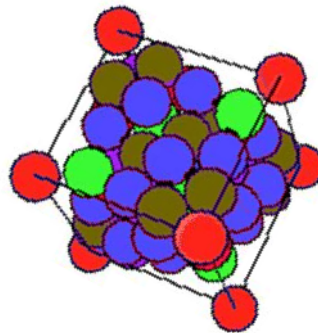# Crystal Structure

Preface

Crystal structure is one of the most important aspects of materials science and engineering as many properties of materials depend on their crystal structures. The basic principles of many materials characterization techniques such as X-ray diffraction (XRD), Transmission electron microscopy (TEM) are based on crystallography. Therefore, understanding the basics of crystal structures is of paramount importance.
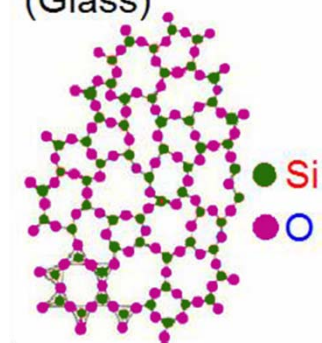
Atomic arrangement

Crystalline SiO₂
(Quartz)

Solid

Amorphous SiO₂
(Glass)

● Si ●O
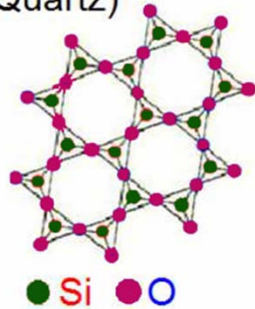
Crystalline   Amorphous

● Si
● O

Crystalline – periodic arrangement of atoms: definite repetitive pattern

Non-crystalline or Amorphous – random arrangement of atoms.

The periodicity of atoms in crystalline solids can be described by a network of points in space called lattice.

Space lattice

➤ A space lattice can be defined as a three dimensional array of points, each of which has identical surroundings.

➤ If the periodicity along a line is a, then position of any point along the line can be obtained by a simple translation, $r_u = ua$.

➤ Similarly $r_{uv} = ua + vb$ will repeat the point along a 2D plane, where u and v are integers.
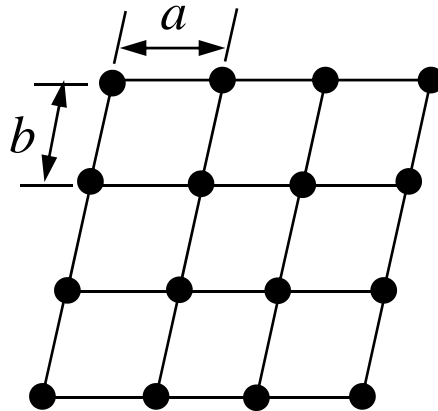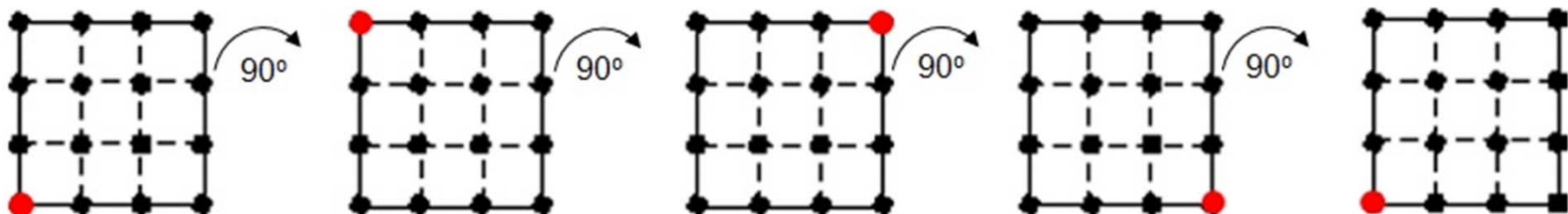
Symmetry

Symmetry

➤ Symmetry refers to certain pattern or arrangement. A body is symmetrical when it is reproduced by certain operation.

➤ The symmetry word (somewhat distorted) itself shows 2-fold rotation symmetry (restored by 180º rotation)
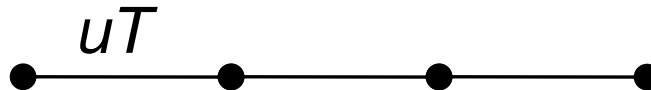
➤ In the picture below the plane looks identical after a 90º rotation. The plane has 4 fold rotation symmetry as it repeats itself 4 times (shown by the red dot) in a full 360º rotation.

Symmetry operations

1. Translation

2. Rotation

3. Reflection

4. Inversion

Translation

uT

The first point is repeated at equal distances along a line by a translation uT, where T is the translation vector and u is an integer.

Translation on a point with coordinates xyz $\rightarrow$ x+a y+b z+c where, a, b and c are the unit vectors in x, y and z directions respectively.

Symmetry operations

Rotation

A rotation can be applied on the translation vector T in all directions, clock or anti-clock wise, through equal angles α in the 2D space.

If two rotation operations, one each in clock and anti-clock direction, are applied on the translation vector T, it will create two more lattice points. Because of the regular pattern, the translation between these two points will be some multiple of T (pT).
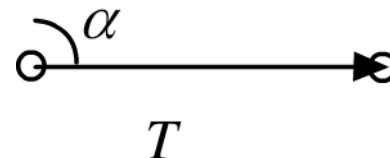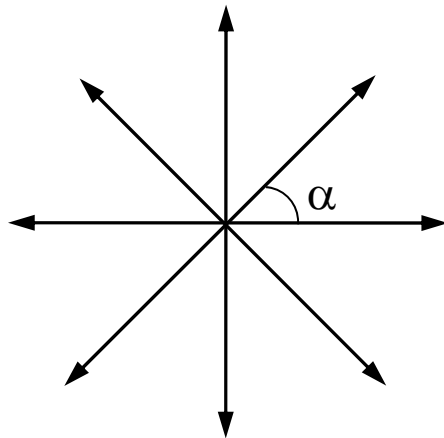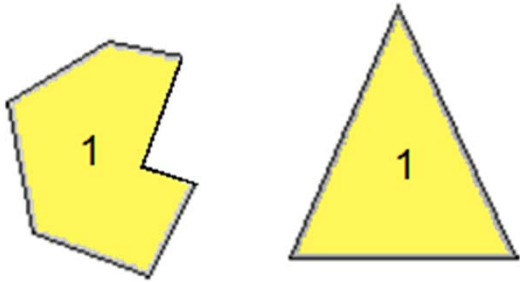
Symmetry operations
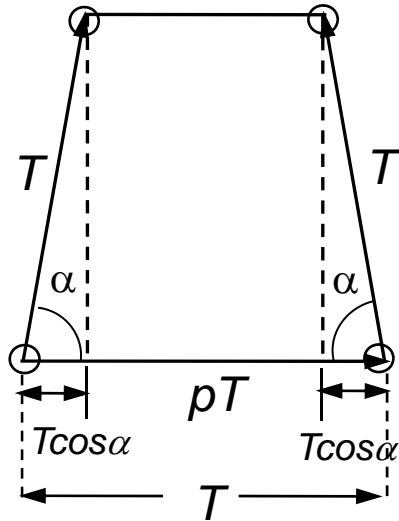
Rotation

$$T = T\cos\alpha + pT + T\cos\alpha = pT + 2T\cos\alpha$$

$$\cos\alpha = (1 - p)/2$$

| p	$\alpha°$	n-fold	Symbol
0	60	6	⬢
1	90	4	■
2	120	3	▲
3	180	2	⬭
-1	0/360	1	

An n-fold rotation symmetry means rotation through an angle of $2\pi/n$ will repeat the object or motif n times in a full $360°$ rotation. n =1 means no symmetry.
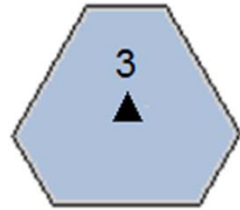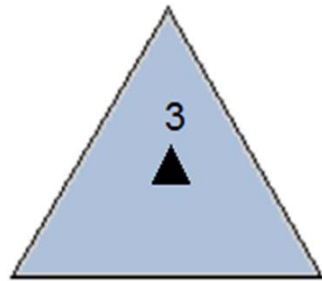
Rotation

1-Fold Rotation Axis - An object that requires rotation of a full 360° to repeat itself has no rotational symmetry.

2-fold Rotation Axis - If an object appears identical after a rotation of 180°, that is twice in a 360° rotation, then it is said to have a 2-fold ($2\pi/180$) rotation symmetry
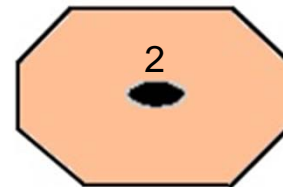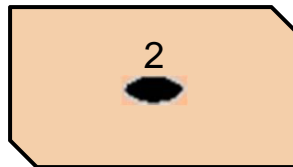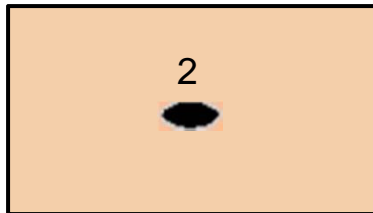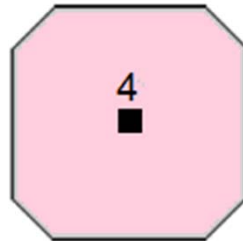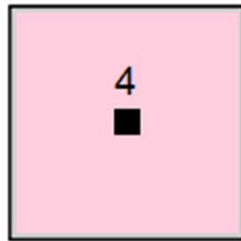
Rotation

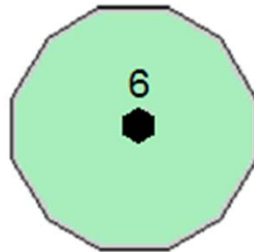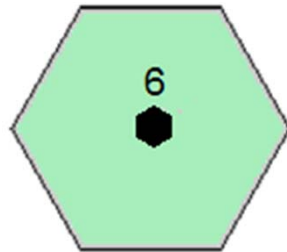Similarly we have 3, 4 and 6-fold rotational symmetry

3 fold – $2\pi/120$

4 fold – $2\pi/90$

6 fold – $2\pi/60$

Rotation

Is it possible to have 5, 7 or 8-fold rotation symmetry?

Objects with 5, 7 and 8 or higher order symmetry do exist in nature, e.g. star fish (5-fold), flowers with 5 or 8-fold symmetry.

However, these are not possible in crystallography as they cannot fill the space completely
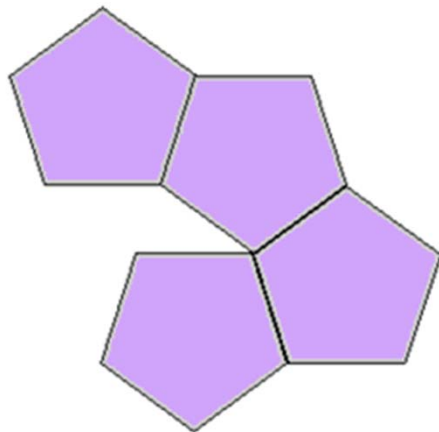
5 fold
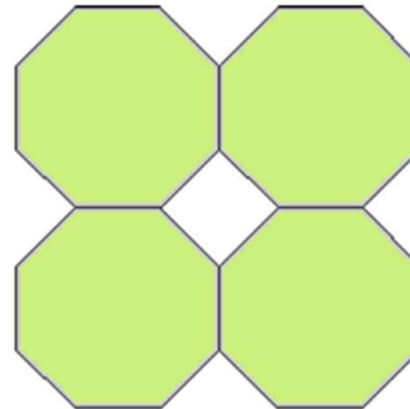
8 fold

Reflection or Mirror symmetry

An object with a reflection symmetry will be a mirror image of itself across a plane called mirror plane (*m*).
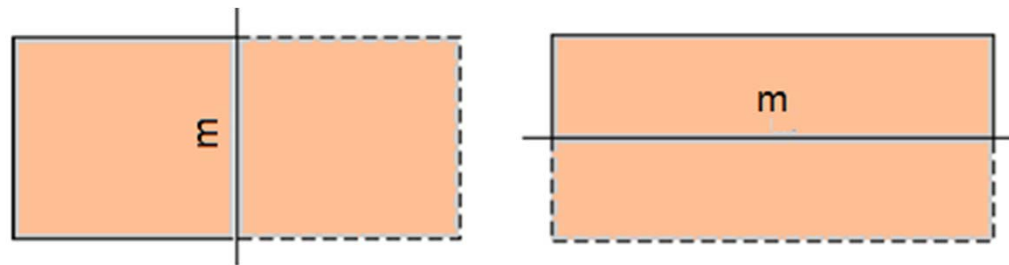
AMAN A PLAN A CANAL PANAMA
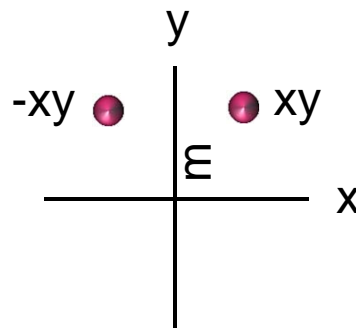
Reflection operation: xyz → -x y z ($\bar{x}$ y z) across a mirror plane perpendicular to x axis

Symmetry and Space lattice

Symmetry elements discussed so far define five types of 2D space lattices. When a translation is applied to the third direction these lattices create a total of 7 crystal systems.
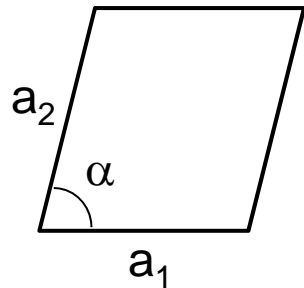
2-fold
Parallelogram
$a_1 \neq a_2$, $\alpha = $ Any
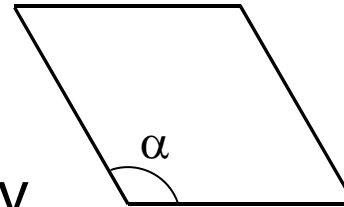
3, 6-fold
Hexagonal
$a_1 = a_2$, $\alpha = 120°$
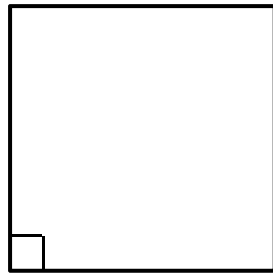
4-fold: Square
$a_1 = a_2$, $\alpha = 90°$
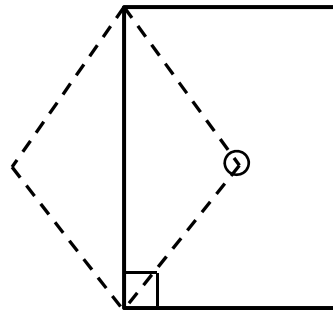
Centered-Rectangular
$a_1 \neq a_2$, $\alpha = 90°$
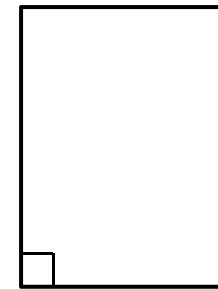
Primitive-Rectangular
$a_1 \neq a_2$, $\alpha = 90°$

Inversion – Center of symmetry

In this operation, every part of the object is reflected through an inversion center called center of symmetry which is denoted as *i*. The object is reproduced inverted from its original position.

$$xyz \xrightarrow{i} -x\ -y\ -z\ (\ \bar{x}\ \bar{y}\ \bar{z})$$
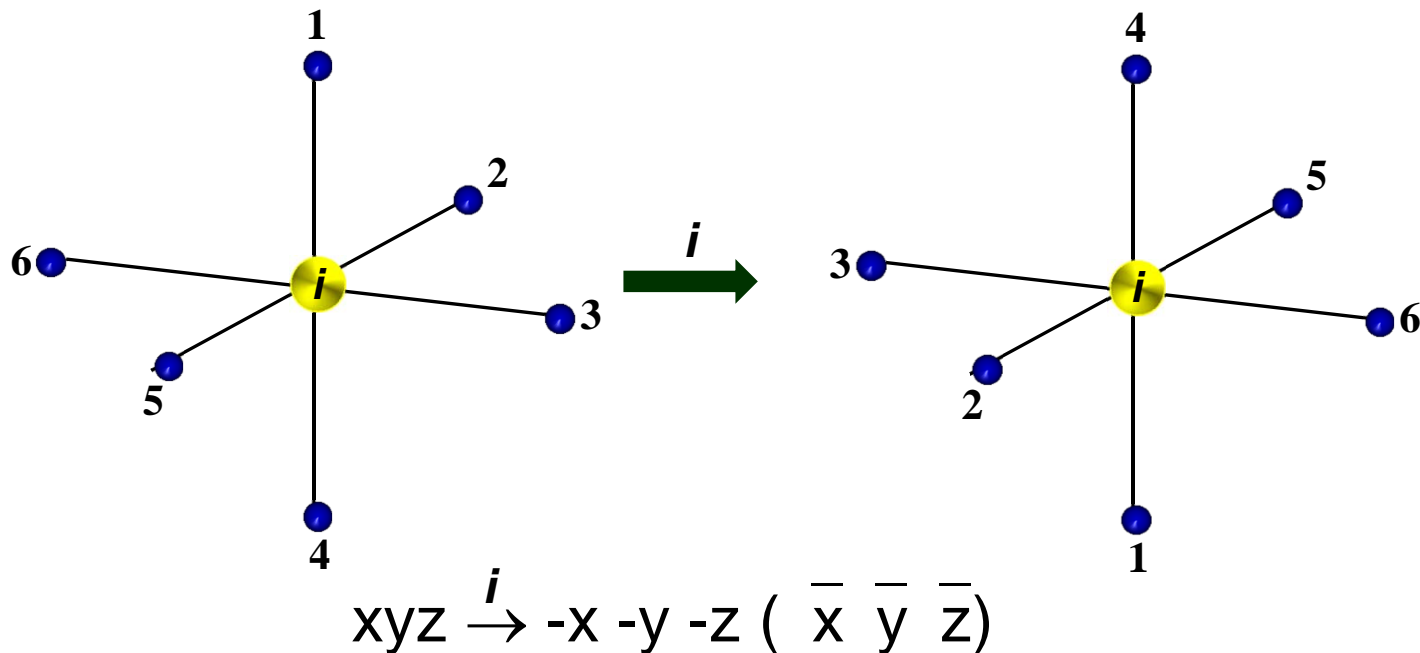
Combined operations

Combined symmetry operations also exist. For example, rotation can be combined with inversion which is called *roto-inversion*. The roto-inversion axis is denoted as $\bar{n}$. For example, a 6-fold roto-inversion ($\bar{6}$) involves rotating the object by 60° (360/6), and inverting through a symmetry center.
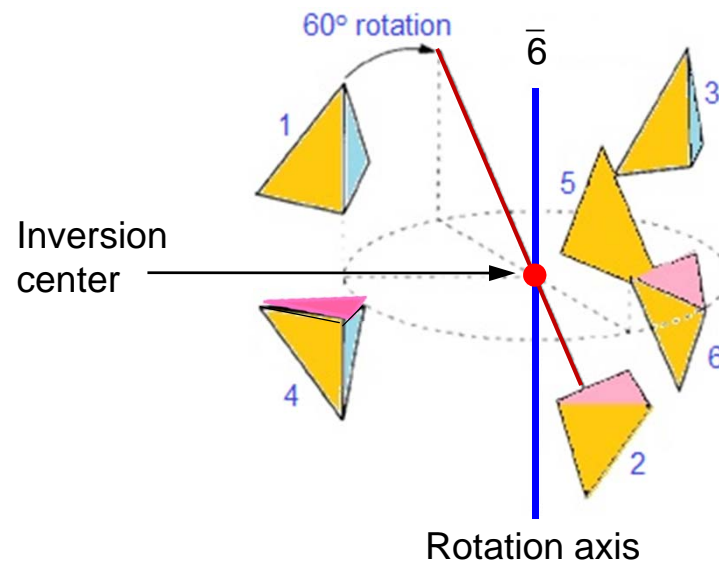
Point and Space groups

Symmetry operations generate a variety of arrangements of lattice points in three dimensions. There are **32** unique ways in which lattice points can be arranged in space. These non-translation elements are called *point-groups*.

A large number of 3D structures are generated when translations [linear translation, translation + reflection (glide plane) and translation + rotation (screw axis)] are applied to the point groups. There are **230** unique shapes which can be generated this way. These are called *space groups*.

Hermann-Mauguin Symbols

➤The 32 point groups are denoted by notations called Hermann-Mauguin symbols. These symbols basically describe the unique symmetry elements present in a body.

➤The shape in Fig.(a) contains 1 4-fold axis, 4 2-fold axes, 5 mirror planes. 3 mirror planes and 2 2-fold axes are unique as others can be produced by a symmetry operation. Therefore, point group symbol for this shape is 4/m2/m2/m. The "/" between 4 or 2 and m indicates that they are perpendicular to each other.

m

m

(a)

4/m2/m2/m

(b)

2/m2/m2/m
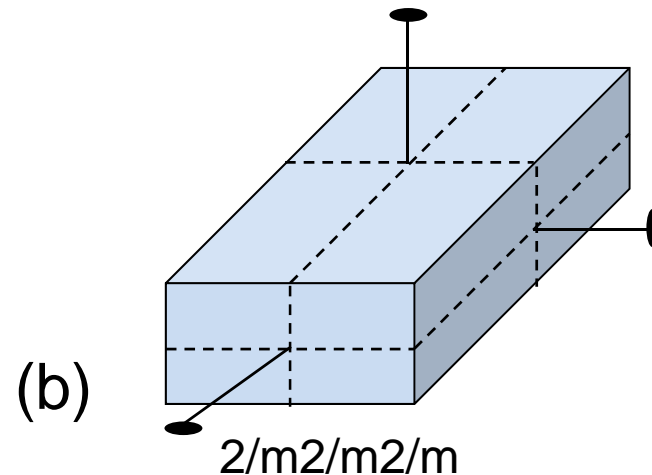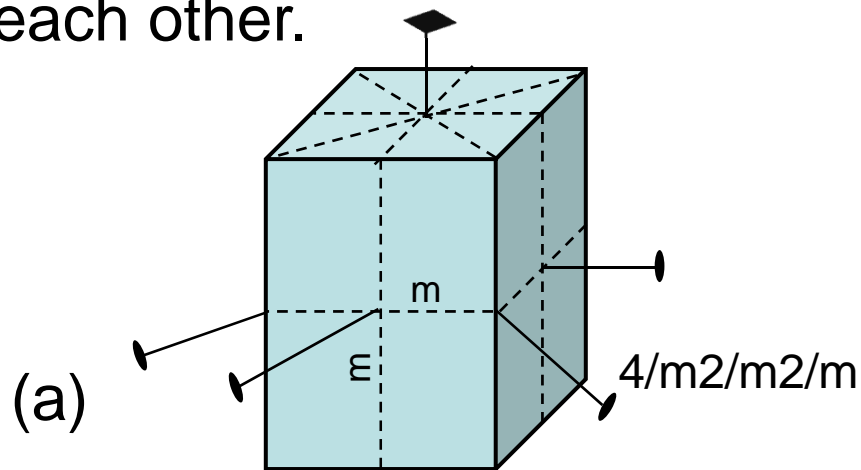
Summary

❑Space lattice is arrangement of points with each point having exactly same surroundings.

❑Symmetry operations restore a body to its original position.

❑There are four symmetry operations – Translation, reflection, rotation and inversion.

❑There are 32 point groups and 230 space groups.

❑Hermann-Mauguin symbols are used to denote point groups.

References
http://www.tulane.edu/~sanelson/eens211/index.html#Lecture Notes
http://www.tulane.edu/~sanelson/eens211/introsymmetry.pdf
http://www.tulane.edu/~sanelson/eens211/32crystalclass.pdf

Crystal Systems

➢The space lattice points in a crystal are occupied by atoms.

➢The position of any atom in the 3D lattice can be described by a vector $r_{uvw} = u a + v b + w c$, where u, v and w are integers.

(a)

(b)
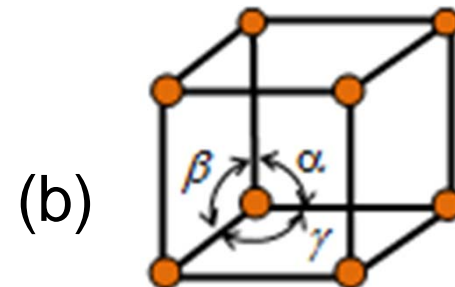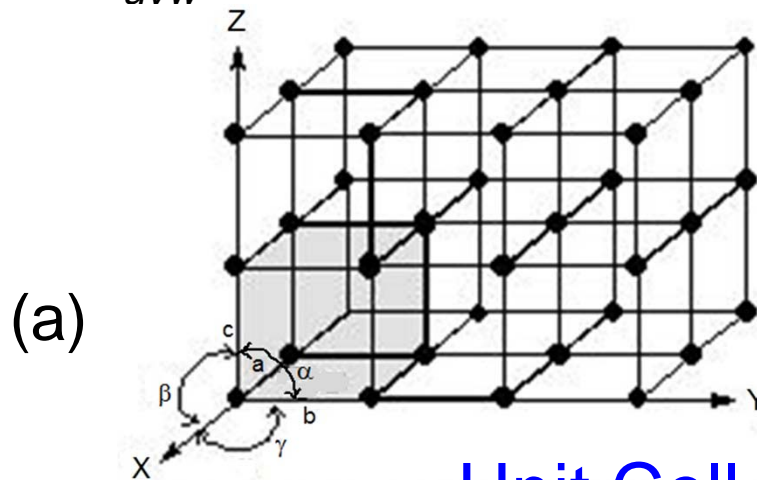
Unit Cell

The three unit vectors, *a*, *b*, *c* can define a cell as shown by the shaded region in Fig.(a) This cell is known as unit cell (Fig. b) which when repeated in the three dimensions generates the crystal structure.

Crystal Systems

Bravais Lattice

The unit vectors *a*, *b* and *c* are called lattice parameters. Based on their length equality or inequality and their orientation (the angles between them, α, β and γ) a total of 7 crystal systems can be defined. With the centering (face, base and body centering) added to these, 14 kinds of 3D lattices, known as ***Bravais lattices***, can be generated.

Crystal Systems

Cubic: $a = b = c$, $\alpha = \beta = \gamma = 90^o$
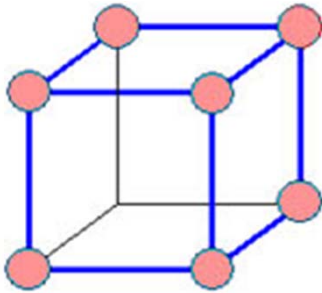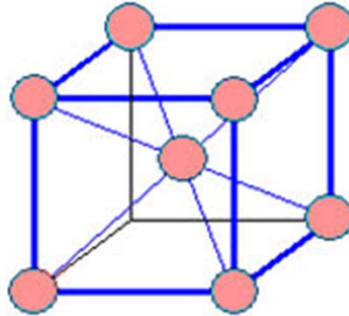
Simple
cubic

Body-centered
cubic (BCC)
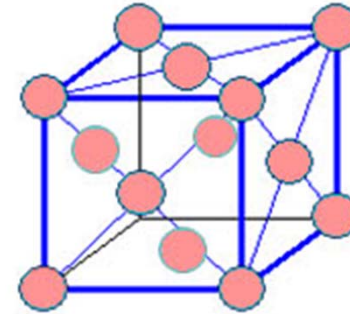
Face-centered
cubic (FCC)

Tetragonal: $a = b \neq c$, $\alpha = \beta = \gamma = 90^o$
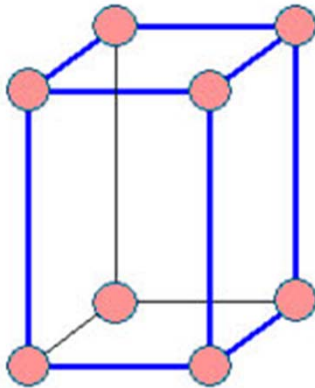
Simple
Tetragonal
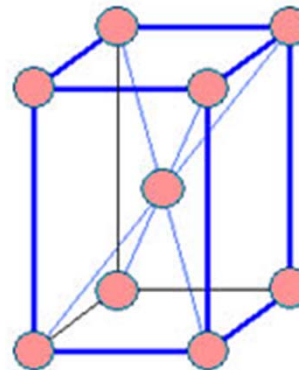
Body-centered
Tetragonal (BCT)

Crystal Systems

Orthorhombic: $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^o$
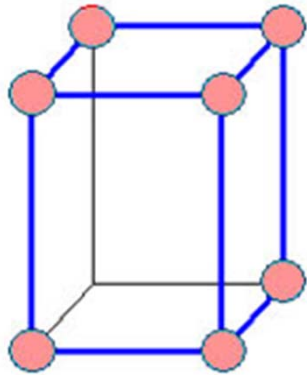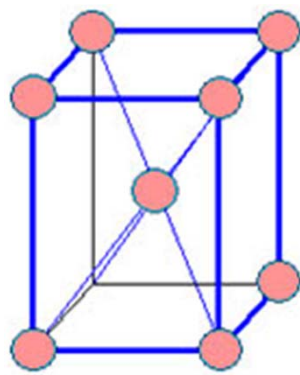
Simple   Body-centered   Base-centered   Face-centered
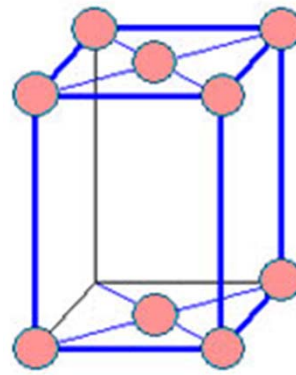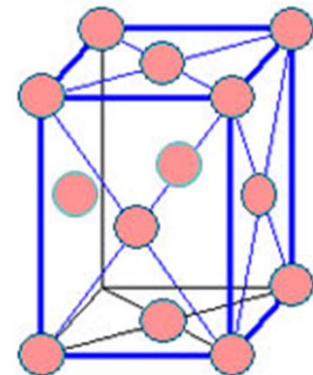
Monoclinic: $a \neq b \neq c$, $\alpha = \gamma = 90^o \neq \beta$
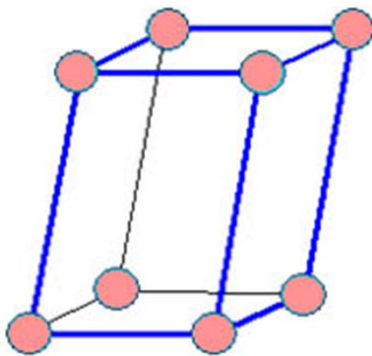
Simple
monoclinic
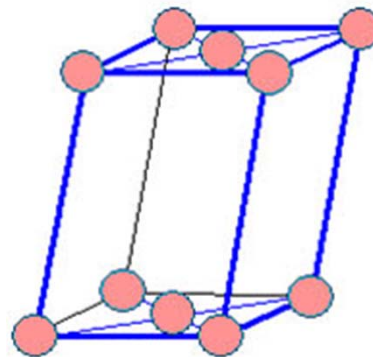
Base-centered
monoclinic

Crystal Systems
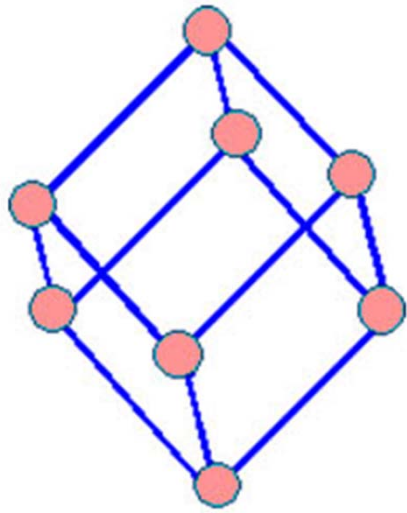
Rhombohedral
$a = b = c$
$\alpha = \beta = \gamma \neq 90^o$
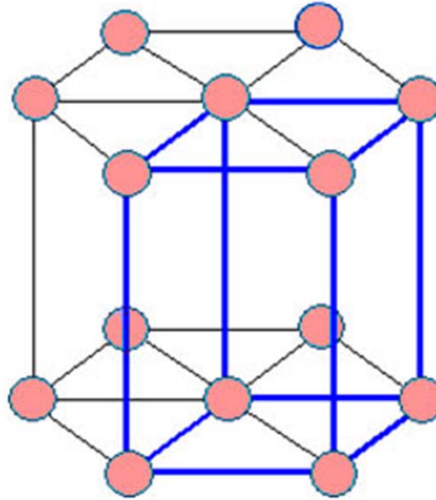
Hexagonal
$a = b \neq c$
$\alpha = \beta = 90^o$ $\gamma = 120^o$
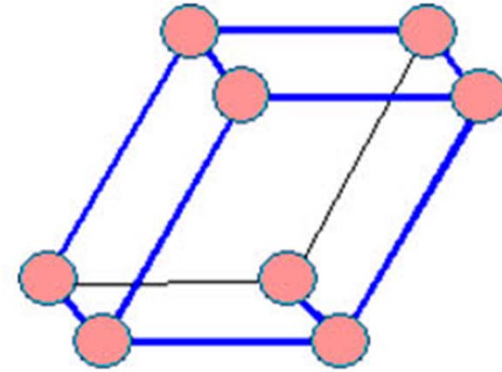
Triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90^o$

Crystal Systems

Crystal system	Example
Triclinic	$K_2S_2O_8, K_2Cr_2O_7$
Monoclinic	As_4S_4, KNO_2, $CaSO_4.2H_2O$, β-S
Rhombohedral	Hg, Sb, As, Bi, $CaCO_3$
Hexagonal	Zn, Co, Cd, Mg, Zr, NiAs
Orthorhombic	Ga, Fe_3C, α-S
Tetragonal	In, TiO_2, β-Sn
Cubic	Au, Si, Al, Cu, Ag, Fe, NaCl

Point Coordinates

Position of any point in a unit cell is given by its coordinates or distances from the x, y and z axes in terms of the lattice vectors a, b and c.

Thus the point located at a/2 along x axis, b/3 along y axis and c/2 along z axis, as shown in the figure below, has the coordinates $\dfrac{1}{2}\dfrac{1}{3}\dfrac{1}{2}$
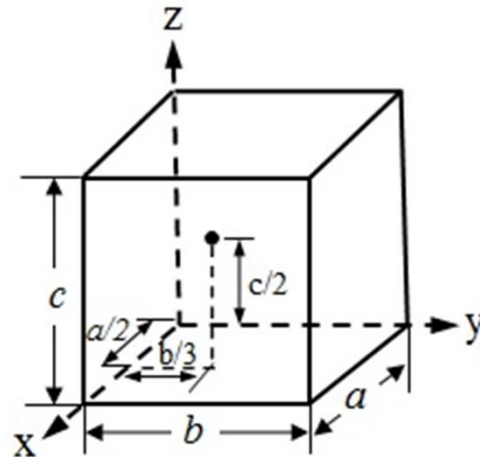
Crystal Planes

Miller Indices

Planes in a crystal are described by notations called Miller indices

❖Miller indices of a plane, indicated by h k l, are given by the reciprocal of the intercepts of the plane on the three axes.

❖The plane, which intersects X axis at 1 (one lattice parameter) and is parallel to Y and Z axes, has Miller indices $h = 1/1 = 1$, $k = 1/\infty = 0$, $l = 1/\infty = 0$. It is written as (hkl) = (100).

❖Miller indices of some other planes in the cubic system are shown in the figures in the next slide

Crystal Planes

$$\frac{h}{1} \quad \frac{k}{1} \quad \frac{l}{1}$$

$$\frac{1}{1} \quad \frac{1}{\infty} \quad \frac{1}{\infty} = (100)$$

$$\frac{h}{1} \quad \frac{k}{1} \quad \frac{l}{1}$$

$$\frac{1}{1} \quad \frac{1}{1} \quad \frac{1}{\infty} = (110)$$

$$\frac{h}{1} \quad \frac{k}{1} \quad \frac{l}{1}$$

$$\frac{1}{1} \quad \frac{1}{1} \quad \frac{1}{1} = (111)$$
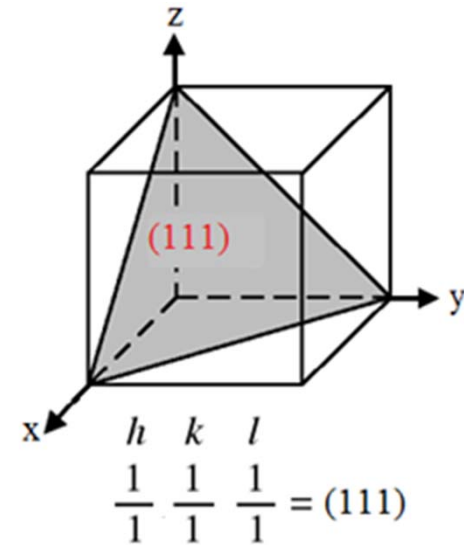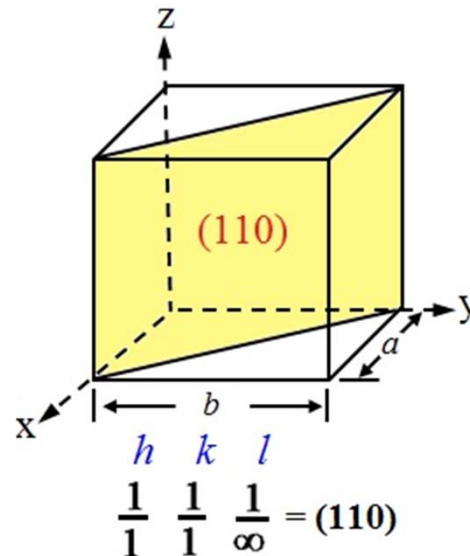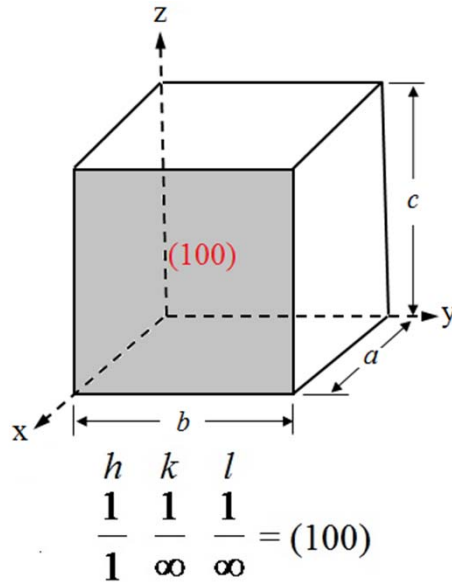
To find the Miller Indices of a plane, follow these steps:

▪Determine the intercepts of the plane along the crystal axes
▪Take the reciprocals
▪Clear fractions
▪Reduce to lowest terms and enclose in brackets ()
Ex: Intercepts on a, b, c : ¾, ½, ¼ (h k l) = (4/3, 2, 4) = (2 3 6)

Crystal Planes

Planes can also have negative intercept e.g. 1, -1/2, 1

h k l = 1 -2 1. This is denoted as $(1\bar{2}1)$

Family of planes $\{hkl\}$

Planes having similar indices are equivalent, e.g. faces of the cube (100), (010) and (001). This is termed as a family of planes and denoted as {100} which includes all the (100) combinations including negative indices. Some other equivalent planes are shown in the next slide.

Equivalent Planes
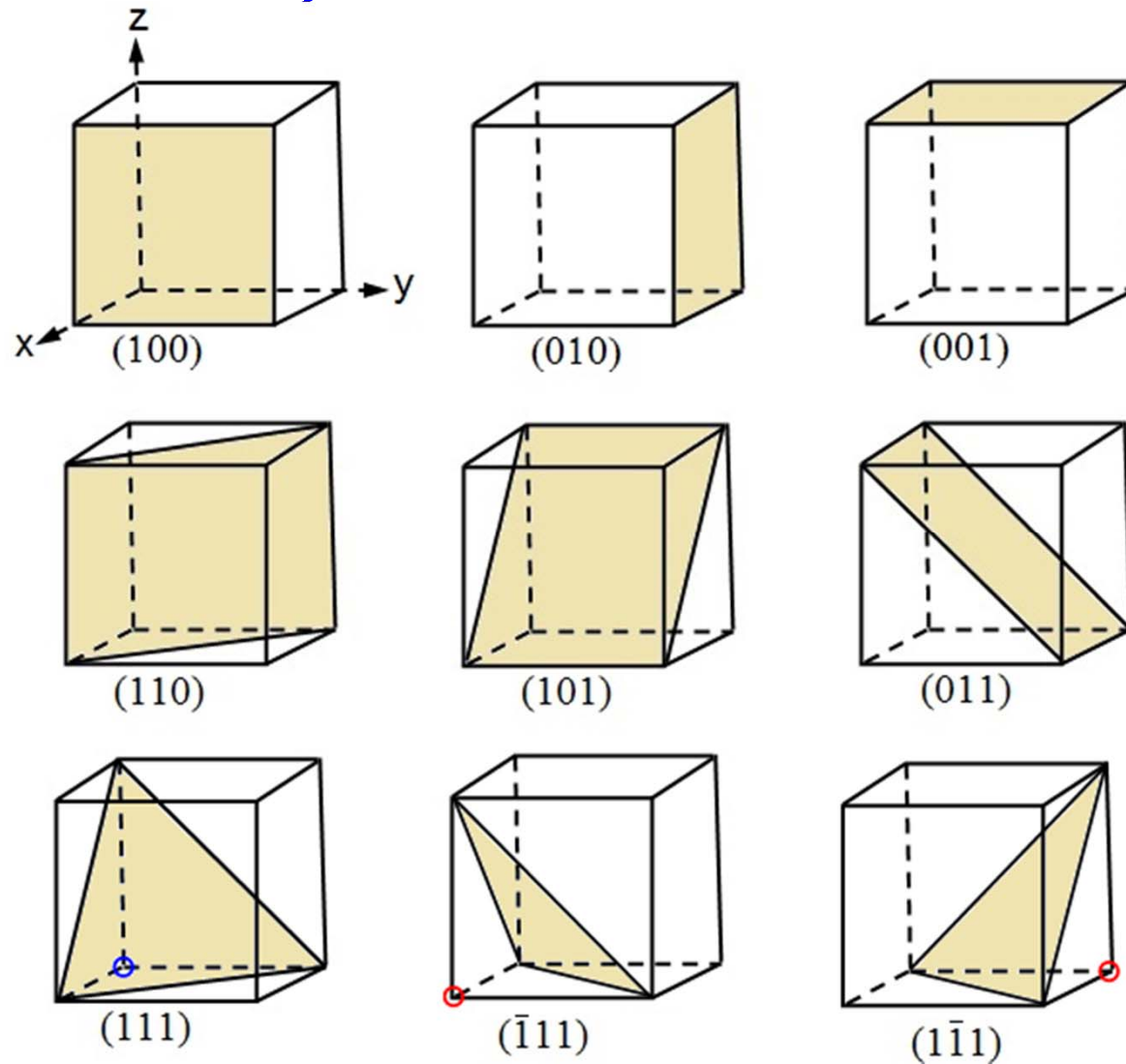
Note the shift of origin from blue to red circle for the negative indices

Planes in Hexagonal system

➢In the cubic system all the faces of the cube are equivalent, that is, they have similar indices.

➢However, this is not the case in the hexagonal system. The six prism faces for example have indices (1 0 0), (0 1 0), ($\bar{1}$ 1 0), ($\bar{1}$ 0 0), (0 $\bar{1}$ 0), (1 $\bar{1}$ 0), which are not same.

In order to address this, a fourth axis (a_3) which is opposite to the vector sum of a_1 and a_2 is used and a corresponding fourth index i is used along with *hkl*. Therefore the indices of a plane is given by *(hkil)* whre $i = -(h+k)$. Sometime i is replaced with a dot and written as (h k . l)
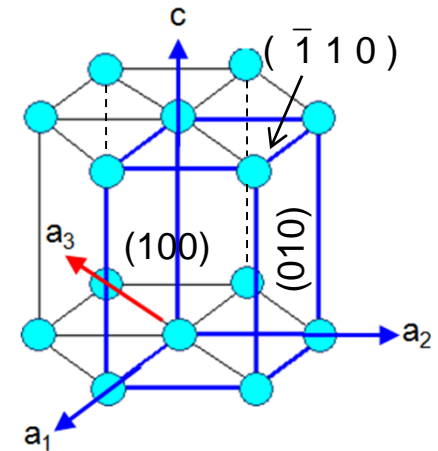
Planes in Hexagonal system

The indices of six faces now become $(1\,0\,\bar{1}\,0)$, $(0\,1\,\bar{1}\,0)$, $(\bar{1}\,1\,0\,0)$, $(\bar{1}\,0\,1\,0)$, $(0\,\bar{1}\,1\,0)$, $(1\,\bar{1}\,0\,0)$ which are now equivalent and belong to the $\{1\,0\,\bar{1}\,0\}$ family of planes.
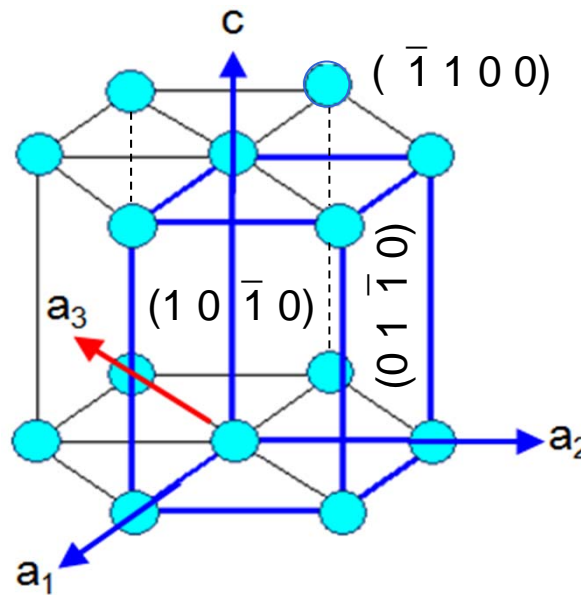
Interplanar spacing

The spacing between planes in a crystal is known as interplanar spacing and is denoted as d_{hkl}

In the cubic system spacing between the (hkl) planes is given as
$$\frac{1}{d^2} = \frac{1}{a^2}\left(h^2 + k^2 + l^2\right)$$

For example, d_{hkl} of {111} planes $d_{111} = a/\sqrt{3}$

In Tetragonal system
$$\frac{1}{d^2_{hkl}} = \frac{1}{a^2}\left(h^2 + k^2\right) + \frac{1}{c^2}l^2$$

In Orthorhombic system
$$\frac{1}{d^2_{hkl}} = \frac{1}{a^2}h^2 + \frac{1}{a^2}k^2 + \frac{1}{c^2}l^2$$

In Hexagonal system
$$\frac{1}{d^2_{hkl}} = \frac{4}{3a^2}\left(h^2 + hk + k^2\right) + \frac{1}{c^2}l^2$$

Crystal Directions

The directions in a crystal are given by specifying the coordinates (u, v, w) of a point on a vector (r_{uvw}) passing through the origin. r_{uvw} = ua + vb + wc. It is indicated as [uvw]. For example, the direction [110] lies on a vector r_{110} whose projection lengths on x and y axes are one unit (in terms of unit vectors *a* and *b*).

Directions of a form or family like [110], [101], [011] are written as <110>
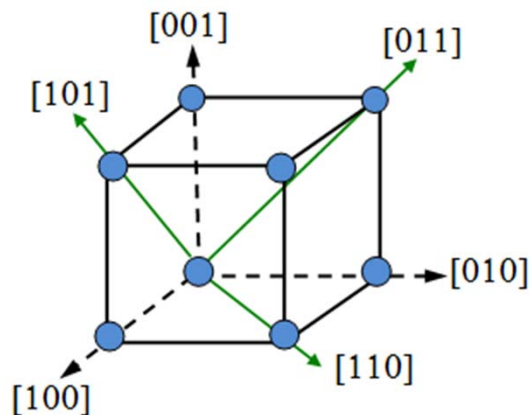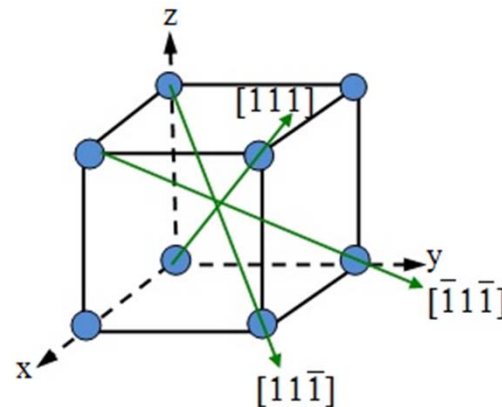
<100> and <110> family   <111> family

Crystal Directions

➢The line which passes through *uvw* will also pass through *2u2v2w* and *½ u ½ v ½ w*. Hence [uvw], [2u2v2w] and [½ u ½ v ½ w] are same and written as [uvw].

➢Fractions are converted in to integers (as shown in the figure below) and reduced to lowest terms.
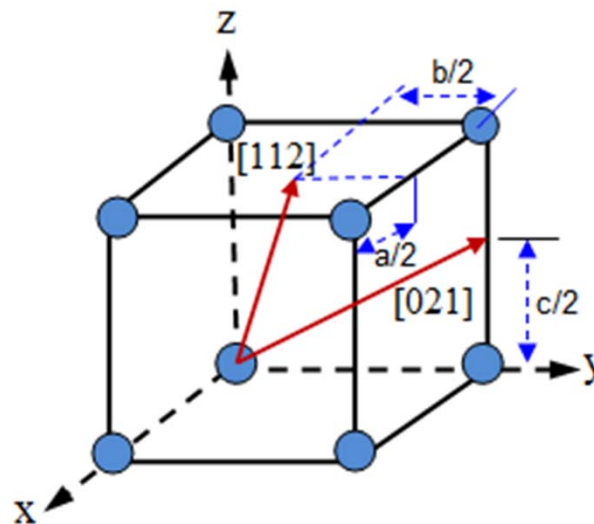
Crystal Directions

To determine a direction of a line in the crystal:

❑Find the coordinates of the two ends of the line and subtract the coordinates (Head – Tail) OR draw a line from the origin parallel to the line and find its projection lengths on x, y and z axis in terms of the unit vectors *a*, *b* and *c*.

❑Convert fractions, if any, in to integers and reduce to lowest term.

❑Enclose in square brackets [uvw]

Directions in Hexagonal Crystal

Like planes, directions in the hexagonal system are also written in terms of four indices as [uvtw].

If [UVW] are indices in three axes then it can be converted to four-axis indices [uvtw] using the following relations.

$U = u - t$ $V = v - t$ $W = w$

$u = (2U-V)/3$ $v = (2V-U)/3$ $t = -(u + v) = -(U + V)/3$

$w = W$

Ex: $[100] = [2\ \bar{1}\ \bar{1}\ 0]$, $[210] = [1\ 0\ \bar{1}\ 0]$

Relationship between direction and planes

In the cubic system planes and directions having same indices are perpendicular to each other i.e. if [uvw] direction is perpendicular to (hkl) plane then h = u, k = v and l = w
Ex: {100} planes and <100> directions are perpendicular to each other.

If [uvw] direction is parallel to (hkl), that is if [uvw] lies in the plane (hkl) then hu + kv + lw = 0. For example, [$\bar{1}$ 1 0] lies in the plane (111) since 1.(-1) + 1.1 + 1.0 = 0
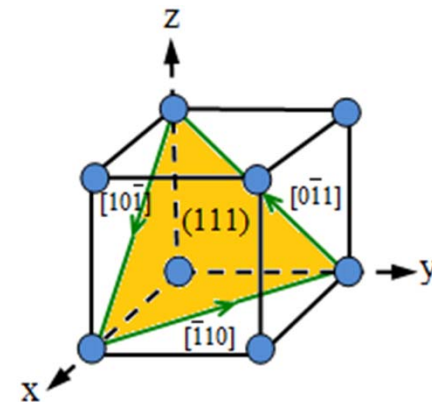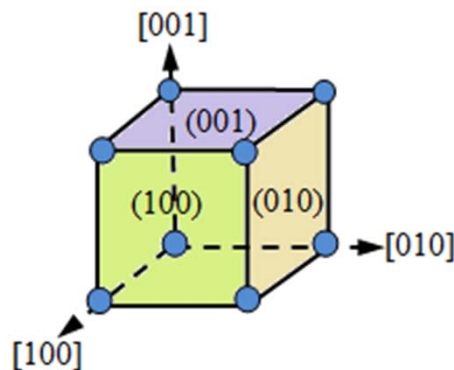
Coordination number

Coordination number is the number of nearest neighbor to a particular atom in the crystal
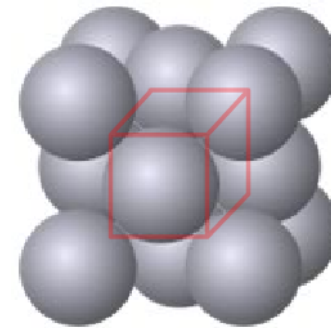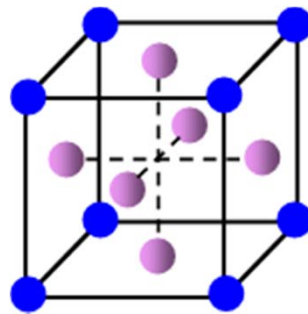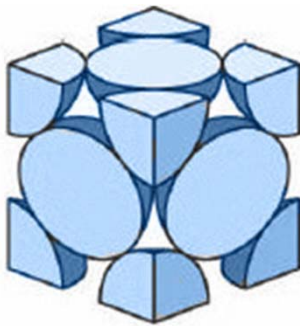
In the FCC lattice each atom is in contact with 12 neighbor atoms. FCC coordination number Z = 12

For example, the face centered atom in the front face is in contact with four corner atoms and four other face-centered atoms behind it (two sides, top and bottom) and is also touching four face-centered atoms of the unit cell in front of it.

Coordination number

The coordination number of BCC crystal is 8.
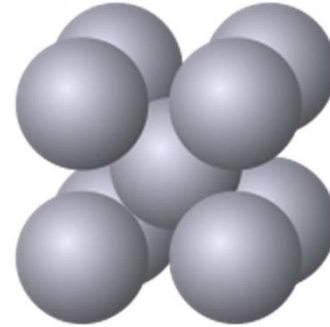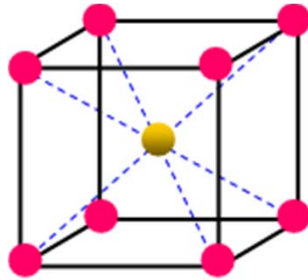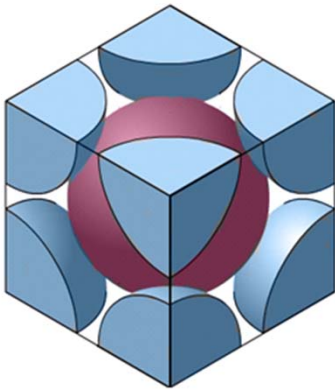
The body centered atom is in contact with all the eight corner atoms. Each corner atom is shared by eight unit cells and hence, each of these atoms is in touch with eight body centered atoms.

Coordination number
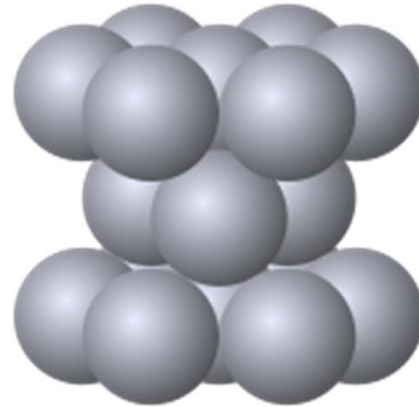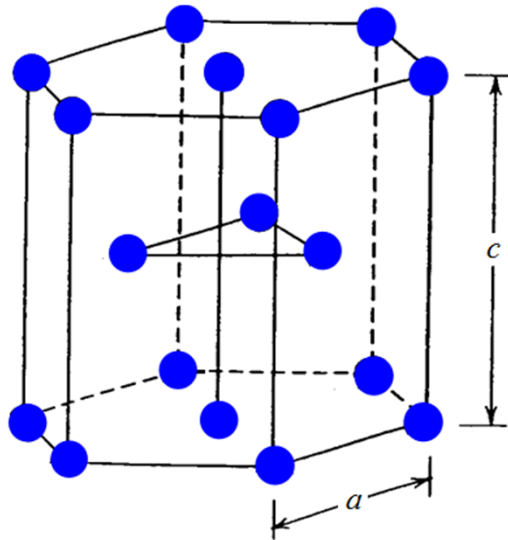
In Hexagonal lattice Z = 12. The center atom of the top face is in touch with six corner atoms, three atoms of the mid layer and other three atoms of the mid layer of the unit cell above it.

Atomic packing factor

Atomic packing factor (APF) or packing efficiency indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and volume of the unit cell

$$APF = \frac{\text{Volme of atoms}}{\text{Volume of unit cell}}$$

Atomic packing factor

FCC lattice

In the FCC unit cell effective number of atoms = 8 corner atoms x (1/8) (each atom is shared by 8 unit cells) + 6 face-centered atoms x1/2 (each shared by two unit cells) = 4
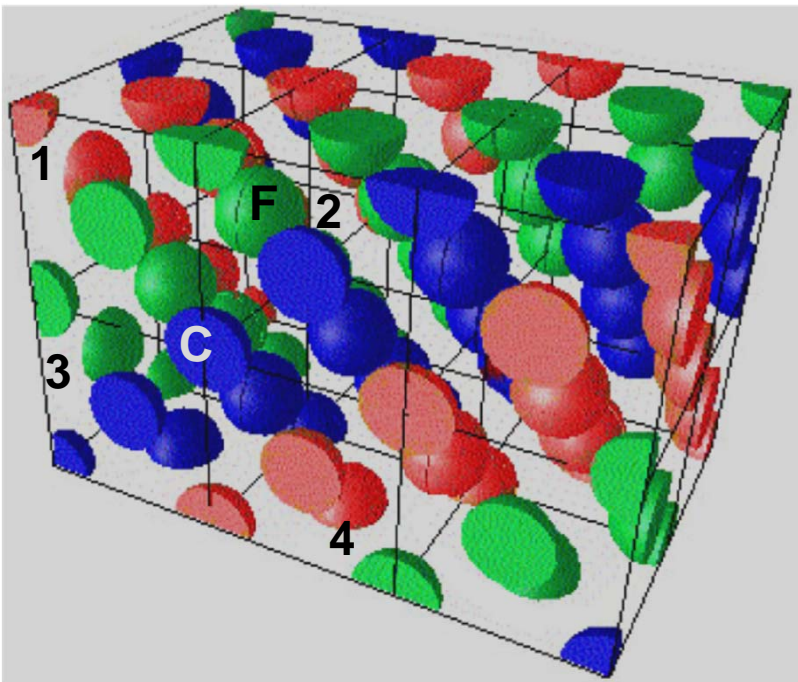
The corner atom *C* is shared by unit cells *1, 2, 3, 4* and four more in front of each of them. The face-centered atom, *F* is shared between cells *1* and *2*.

Click here for animation

Atomic packing factor

FCC lattice

Considering the atoms as hard spheres of radius R

Total volume of atoms $= 4 \times \dfrac{4}{3}\pi R^3$

The relation between R and the FCC cell side a as shown in the figure below is $\sqrt{2}a = 4R$
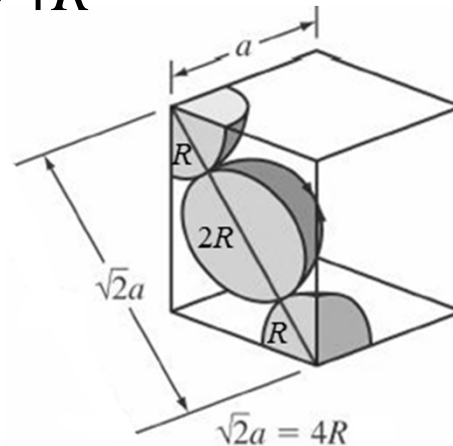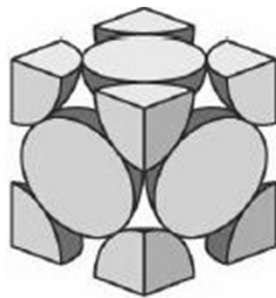
$$APF(FCC) = \frac{4 \times \dfrac{4}{3}\pi R^3}{a^3} = \frac{16 \times 2\sqrt{2}\pi \, a^3}{3 \times 64 a^3} = 0.74$$

Atomic packing factor

BCC

For BCC crystals effective number of atoms per unit cell is 8 x 1/8 + 1 = 2 and the relation between R and a is

$$\sqrt{3}a = 4R$$
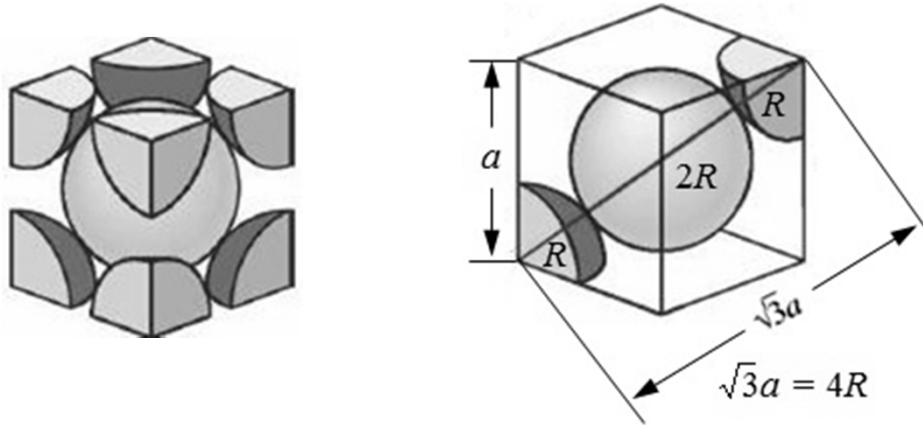
$$APF(BCC) = \frac{2 \times \frac{4}{3}\pi R^3}{a^3} = \frac{8 \times 3\sqrt{3}\pi\, a^3}{3 \times 64 a^3} = 0.68$$

Atomic packing factor

Hexagonal lattice

In the Hexagonal unit cell, number of atoms = 12 corner atoms x 1/6 (shared by six unit cells) + Two face atoms x 1/2 + 3 interior = 6.

$$2R = a$$

Unit cell volume = (6 x ½ x a x h) x c = (3 x a x a sin60°) x c = $3a^2$ c sin60°
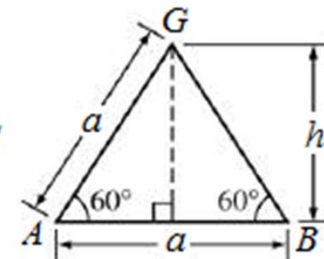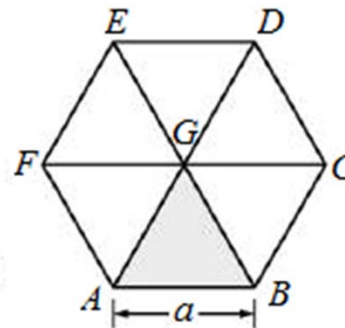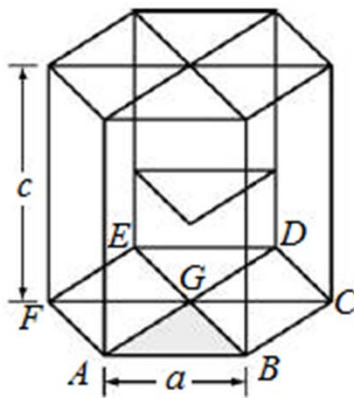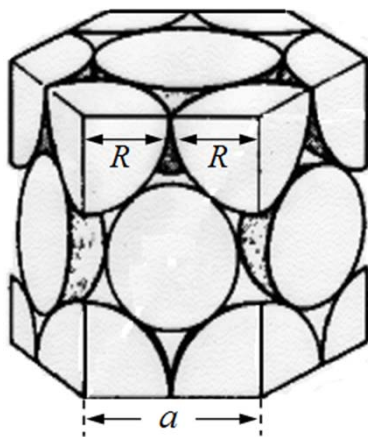
Atomic packing factor
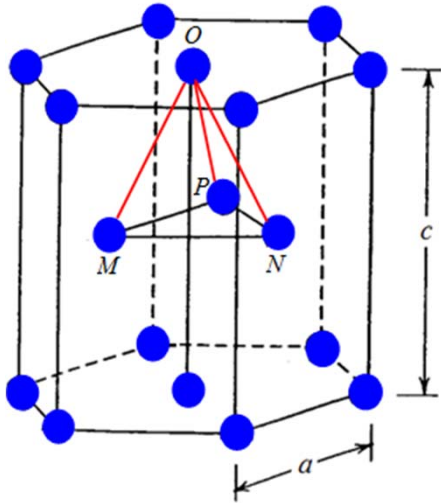
The face-centered atom and the three mid-layer atoms form a tetrahedron MNOP which has sides equal to a (as atoms at vertices touch each other) and height of c/2. Using this tetrahedron it can be shown that for an ideal hexagonal crystal c/a ratio = 1.633

$$APF(HCP) = \frac{6 \times \frac{4}{3}\pi R^3}{3a^2 c \sin 60°} = \frac{8\pi a^3}{3 \times 8 \times 1.414 a^3} = 0.74$$

Planar density

Planar density (PD) refers to density of atomic packing on a particular plane.

$$\text{Planar Density} = \frac{\text{Number of atoms on a plane}}{\text{Area of plane}}$$

For example, there are 2 atoms (1/4 x 4 corner atoms + 1/2 x 2 side atoms) in the {110} planes in the FCC lattice. Planar density of {110} planes in the FCC crystal
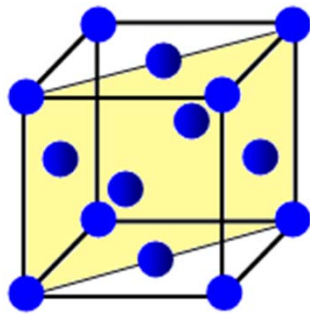
$$PD_{(110)} = \frac{2}{a\sqrt{2}a} = \frac{\sqrt{2}}{a^2}$$
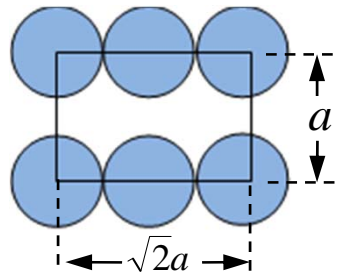
Planar density

In the {111} planes of the FCC lattice there are 2 atoms (1/6 x 3 corner atoms + 1/2 x 3 side atoms). Planar density of {111} planes in the FCC crystal

$$PD_{(111)} = \frac{2}{\frac{1}{2}\sqrt{2}a \times \sqrt{2}a \frac{\sqrt{3}}{2}} = \frac{4}{\sqrt{3}a^2}$$

This is higher than {110} and any other plane. Therefore, {111} planes are most densely packed planes in the FCC crystal
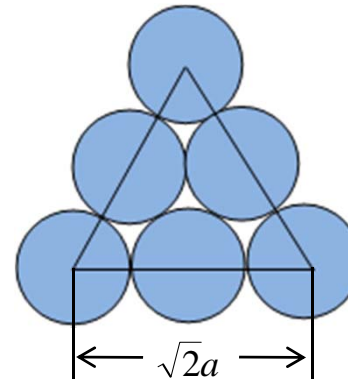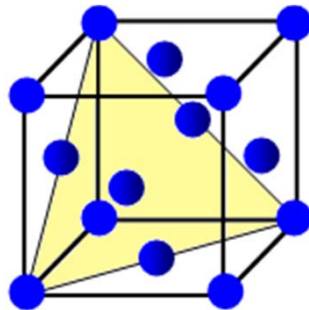
Linear Density

Linear density (LD) is the number of atoms per unit length along a particular direction

$$\text{Linear Density} = \frac{\text{Number of atoms on the direction vector}}{\text{Length of the direction vector}}$$

<110> directions in the FCC lattice have 2 atoms (1/2 x 2 corner atoms + 1 center atom) and the length is $\sqrt{2}a$

$$LD_{[110]} = \frac{2}{\sqrt{2}a} = \frac{\sqrt{2}}{a}$$

This is the most densely packed direction in the FCC lattice
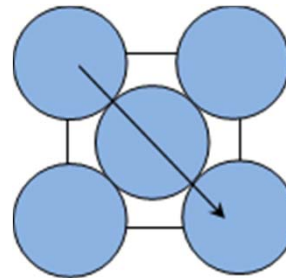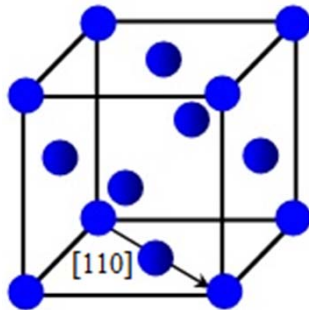
Close-Packed Structure

➤FCC and hexagonal crystal structures are most highly packed with packing efficiency of 74% (APF= 0.74). Such structures can be described in terms of close-packed atomic planes.

➤In FCC, {111} planes are close-packed and the basal plane (0001) is the close-packed one in hexagonal close-packed (HCP) system. Therefore, both of these structures can be generated by stacking of these planes. A portion of such a stack is shown in the picture below.
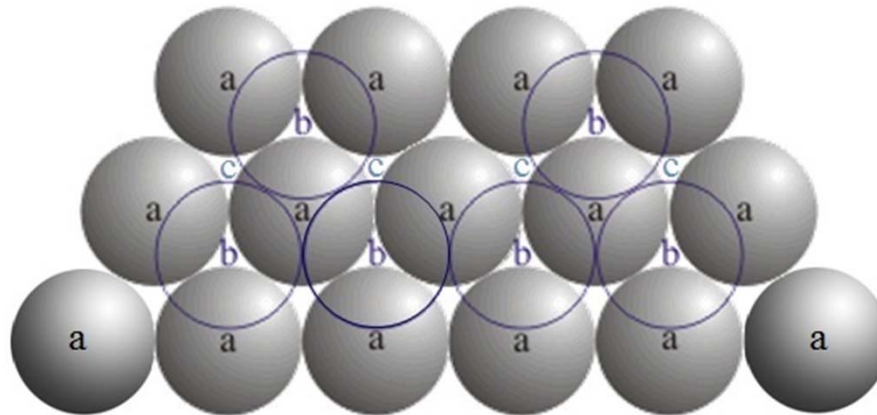
Close-Packed Structure

➤There are two types of voids between the atoms – vertex up (*b*), and vertex down (*c*). The atoms in the next layer sit on the *b* sites (See animation below).

➤In FCC, atoms in the third layer sit over the *c* sites and this repeats giving rise to ABC ABC ABC type of stacking.
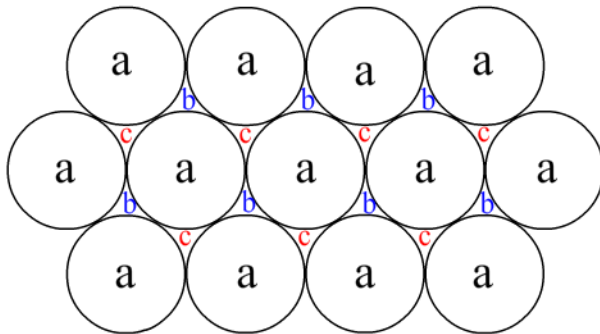
Close-Packed Structure

➤In HCP system, centers of atoms of the third layer lie directly over centers of atoms of the first layer (a positions) giving rise to AB AB AB type of stacking.

HCP
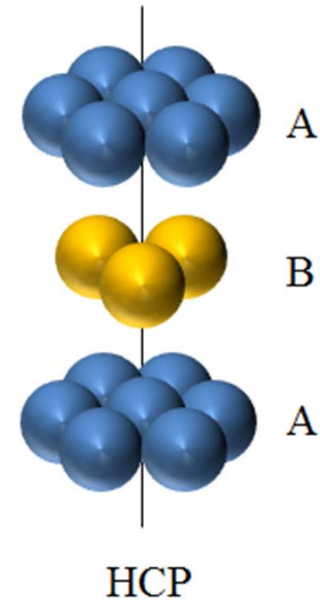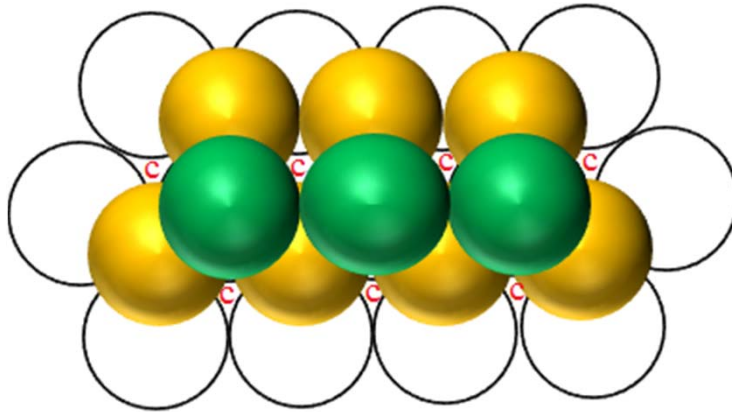
Structure-Property correlation

Aluminium (Al) is ductile while iron (Fe) and magnesium (Mg) are not. This can be explained from their crystal structures.

Al is FCC where as Fe is BCC and Mg is HCP.

Plastic deformation in metals takes place mainly by a process called slip. Slip can broadly be visualized as sliding of crystal planes over one another. Slip occurs on most densely packed planes in the most closely packed directions lying on that plane.

The slip plane and the direction together is called a
Slip system

Structure-Property correlation

❑In FCC, {111} planes are close-packed and there are four unique {111} planes. Each of these planes contains three closely packed <110> directions. Therefore, there are 4 x 3 = 12 slip systems

❑In HCP, the basal plane, (0001) is the close-packed and it contains three <1 1 $\bar{2}$ 0> directions. Hence, number of slip system = 1 x 3 = 3

❑Slip in more number of slip systems allows greater plastic deformation before fracture imparting ductility to FCC materials
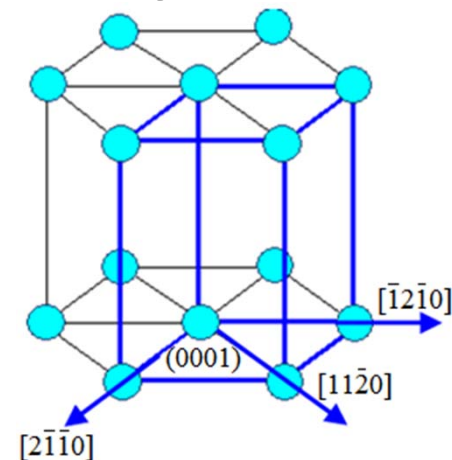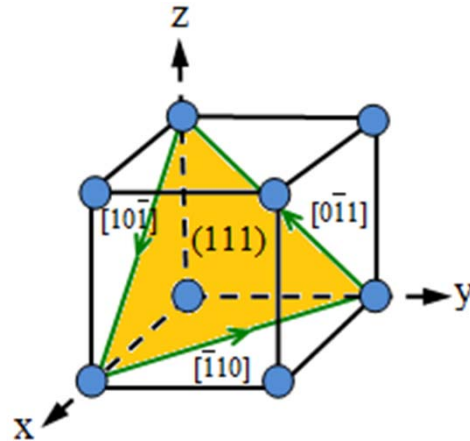
Structure-Property correlation

❑Close-packed planes are also planes with greatest interplanar spacing and this allows slip to take place easily on these planes.

❑BCC structure on the other hand has 48 possible slip systems. However, there is no close-packed plane. Hence, plastic deformation before fracture is not significant. Slip might occur in {110}, {112} and {123} planes in the <111> directions.

Evaluation

At the end of this chapter on crystallography, one should be able to

➢Understand Space lattice, Unit cells,7 crystal structure and 14 Bravais lattices.

➢Understand atomic arrangement and packing in different unit cells.

➢Derive point coordinates

➢Find out miller indices of crystallographic planes and directions.

➢Correlate some properties to crystal structure.

Web References

http://www.youtube.com/watch?v=qh29mj6uXoM&feature=relmfu
http://www.youtube.com/watch?v=8zWySdeXB0M&feature=relmfu
http://www.youtube.com/watch?v=Rm-i1c7zr6Q&feature=related
http://www.youtube.com/watch?v=PWQ89UoxOK8&feature=related
http://www.youtube.com/watch?v=mQy2CdKYqX0&feature=related

Key words: Symmetry; Space lattice; Crystal structure; Miller indices; Close pack structure; Slip system

Examples

Ex. 1: Theoretical density calculation from crystal structure.

Theoretical density, $\rho = \dfrac{nA}{V_C N_A}$

n = number of atoms in the unit cell
A = atomic weight
V_C = volume of unit cell
N_A = Avogadro's number (6.023 x 10^{23} atoms/mol)

Calculate the theoretical density of Al.

Al is FCC, lattice parameter, a = 4.05 Å, n = 4.
Atomic weight of Al is 26.98 g/mol

$$\rho = \frac{4 \times 26.98}{\left(4.05 \times 10^{-8}\right)^3 \times 6.023 \times 10^{23}} = 2.697 \, g/cc$$

Examples

Ex. 2: Show the point having coordinates 1/2, 1, 1/3 .

Solution: Select one of the corners of the unit cell as the origin. Move a/2 from the origin along the x axis and mark this point. From this point move b units along the y axis and then c/3 units along the z axis.

Ex. 3: Draw the plane (3 $\overline{1}$ 2) in a cubic unit cell.
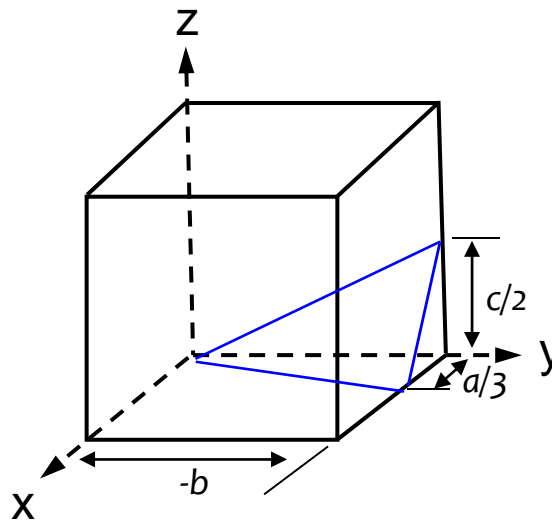
Examples

Ex. 4: Draw the directions [236] and [203] and [2 $\bar{1}$ 1] in a cubic unit cell.
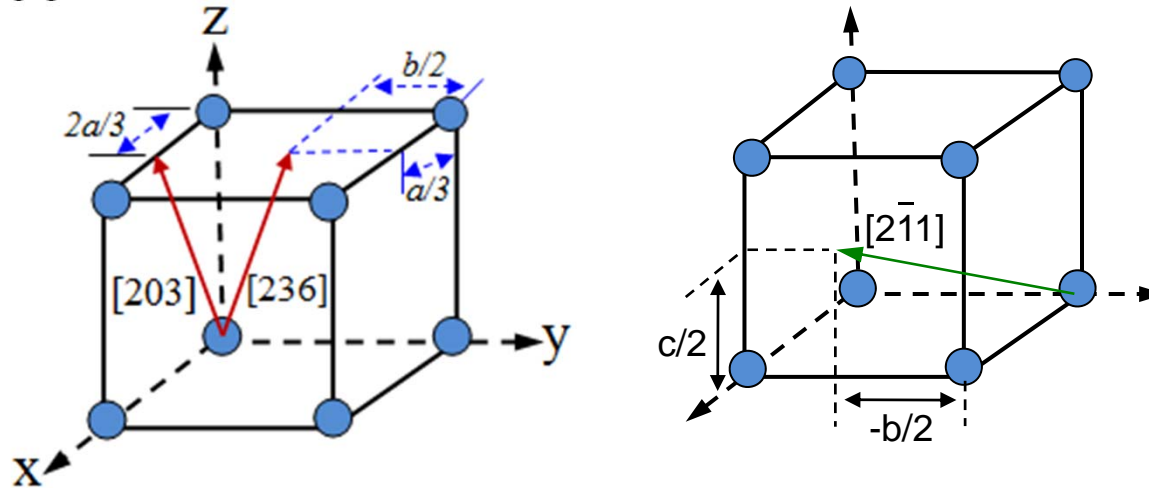
Ex. 5: The atomic radius of Fe is 0.124 nm. Find the lattice parameter of Fe.

Solution: Fe is BCC at room temperature. Therefore,

$$\sqrt{3}a = 4R \quad \text{and} \quad a = \frac{4R}{\sqrt{3}} = \frac{4 \times 0.124}{\sqrt{3}} = 0.286 \text{ nm}$$

Quiz

1. Show that only four types of rotational symmetry are possible.
 2. Why it is not possible to have 5, 7 or higher order symmetry in crystallography?
3. What is point group? How many point-groups are possible?
4. Find out the Hermann-Mauguin symbol for a cube.
5. For a point at xyz write a translation, a reflection and an inversion operation.
5. What is unit cell? What is lattice parameter?
6. What is Bravais lattice? How are the Bravais lattices obtained from the primitive cell? How many types of Bravais lattices are there?
7. What is the effective number of atoms in a simple cubic unit cell?

Quiz

8. What is coordination number (CN)? Show that CN for FCC and HCP structure is 12 while it is 8 for BCC.

9. Show that packing efficiency of FCC is 74% and that of BCC is 68%.

10. Show that the ideal c/a ratio in a hexagonal unit cell is 1.633 and calculate the packing efficiency.

11. What are the coordinates of the center atom in the BCC unit cell.

12. What is miller index? How is it obtained?

13. Draw the planes ($\bar{1}$ $\bar{1}$ 0), (1 $\bar{2}$ 1), (2 $\bar{3}$ 4), ($\bar{1}$ 12) and directions[1 1 $\bar{1}$], [123], [120], [1 $\bar{2}$ 1] in a cubic unit cell.

14. Why it is necessary to include a fourth miller index in the hexagonal system?

15. Convert the directions [112], [1 $\bar{2}$ 3], [110], [111], [130] to four indices in a hexagonal lattice.

Quiz

16. What is family of planes? Draw the {111} family of planes in cubic system?

17. What is linear density? What is planar density?

18. Find the planar of density {111} planes and linear density of <110> directions in FCC system.

19. What is the linear density of <111> directions in the BCC crystal.

20. What is interplanar spacing? Find the interplanar spacing of the vertical planes in the HCP system?

21. What is the stacking sequence of FCC and HCP crystals?

22. What is slip system?

23. Why FCC metals are ductile while BCC and HCP metals are not?

24. Calculate the theoretical density of Cu from its crystal structure.

Quiz

25. Lattice constant of Al is 4.05 Å. What is the atomic radius of Al?

26. Calculate the theoretical density of Mg, Cu and Fe and compare them to the standard values.

27. A metal has a density of 10.22 g/cc, atomic weight of 95.94 and atomic radius of 0.136 nm. Is it BCC or FCC?

28. Calculate the volume of the unit cell of Zn crystal. a and c of Zn are 266.5 pm and 494.7 pm respectively.

29. Calculate the planar density of {110} planes in α-Fe (BCC) crystal. $a = 0.287$ nm.

30. Calculate the linear density of [110] direction in a Cu crystal. $a = 0.361$ nm.