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M. Sc. Chemistry Semester –I
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Crystallography : Unit -IV

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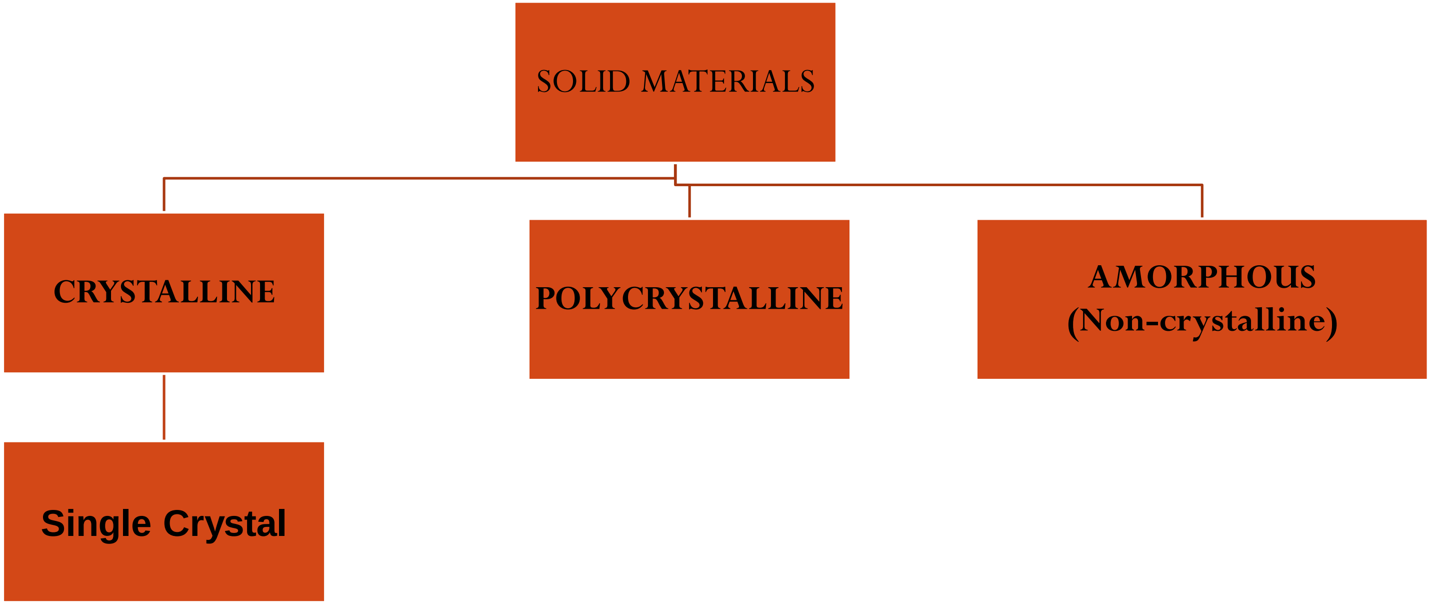
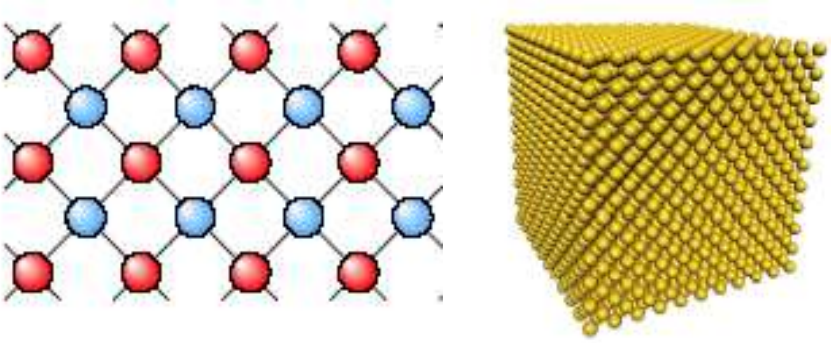


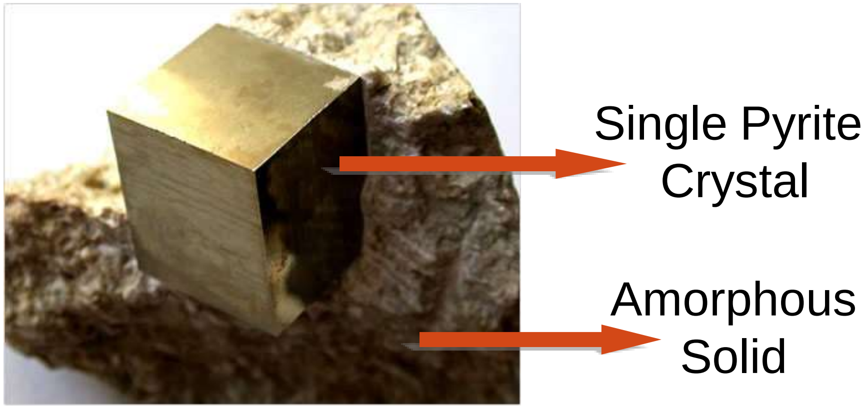
SOLID MATERIALS

- CRYSTALLINE
  - Single Crystal
- POLYCRYSTALLINE
- AMORPHOUS (Non-crystalline)

A) Crystalline Solid

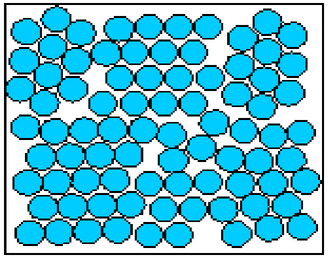
- Crystalline Solid is the solid form of a substance in which the ***atoms or molecules*** are arranged in a definite, repeating pattern in three dimension.
- Single crystals, ideally have a high degree of order, or regular geometric periodicity, throughout the ***entire volume of the material***.



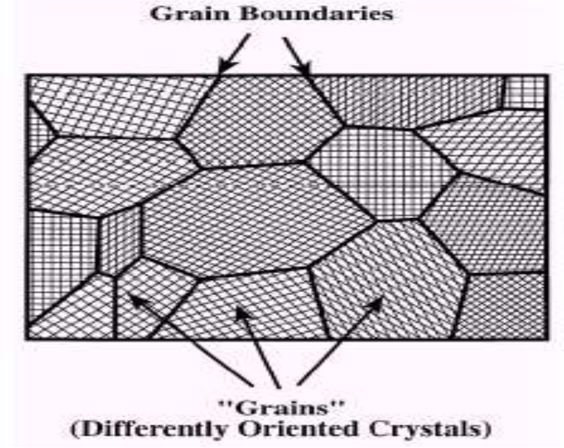


B) Polycrystalline Solid

- Polycrystal is a material made up of an aggregate of *many small single crystals* (also called crystallites or grains).
- Polycrystalline material have a high degree of order over many atomic or molecular dimensions.
- These *ordered regions,* or single crytal regions, vary in size and orientation wrt one another.
- These regions are called as *grains (domain)* and are separated from one another by *grain boundaries. The atomic order can vary from one domain to the next*.
- The grains are usually *100 nm - 100 microns in diameter*. Polycrystals with grains that are <10 nm in diameter are called nanocrystalline

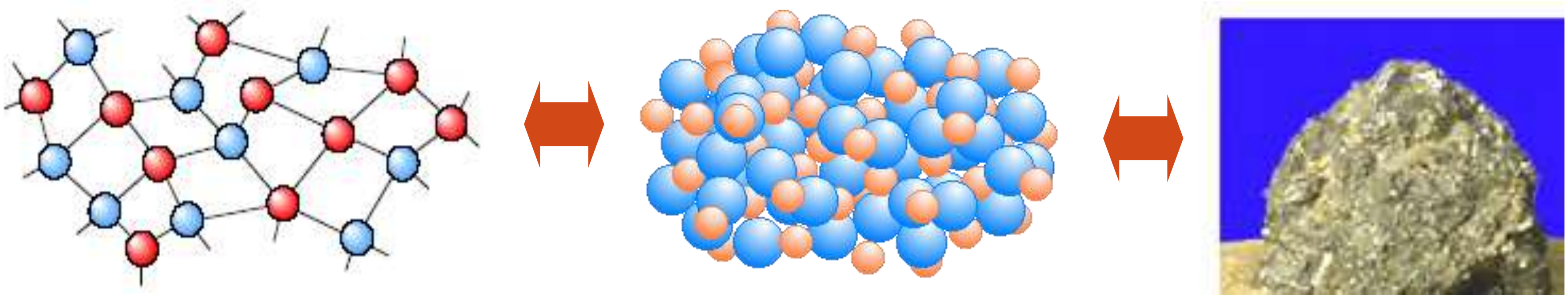


Polycrystalline
Pyrite form
(Grain)

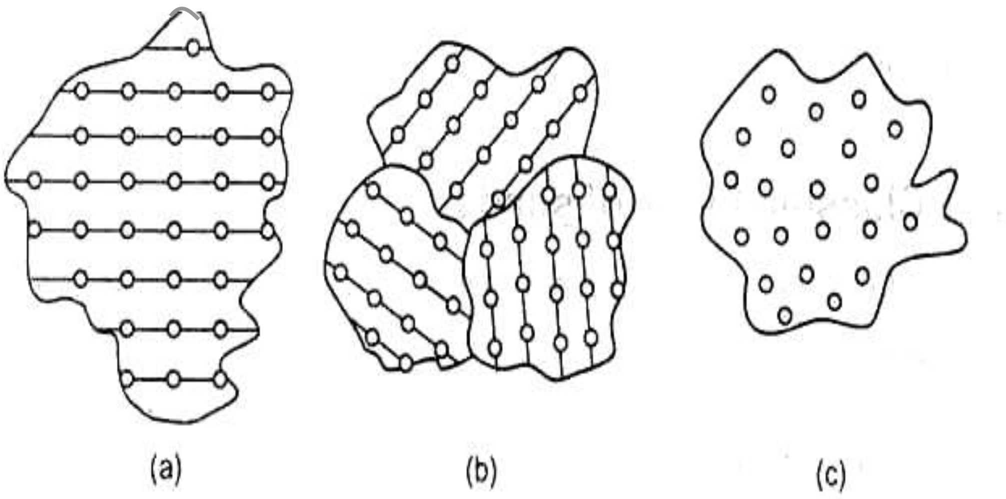


C) Amorphous Solid

- Amorphous (Non-crystalline) Solid is composed of randomly orientated atoms , ions, or molecules that do not form defined patterns or lattice structures.
- Amorphous materials have order only within a few atomic or molecular dimensions.
- Amorphous materials do not have any long-range order, but they have varying degrees of short-range order.
- Examples to amorphous materials include amorphous silicon, plastics, and glasses.
- Amorphous silicon can be used in solar cells and thin film transistors.



ATOMIC ARRANGEMENT IN CRYSTALS



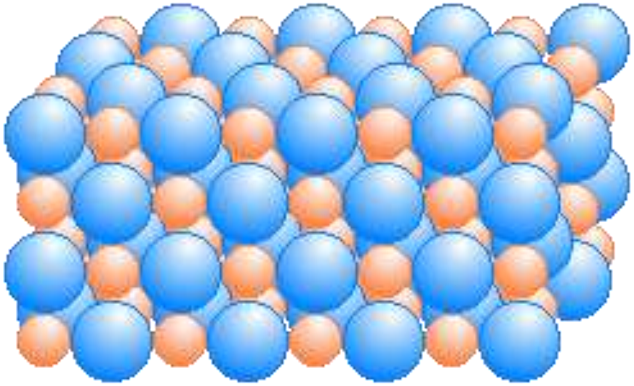
(a) mono (or) single crystals

(b) polycrystalline solids

(c) amorphous solids

❑ Perfect Crystal

- Strictly speaking, one cannot prepare a perfect crystal. For example, even the surface of a crystal is a kind of imperfection because the periodicity is interrupted there.
- Another example concerns the thermal vibrations of the atoms around their equilibrium positions for any temperature T>0°K.



- As a third example, actual crystal always contains some foreign atoms, i.e., impurities. These impurities spoils the perfect crystal structure.

❑ Crystals

- The periodic array of atoms, ions, or molecules that form the solid is called ***Crystal Structure***

  Crystal Structure = Space (Crystal) Lattice + Basis

  - **Space (Crystal) Lattice** is a regular periodic arrangement of ***points*** in space, and is purely ***mathematical abstraction***
  - **Crystal Structure** is formed by "putting" the identical atoms (group of atoms) in the points of the space lattice
  - This group of atoms is the ***Basis***

❑ Crystal Lattice

Mathematically,

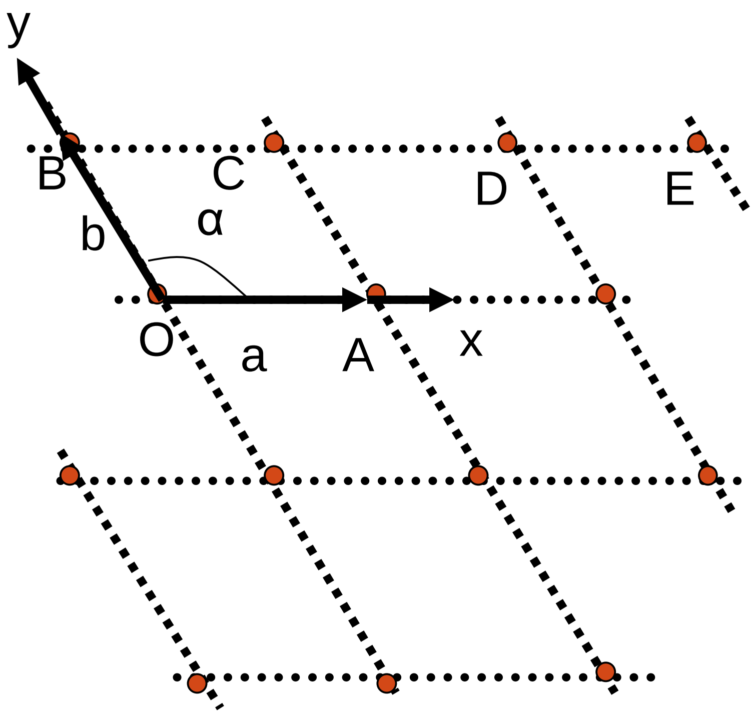
A Lattice is defined as an Infinite Array of Points in Space in which Each point has identical surroundings To all others.

The points are arranged exactly in a Periodic manner.

2 Dimensional Example

↓

↓



- The structure of an ***Ideal Crystal*** can be described in terms of a mathematical construction called a **Lattice**.

A Lattice ≡

- A 3-dimensional periodic array of points in space. For a particular solid, the smallest structural unit, which when repeated for every point in the lattice is called the **Basis**.
- The ***Crystal Structure*** is defined once both the lattice & the basis are specified. That is

Crystal Structure ≡ **Lattice** + **Basis**

- A crystal lattice can be divided in to two categories,

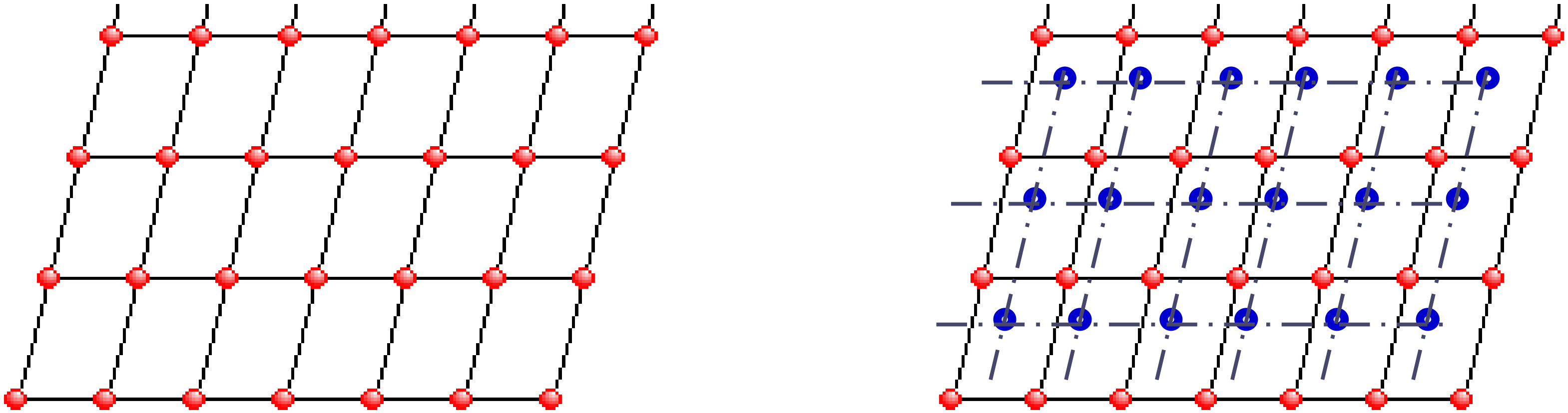
Crystal Lattice

Bravais Lattice (BL)

§ All atoms are of the same kind
§ All lattice points are equivalent

Non-Bravais Lattice (non-BL)

§ Atoms can be of different kind
§ Some lattice points are not equivalent
§A combination of two or more BL

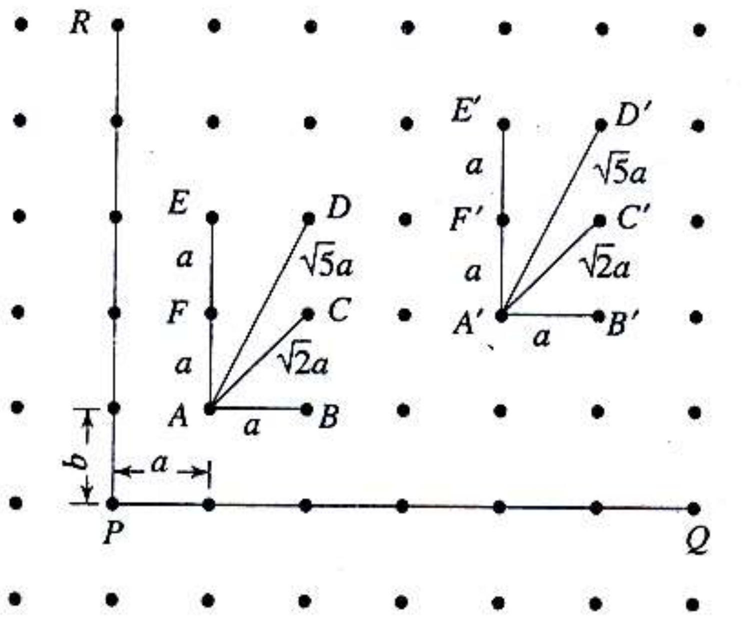


❑ Space Lattice

- A lattice is a regular and periodic arrangement of points in three dimension.

- It is defined as an infinite array of points in three dimension in every point has surroundings identical to that of every other point in the array.

- The Space lattice is otherwise called the Crystal lattice



Two Dimentional Space Lattice

❑ Basis

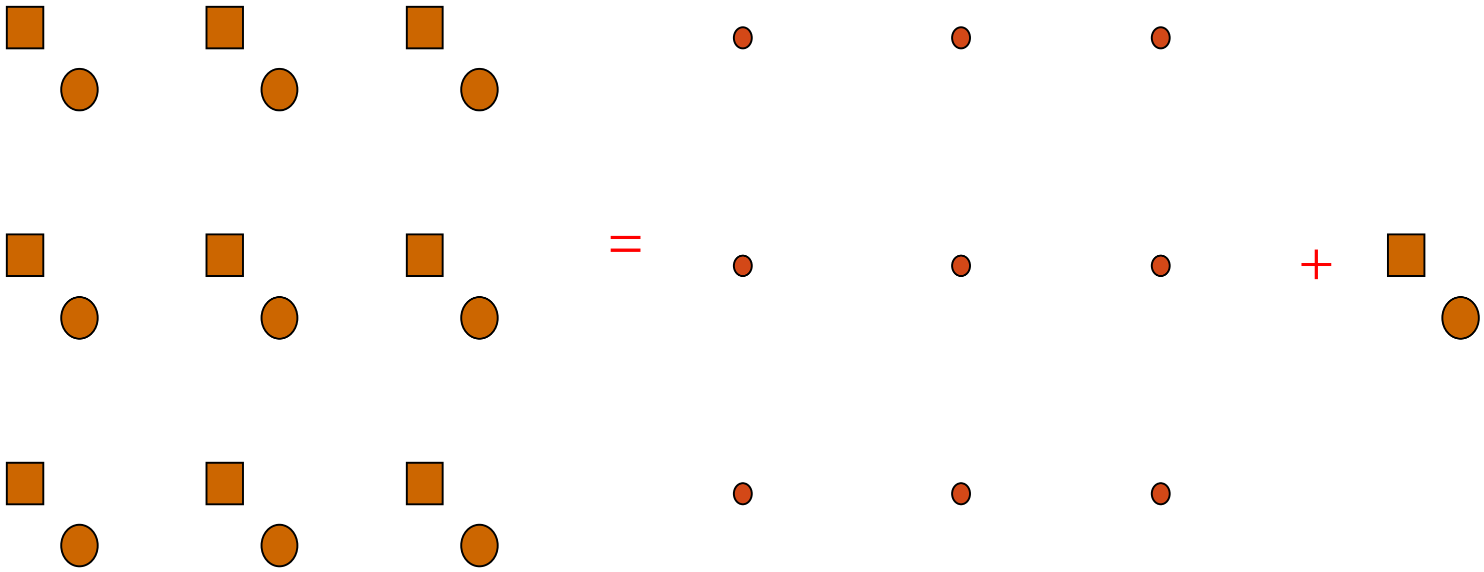
- A crystal structure is formed by associating every lattice point with an unit assembly of atoms or molecules identical in composition, arrangement and orientation.

- 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.

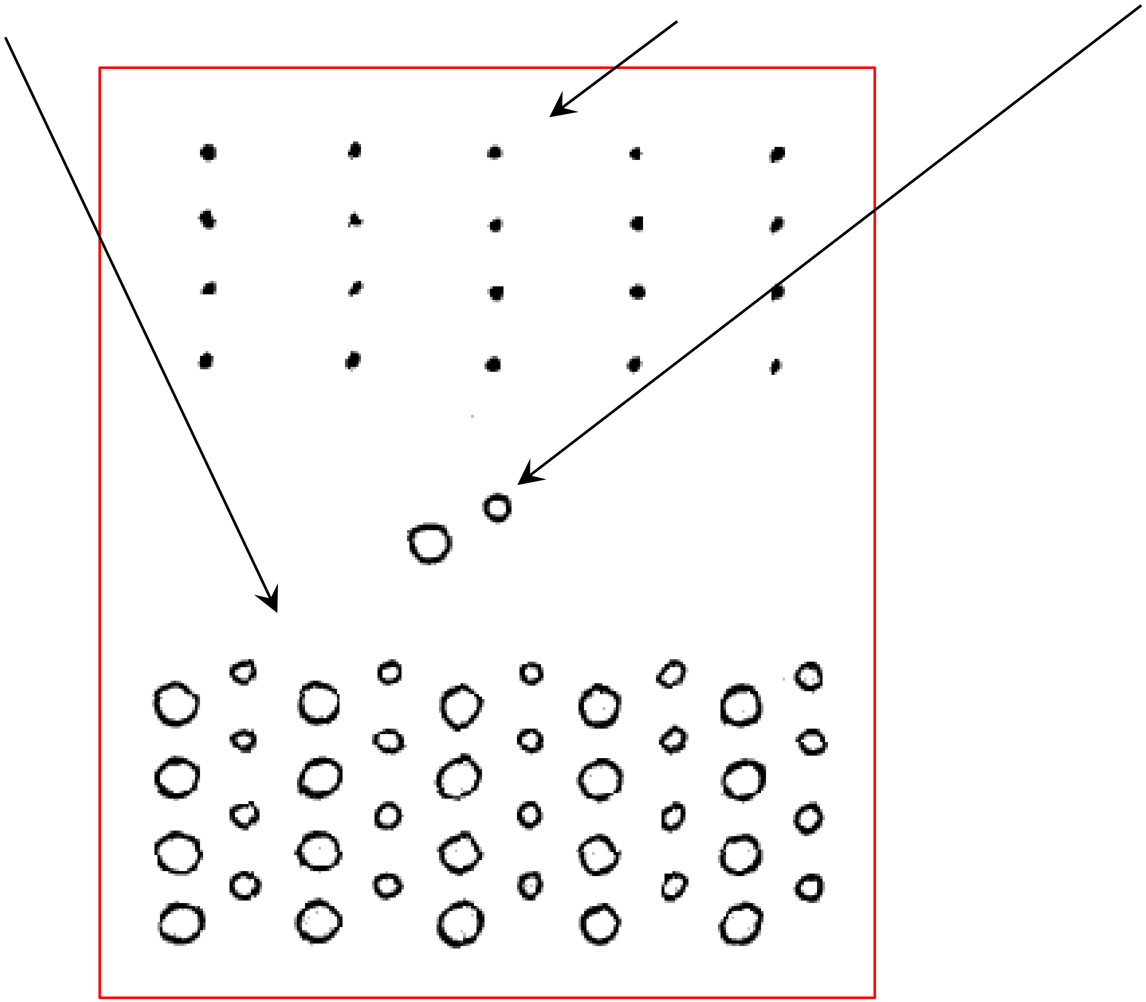
❑ Crystal Structure



Crystal structure = Lattice + Basis

❑ Crystals

Crystal Structure = Space Lattice + Basis

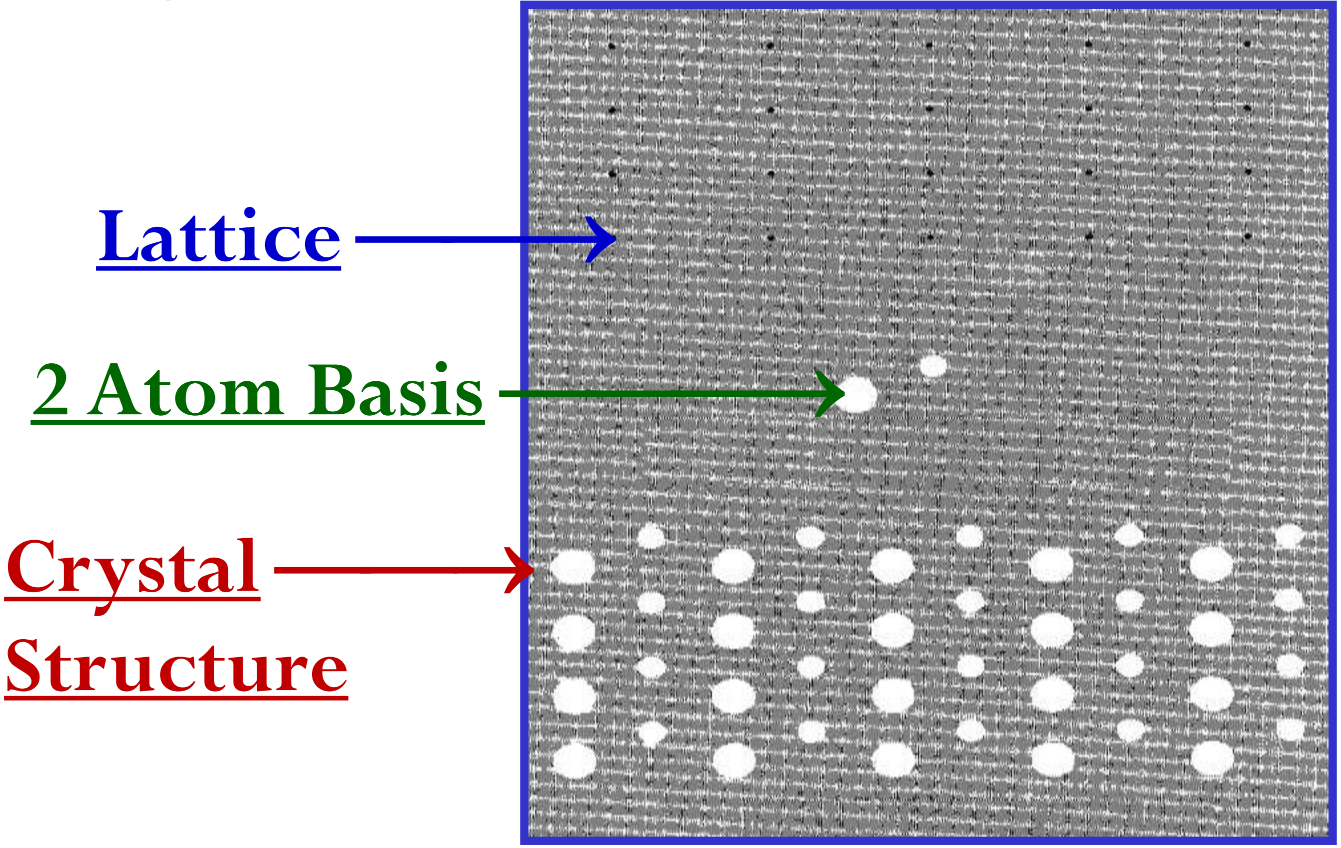


Crystalline Periodicity

- In a crystalline material, the equilibrium positions of all the atoms form a crystal

Crystal Structure ≡ Lattice + Basis

For example, see **Fig**.



Lattice

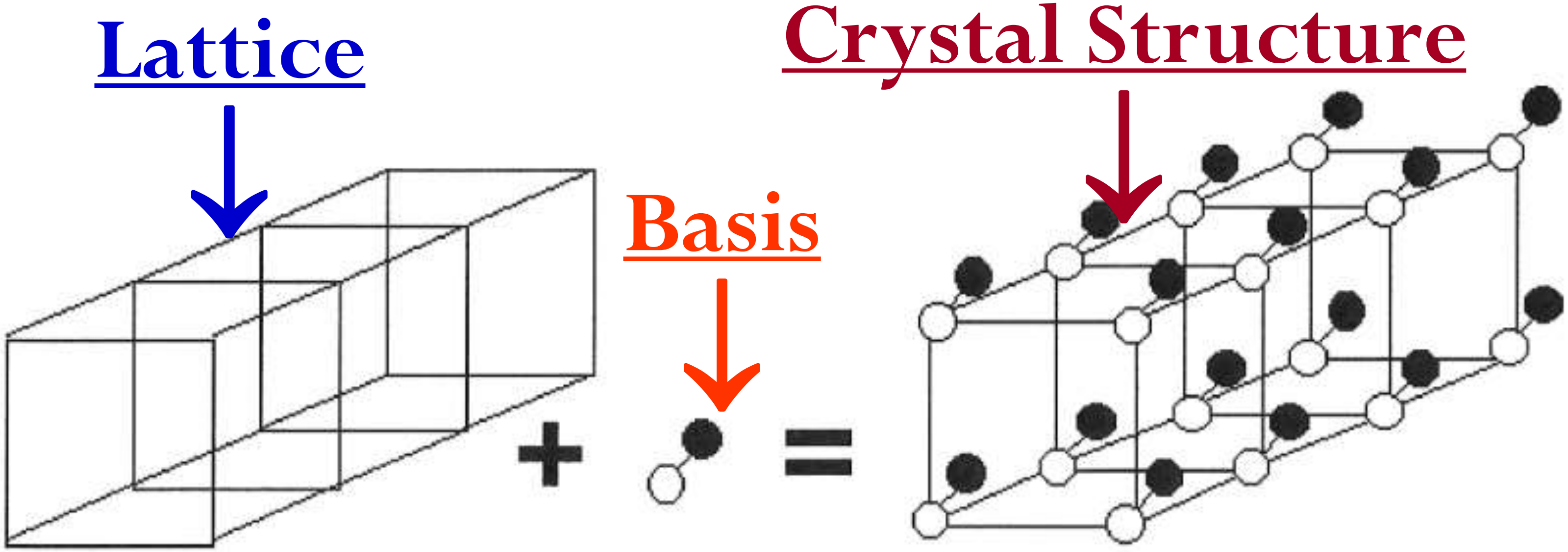
2 Atom Basis

Crystal Structure

❑ Crystalline Periodicity

Crystal Structure ≡ Lattice + Basis

For another example, see the figure.



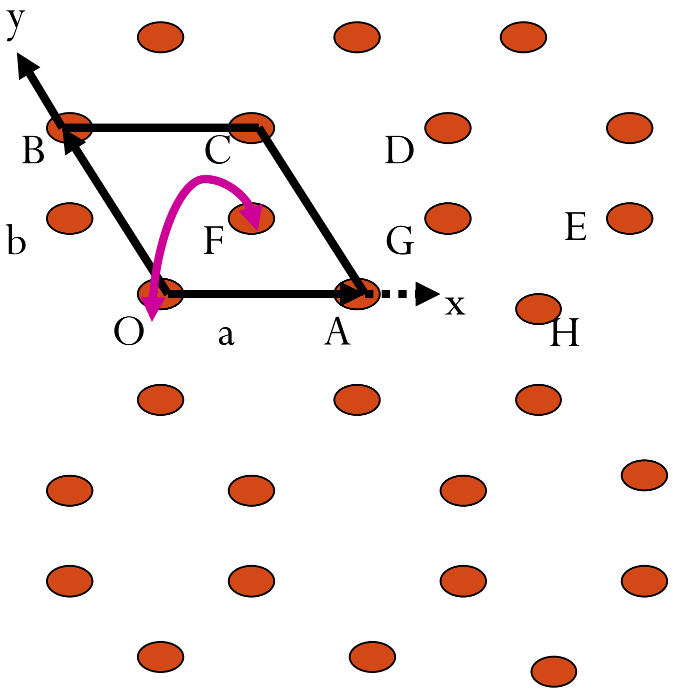
Lattice

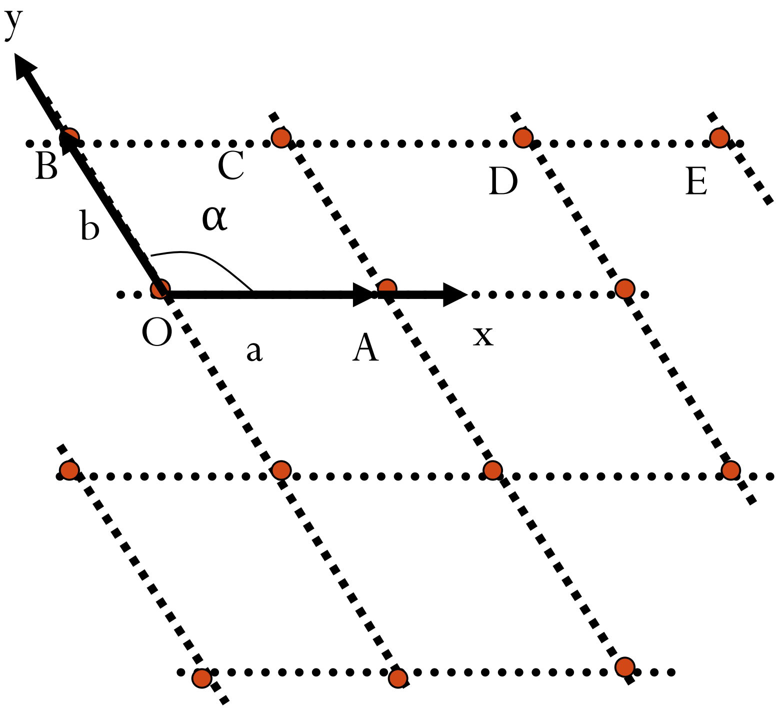
Basis

Crystal Structure

2-Dimensional Lattice

Lattice with atoms at the corners of regular hexagons

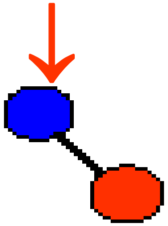




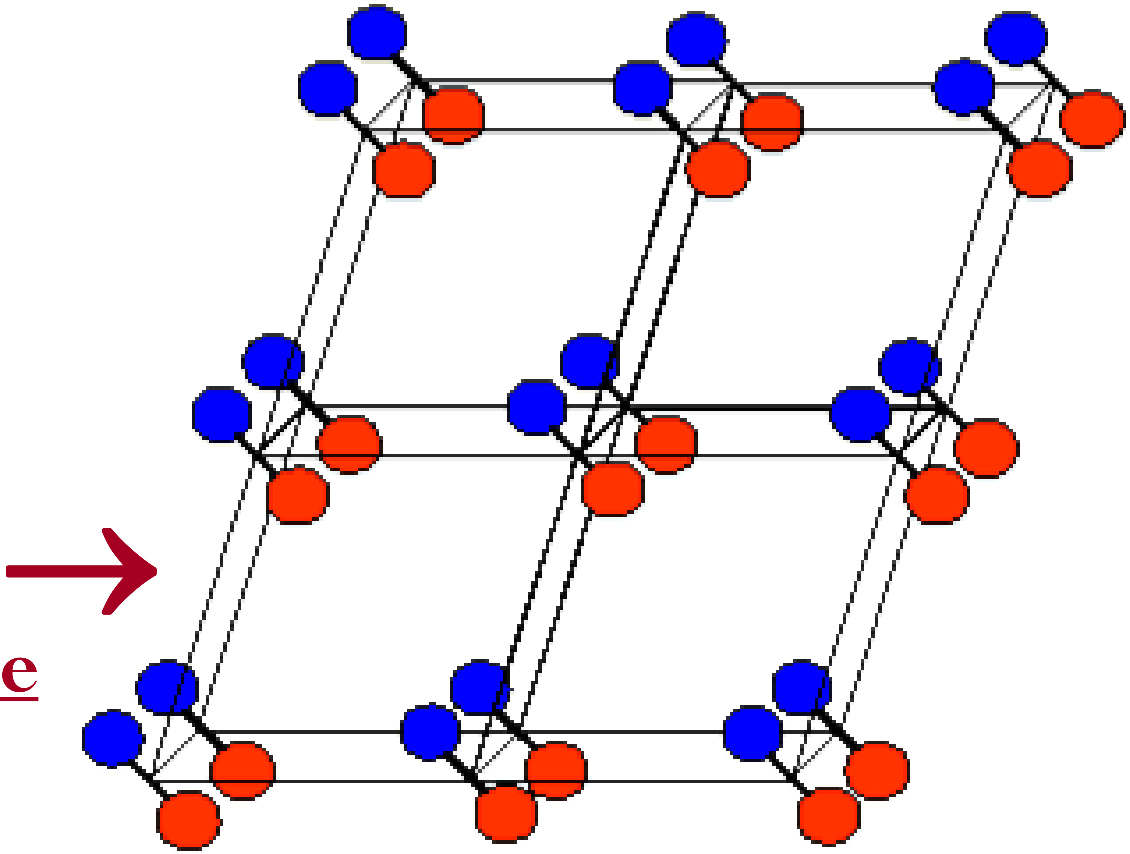
- The atoms do not necessarily lie at lattice points!!!

Crystal Structure = Lattice + Basis

Basis

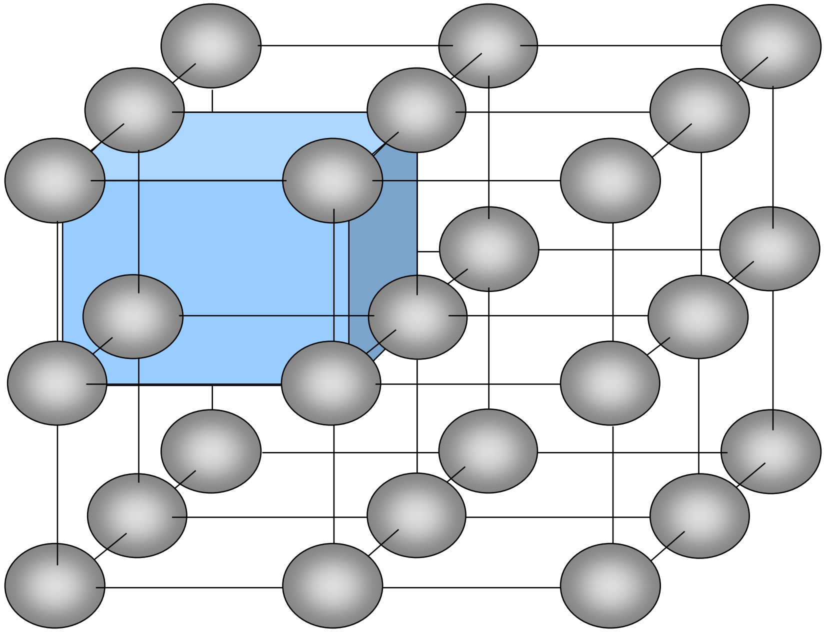


Crystal Structure



❑ Unit Cell

- The simplest repeating unit in a crystal is called a **unit cell**.
- Opposite faces of a unit cell are parallel.
- The edge of the unit cell connects equivalent points.
- Not unique. There can be several unit cells of a crystal.
- The smallest possible unit cell is called **primitive unit cell** of a particular crystal structure.

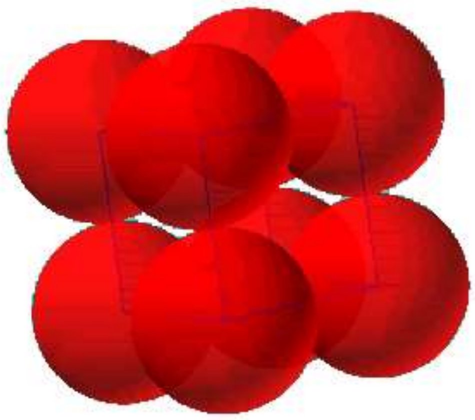


❑ Crystal Structure for Metallic Elements

(1-a): Simple Cubic Structure (SC)

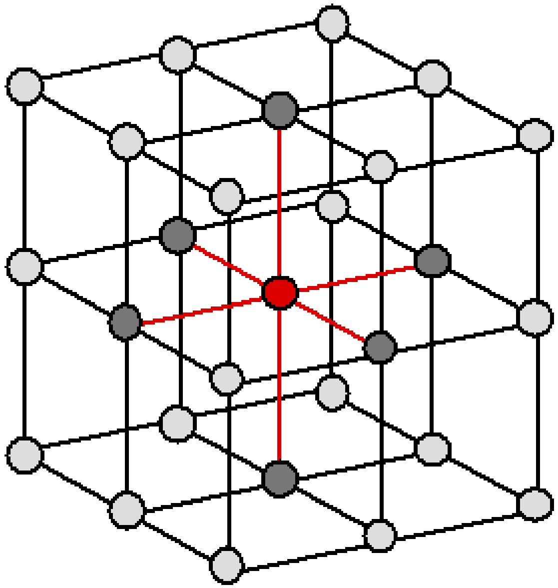
- Rare due to poor packing (only Po has this structure)
- Close-packed directions are cube edges.

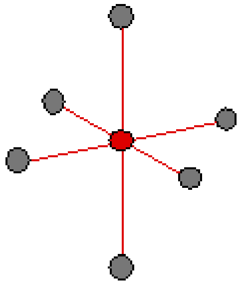
1 atom/unit cell



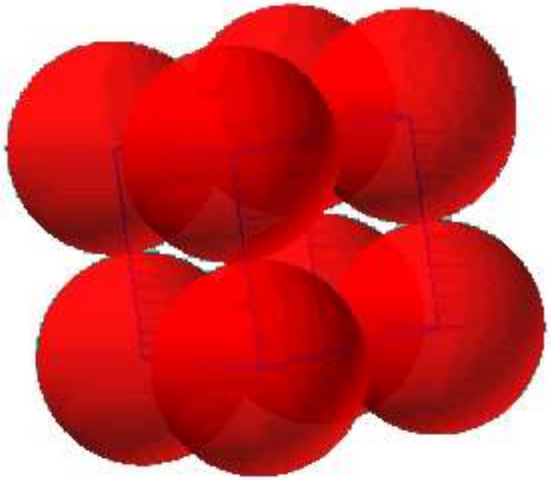
Coordination # = 6

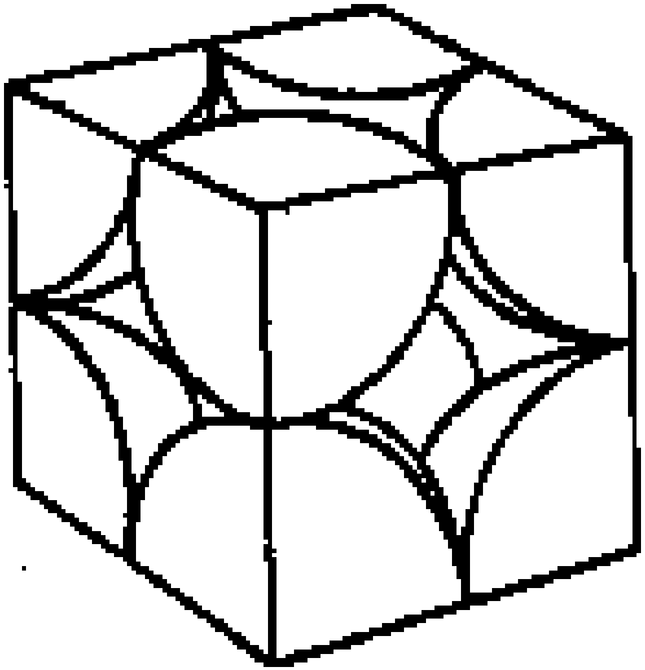
nearest neighbors)





One atom per unit cell



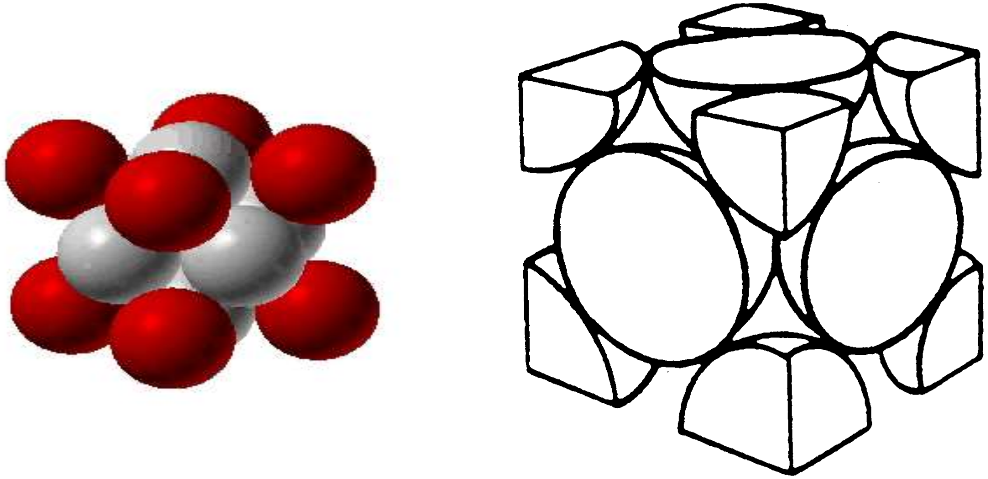


$1/8 \times 8 = 1$

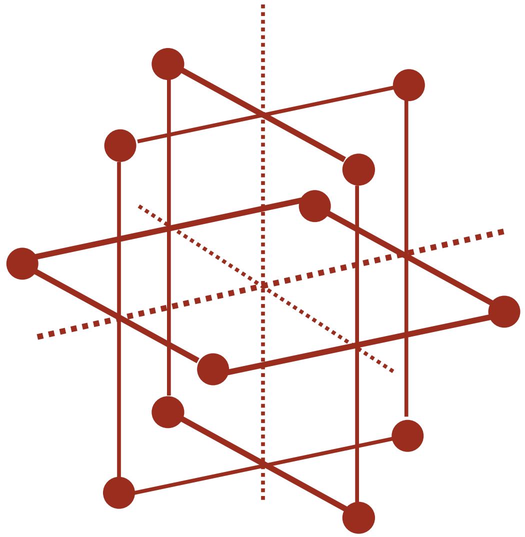
(1-b): Face Centered Cubic Structure (FCC)

- Exhibited by Al, Cu, Au, Ag, Ni, Pt
- Close packed directions are face diagonals.
- Coordination number = 12
- 4 atoms/unit cell

All atoms are identical



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

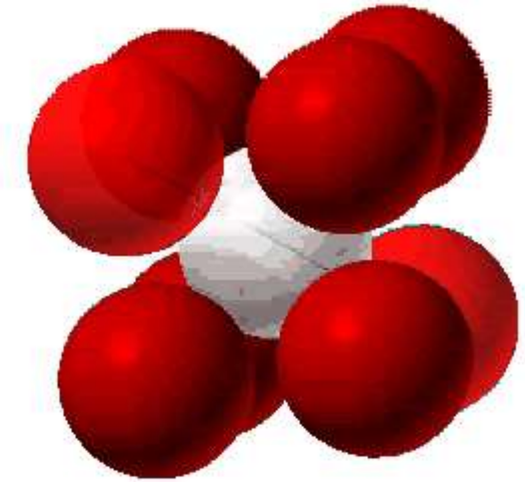


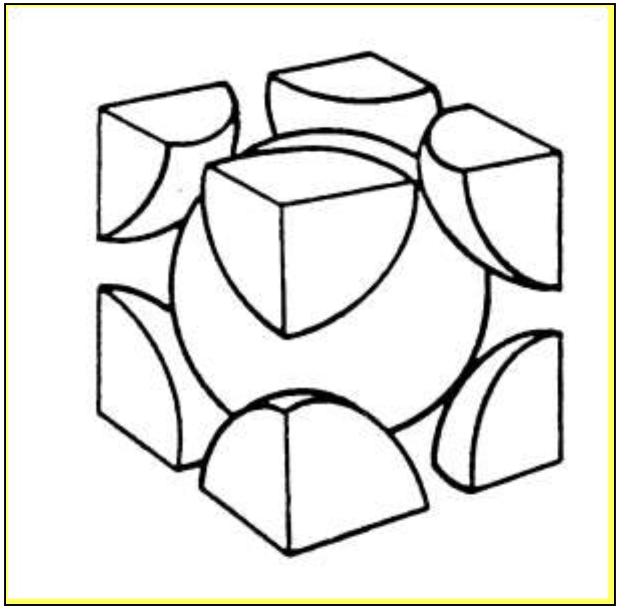
FCC
Coordination number = 12
3 mutually perpendicular planes.
4 nearest neighbors on each of the three planes.

(1-c): Body Centered Cubic Structure (BCC)

- Exhibited by Cr, Fe, Mo, Ta, W
- Close packed directions are cube diagonals.
- Coordination number = 8

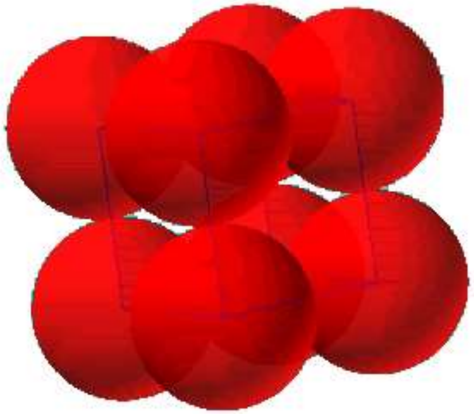
All atoms are identical

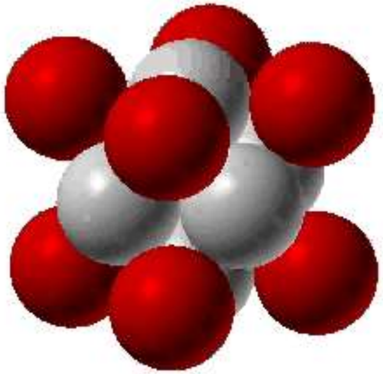


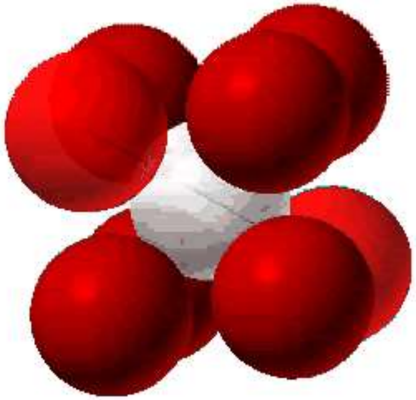


2 atoms/unit cell

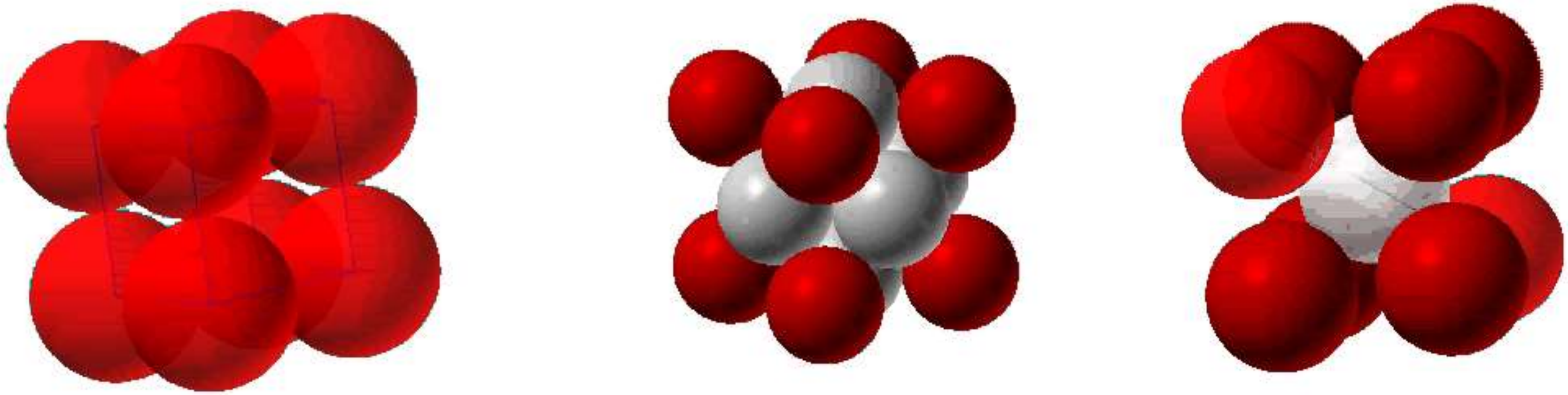
Which one has most packing ?







Which one has most packing ?



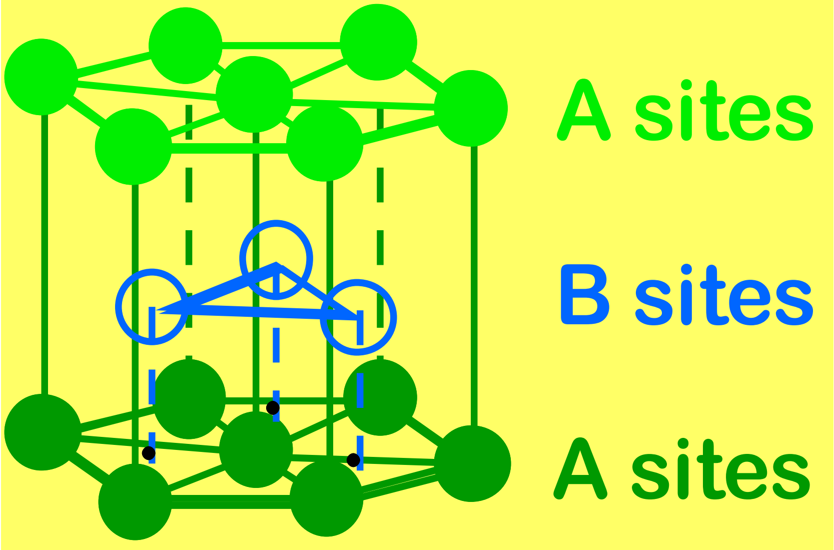
For that reason, FCC is also referred to as cubic closed packed (CCP)

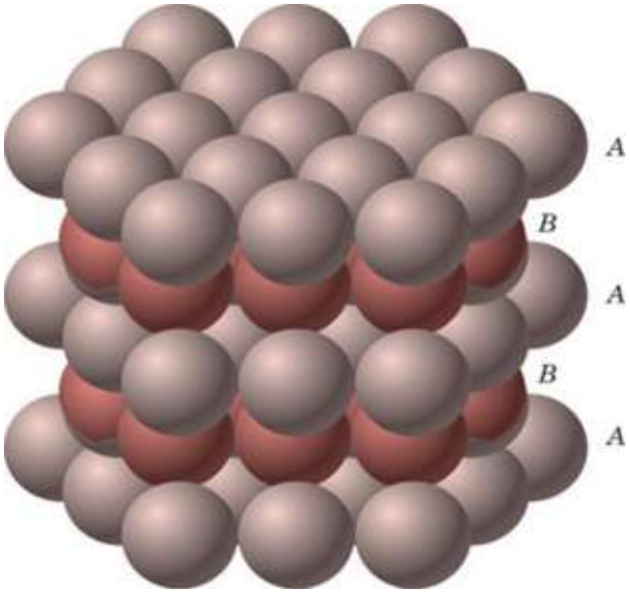
Hexagonal Closed Packed Structure (HCP)

- Exhibited by ….
- ABAB… Stacking Sequence
- Coordination # = 12

2D Projection

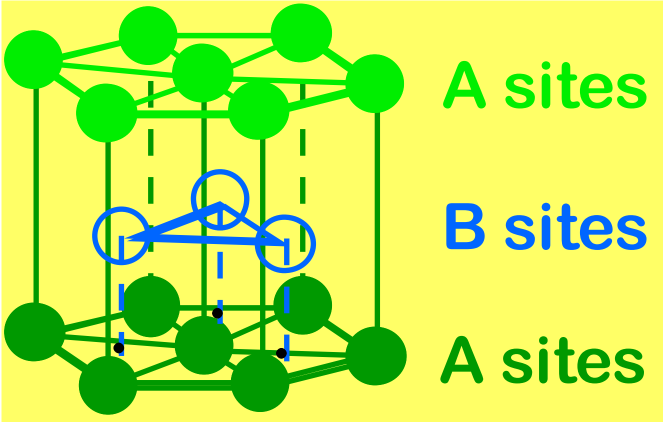
3D Projection

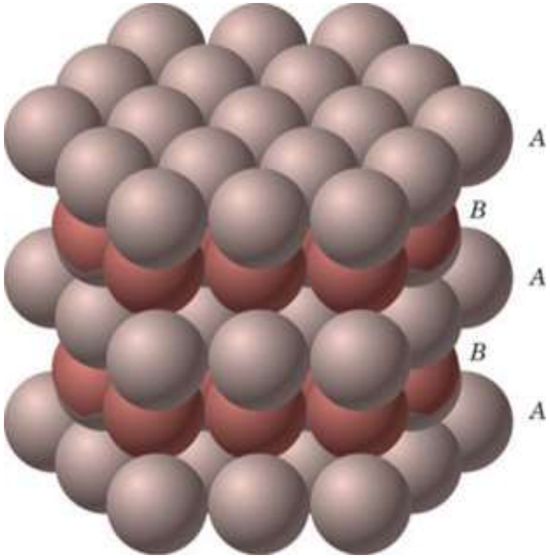




Layer Stacking Sequence

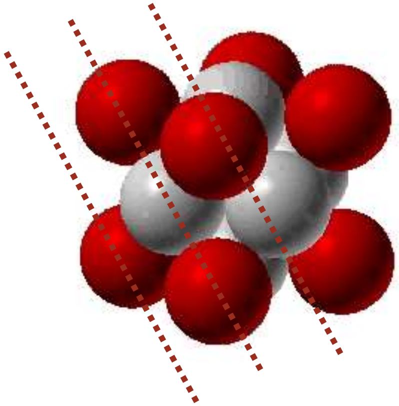
HCP





= ABAB…

FCC



= ABCABC..

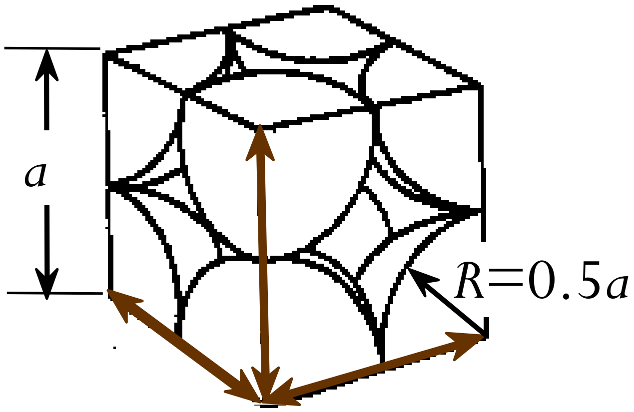
❑ Atomic Packing Factor

Atomic Packing Factor (APF) is defined as the volume of atoms within the unit cell divided by the volume of the unit cell.

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

*(assume hard spheres)

- APF for a simple cubic structure = 0.52



close-packed directions

contains (8 x 1/8) =

1 atom/unit cell

Adapted from Fig. 3.23, *Callister 7e.*

$\frac{\text{atoms}}{\text{unit cell}}$ $\frac{\text{volume}}{\text{atom}}$

$$\text{APF} = \frac{1 \quad \frac{4}{3}\pi\,(0.5a)^3}{a^3}$$

$\frac{\text{volume}}{\text{unit cell}}$

Here: a = R_{at}*2

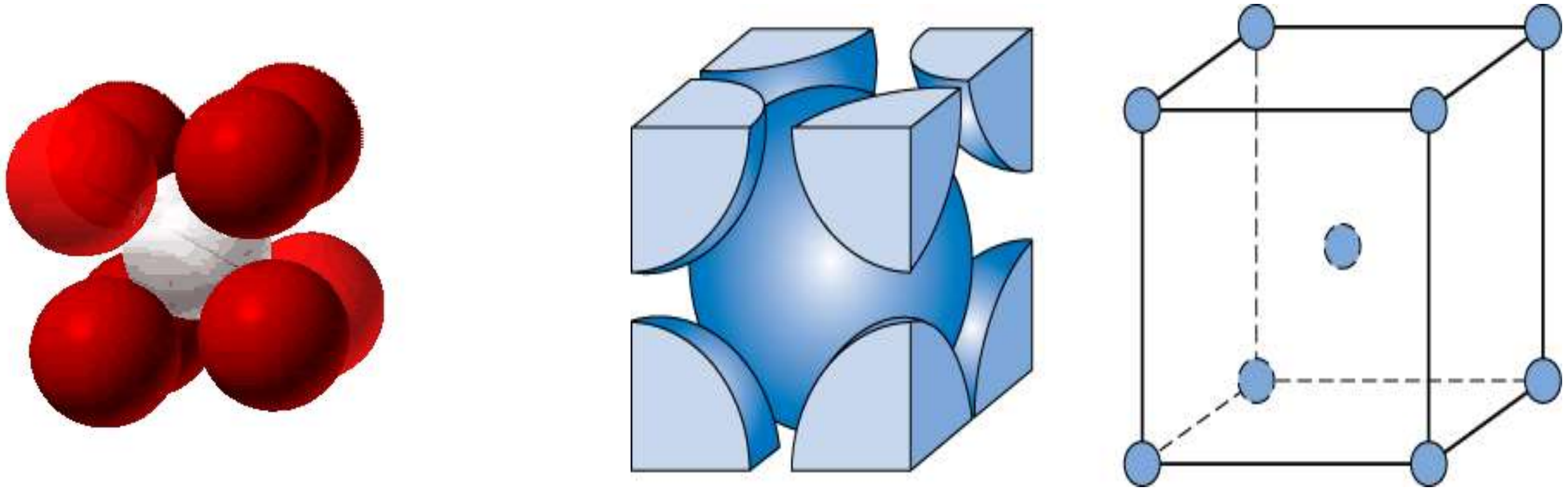
Where R_{at} is the 'handbook' atomic radius

A] Body Centered Cubic Structure (BCC)

- Atoms touch each other along *cube diagonals within a unit cell*.

Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

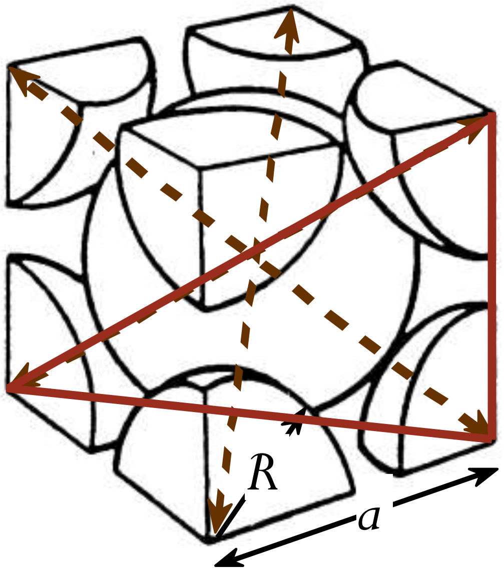
ex: Cr, W, Fe (α), Tantalum, Molybdenum

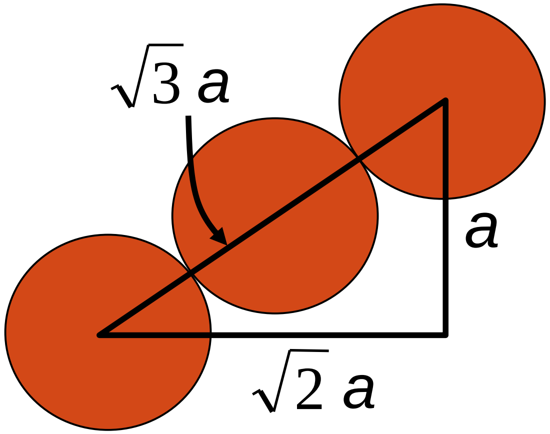


- Coordination # = 8

2 atoms/unit cell: (1 center) + (8 corners x 1/8)

Atomic Packing Factor: BCC





Close-packed directions:
length = $4R = \sqrt{3}\,a$

$\frac{\text{atoms}}{\text{unit cell}}$

$\frac{\text{volume}}{\text{atom}}$

$$\text{APF} = \frac{2 \;\; \frac{4}{3}\pi(\sqrt{3}\,a/4)^3}{a^3}$$

$\frac{\text{volume}}{\text{unit cell}}$

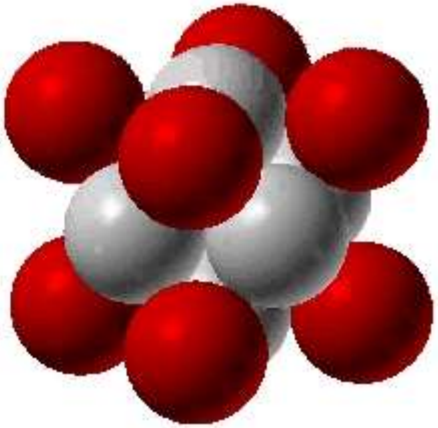
- APF for a body-centered cubic structure = 0.68

B] Face Centered Cubic Structure (FCC)

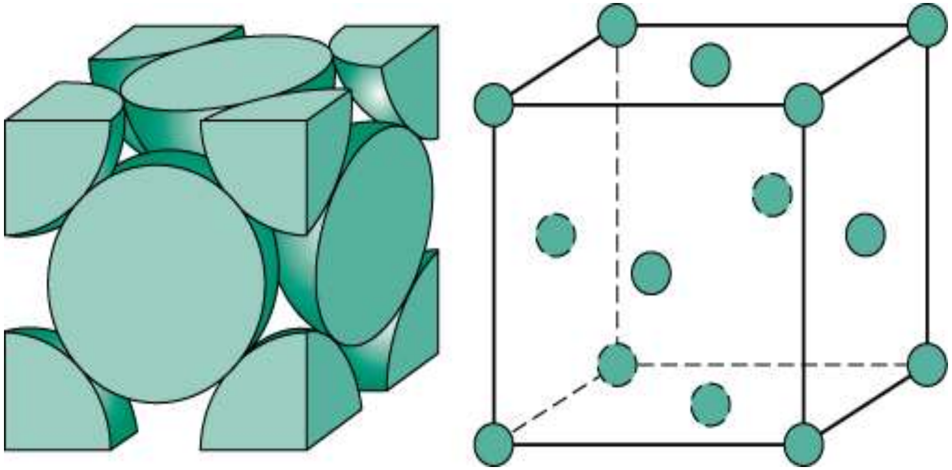
- Atoms touch each other along *face diagonals*.

Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ex: Al, Cu, Au, Pb, Ni, Pt, Ag



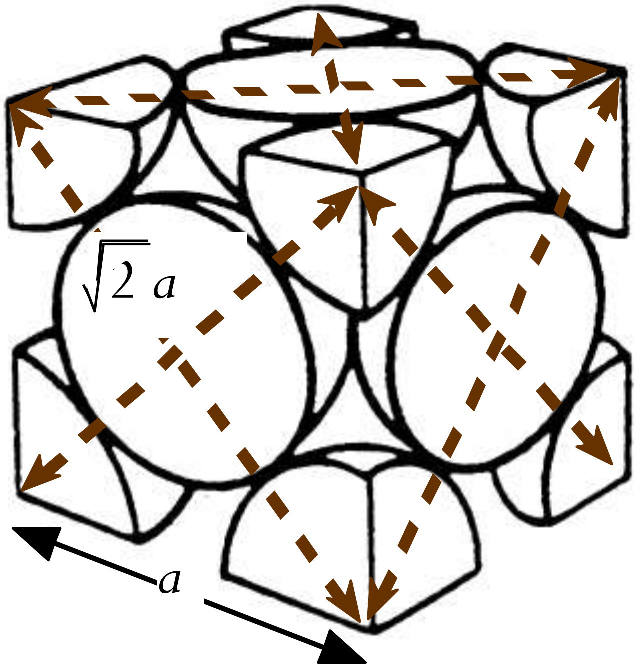
Coordination # = 12



4 atoms/unit cell: (6 face x ½) + (8 corners x 1/8)

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74



The maximum achievable APF!

Close-packed directions:

length = $4R = \sqrt{2}\,a$

(a = 2√2*R)

Unit cell contains:

6 x 1/2 + 8 x 1/8

= 4 atoms/unit cell

$$\text{APF} = \frac{4\ \frac{4}{3}\pi\left(\sqrt{2}\,a/4\right)^{3}}{a^{3}}$$

atoms / unit cell → 4

volume / atom → $\frac{4}{3}\pi\left(\sqrt{2}\,a/4\right)^{3}$

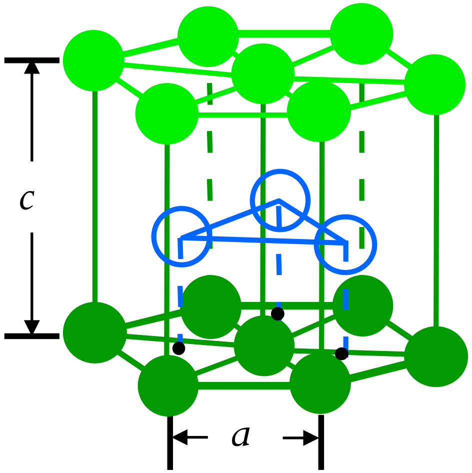
volume / unit cell → a^3

C] Hexagonal Close-Packed Structure (HCP)

ex: Cd, Mg, Ti, Zn

- ABAB... Stacking Sequence

- 3D Projection

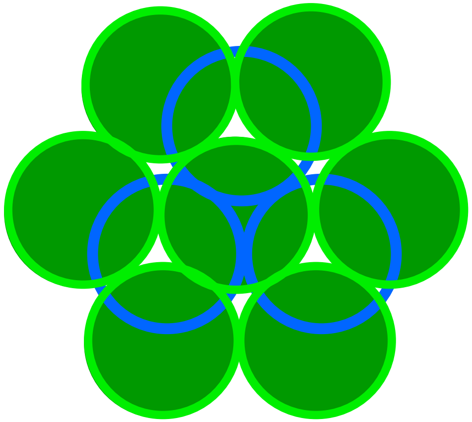


A sites

B sites

A sites

- 2D Projection



Top layer

Middle layer

Bottom layer

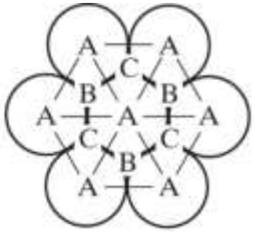
- Coordination # = 12

6 atoms/unit cell

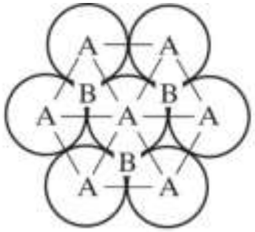
- APF = 0.74

- $c/a = 1.633$ *(ideal)*

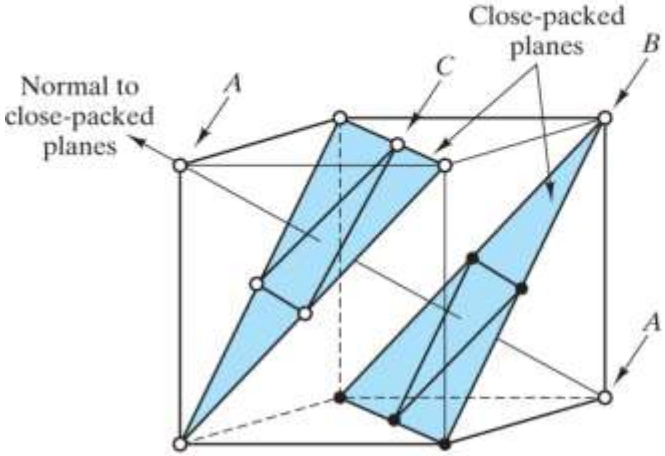
We find that both FCC & HCP are highest density packing schemes (APF = .74) – this illustration shows their differences as the closest packed planes are "built-up"



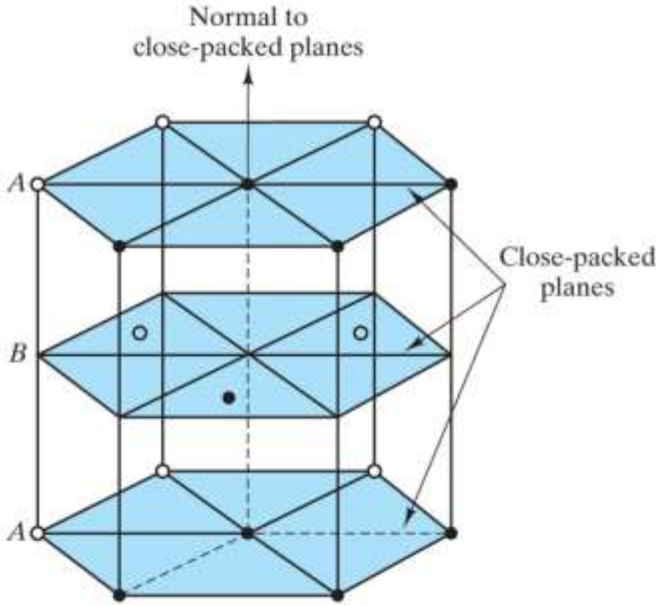
(a) Stacking of close-packed planes



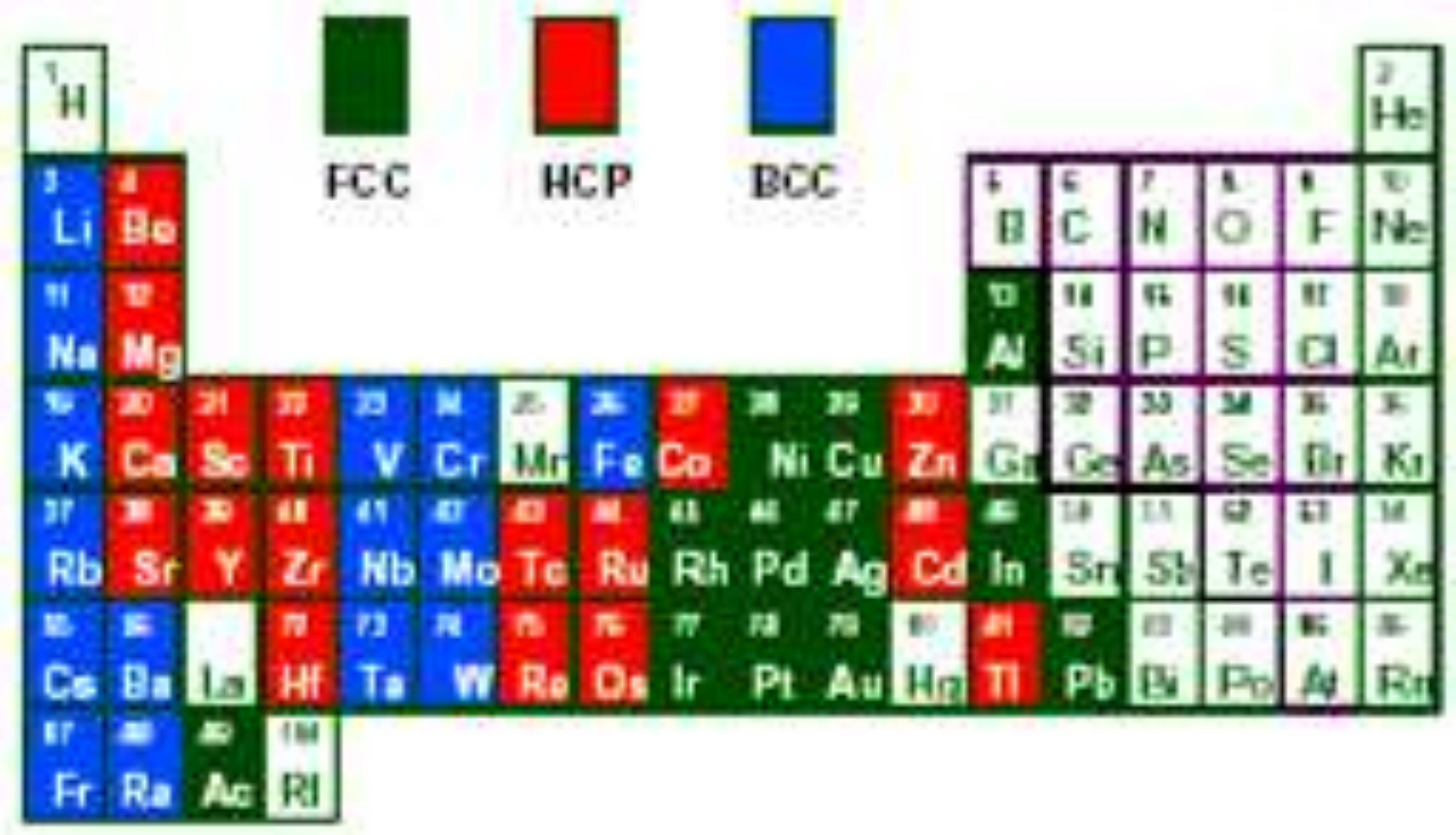
(b) Stacking of close-packed planes



(c) Face-centered cubic



(d) Hexagonal close packed



🟩 FCC 🟥 HCP 🟦 BCC

H																	He
🟦 Li	🟥 Be											B	C	N	O	F	Ne
🟦 Na	🟥 Mg											🟩 Al	Si	P	S	Cl	Ar
🟦 K	🟥 Ca	🟥 Sc	🟥 Ti	🟦 V	🟦 Cr	Mn	🟦 Fe	🟥 Co	🟩 Ni	🟩 Cu	🟥 Zn	Ga	Ge	As	Se	Br	Kr
🟦 Rb	🟥 Sr	🟥 Y	🟥 Zr	🟦 Nb	🟦 Mo	🟥 Tc	🟥 Ru	🟩 Rh	🟩 Pd	🟩 Ag	🟥 Cd	🟩 In	Sn	Sb	Te	I	Xe
🟦 Cs	🟦 Ba	La	🟥 Hf	🟦 Ta	🟦 W	🟥 Re	🟥 Os	🟩 Ir	🟩 Pt	🟩 Au	Hg	🟥 Tl	🟩 Pb	Bi	Po	At	Rn
🟦 Fr	🟦 Ra	🟩 Ac	Rl														

❑ Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

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

Where,

n = number of atoms/unit cell

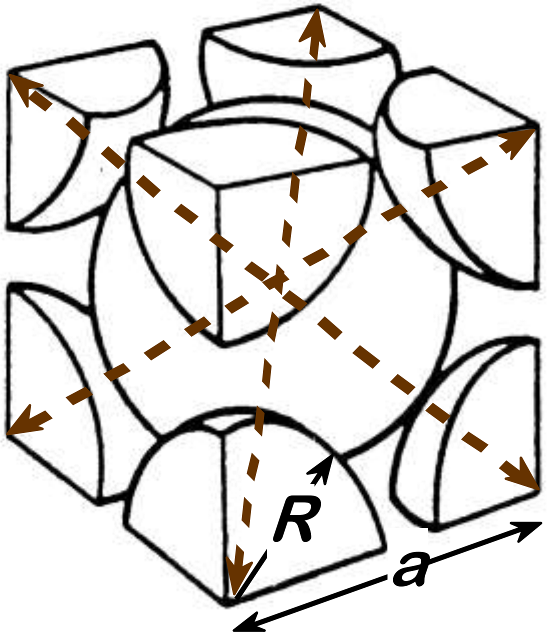
A = atomic weight

V_C = Volume of unit cell = a^3 for cubic

N_A = Avogadro's number

= 6.023×10^{23} atoms/mol

Theoretical Density, ρ



- Ex: Cr (BCC)

$A = 52.00 \text{ g/mol}$

$R = 0.125 \text{ nm}$

$n = 2$

$\therefore a = 4R/\sqrt{3} = 0.2887 \text{ nm}$

$$\rho = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{2}\ \overset{\frac{\text{g}}{\text{mol}}}{52.00}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^3}\ \underset{\frac{\text{atoms}}{\text{mol}}}{6.023 \text{ x } 10^{23}}}$$

$\rho_{\text{theoretical}} = 7.18 \text{ g/cm}^3$

$\rho_{\text{actual}} = 7.19 \text{ g/cm}^3$

❑ Crystal Symmetry

- Crystals, and therefore minerals, have an ordered internal arrangement of atoms.

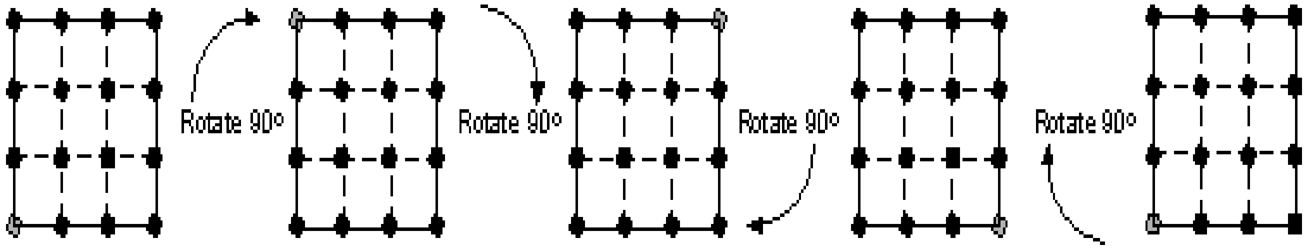
- This ordered arrangement shows symmetry, i.e. the atoms are arranged in a symmetrical fashion on a three dimensional network referred to as a ***lattice***.

- When a crystal forms in an environment where there are no impediments to its growth, crystal faces form as smooth planar boundaries that make up the surface of the crystal.

- These crystal faces reflect the ordered internal arrangement of atoms and thus reflect the symmetry of the crystal lattice.

Crystal Symmetry

- To see this, imagine a small 2 dimensional crystal composed of atoms in an ordered internal arrangement as shown below.
- Although all of the atoms in this lattice are the same, one of them is gray so that its position can be tracked.
- If we rotate the simple crystals by 90° notice that the lattice and crystal look exactly the same as what we started with.
- Rotate it another 90° and again its the same. Another 90° rotation again results in an identical crystal, and another 90° rotation returns the crystal to its original orientation.
- Thus, in 1 360° rotation, the crystal has repeated itself, or looks identical 4 times. We thus say that this object has 4-fold rotational symmetry.



Crystal Symmetry

- There are four elements of symmetry for a crystal.

- These include :

  A] Axes of symmetry

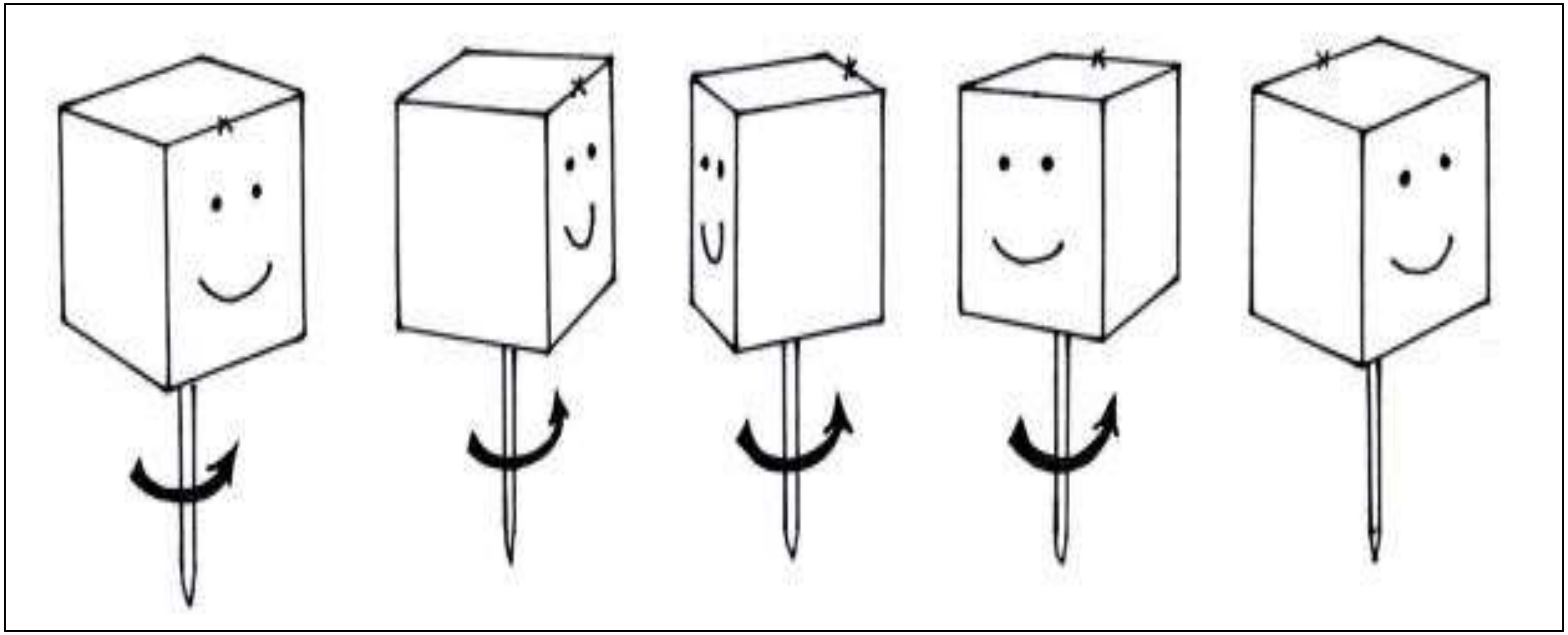
  B] Plane of symmetry

  C] Center of symmetry

- These symmetry elements may be or may not be combined in the same crystal. Indeed, we will find that one crystal class or system has only one of these elements.

A] Axes of Symmetry/Rotational Symmetry

- If an object can be rotated about an axis and repeats itself every 90° of rotation then it is said to have an axis of 4-fold rotational symmetry.
- The axis along which the rotation is performed is an element of symmetry referred to as a rotation axis.

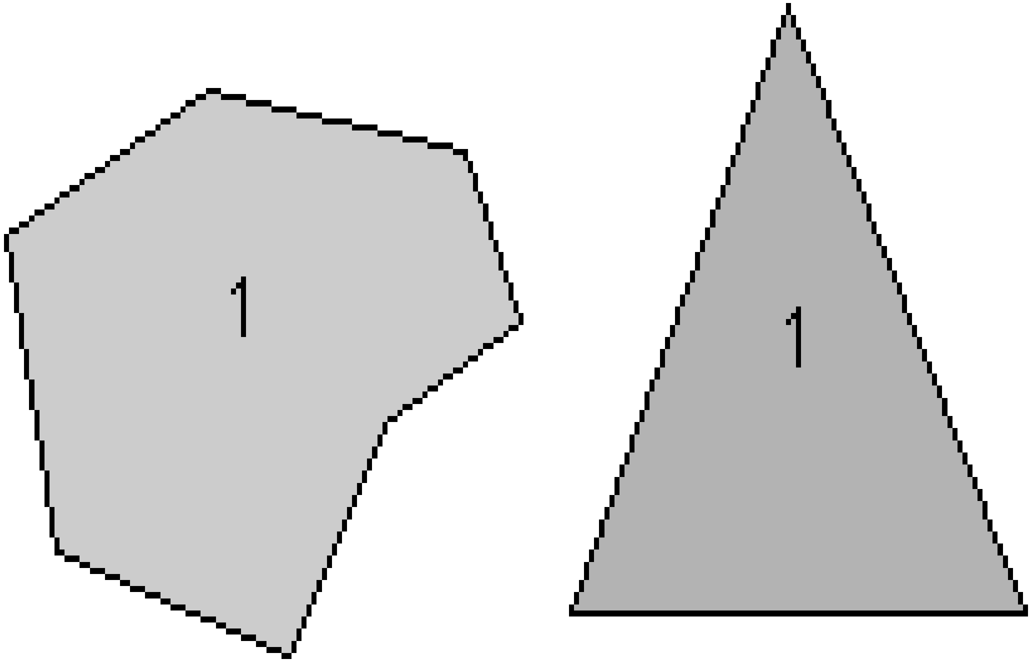


Axes of Symmetry/Rotational Symmetry

- When rotation repeats form every 60 degrees, then we have sixfold or **HEXAGONAL SYMMETRY**. A filled hexagon symbol is noted on the rotational axis.
- When rotation repeats form every 90 degrees, then we have fourfold or **TETRAGONAL SYMMETRY**. A filled square is noted on the rotational axis.
- When rotation repeats form every 120 degrees, then we have threefold or **TRIGONAL SYMMETRY**. A filled equilateral triangle is noted on the rotational axis.
- When rotation repeats form every 180 degrees, then we have twofold or **BINARY SYMMETRY**. A filled oval is noted on the rotational axis.
- When rotation repeats form every 360 degrees, then we use a filled circle as notation. This one I consider optional to list as almost any object has this symmetry. If you really want to know the truth, this means **NO SYMMETRY**!

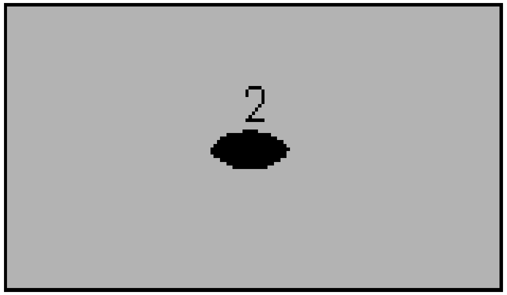
Axes of Symmetry/Rotational Symmetry

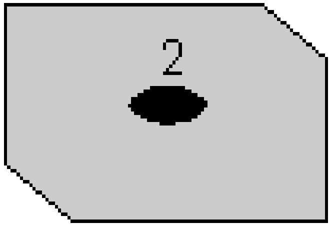
- The following types of rotational symmetry axes are possible in crystals.
- ***1-Fold Rotation Axis*** - An object that requires rotation of a full 360° in order to restore it to its original appearance has no rotational symmetry.
- Since it repeats itself 1 time every 360° it is said to have a 1-fold axis of rotational symmetry.

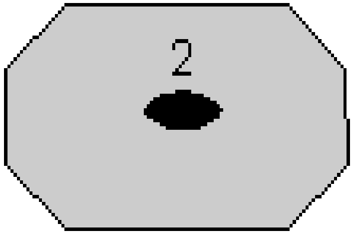


Axes of Symmetry/Rotational Symmetry

- ***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 rotation axis (360/180 = 2).
- Note that in these examples the axes we are referring to are imaginary lines that extend toward you perpendicular to the page or blackboard.
- A filled oval shape represents the point where the 2-fold rotation axis intersects the page.

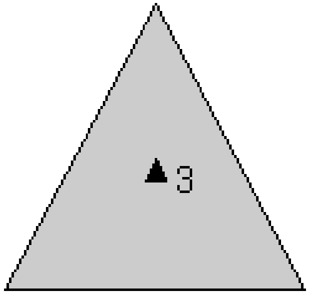


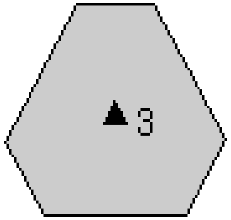


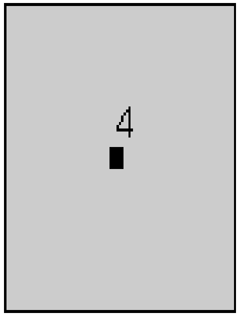


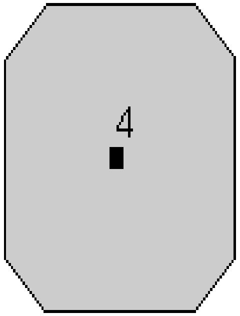
Axes of Symmetry/Rotational Symmetry

- ***3-Fold Rotation Axis***- Objects that repeat themselves upon rotation of 120° are said to have a 3-fold axis of rotational symmetry (360/120 =3), and they will repeat 3 times in a 360° rotation.
- A filled triangle is used to symbolize the location of 3-fold rotation axis.
- ***4-Fold Rotation Axis*** - If an object repeats itself after 90° of rotation, it will repeat 4 times in a 360° rotation, as illustrated previously.
- A filled square is used to symbolize the location of 4-fold axis of rotational symmetry.



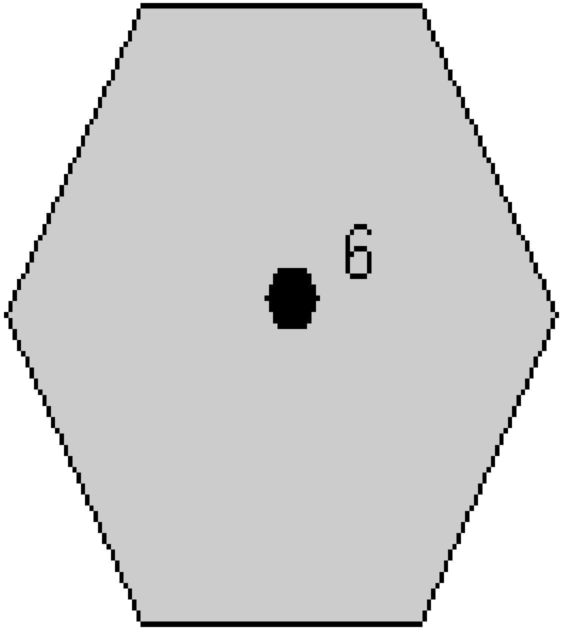


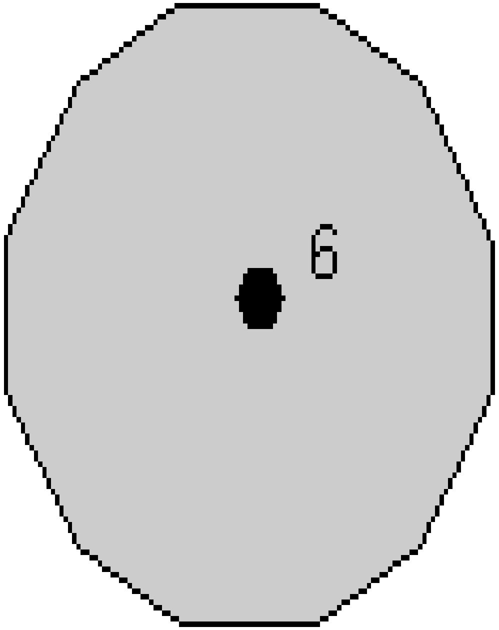




Axes of Symmetry/Rotational Symmetry

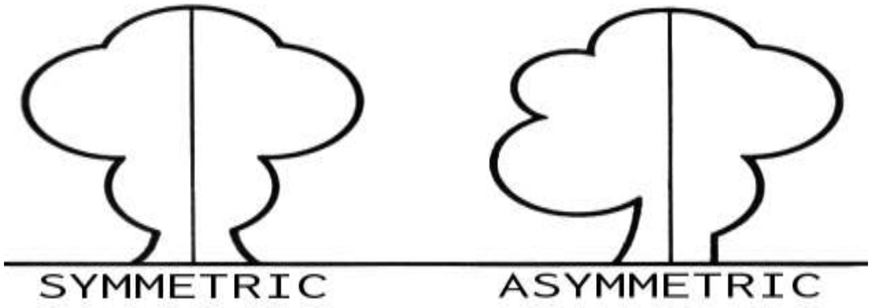
- ***6-Fold Rotation Axis*** - If rotation of 60° about an axis causes the object to repeat itself, then it has 6-fold axis of rotational symmetry (360/60=6).
- A filled hexagon is used as the symbol for a 6-fold rotation axis.





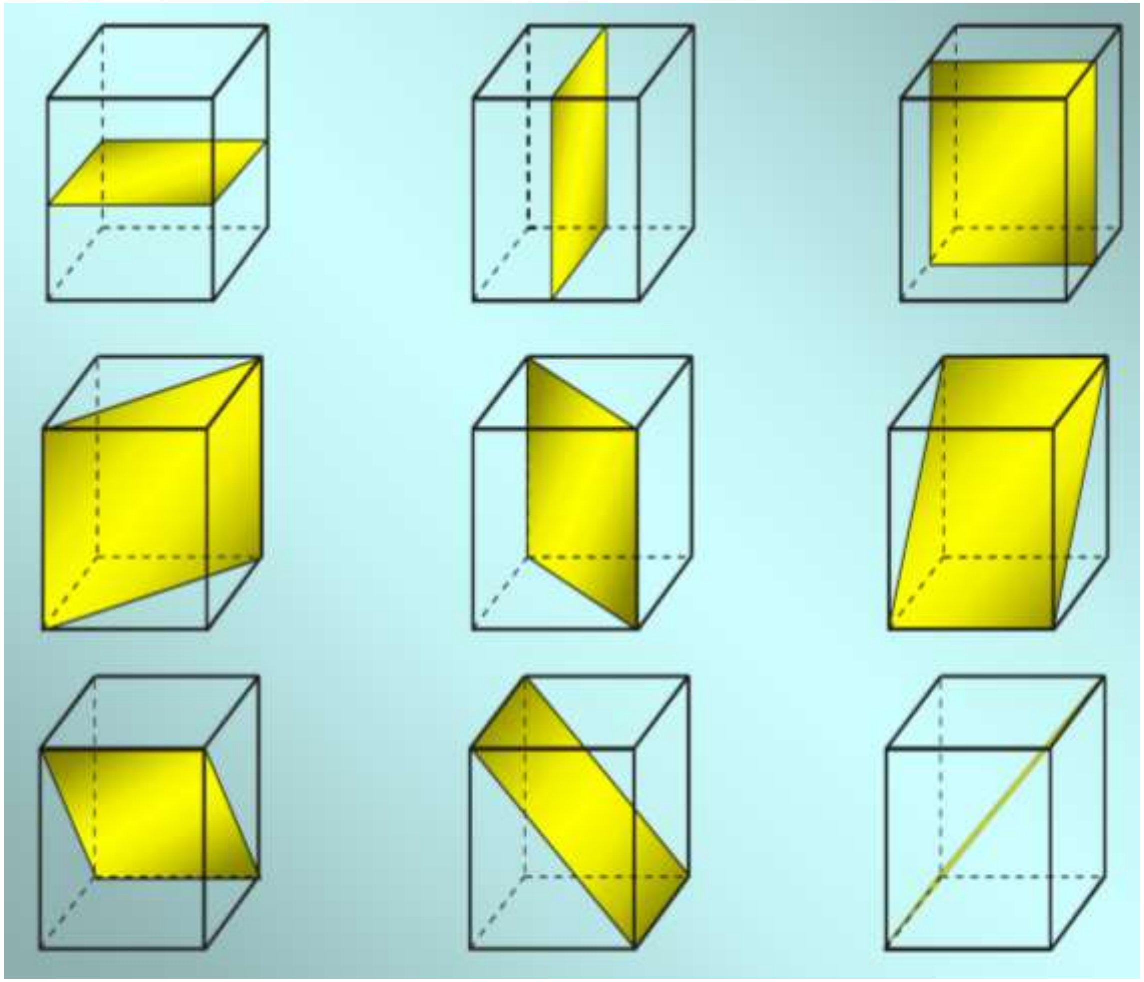
B] Plane of Symmetry/Reflection Symmetry/ Mirror Symmetry

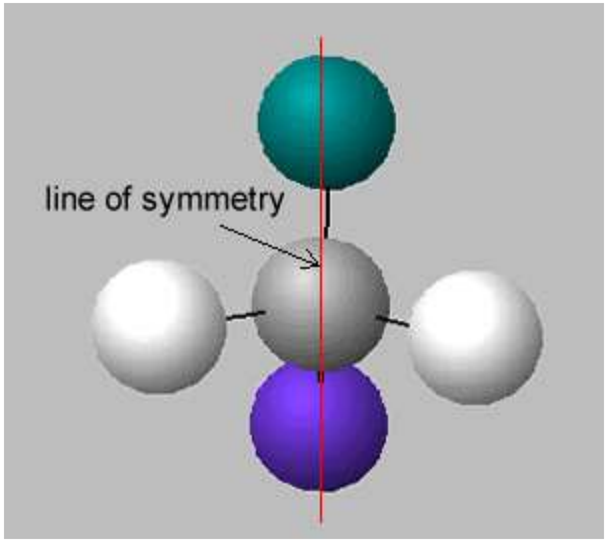
- Any two dimensional surface that, when passed through the center of the crystal, divides it into two symmetrical parts that are **MIRROR IMAGES** is a **PLANE OF SYMMETRY**.
- A mirror symmetry operation is an imaginary operation that can be performed to reproduce an object.
- The operation is done by imagining that you cut the object in half, then place a mirror next to one of the halves of the object along the cut.
- If the reflection in the mirror reproduces the other half of the object, then the object is said to have mirror symmetry.
- The plane of the mirror is an element of symmetry referred to as a ***mirror plane***, and is symbolized with the letter **m**.
- As an example, the human body is an object that approximates mirror symmetry,



Plane of Symmetry/Reflection Symmetry/ Mirror Symmetry

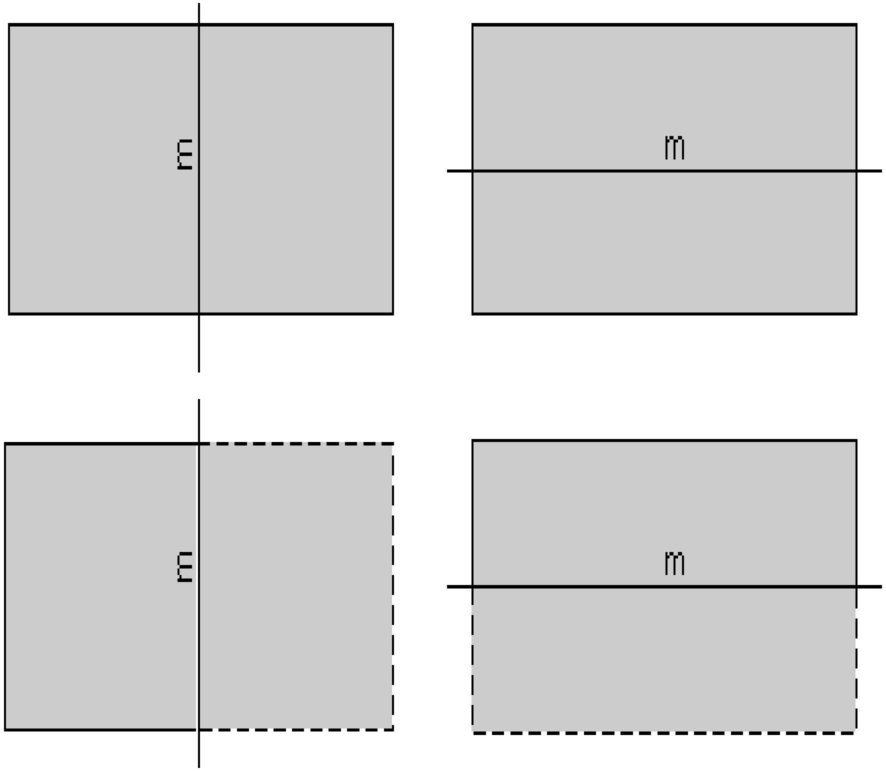
Plane of Symmetry for the crystals in cubic system





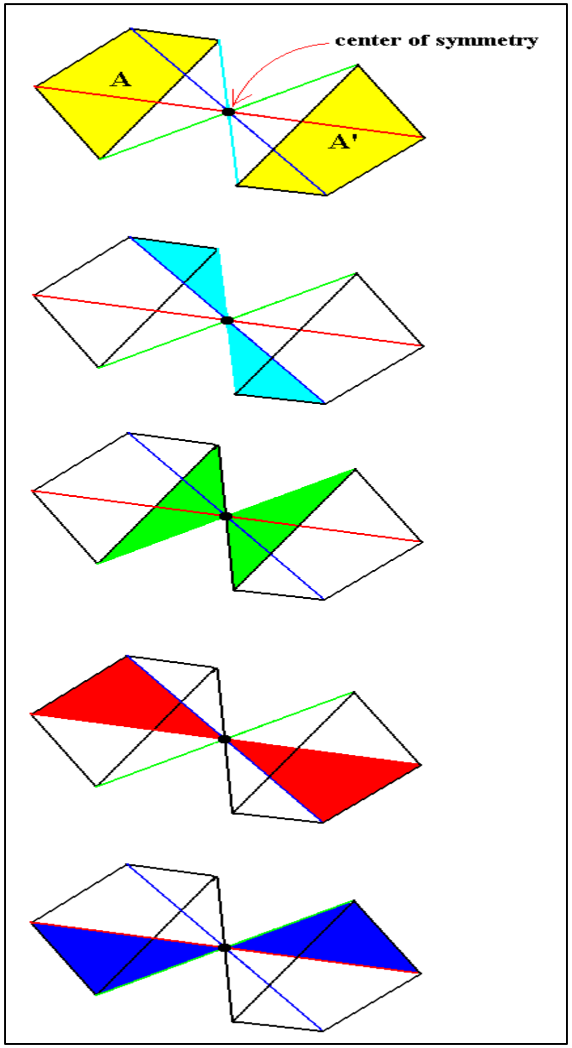
Plane of Symmetry/Reflection Symmetry/ Mirror Symmetry

- The rectangles shown here have two planes of mirror symmetry.
- The rectangle on the left has a mirror plane that runs vertically on the page and is perpendicular to the page.
- The rectangle on the right has a mirror plane that runs horizontally and is perpendicular to the page.
- The dashed parts of the rectangles below show the part the rectangles that would be seen as a reflection in the mirror



C] Center of Symmetry/Inversion Symmetry

- Most crystals have a **center of symmetry**, even though they may not possess either planes of symmetry or axes of symmetry.
- If you can pass an imaginary line from the surface of a crystal face through the center of the crystal (the axial cross) and it intersects a similar point on a face equidistance from the center, then the crystal has a center of symmetry.
- In this operation lines are drawn from all points on the object through a point in the center of the object, called a symmetry center (symbolized with the letter "i").
- The lines each have lengths that are equidistant from the original points.
- When the ends of the lines are connected, the original object is reproduced inverted from its original appearance.



❑ Crystal System

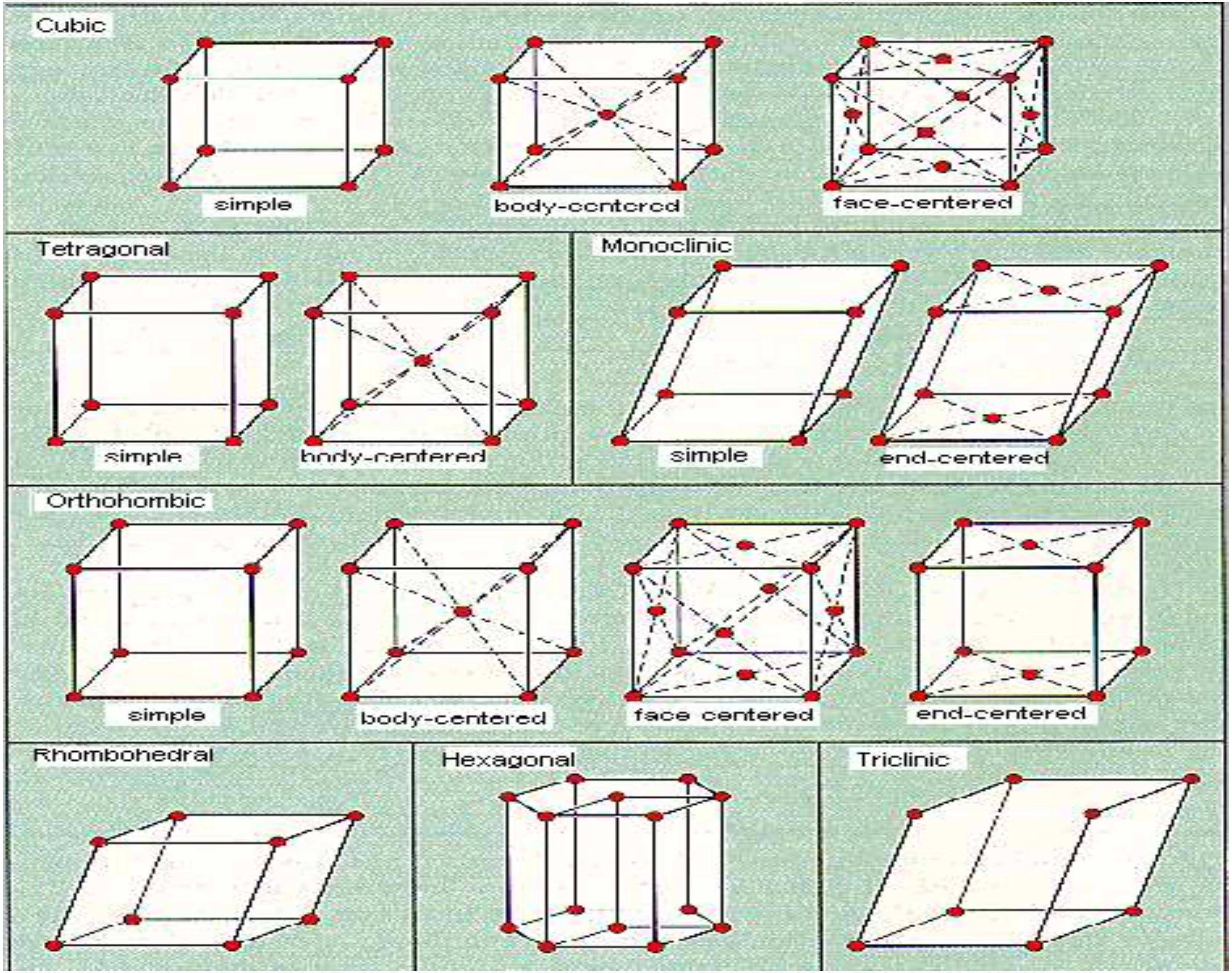
- The **crystal system:** Set of rotation and reflection symmetries which leave a lattice point fixed.
- There are seven unique crystal systems: the cubic (isometric), hexagonal, tetragonal, rhombohedral (trigonal), orthorhombic, monoclinic and triclinic.

▪ Bravais Lattice and Crystal System

Crystal structure: contains atoms at every lattice point.

- The symmetry of the crystal can be more complicated than the symmetry of the lattice.

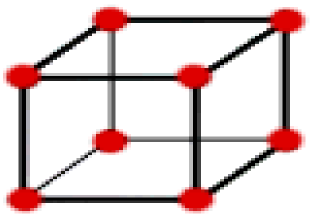
- Bravais lattice points do not necessarily correspond to real atomic sites in a crystal. A Bravais lattice point may be used to represent a group of many atoms of a real crystal. This means more ways of arranging atoms in a crystal lattice.

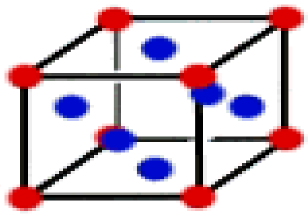

Cubic
simple
body-centered
face-centered
Tetragonal
simple
body-centered
Monoclinic
simple
end-centered
Orthohombic
simple
body-centered
face centered
end-centered
Rhombohedral
Hexagonal
Triclinic

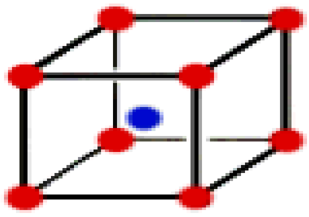
1. Cubic (Isometric) System

- This is also known as the isometric crystal system
- The cubic (Isometric) crystal system is characterized by its total symmetry
- The Cubic system has three crystallographic axes that are all perpendicular to each other, and equal in length.
- The three crystallographic axes a1, a2, a3 (or a, b, c) are all equal in length and intersect at right angles (90 degrees) to each other.

3 Bravais lattices


Simple cubic

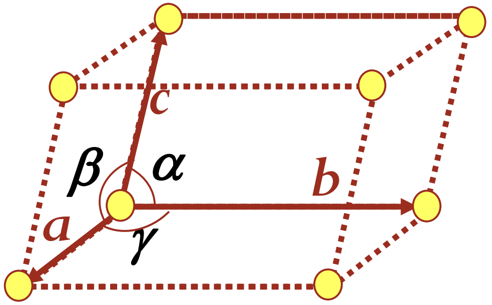

Face-centered cubic


Body-centered cubic

Symmetry elements: Four 3-fold rotation axes along cube diagonals

a = b = c

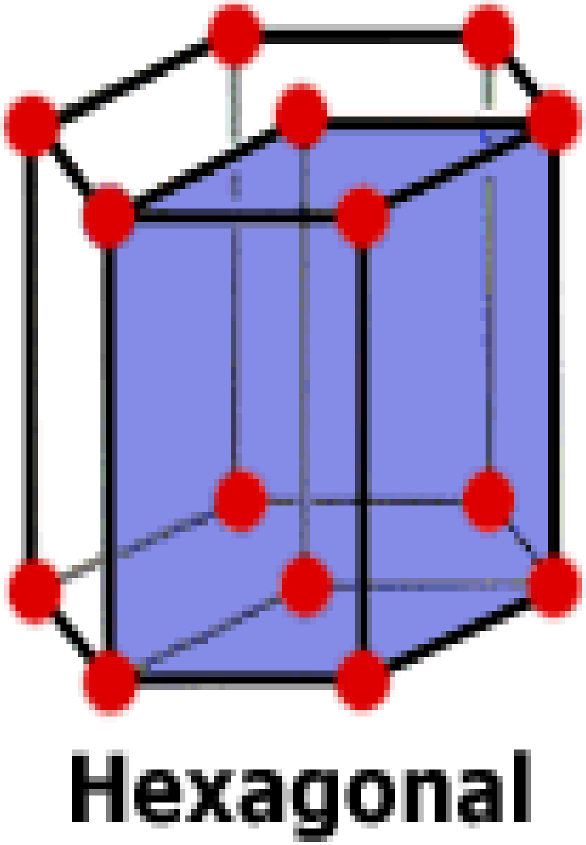
$\alpha = \beta = \gamma = 90^o$



2. Hexagonal System

- The hexagonal crystal system has four crystallographic axes consisting of three equal horizontal or equatorial (a, b, and d) axes at 120°, and one vertical (c) axis that is perpendicular to the other three.

- The (c) axis can be shorter, or longer than the horizontal axes.



Only one Bravais lattice

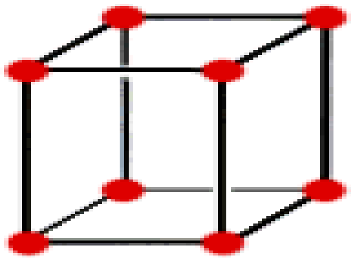
Symmetry element: One 6-fold rotation axis
$a = b \neq c$
$\alpha = 120^{o}$
$\beta = \gamma = 90^{o}$

3. Tetragonal System

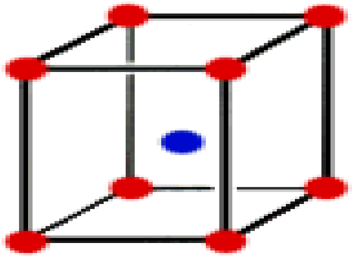
- A tetragonal crystal is a simple cubic shape that is stretched along its (c) axis to form a rectangular prism.
- The tetragonal crystal will have a square base and top, but a height which is taller.
- Three axes, all at right angles, two of which are equal in length (a and b) and one (c) which is different in length (Shorter or Longer)

Note: If c was equal in length to a or b, then we would be in the cubic system!

Two Bravais lattices



Simple tetragonal



Body-centered tetragonal

Symmetry element: One 4-fold rotation axis

$a = b \neq c$

$\alpha = \beta = \gamma = 90^o$

4. Trigonal (Rhombohedral) System

- A rhombohedron has a three-dimensional shape that is similar to a cube, but it has been skewed or inclined to one side making it oblique.
- It is also known as the Trigonal crystal system.
- A rhombohedral crystal has six faces, 12 edges, and 8 vertices.
- If all of the non-obtuse internal angles of the faces are equal (flat sample, below), it can be called a trigonal-trapezohedron

One Bravais lattice

Symmetry element: One 3-fold rotation axis

$a = b \neq c$

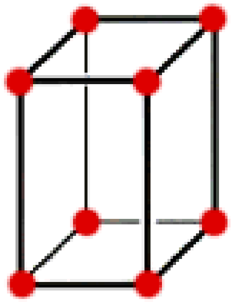
$\alpha = 120^{o}$

$\beta = \gamma = 90^{o}$

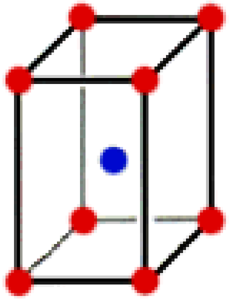
5. Orthorhombic System

- Minerals that form in the orthorhombic (aka rhombic) crystal system have three mutually perpendicular axes, all with different, or unequal lengths.
- The orthorhombic crystal system is also known as Rhombic crystal system
- Three axes, all at right angles, and all three of different lengths.
- Note: If any axis was of equal length to any other, then we would be in the tetragonal system!

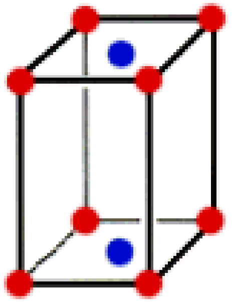
Four Bravais lattices



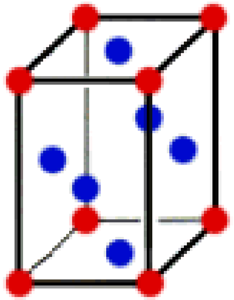
Simple orthorhombic



Body-centered orthorhombic



Base-centered orthorhombic



Face-centered orthorhombic

Symmetry element: Three mutually perpendicular 2-fold rotation axes

$a \neq b \neq c$

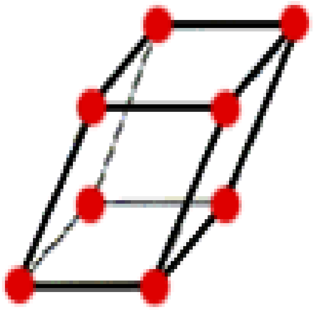
$\alpha = \beta = \gamma = 90^o$

6. Monoclinic System

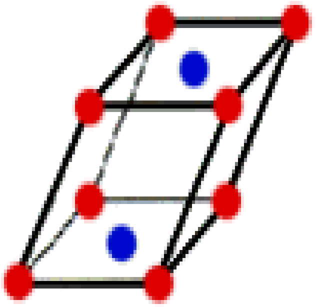
- Crystals that form in the monoclinic system have three unequal axes.
- The (a) and (c) crystallographic axes are inclined toward each other at an oblique angle, and the (b) axis is perpendicular to a and c.
- The (b) crystallographic axis is called the "ortho" axis.

Note: If a and c crossed at 90 degrees, then we would be in the orthorhombic system!

Two Bravais lattices



Simple Monoclinic



Base-centered monoclinic

Symmetry element: One 2-fold rotation axis

$\mathbf{a \neq b \neq c}$

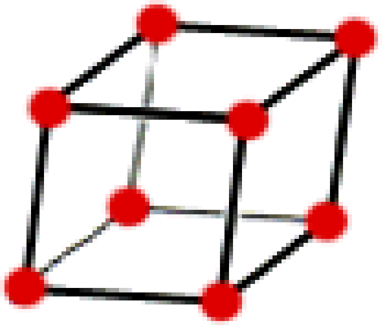
$\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$

7. Triclinic System

- Crystals that form in the triclinic system have three unequal crystallographic axes, all of which intersect at oblique angles.
- Triclinic crystals have a 1-fold symmetry axis with virtually no discernible symmetry, and no mirrored or prismatic planes.

Note: If any two axes crossed at 90 degrees, then we would be describing a monoclinic crystal!

One Bravais lattice



Triclinic

Symmetry element: None

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90^o$

❑ Miller Indices

Miller Indices are a symbolic vector representation for the orientation of an atomic plane in a crystal lattice and are defined as the reciprocals of the fractional intercepts which the plane makes with the crystallographic axes.

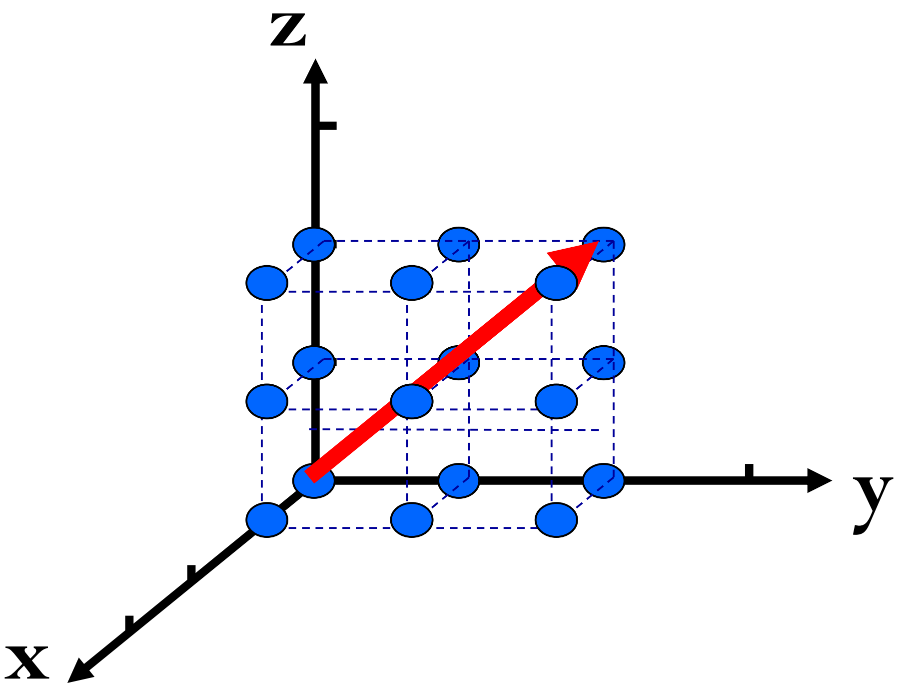
To determine Miller indices of a plane, take the following steps;

1) Determine the intercepts of the plane along each of the three crystallographic directions

2) Take the reciprocals of the intercepts

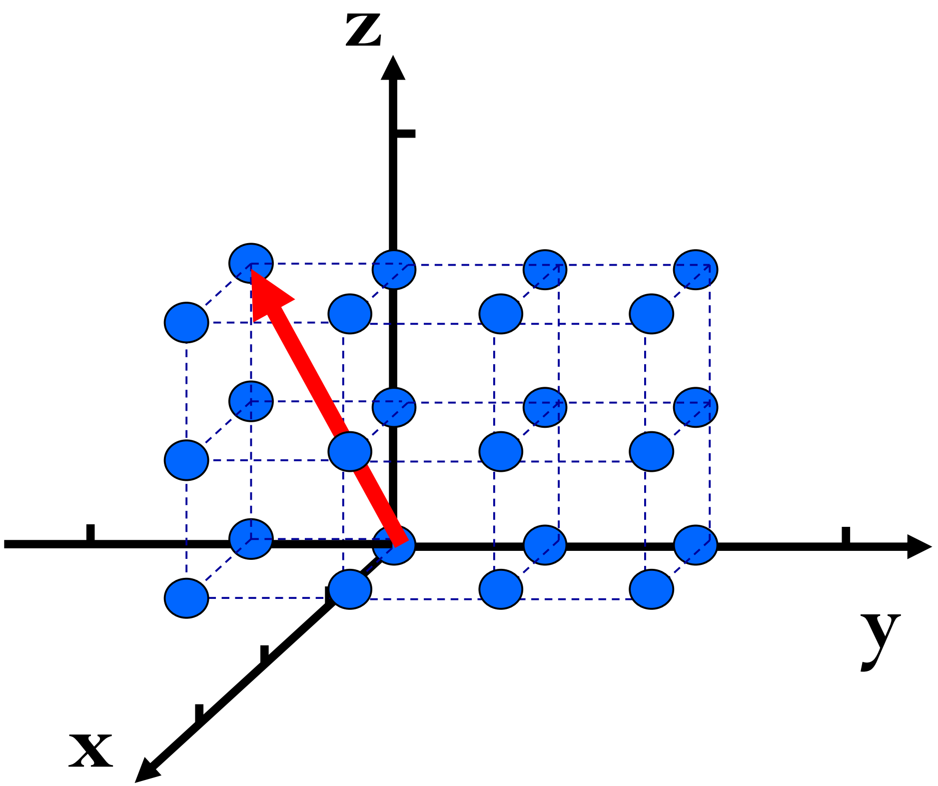
3) If fractions result, multiply each by the denominator of the smallest fraction

Miller Indices: Directions



	x	y	z
[1] Draw a vector and take components	0	2a	2a
[2] Reduce to simplest integers	0	1	1
[3] Enclose the number in square brackets	[0 1 1]		

Negative Directions



	x	y	z
[1] Draw a vector and take components	0	-a	2a
[2] Reduce to simplest integers	0	-1	2
[3] Enclose the number in square brackets			

$$\left[0\,\bar{1}\,2\right]$$

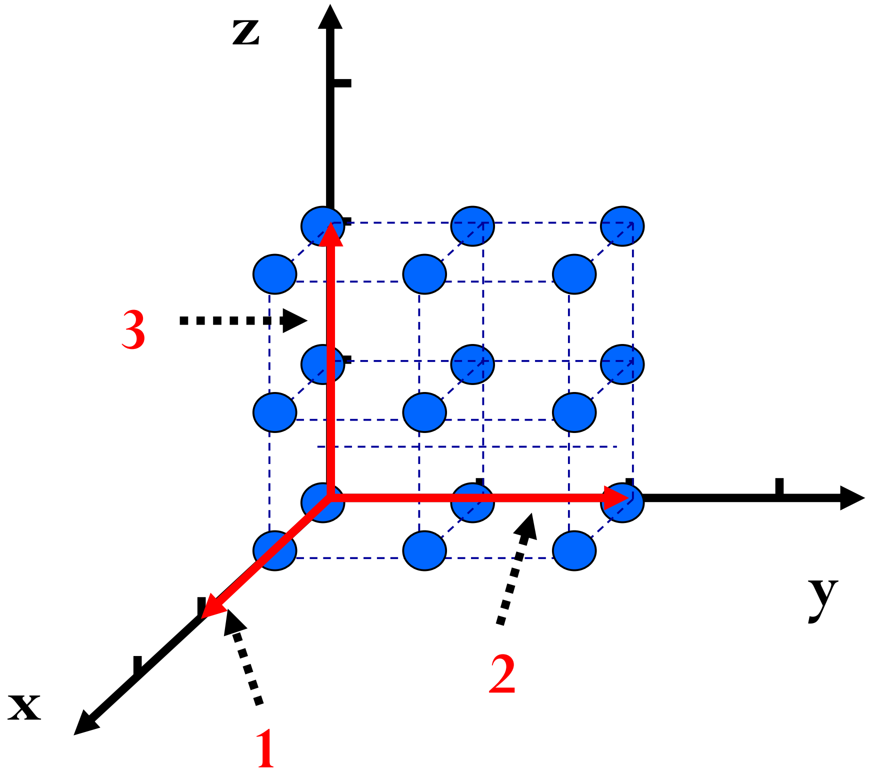
Equivalent Directions

Equivalent directions due to crystal symmetry:

1: [100]

2: [010]

3: [001]



Notation <100> used to denote all directions equivalent to [100]

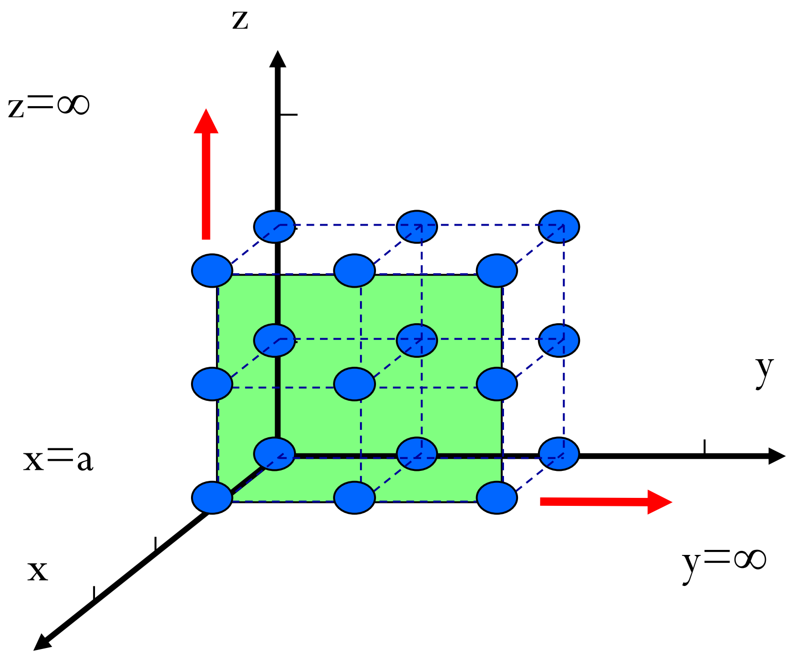
The intercepts of a crystal plane with the axis defined by a set of unit vectors are at 2a, -3b and 4c. Find the corresponding Miller indices of this and all other crystal planes parallel to this plane.

The Miller indices are obtained in the following three steps:

1. Identify the intersections with the axis, namely 2, -3 and 4.
2. Calculate the inverse of each of those intercepts, resulting in 1/2, -1/3 and 1/4.
3. Find the smallest integers proportional to the inverse of the intercepts. Multiplying each fraction with the product of each of the intercepts (24 = 2 x 3 x 4) does result in integers, but not always the smallest integers.
4. These are obtained in this case by multiplying each fraction by 12.
5. Resulting Miller indices is
6. Negative index indicated by a bar on top.

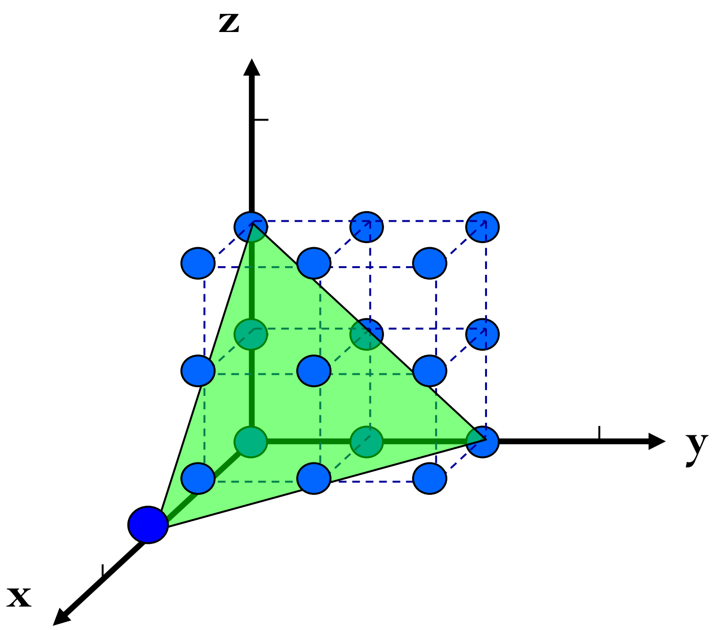
$$\left(6\ \bar{4}\ 3\right)$$

Miller Indices of Planes



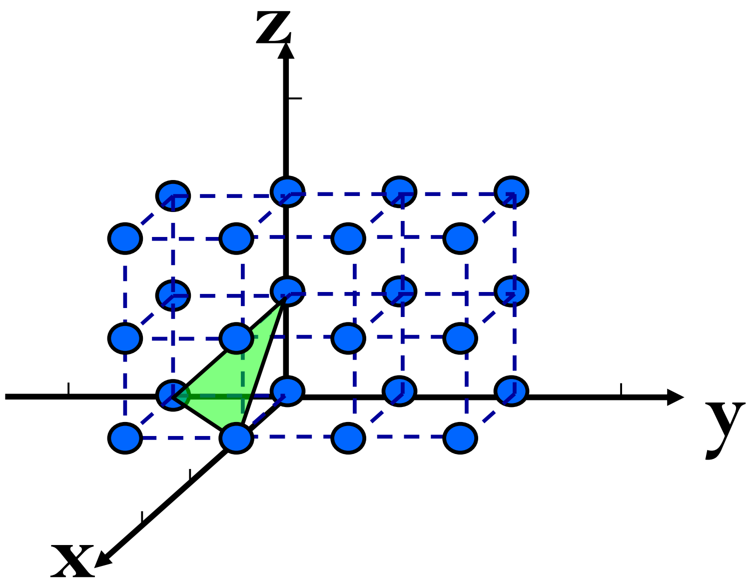
	x	y	z
[1] Determine intercept of plane with each axis	a	∞	∞
[2] Invert the intercept values	1/a	1/∞	1/∞
[3] Convert to the smallest integers	1	0	0
[4] Enclose the number in round brackets		(1 0 0)	

Miller Indices of Planes



	x	y	z
[1] Determine intercept of plane with each axis	2a	2a	2a
[2] Invert the intercept values	1/2a	1/2a	1/2a
[3] Convert to the smallest integers	1	1	1
[4] Enclose the number in round brackets		(1 1 1)	

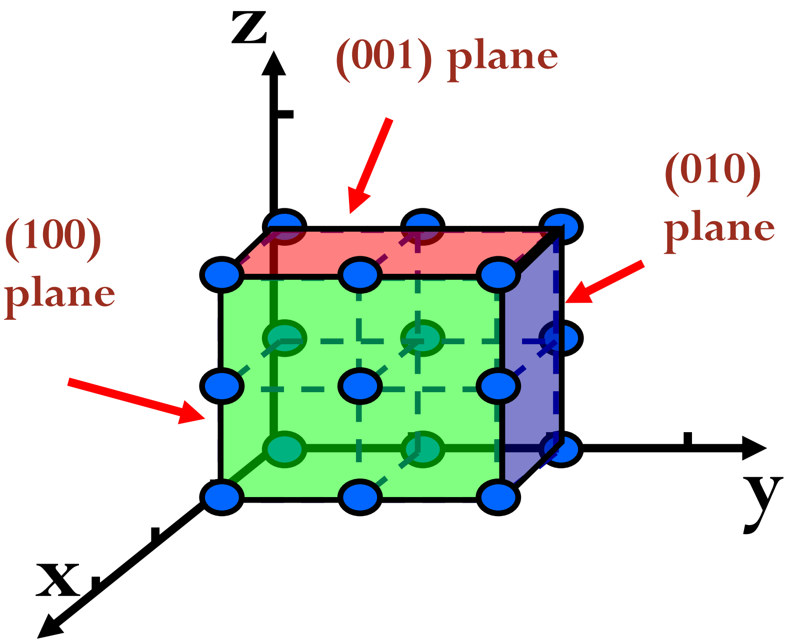
Planes with Negative Indices



	x	y	z
[1] Determine intercept of plane with each axis	a	-a	a
[2] Invert the intercept values	1/a	-1/a	1/a
[3] Convert to the smallest integers	1	-1	-1
[4] Enclose the number in round brackets			

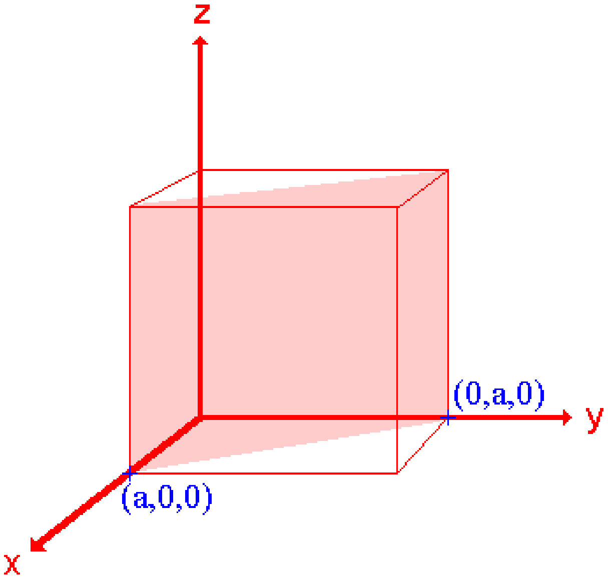
$$\left(1\bar{1}1\right)$$

Equivalent Planes



- Planes (100), (010), (001), (100), (010), (001) are equivalent planes. Denoted by {1 0 0}.
- Atomic density and arrangement as well as electrical, optical, physical properties are also equivalent.

In the cubic system the (*hkl*) plane and the vector [*hkl*] are normal to one another.
This characteristic is unique to the cubic crystal system and does not apply to crystal systems of lower symmetry.



The (110) surface

Assignment

Intercepts : *a* , *a* , ∞

Fractional intercepts : 1 , 1 , ¥

Miller Indices : **(110)**

The (100), (110) and (111) surfaces considered above are the so-called low index surfaces of a cubic crystal system (the "low" refers to the Miller indices being small numbers - 0 or 1 in this case).

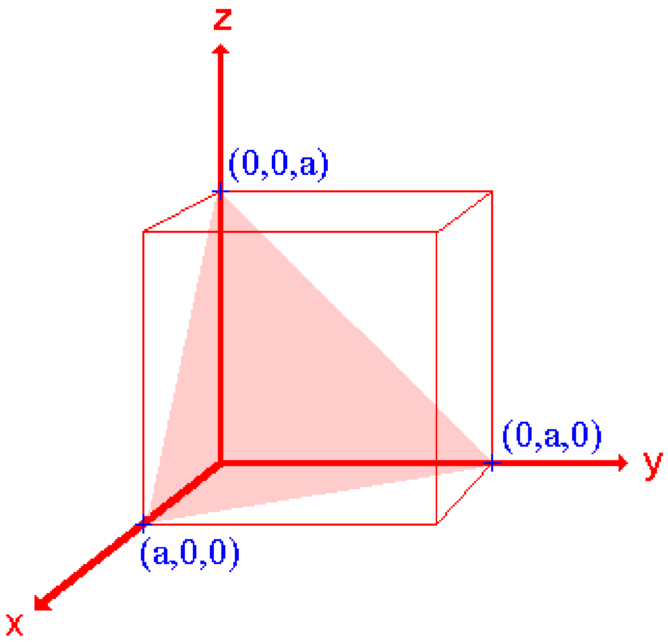
The (111) surface

Assignment

Intercepts : *a* , *a* , *a*

Fractional intercepts : 1 , 1 , 1

Miller Indices : **(111)**



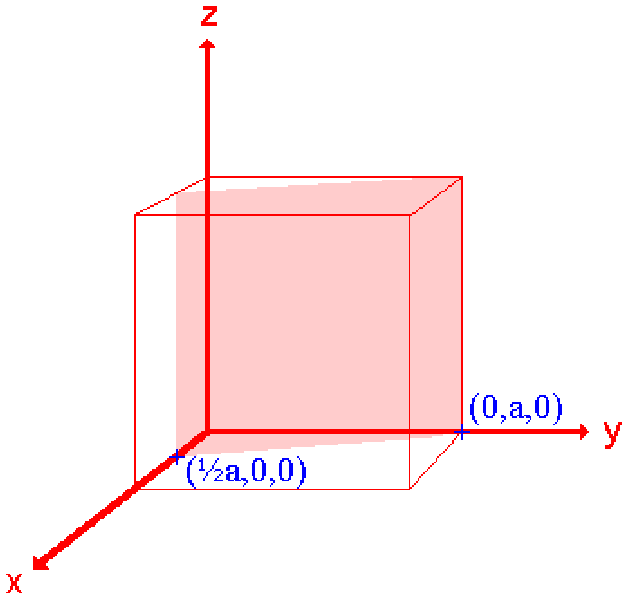
The (210) surface

Assignment

Intercepts : ½ *a* , *a* , ∞

Fractional intercepts : ½ , 1 , ∞

Miller Indices : **(210)**



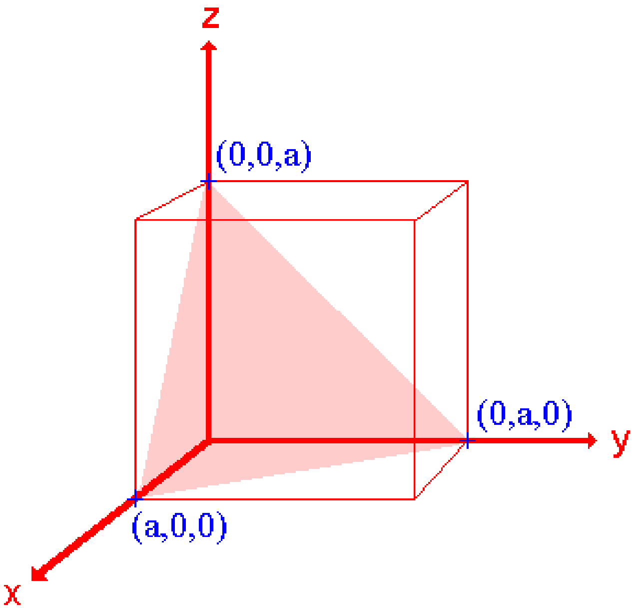
The (111) surface

Assignment

Intercepts : *a* , *a* , *a*

Fractional intercepts : 1 , 1 , 1

Miller Indices : **(111)**



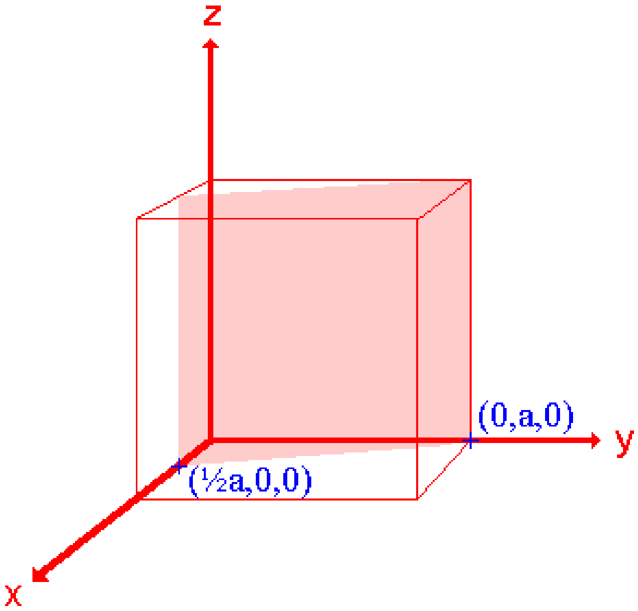
The (210) surface

Assignment

Intercepts : ½ *a* , *a* , ∞

Fractional intercepts : ½ , 1 , ∞

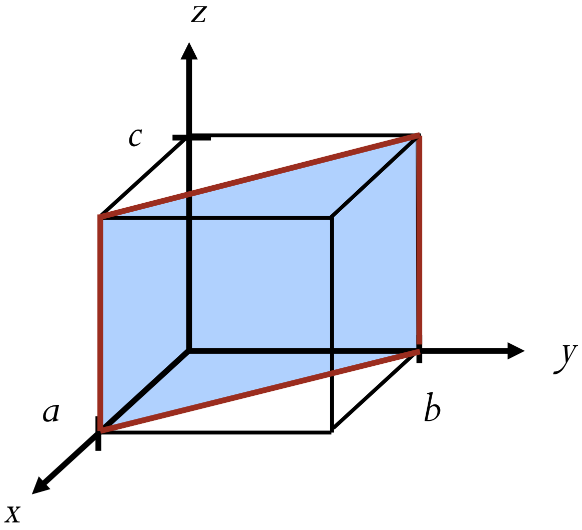
Miller Indices : **(210)**



Crystallographic Planes

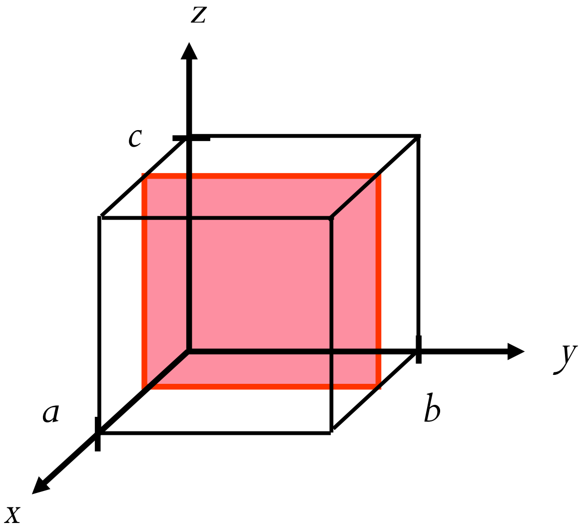
example		*a*	*b*	*c*
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0

4. Miller Indices (110)



example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	1	0	0

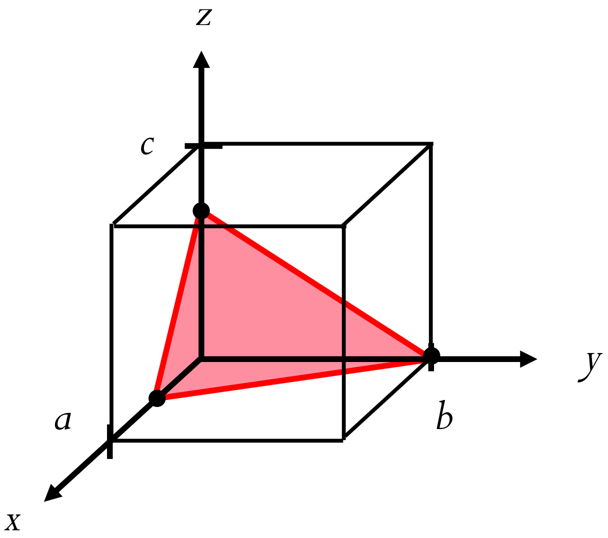
4. Miller Indices (100)



Crystallographic Planes

<u>example</u>	a	b	c
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/½	1/1	1/¾
	2	1	4/3
3. Reduction	6	3	4

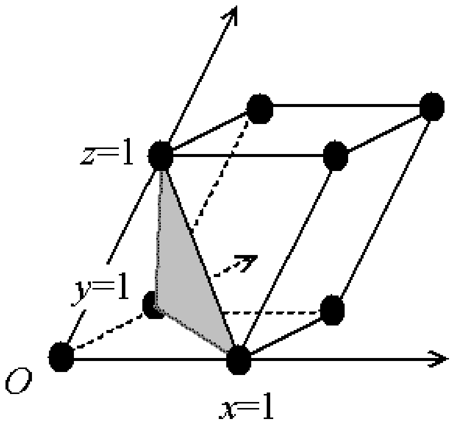
4. Miller Indices (634)



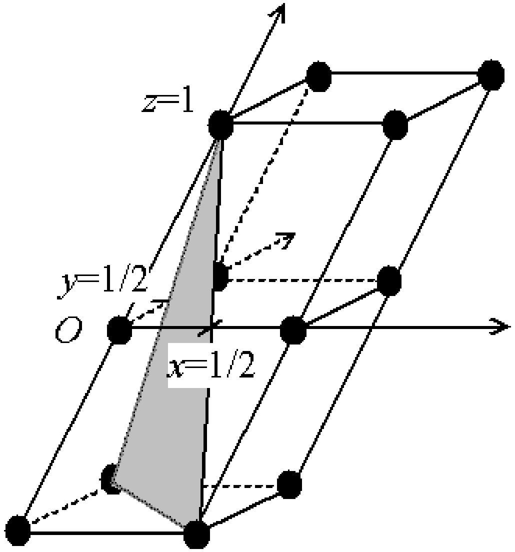
Family of Planes $\{hkl\}$

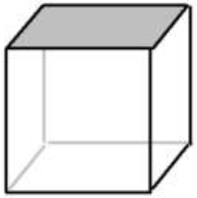
Ex: $\{100\} = (100),\quad (010),\quad (001),\quad (\bar{1}00),\quad (0\bar{1}0),\quad (001)^{-}$

plan (111)

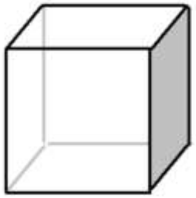


plan (221)

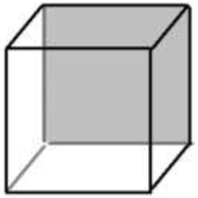




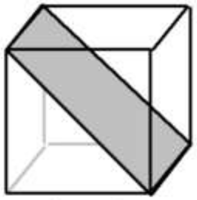
(001)



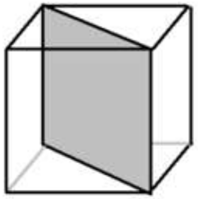
(100)



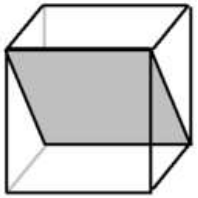
(010)



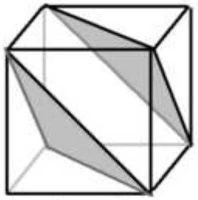
(101)



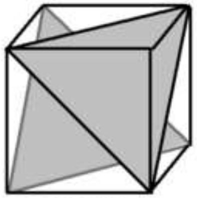
(110)



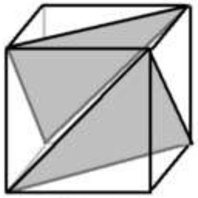
(011)



(111)



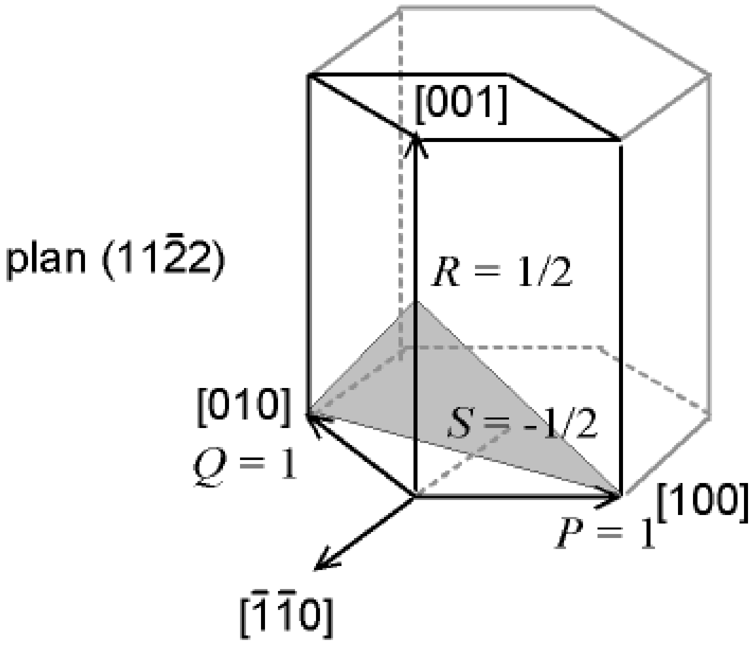
$(1\bar{1}1)$



$(\bar{1}11)$

Miller Index for Hexagonal Crystal System

- Four principal axes used, leading to four Miller Indices:
- Directions [h k i l]; Planes (h k i l), e.g. (0001) surface.
- First three axes/indices are related: h + k + i = 0 or i = -h-k.
- Indices *h*, *k* and *l* are identical to the Miller index.
- Rhombohedral crystal system can also be identified with four indices.

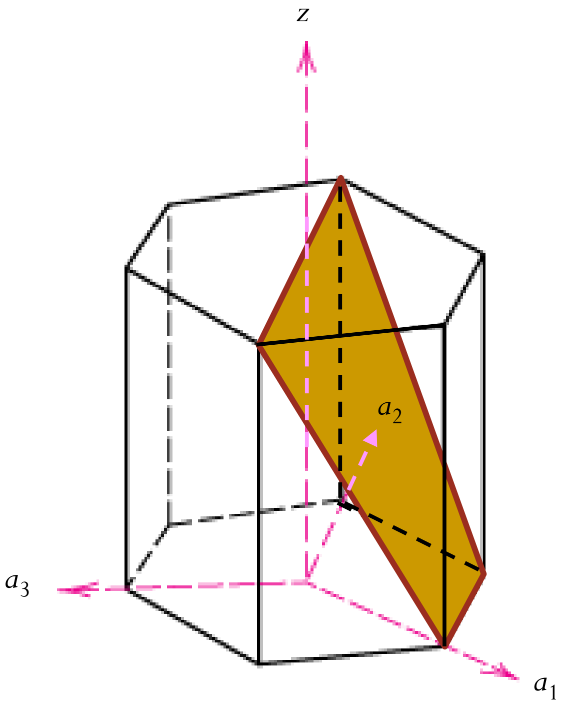


Crystallographic Planes (HCP)

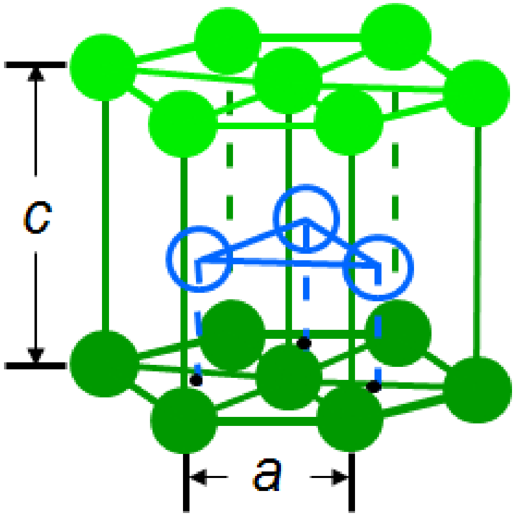
- In hexagonal unit cells the same idea is used

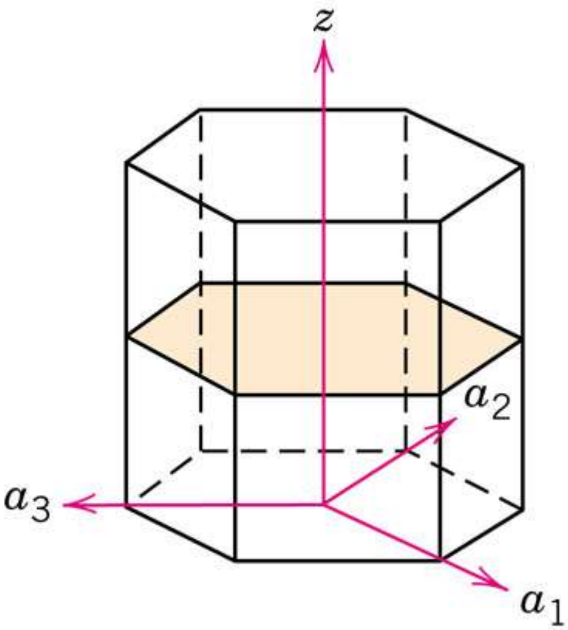
<u>example</u>		a_1	a_2	a_3	c
1.	Intercepts	1	∞	-1	1
2.	Reciprocals	1	$1/\infty$	-1	1
		1	0	-1	1
3.	Reduction	1	0	-1	1

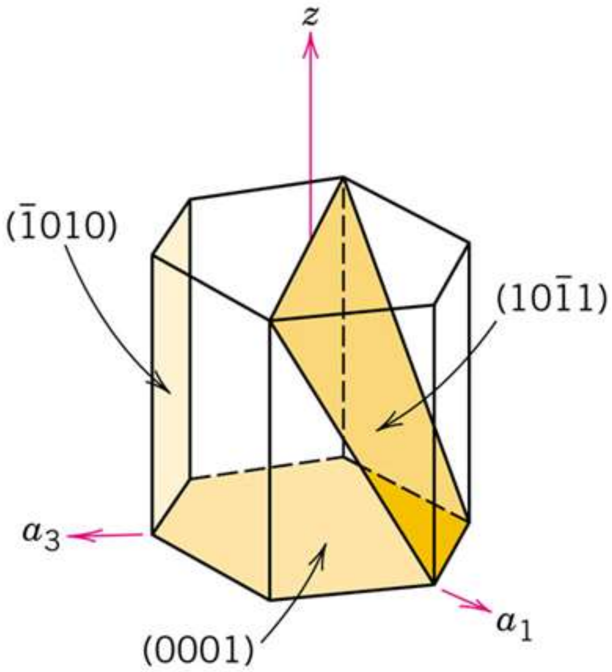
4. Miller-Bravais Indices $(10\bar{1}1)$



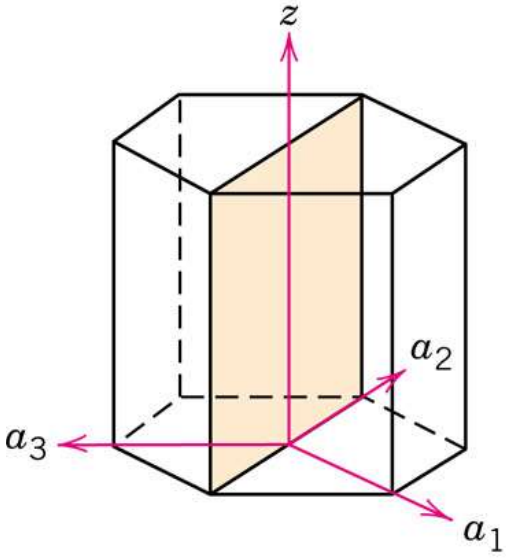
Determine the indices for the planes shown in the hexagonal unit cells below:

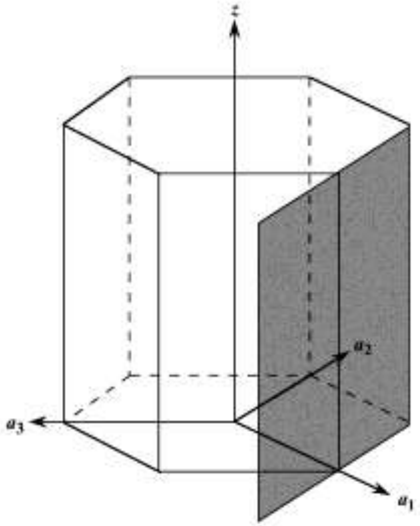


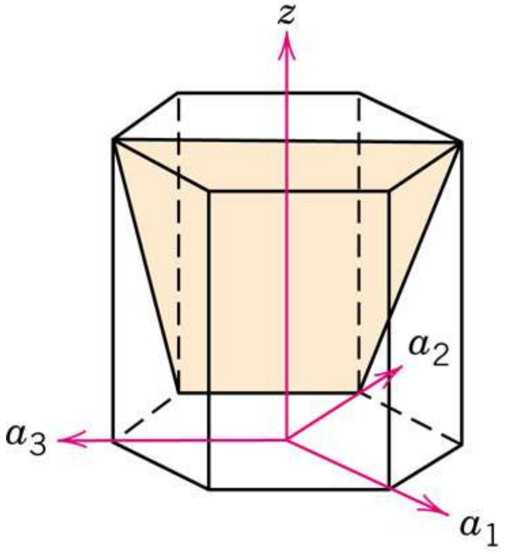


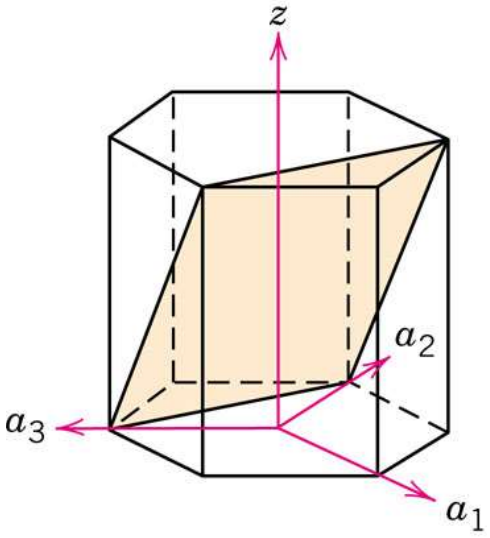


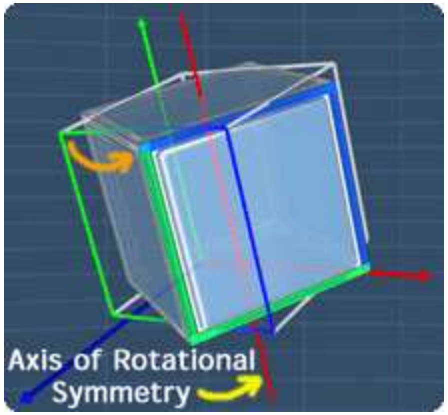
Determine the indices for the planes shown in the hexagonal unit cells below:

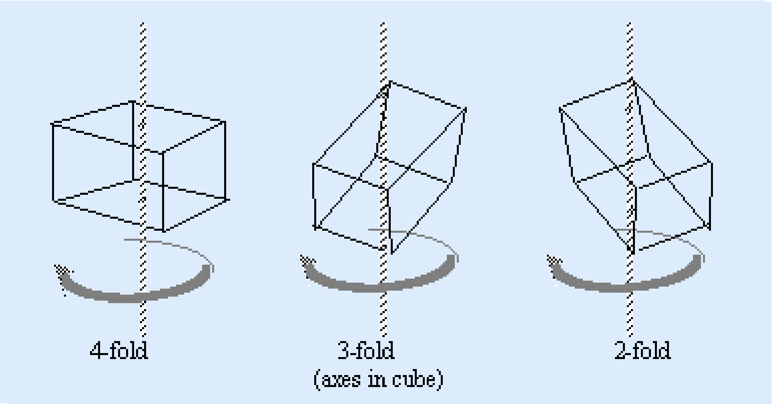


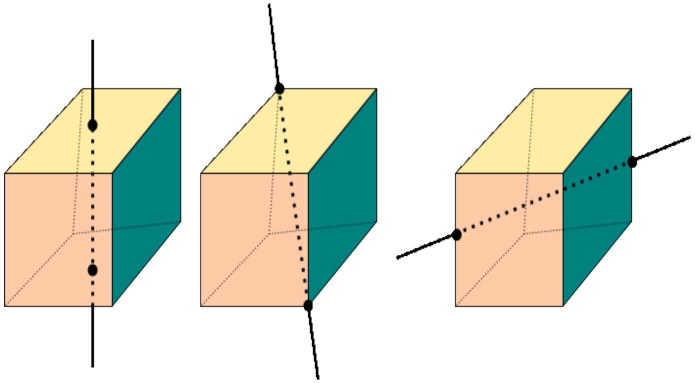


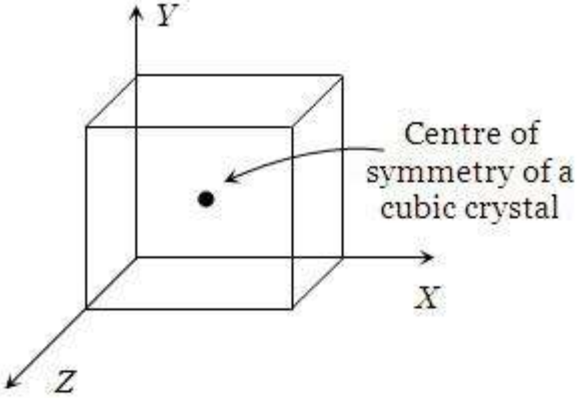


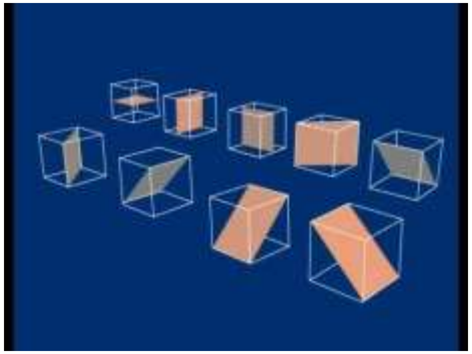


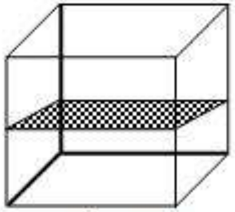




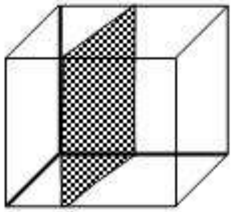




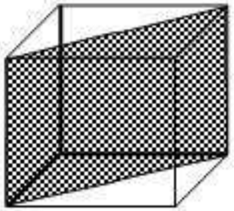




Plane of symmetry



Rectangular plane of symmetry



Diagonal plane of symmetry

Thank You