IV. CONDENSED MATTER PHYSICS

UNIT –I CRYSTAL PHYSICS

Lecture - I

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Semester-I

IV. CONDENSED MATTER PHYSICS

UNIT –I CRYSTAL PHYSICS

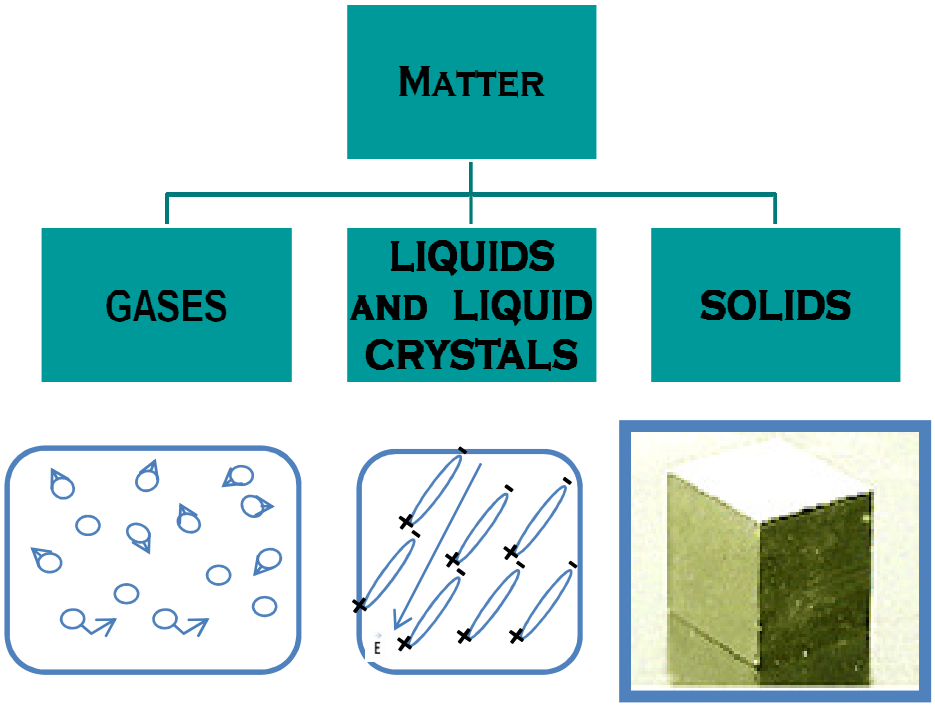
Crystalline state of solids, simple crystal structures, Bragg condition, Brillouin zones, reciprocal lattice, structure factor; comparison of X-ray, electron and neutron diffraction methods; types of bonding.

CRYSTAL PHYSICS

- **INTRODUCTION TO CRYSTAL PHYSICS**
- **CRYSTALLINE AND NONCRYSTALLINE SOLIDS**
- **SPACE LATTICE**
- **CRYSTAL STRUCTURE**
- **LATTICE PARAMETERS**
- **CRYSTAL SYSTEMS**
- **BRAVAIS LATTICES**

INTRODUCTION TO CRYSTAL PHYSICS

Crystal Physics' or ***'Crystallography'*** is a branch of physics that deals with the study of all possible types of crystals and the physical properties of crystalline solids by the determination of their actual structure by using X-rays, neutron beams and electron beams.



- Matter exists in three different states – solids, liquids and gases.
- All these states are composed of atoms and molecules.
- When we focus the solids, they are classified into many types based on several properties like electrical, mechanical, magnetic, optical, thermal etc.,
- The main reason for these different properties of solids is their crystal structure.

CLASSIFICATION OF SOLIDS

- Solids can broadly classified into two types based on the arrangement of units of matter. The units of matter may be atoms, molecules or ions. They are,
  - Crystalline solids and
  - Non-crystalline (or) Amorphous solids

- A substance is said to be crystalline when the arrangement of units of matter is regular and periodic.

- A crystalline material has directional properties and therefore called as anisotropic substance.

- A crystal has a sharp melting point.

- It possesses a regular shape and if it is broken, all broken pieces have the same regular shape.

CRYSTALLINE SOLIDS

- A crystalline material can either be a single (mono) crystal or a polycrystal.

- A single crystal consists of only one crystal, whereas the polycrystalline material consists of many crystals separated by well-defined boundaries.

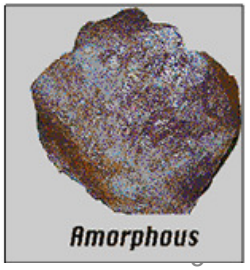
Examples - Metallic crystals – Cu, Ag, Al, Mg etc,
Non-metallic crystals – Carbon,Silicon,Germanium,

NON CRYSTALLINE SOLIDS

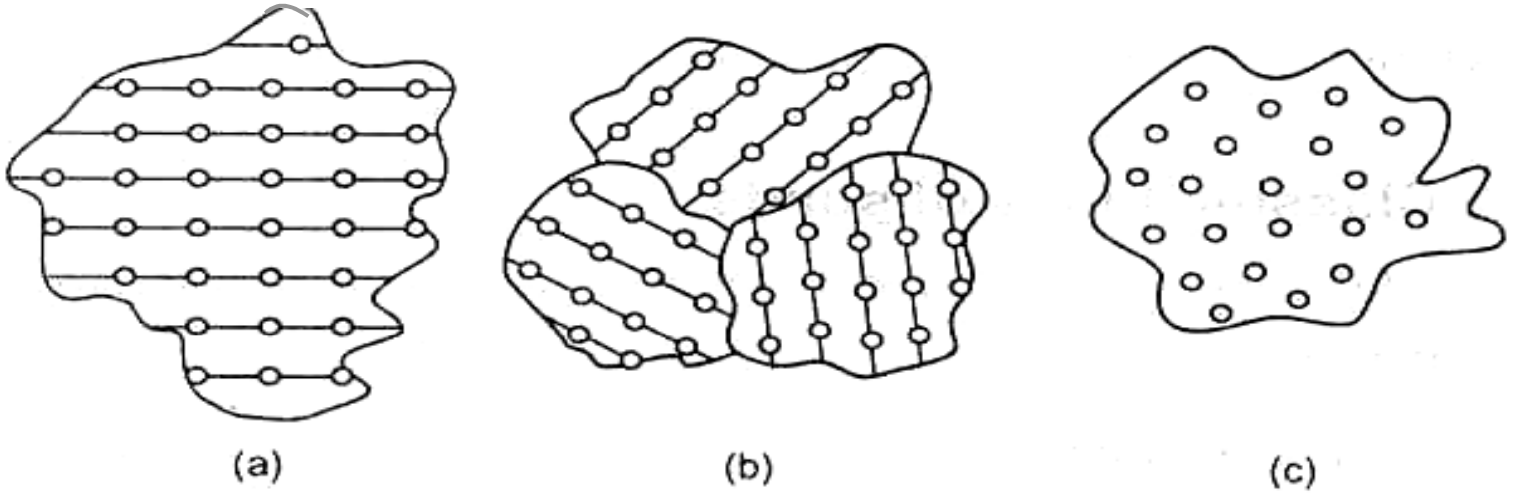
- In amorphous solids, the constituent particles are not arranged in an orderly manner. They are randomly distributed.

- They do not have directional properties and so they are called as `isotropic' substances.

- They have wide range of melting point and do not possess a regular shape.
Examples: Glass, Plastics, Rubber etc.,



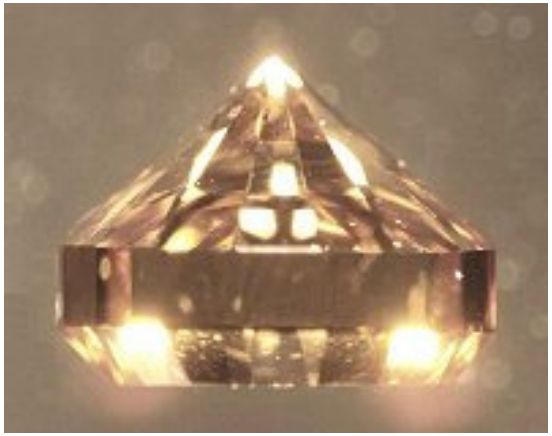
ATOMIC ARRANGEMENT IN CRYSTALS



(a) mono (or) single crystals **(b) polycrystalline solids** **(c) amorphous solids**

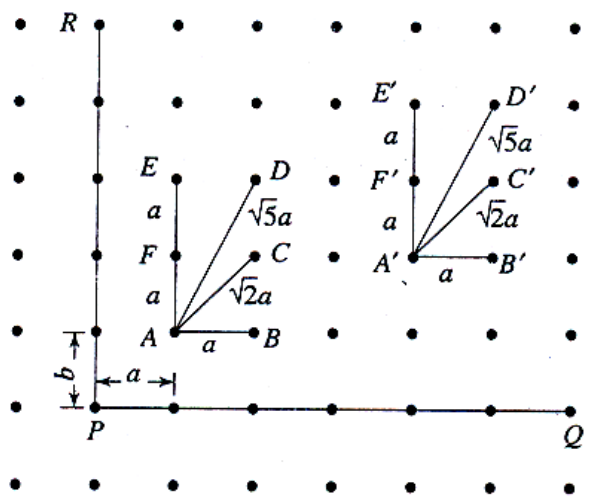
CRYSTALS

➢ It is a substance in which the constituent particles are arranged in a systematic geometrical pattern.



SPACE LATTICE

The regular and periodic arrangement of infinite number of points in a space is called space lattice. It is also called as Crystal lattice.



- Consider the points P, Q and R.
- Let us join the points P and Q by a straight line, and the point P and R by another straight line.
- The line PQ is taken as X-axis and the line PR is taken as Y-axis.
- The distance between any two successive lattice points in the X-direction is taken as `a'.

- Similarly, the distance between any two successive lattice points along the Y-direction is taken as `b'.

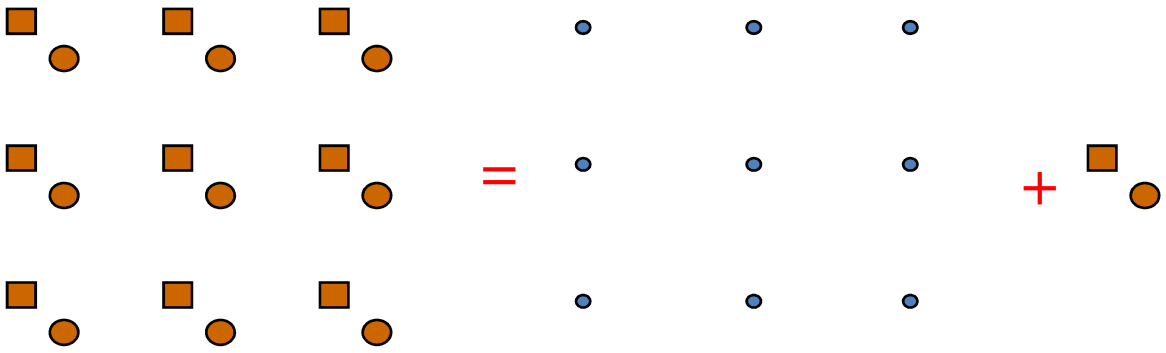
- Here a and b are said to be lattice translational vectors. Consider a square lattice in which a=b.

BASIS AND CRYSTAL STRUCTURE

- A crystal structure is formed by associating every lattice point with an unit assembly of atoms or molecules identical in composition, arrangement and orientation. This unit assembly is called the `***basis***'.

- When the basis is repeated with correct periodicity in all directions, it gives the actual crystal structure.

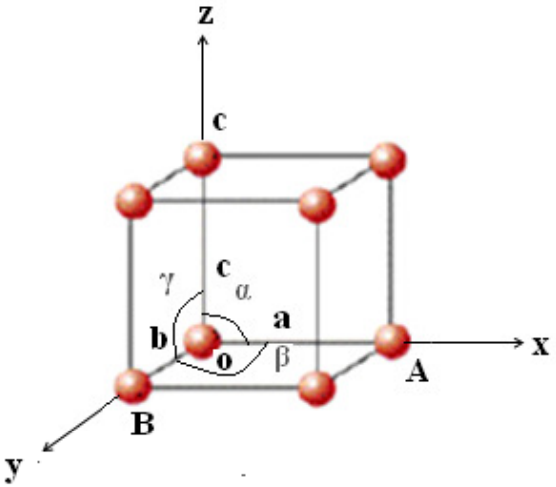
- The crystal structure is real, while the lattice is imaginary.

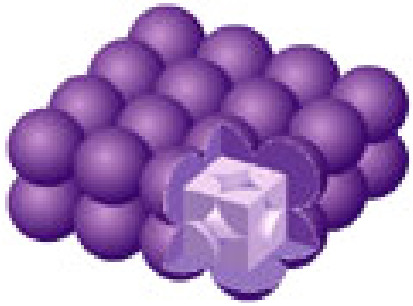


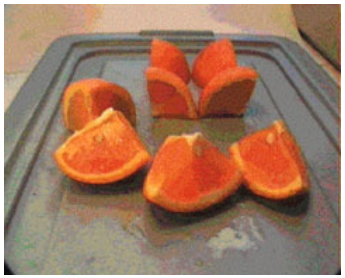
Crystal structure = Lattice + Basis

UNIT CELL

A unit cell is defined as a fundamental building block of a crystal structure, which can generate the complete crystal by repeating its own dimensions in various directions.



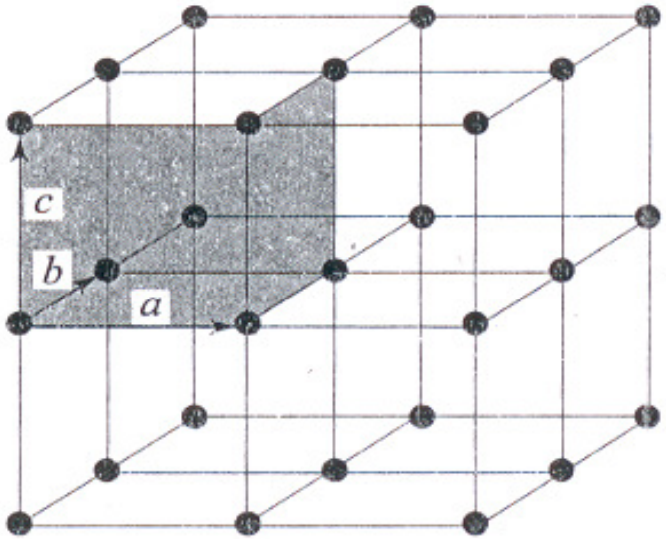




- Consider a unit cell consisting of three mutually perpendicular edges OA, OB and OC as shown in figure. Draw parallel lines along the three edges.
- These lines are taken as crystallographic axes and they are denoted as X, Y and Z axes.
- These intercepts are known as ***primitives***. In crystallography the intercepts OA, OB and OC are represented as $\vec{a}$, $\vec{b}$ and $\vec{c}$. The angle between X and Y axes is represented as β.
- Similarly the angles between Y and Z and Z and X axes are denoted by ′γ′ and ′α′ respectively as shown in the figure. These angles α, β and γ are called as ***interaxial angles or interfacial angles***.
- To represent a lattice, the three interfacial angles and their corresponding intercepts are essential. These six parameters are said to be ***lattice parameters***.

PRIMITIVE CELL

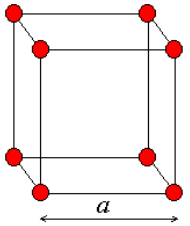
It is the smallest unit cell in volume constructed by primitives. It consists of only one full atom



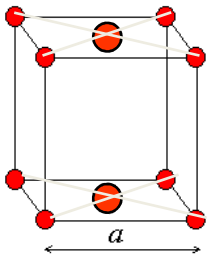
- A primitive cell is one, which has got the points or atoms only at the corners of the unit cell.
- If a unit cell consists of more than one atom, then it is not a primitive cell.
- Example for primitive cell :Simple Cubic unit cell.
- Examples for non-primitive cell:BCC and FCC unit cell.

Unit Cell Configurations

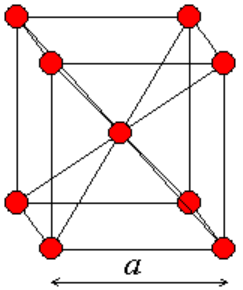
The space lattices formed by unit cells are marked by the following symbols.



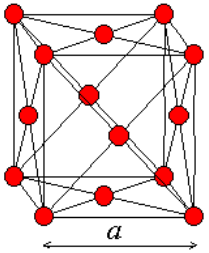
➢ Primitive lattice:P → having lattice points only at the corners of the unit cell.



➢Base centred lattice:C → having lattice points at the corners as well as at the top and bottom base centres of the unit cell.



➢ Body centred lattice:I → having lattice points at the corners as well as at the body centre of the unit cell.



➢Face centred lattice:F → having lattice points at the corners as well as at the face centres of the unit cell.

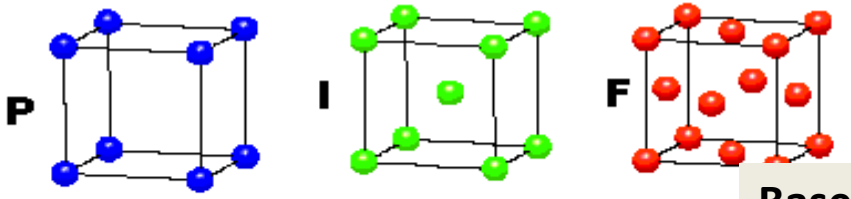
CRYSTALS SYSTEMS

- Cubic (isometric)
- Tetragonal
- Orthorhombic
- Trigonal (rhombohedral)
- Hexagonal
- Monoclinic and
- Triclinic

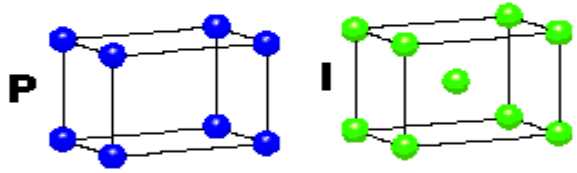
➢ Bravais in 1948 showed that 14 types of unit cells under seven crystal systems are possible. They are commonly called as ***`Bravais lattices***

CRYSTAL SYSTEM

CUBIC
$a = b = c$
$\alpha = \beta = \gamma = 90°$

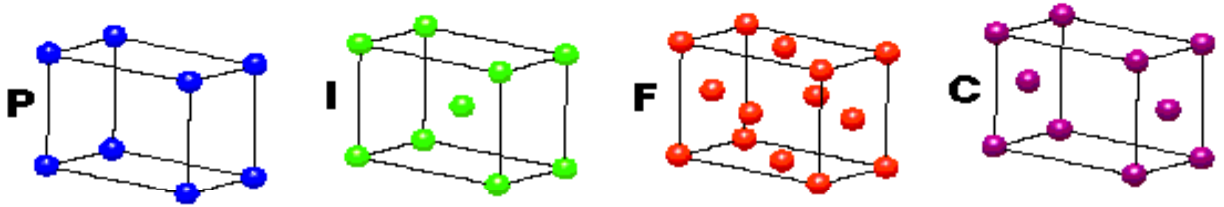


TETRAGONAL
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

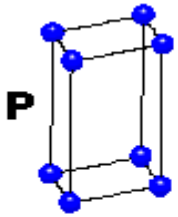


Based on unit cell configurations and atomic arrangements

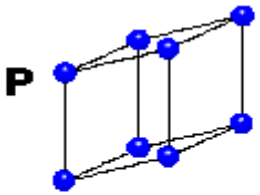
ORTHORHOMBIC
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$



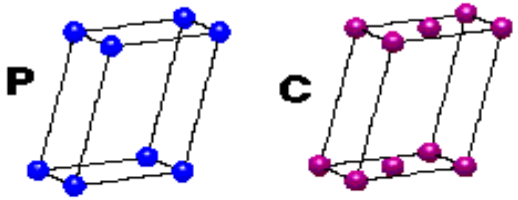
HEXAGONAL
$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$



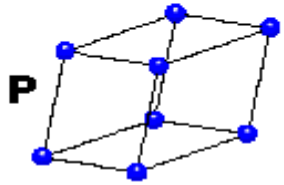
TRIGONAL
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$



MONOCLINIC
$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$

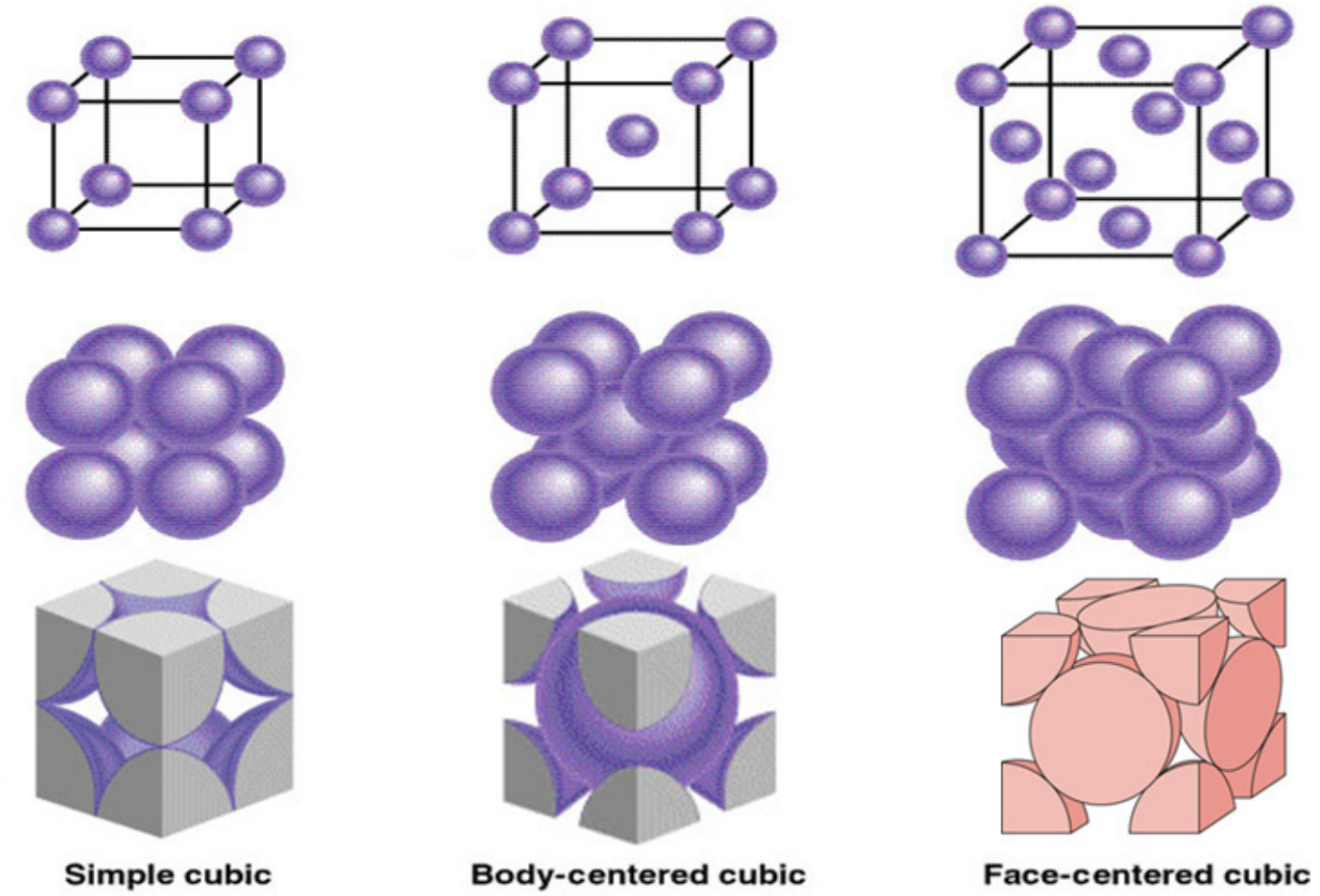


TRICLINIC
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

NUMBER OF ATOMS PER UINT CELL

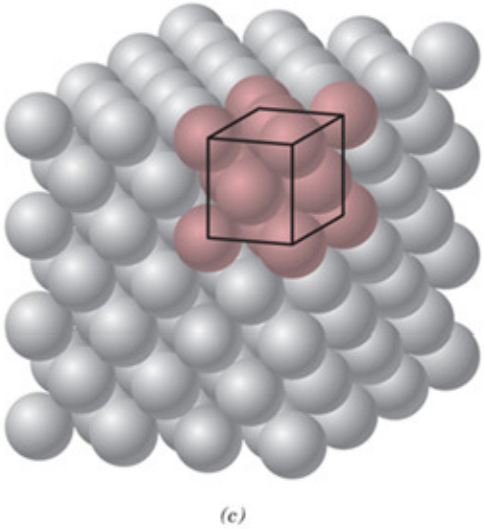


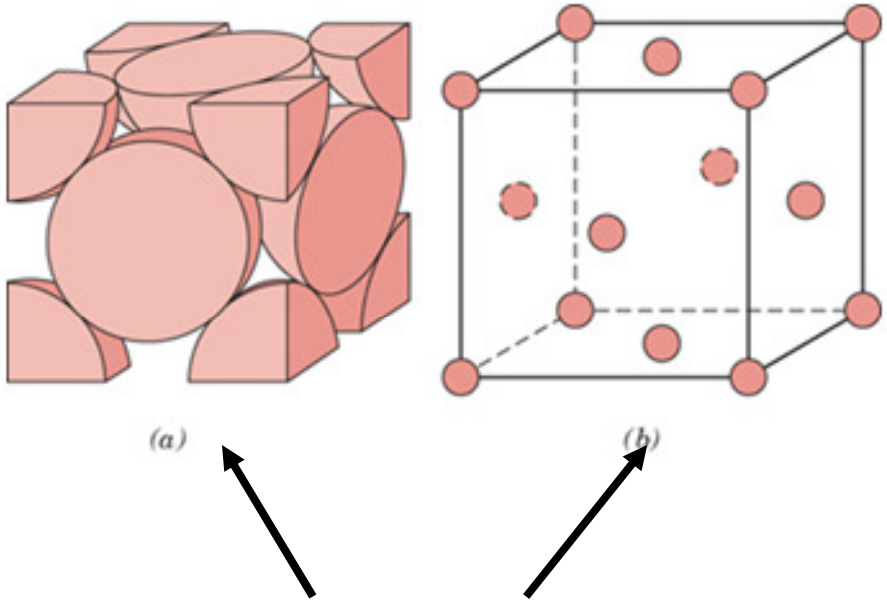
1 atom/unit cell
(8 x 1/8 = 1)

2 atoms/unit cell
(8 x 1/8 + 1 = 2)

4 atoms/unit cell
(8 x 1/8 + 6 x 1/2 = 4)

Face Centered Cubic (FCC) Structure





Two representations of a unit cell

How many atoms are in the fcc unit cell?

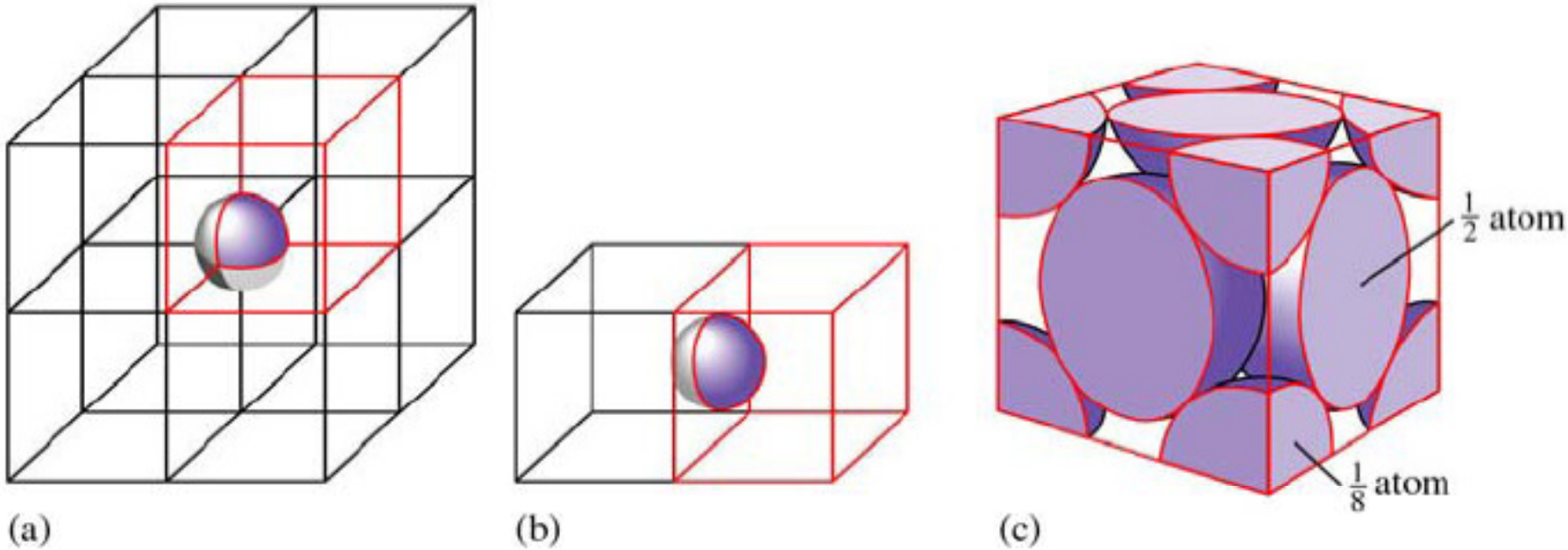


Figure 16.17

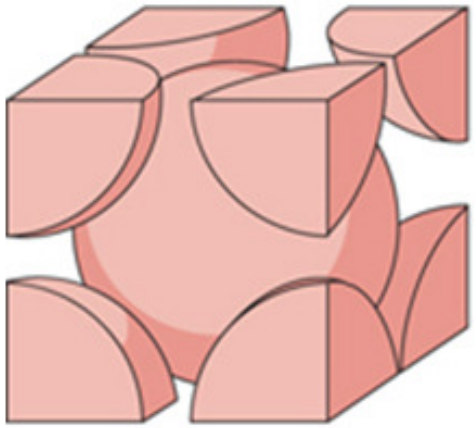
6(atoms on faces) + 8(atoms on corners)

= 6(1/2) + 8(1/8)

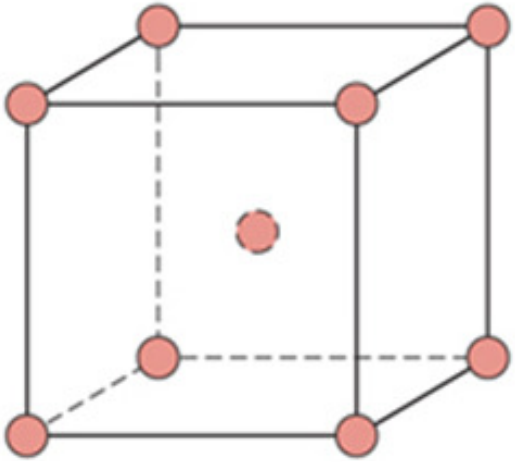
= 3 + 1

= 4

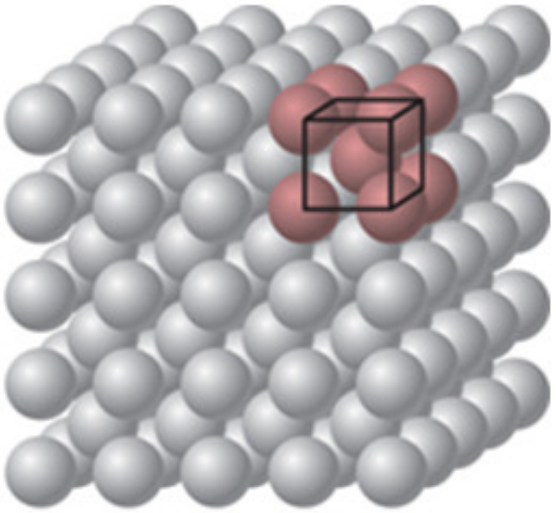
Body Centered Cubic (BCC) Structure



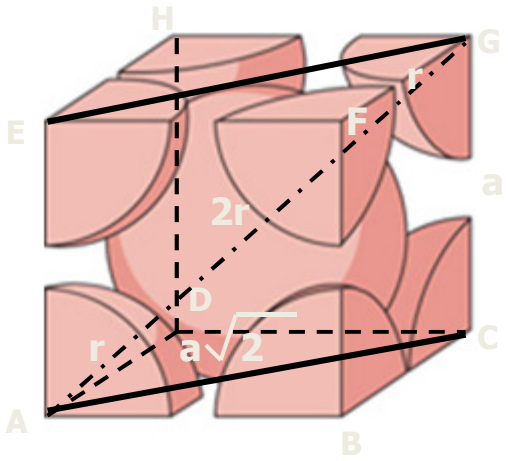
(a)



(b)

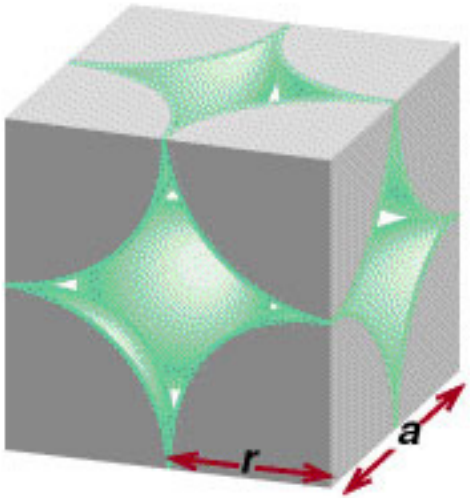


(c)



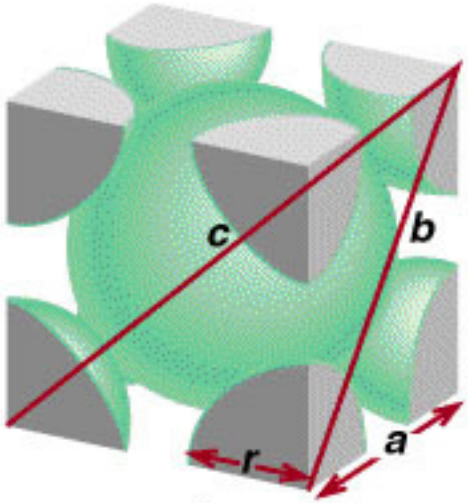
How many atoms are there in BCC structure?

Relationship Between the Atomic Radius and the Edge Length in Three Different Unit Cells



scc

$a = 2r$



bcc

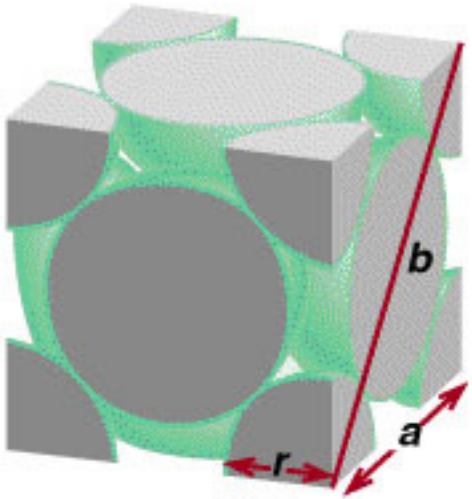
$b^2 = a^2 + a^2$

$c^2 = a^2 + b^2$

$= 3a^2$

$c = \sqrt{3}a = 4r$

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



fcc

$b = 4r$

$b^2 = a^2 + a^2$

$16r^2 = 2a^2$

$a = \sqrt{8}r$

MILLER INDICES OF LATTICE PLANE

In crystel there exist directions and planes which contain a large concentration of atoms. It is necessary to locate these directions and planes for crystal analysis. To recognize the orientation of planes and directions was discovered by Miller. Miller developed a method to designate a plane in a crystal by three number (hkl) known as Miller indices.

It is also a ratio of crystal axes but for the sake of brevity the ratio sign is omitted. It uses the relative intercepts of the faces with the axes.

Miller indices is a reciprocals of parameters. The expression of Miller indices by the whole number and zero is called "The law of rational indices"

Some characteristic:

1- In all crystal systems (except hexagonal) they are three digit , (hkl).

2- In hexagonal system they are four digit , (hkil).

i= -(h+k)

h+k+i=0

The Miller Index for a crystal face is found by

1-first determining the parameters

2-second inverting the parameters, and

3-third clearing the fractions.

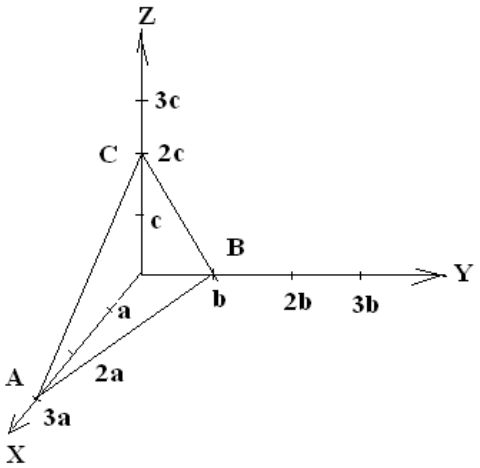
For example, if the face has the parameters 1 a, 1 b, ∞ c

inverting the parameters would be 1/1, 1/1, 1/ ∞

this would become 1, 1, 0

the Miller Index is written inside parentheses with no commas - thus (110)

Procedures to find miller indices of planes



Consider the plane ABC . This plane cuts the crystallographic axes x, Y, Z with intercepts 3a, b, 2c

Step –I Determine the intercept made by plane with crystallographic axis x,y,z

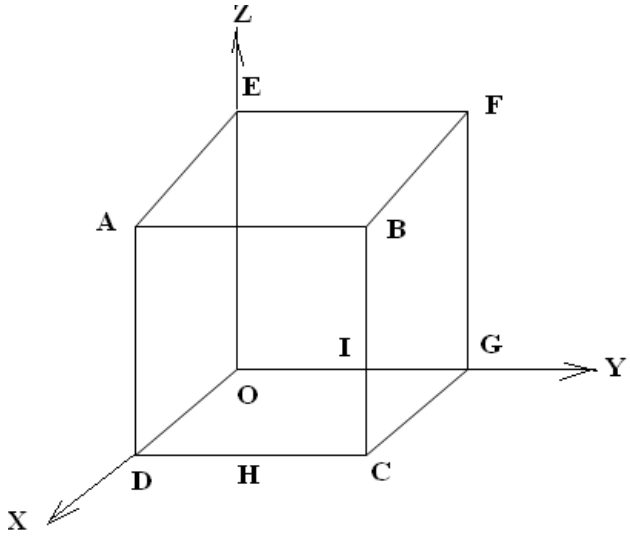
3a , b, 2c

Let pa, qb, rc

For above plane ABC, p= 3, q = 1, r = 2

Step –II Take reciprocal of numerical intercept values

1/3, 1/1 1/2



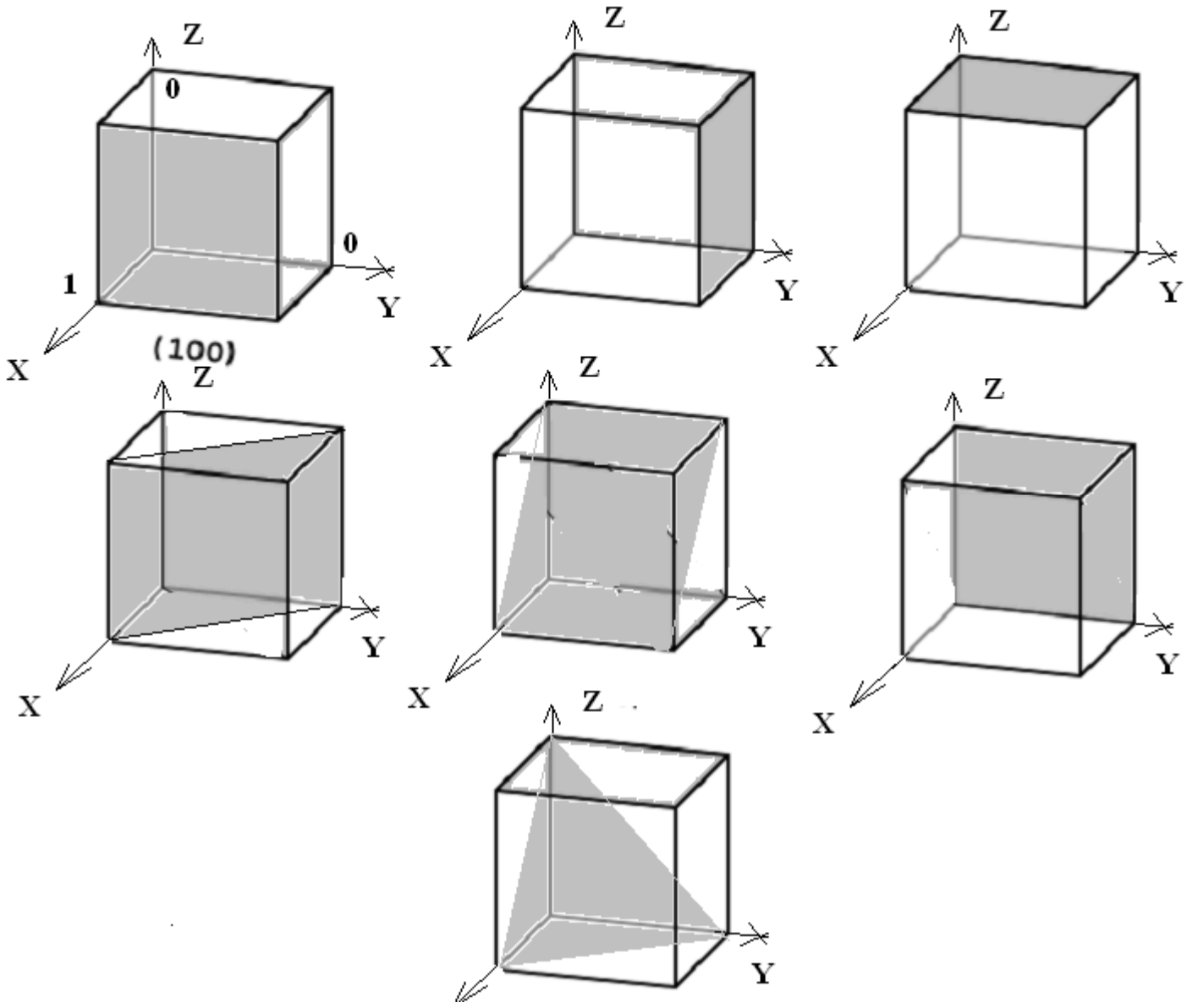
Step –III Convert these reciprocal into whole number by multipying each with their LCM

For above plane LCM = 6

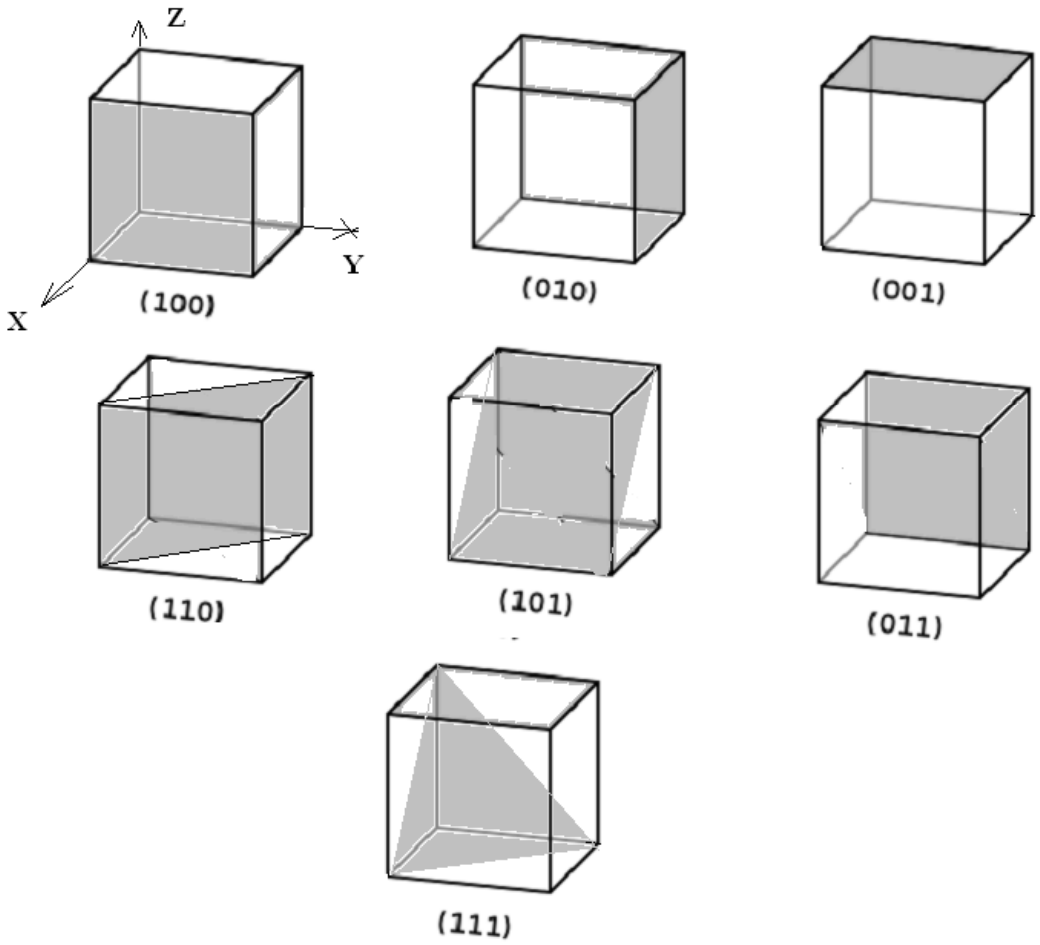
6x1/3 , 6x 1/1, 6x 1/2

2 6 3

Step –IV Enclose these number into bracket . This represents inices of given plane (2 6 3) .


Z
0
0
1
Y
X
(100)
Z
Y
X
Z
Y
X
Z
Y
X
Z
Y
X
Z
Y
X

Different types of Miller indices



Examples

Face	a	b	c	Parameters	Reciprocal	Miller index
AKP	1	1	1	1a:1b:1c	1/1 : 1/1 : 1/1	(111)
XYZ	2	2	2	1a:2b:2c	1/2 : ½ : ½	(111)
ABC	1	4	3	1a:4b:3c	1/1 : ¼ : 1/3	?
	1	3	∞	1a:3b:∞c	1/1 : 1/3 : 1/ ∞	?
	3/2	3	∞	2/3a:3b:∞c	2/3 : 1/ 3: 1/ ∞	?
	3	3	3	3a:3b:3c	1/3 : 1/3 : 1/3	?

EQUIVALENT SITES (ATOMIC POSITIONS) IN CUBIC UNIT CELLS

Simple Cubic, SC - one per unit cell - corner atoms only

(0,0,0) (1,0,0) (1,1,0) (0,1,0)

(0,0,1) (1,0,1) (1,1,1) (0,1,1)

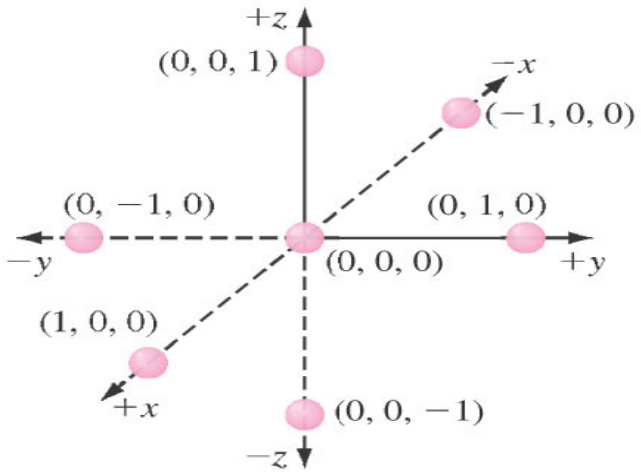
Body Centered Cubic, BCC - two per unit cell - corner atoms as above, plus

(1/2, 1/2, 1/2)

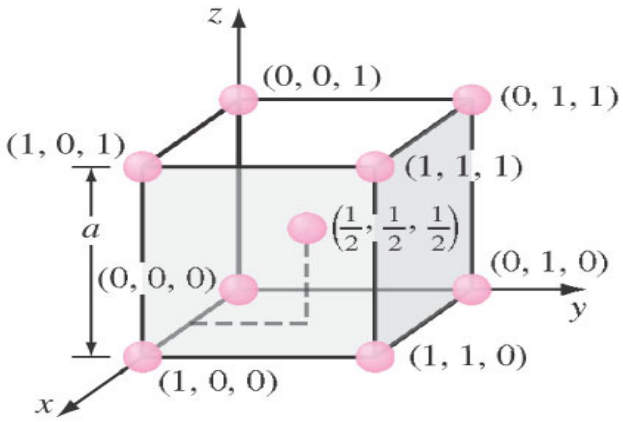
Face Centered Cubic, FCC - four per unit cell - corner atoms as above plus

(1/2, 1/2, 0) (1/2, 0, 1/2) (0, 1/2, 1/2)

(1, 1/2, 1/2) (1/2, 1, 1/2) (1/2, 1/2, 1)



(a)



(b)