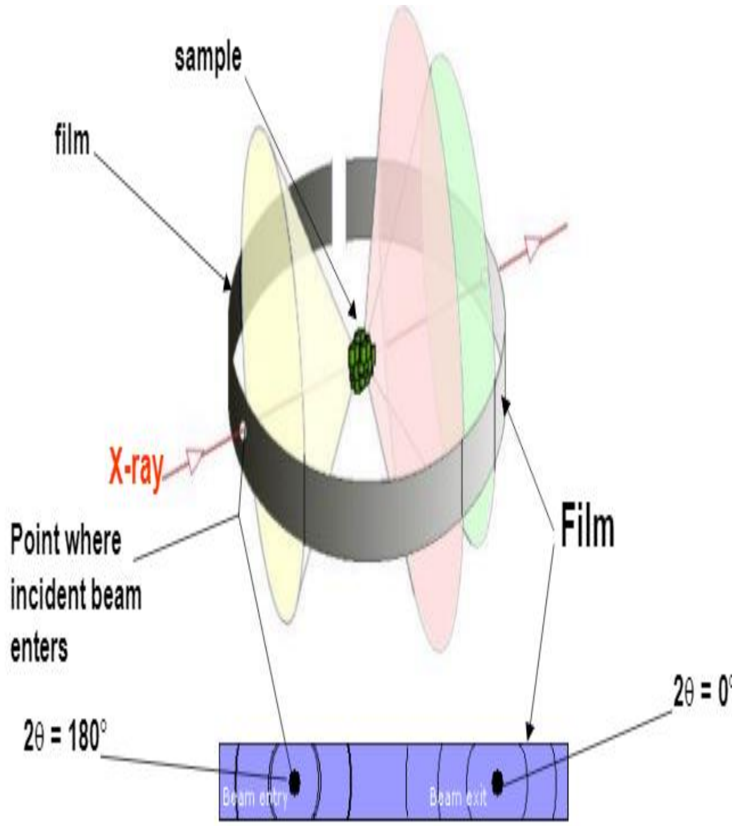
✓ Pencil beam of X rays are diffracted by the powder

✓Diffracted rays are recorded by a photogrphic film as a series of varying curves

✓The distane S between two corresponding arcs in photographic plate measures full opening angle 4θ of diffraction cone

❑4θ = S / R radians, where

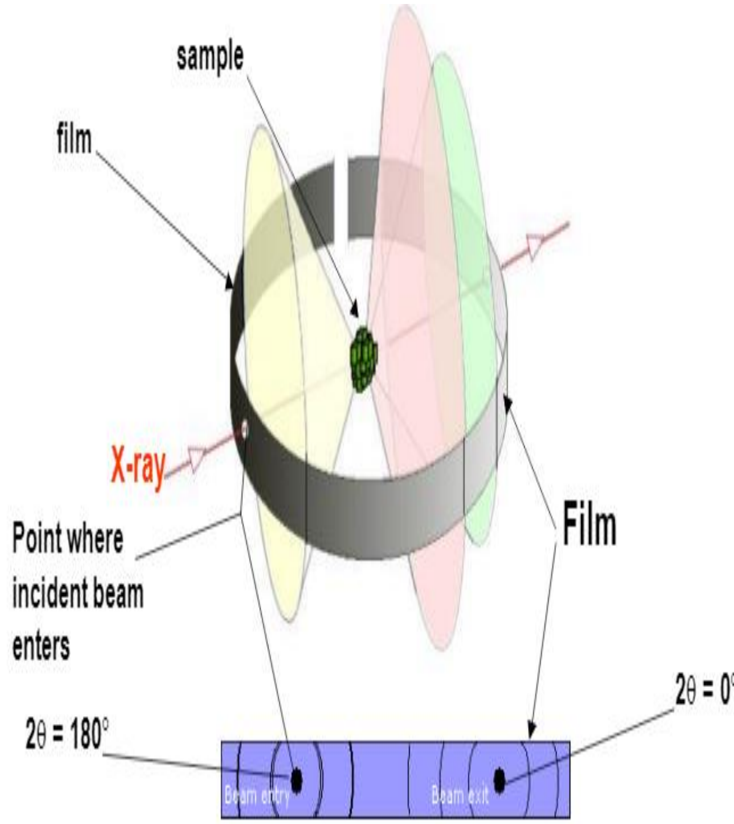
❑R – Specimen to film distance



✓Using the S values of S , values of θ can be tabulated

✓Using the values of θ and λ , interplanar spacing "d" can be determined

✓Using the "d" values between the planes, indexing for reflection and unit cell parameters can be obtained.



Lattice defects – Qualitative ideas of point, line, surface and volume defects

Crystal defects (or) Imperfections

Minor deviation from the periodicity of arrangement of atoms at the surface or inside a crystal is called defect or imperfection.

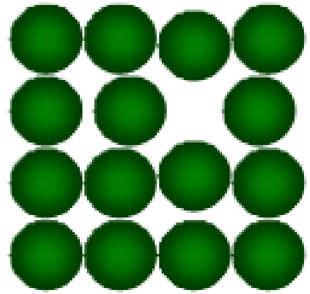
Many crystal properties are defect centric.

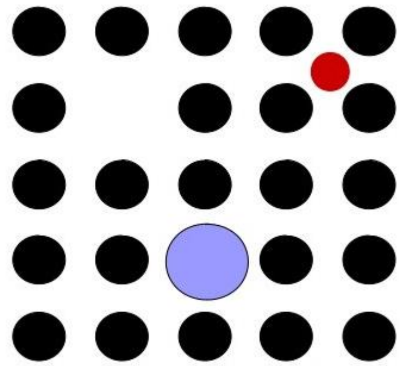
Various crystalline imperfections

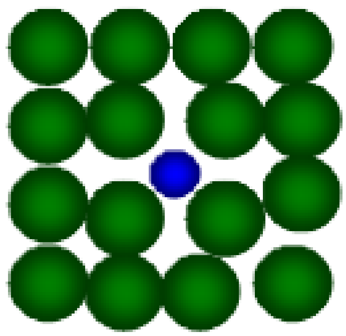
- **Point Imperfection**
- **Line imperfection**
- **Surface imperfection**
- **Volume imperfection**

Point Imperfections

- These are also called as zero dimensional imperfections
- Imperfections are point like regions at the Size of one or two atom size
- Unnecessary presence or absence of atoms result in imperfections

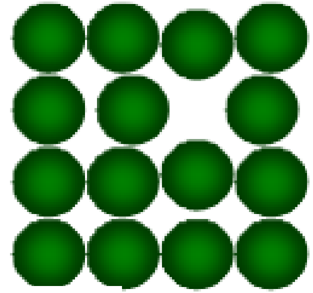






https://www.askiitians.com/iit-jee-solid-state/imperfections-in-solids-and-defects-in-crystals/

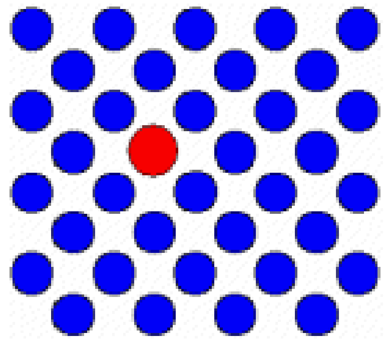
Types of Point Imperfections



Vacancy

Refers to the missing of an atom from its actual place in lattice

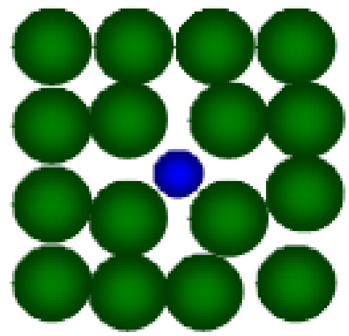
Substitutional Impurity



Refers to a foreign atom that replaces a parent atom in the crystal lattice

Ex: doping of pentavalent or trivalent atoms in semiconductor

Interstitial Impurity

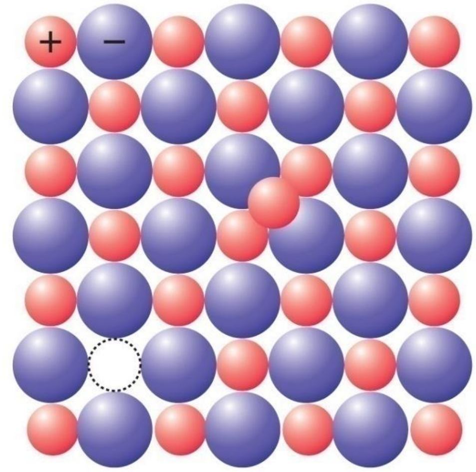


Refers to a small foreign atom which occupies the interstitial space in the lattice without affecting the parent atoms from the their regular place

https://www.askiitians.com/iit-jee-solid-state/imperfections-in-solids-and-defects-in-crystals/

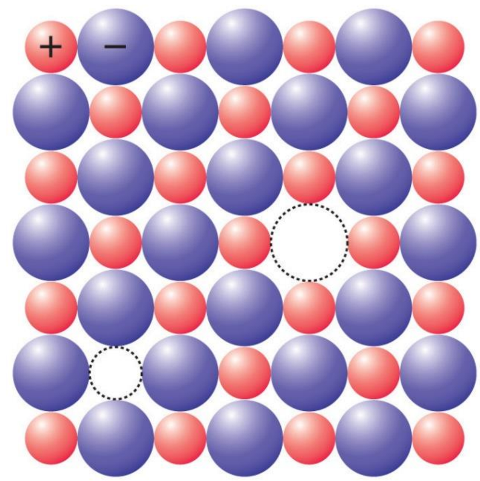
http://studytronics.weebly.com/crystal-structure--defects.html

Interstitial Impurity



❑ Frenkel effect

- Occurs in ionic crystals
- Due to displacement of cations from their regular sites to interstitial sites
- Since cations are smaller, does not affect the lattice



❑ Schottkey effect

- Occurs due to the missing of a pair of anion and cation from their regular place in a lattice

https://www.askiitians.com/iit-jee-solid-state/imperfections-in-solids-and-defects-in-crystals/

Line Imperfections

- One dimensional imperfections
- Also called as **dislocations**

Types

- **Edge dislocation**
- **Screw dislocation**

Edge dislocation

✓Consider a crystal space lattice as shown in fig.1.

✓The image at the bottom of **fig.1** represents the front side atomic arrangement.

✓The arrangement shows the periodic arrangement of atoms in all vertical lines of lattice

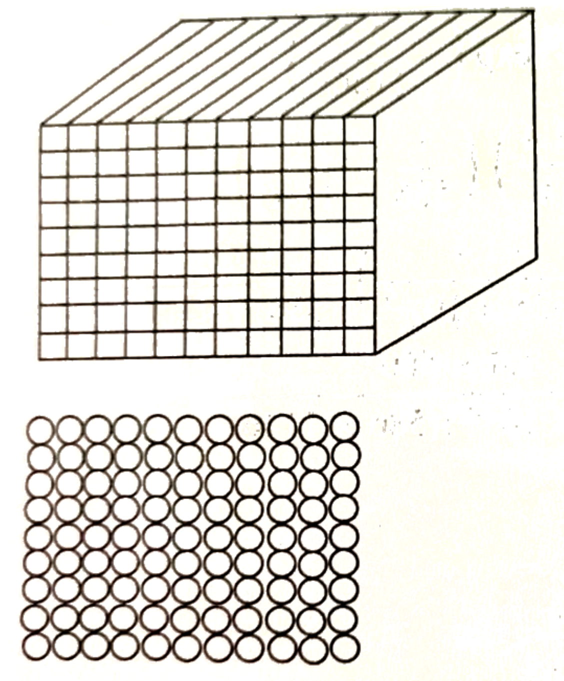


Fig.1

Line Imperfections

Edge dislocation

- In fig.2 there is a discontinuity in atomic ordering in one of the line.
- This type of missing of atoms in a line is called line imperfection
- Above the imperfection the atoms are compressed and below the imperfection the atoms are dragged out and in a state of tension.
- This distorted configuration extends up to the edge of the crystal as shown in fig.2

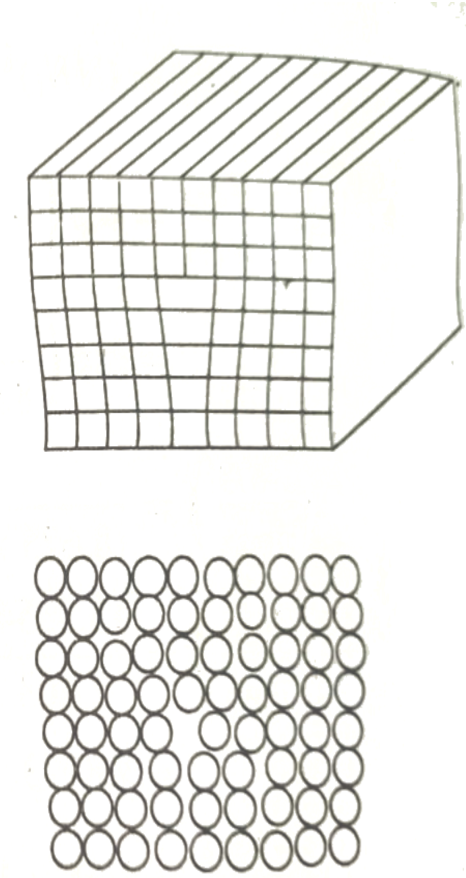
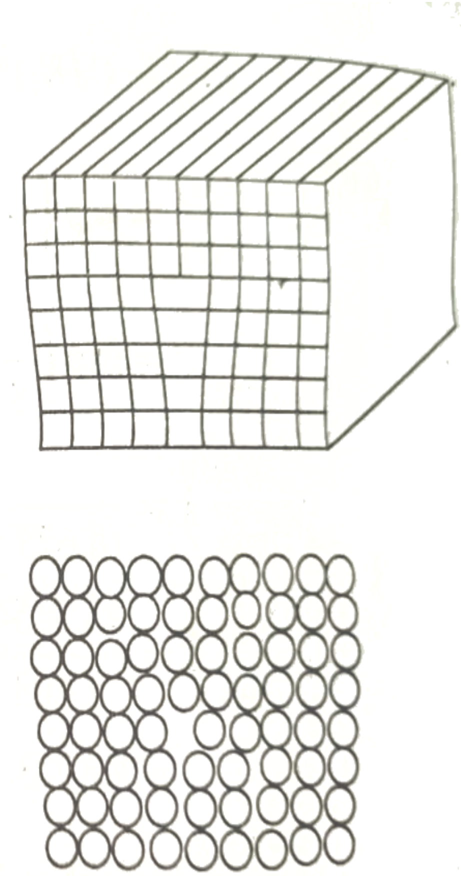


Fig.2

Line Imperfections

Edge dislocation

Positive and negative edge dislocations



- When the incomplete plane starts from the top of crystal it is positive edge location

- If it is from bottom of crystal it is negative edge dislocation

Line Imperfections

Edge dislocation

Burgers Vector

The magnitude and direction of displacement is called Burger vector.

Fig.3 shows a perfect crystal

- **A vector line is drawn from P.**
- **It travels through 6 atoms top**
- **Then travels through 5 atoms right**
- **Then travels through 5 atoms down**
- **Then travel through 6 atoms left and reaches the point P.**
- **Burger circuit is closed**

Fig.3

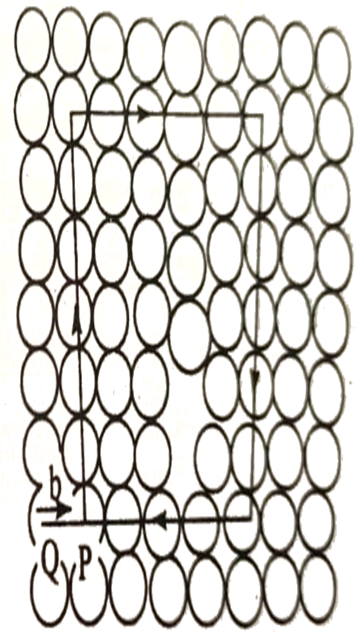


Fig.4

Line Imperfections

Edge dislocation

Burgers Vector

- Fig.4 shows a crystal with edge dislocation
- When the above operation is repeated, the vector ends up in Q instead of P
- To reach P , we have toreturn through QP
- The vector QP is the Burger vector
- Burger Vector BV = QP = b

Fig.3

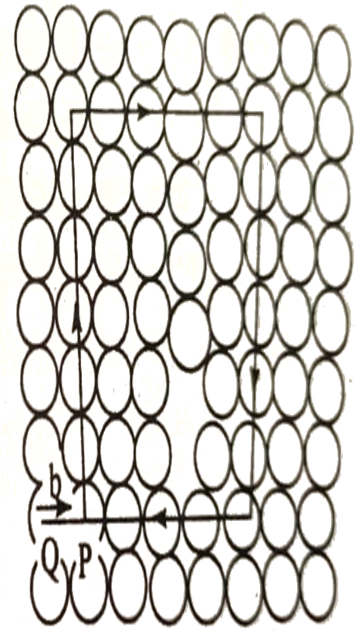


Fig.4

Line Imperfections

Screw dislocation

- Fig.5 shows a crystal with screw dislocation
- It is due to the displacement of atoms in one part of a crystal relative to the other part.
- This creates a spiral ramp at the line of dislocation
- b is the burger vector at the edge dislocation
- Burger circuit is drawn as shown in the fig5.

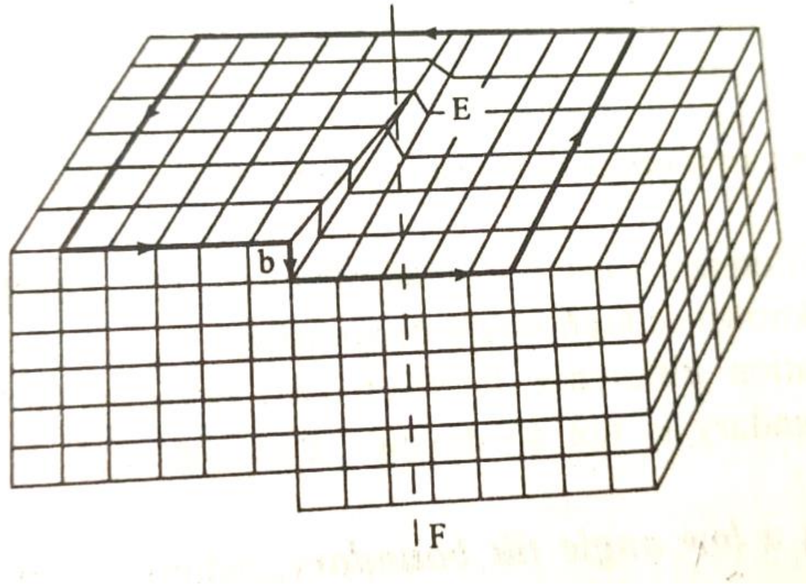


Fig.5

Surface Imperfections

- ❑Distortions at the crystal surface of few atomic diameter thickness
- ❑Occurs due to the termination of atomic bonds at the surface
- ❑Also occurs inside the crystal during recrystallization process
- ❑In recrysatallization, the grains of crystal grow in different orientations as shown in fig.6

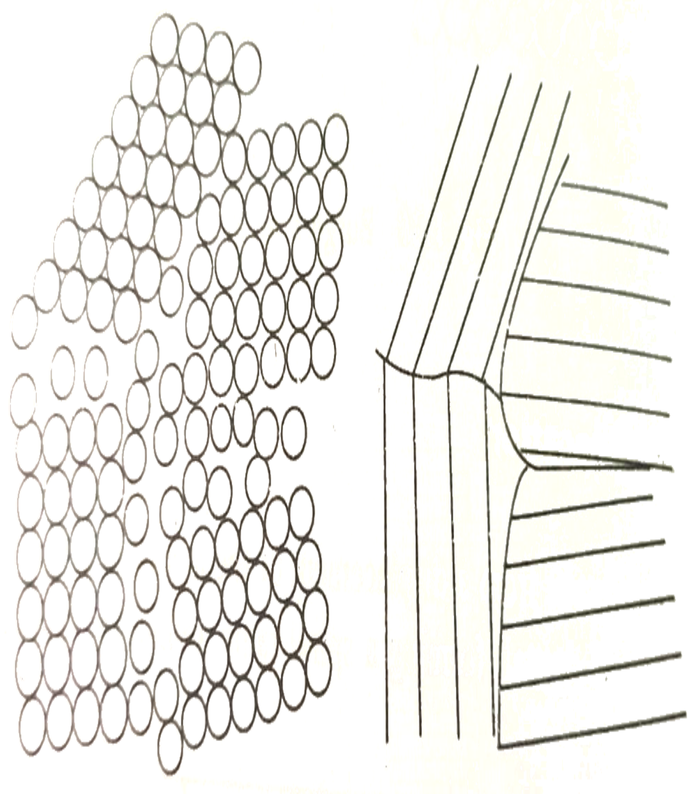


Fig. 6

Surface Imperfections

- One grain compress the another one and atoms at boundary displaced to equilibrium due to varying forces at the boundary
- The regions are called grain boundaries
- They have thickness of few atomic diameter
- The misalignment of grains result in a sharp change of crystal orientation at the boundary as shown in fig.6

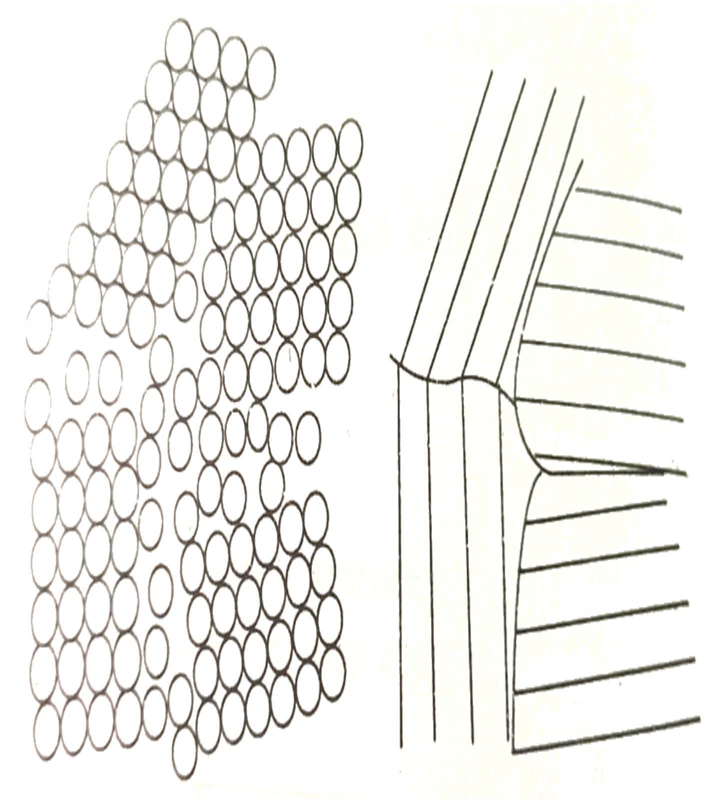


Fig.6

Surface Imperfections

High angle and Low angle boundaries

High angle boundaries

❑If the orientation difference between the grains (crystals) is greater than 10 degrees (Fig.6)

Low angle tilt boundaries

❑The orientation difference is less than 10 degrees. The tilt boudary is shown in Fig.7

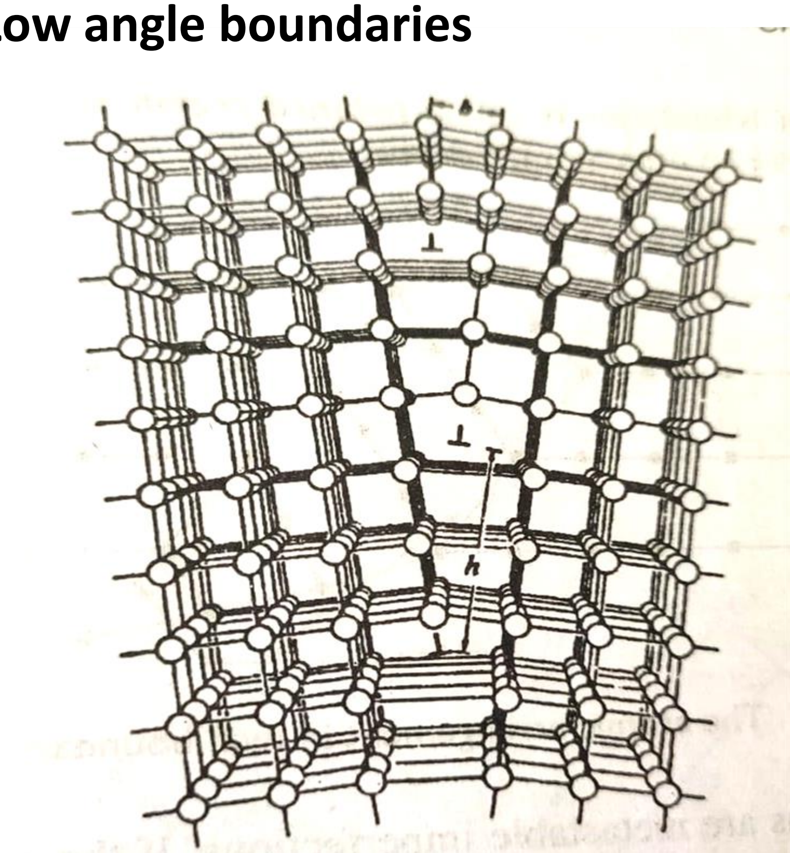


Fig.7

Surface Imperfections

Stacking Faults

❖Planar surface imperfection

❖Occurs due to the fault in the stacking sequence of atomic planes in crystals

Twin Boundaries

❖Planar surface imperfection

❖Atomic arrangements in one side of boundary is the mirror image of other side of boundary

❖The intermediate region is called twinned region (Fig.8)

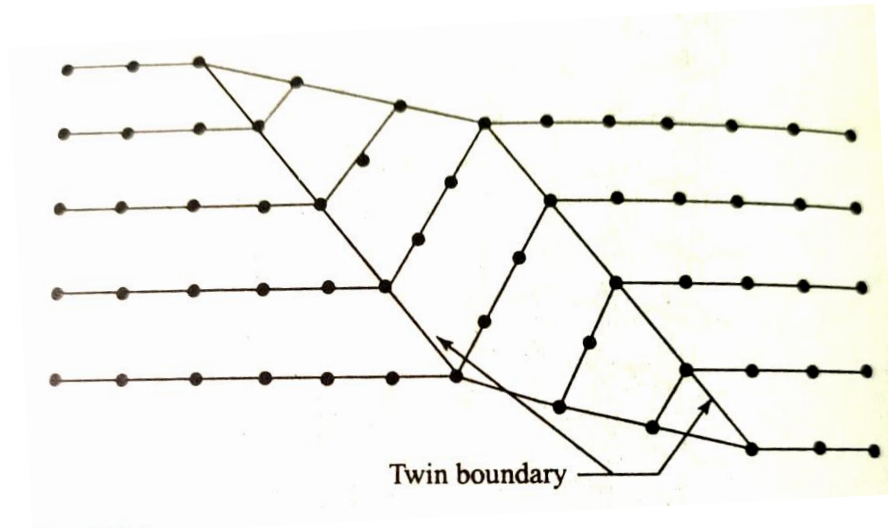


Fig.8

Volume Imperfections

Cracks in a crystal is a volume defect

❖**Cracks may occur during growth**

❖**Cracks can occur due to the electrostatic dissimilarity produced between layers of crystal during growth**

❖**Cracks may occur when crystal is subjected to an external stimulus**

Missing a cluster of atoms inside the crystal

❖**Large void in the crystal is also a volume defect**

When the crystal is grown, chances are there for the setting up of non crystalline regions of considerable size inside the crystal.