

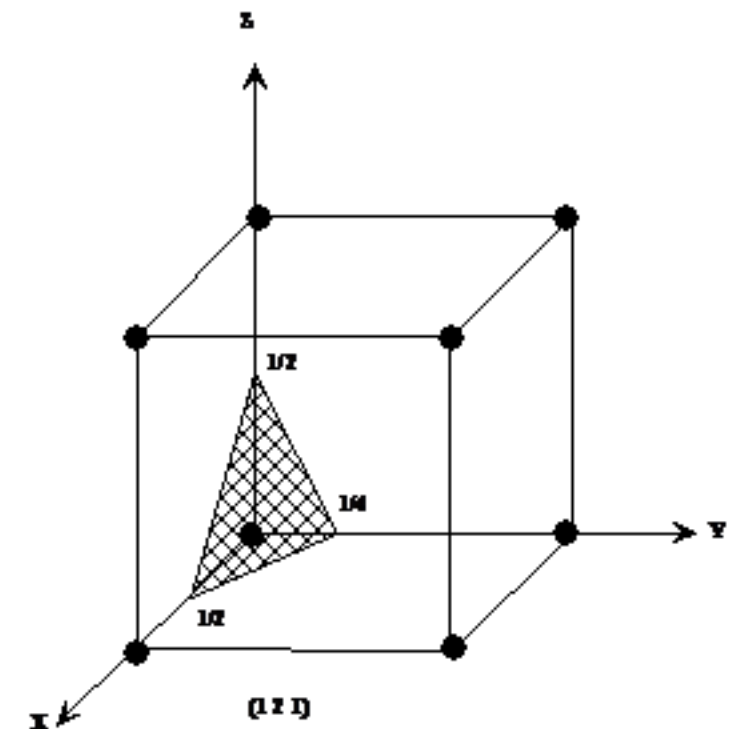
STRUKTUR KRISTAL

Indeks Bidang
Jarak Antar Bidang
Kristal Sederhana

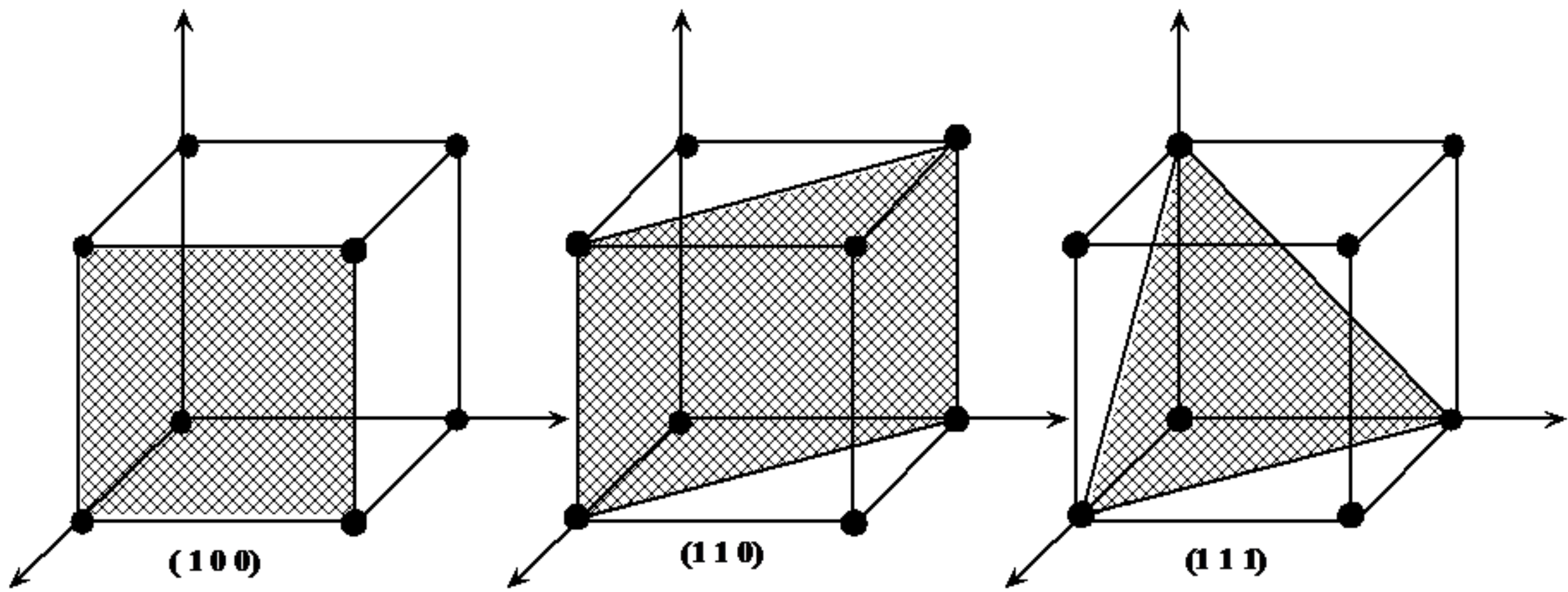
Rita Prasetyowati
Fisika FMIPA UNY
2012

CRYSTALLOGRAPHIC PLANES

- ▶ Crystallographic planes specified by 3 **Miller indices** as (hkl)
- ▶ Procedure for determining h, k and l :
 - If plane passes through origin, translate plane or choose new origin
 - Determine intercepts of planes on each of the axes in terms of unit cell edge lengths (lattice parameters). Note: if plane has no intercept to an axis (i.e., it is parallel to that axis), intercept is infinity ($\frac{1}{2}$ $\frac{1}{4}$ $\frac{1}{2}$)
 - Determine reciprocal of the three intercepts (2 4 2)
 - If necessary, multiply these three numbers by a common factor which converts all the reciprocals to small integers (1 2 1)
 - The three indices are not separated by commas and are enclosed in curved brackets: (hkl) (121)
 - If any of the indices is negative, a bar is placed in top of that index



THREE IMPORTANT CRYSTAL PLANES



THREE IMPORTANT CRYSTAL PLANES

- ▶ Parallel planes are equivalent

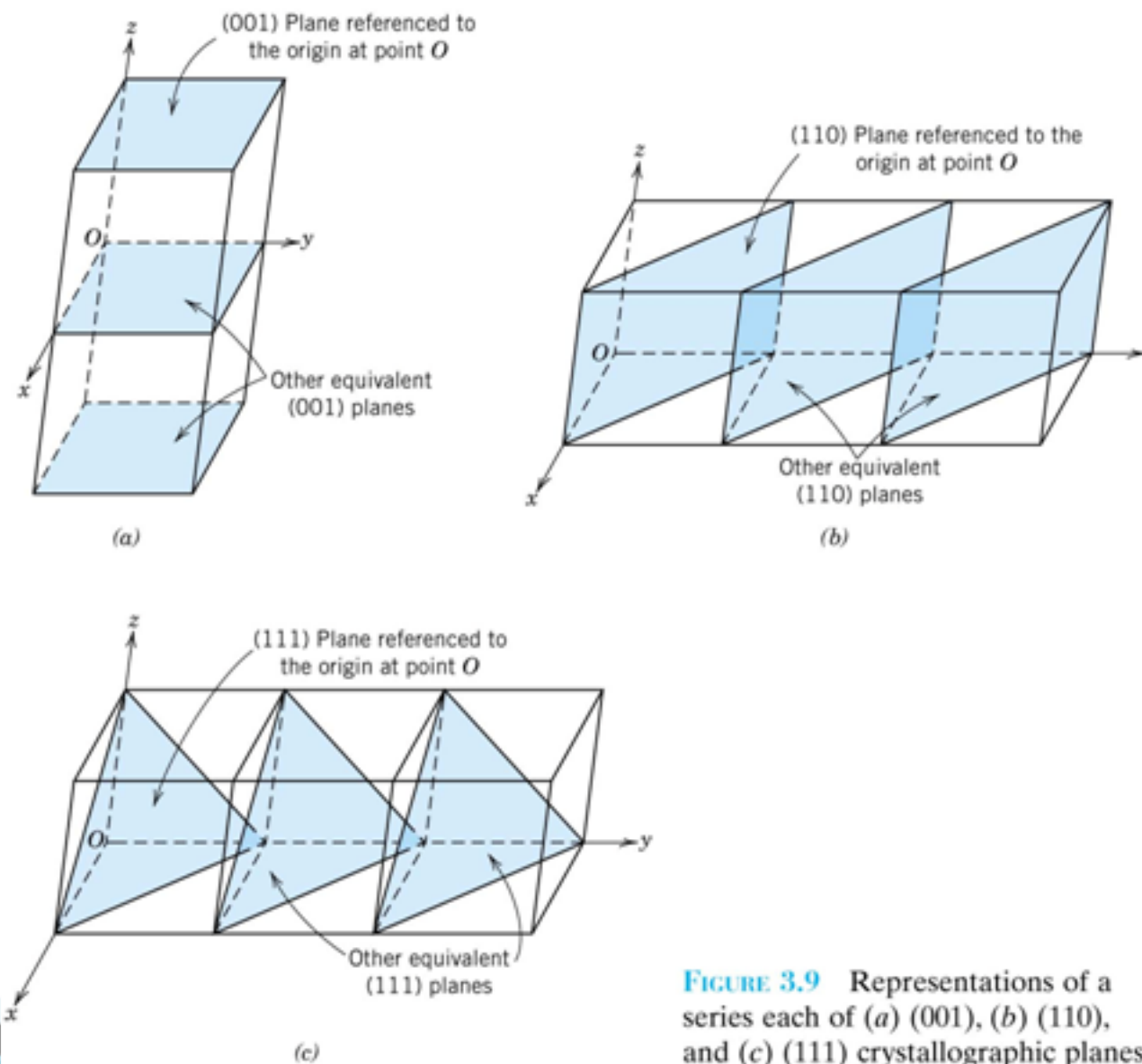
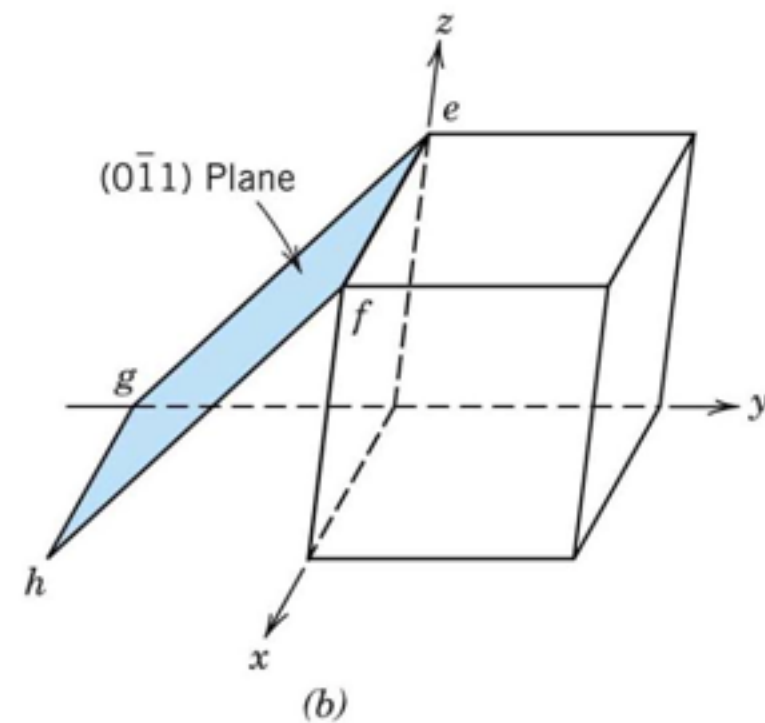
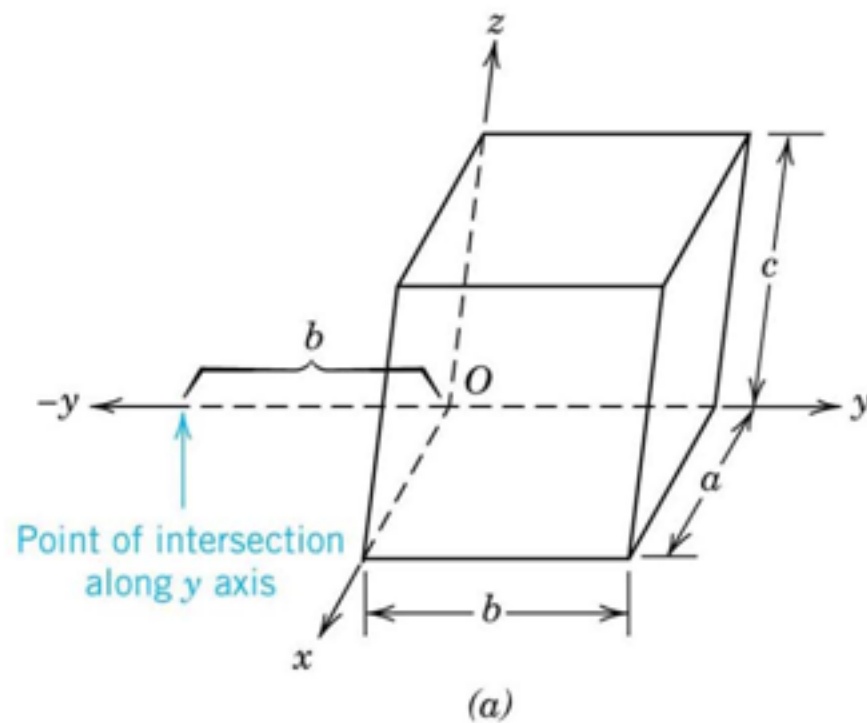


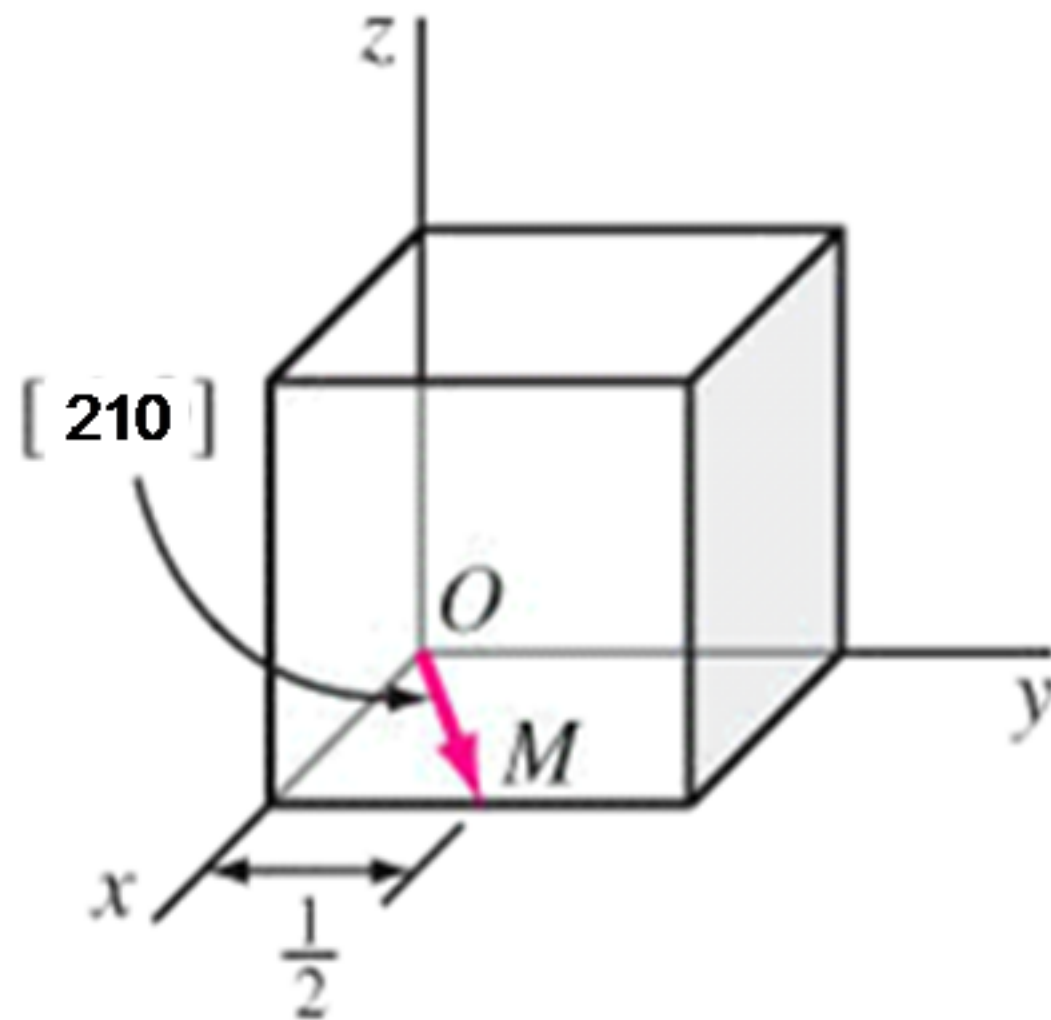
FIGURE 3.9 Representations of a series each of (a) (001), (b) (110), and (c) (111) crystallographic planes.

EXAMPLE: CRYSTAL PLANES

- ▶ Construct a $(0, -1, 1)$ plane

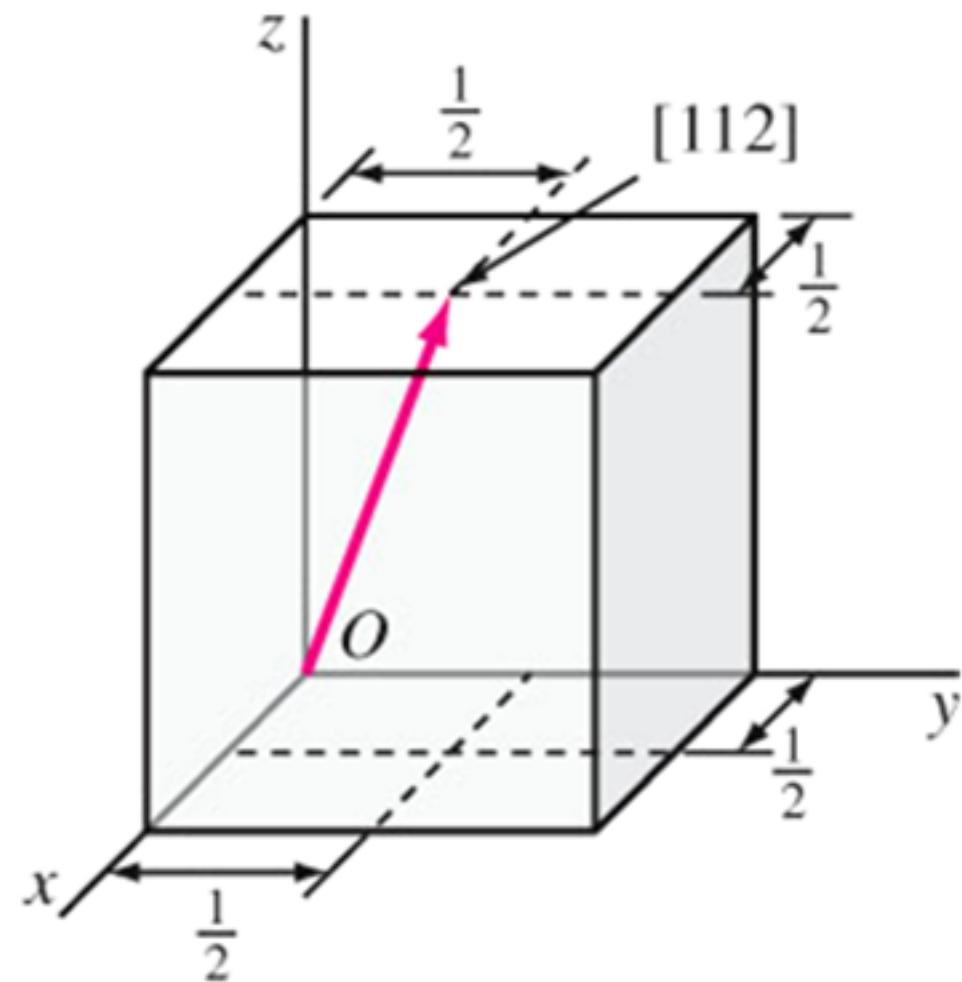


Examples



$$X = 1, Y = \frac{1}{2}, Z = 0$$

$$[1 \frac{1}{2} 0] \rightarrow [2 1 0]$$



$$X = \frac{1}{2}, Y = \frac{1}{2}, Z = 1$$

$$[\frac{1}{2} \frac{1}{2} 1] \rightarrow [1 1 2]$$

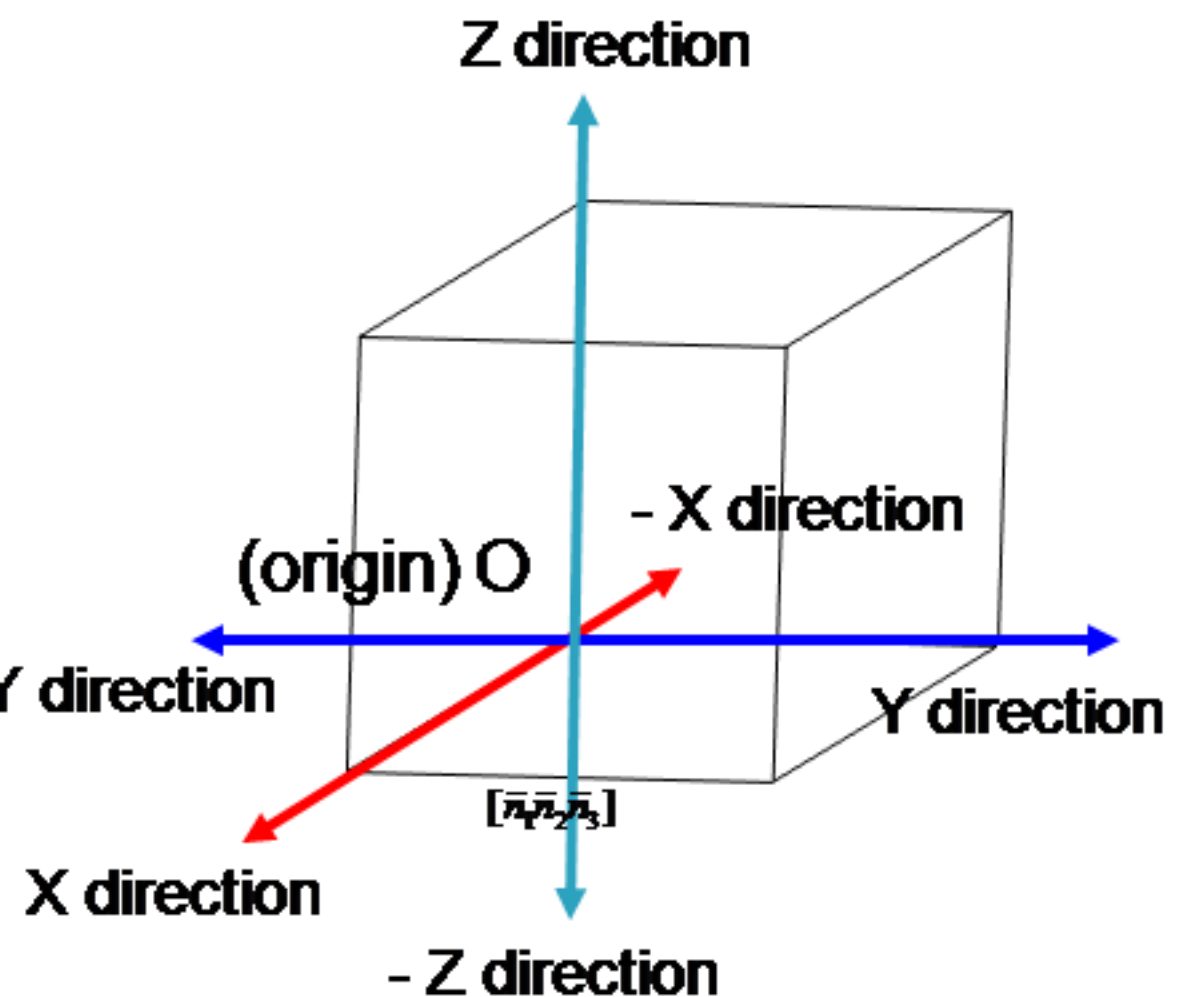
Negative directions

- ▶ When we write the direction $[n_1 n_2 n_3]$ depend on the origin, negative directions can be written as

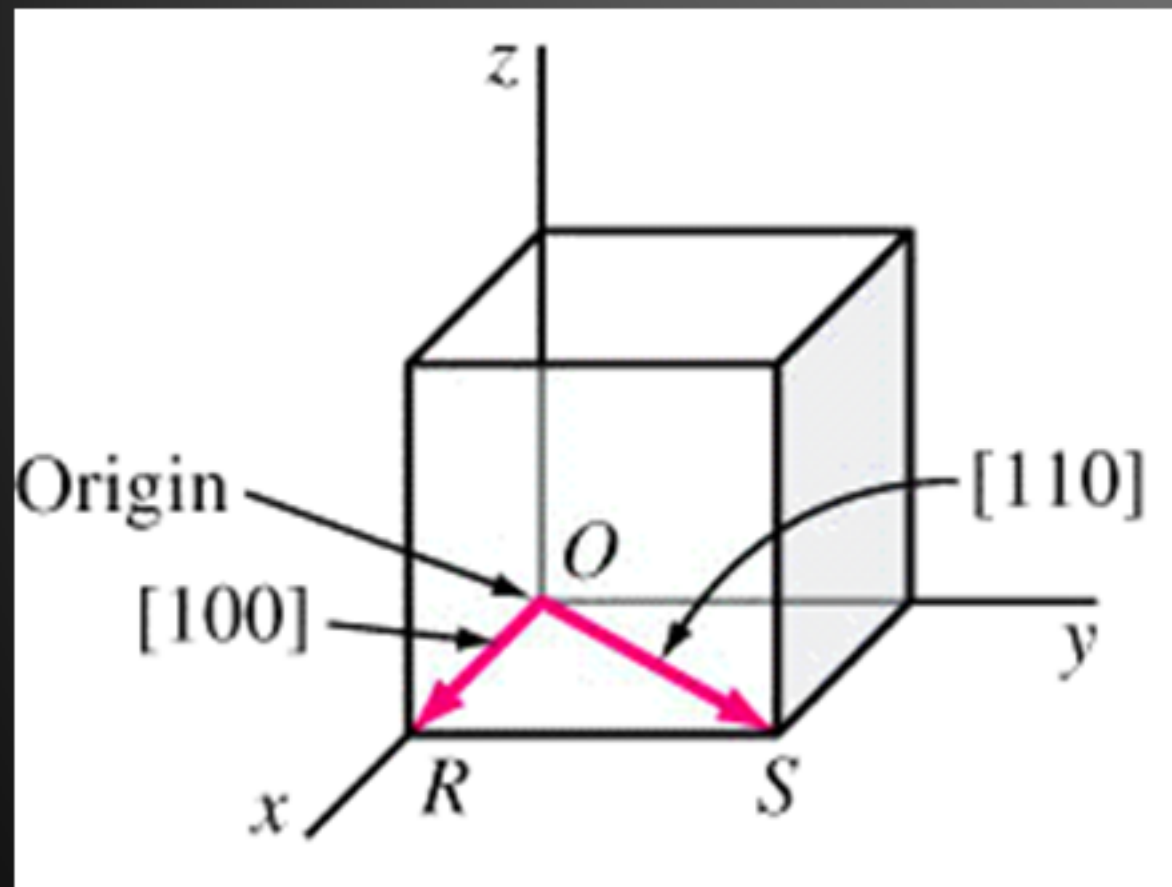
$$\bar{[n_1 \bar{n}_2 \bar{n}_3]}$$

- ▶ $R = n_1 a + n_2 b + n_3 c$

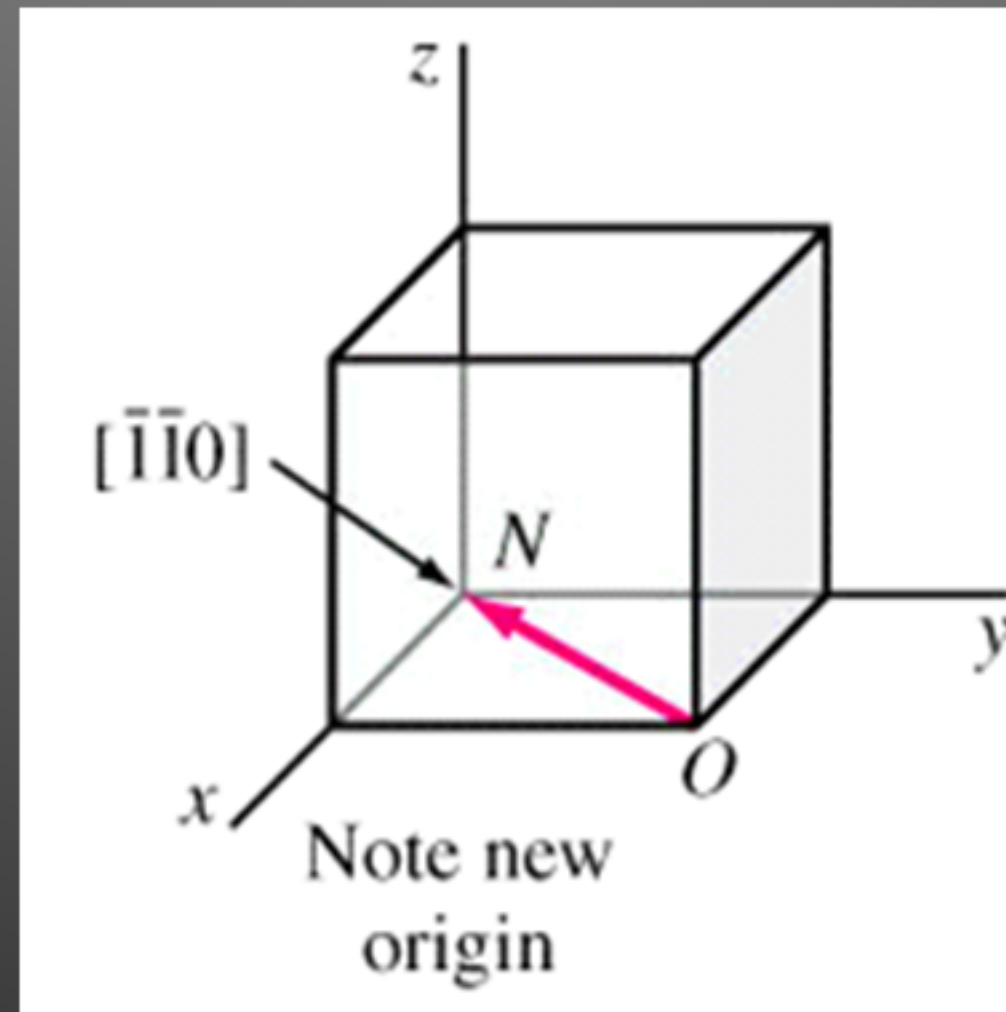
Direction must be smallest integers.



Examples of crystal directions



$$X = 1, Y = 0, Z = 0 \rightarrow [100]$$

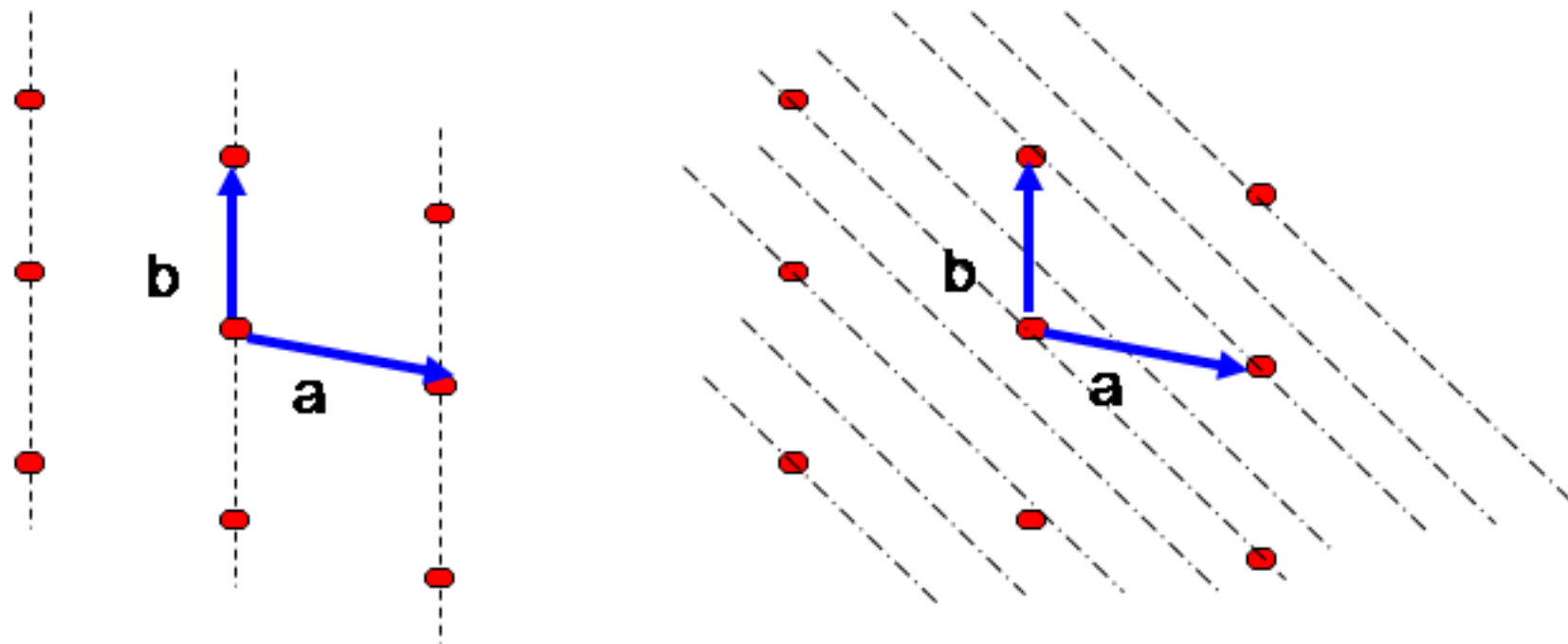


$$X = -1, Y = -1, Z = 0 \rightarrow [\bar{1}\bar{1}0]$$

Crystal Planes

- ▶ Within a crystal lattice it is possible to identify sets of equally spaced parallel planes. These are called **lattice planes**.
- ▶ In the figure density of **lattice points on each plane of a set is the same** and all lattice points are contained on each set of planes.

The set of planes in 2D lattice.



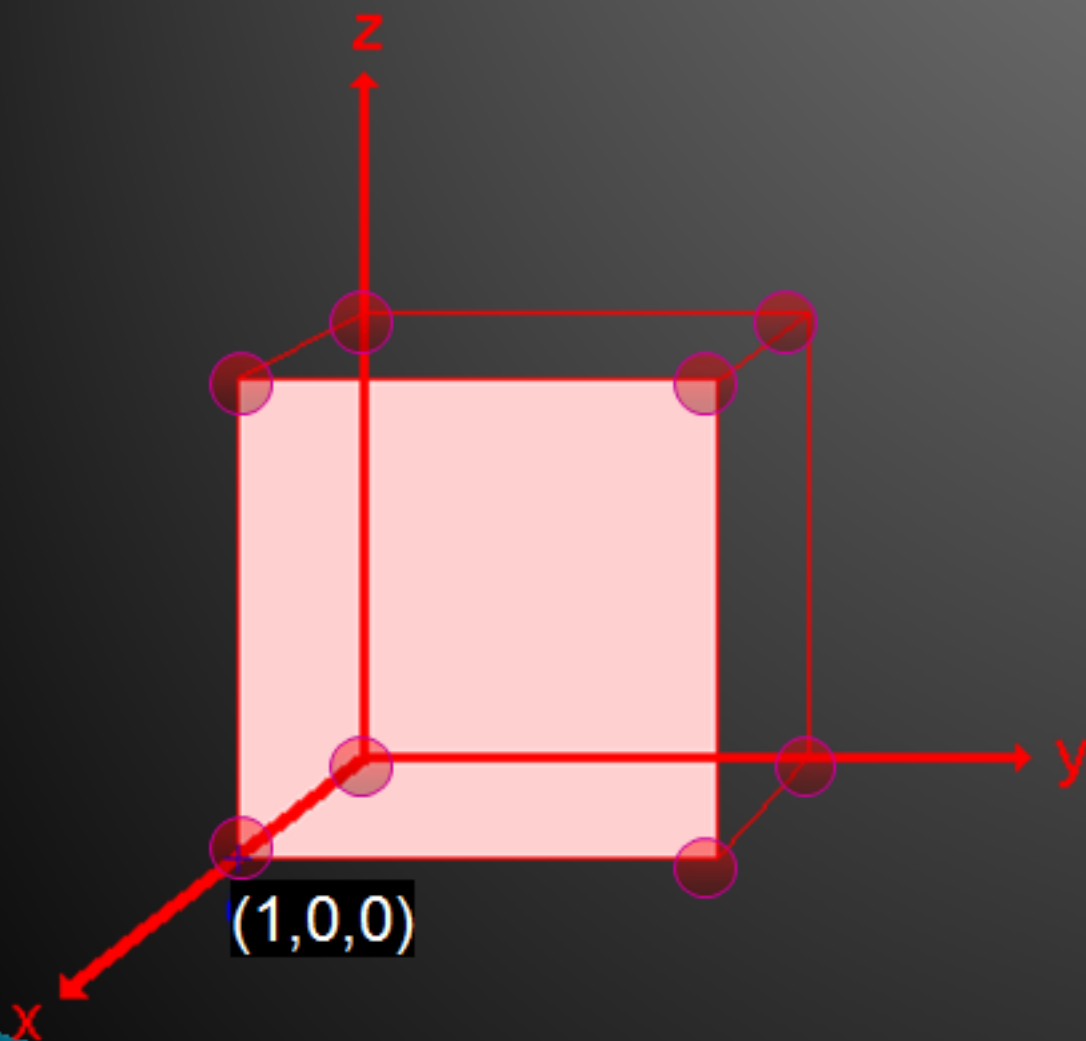
Miller Indices

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

Example-1



Axis	X	Y	Z
Intercept points	1	∞	∞
Reciprocals	1/1	1/ ∞	1/ ∞
Smallest Ratio	1	0	0
Miller indices	(100)		

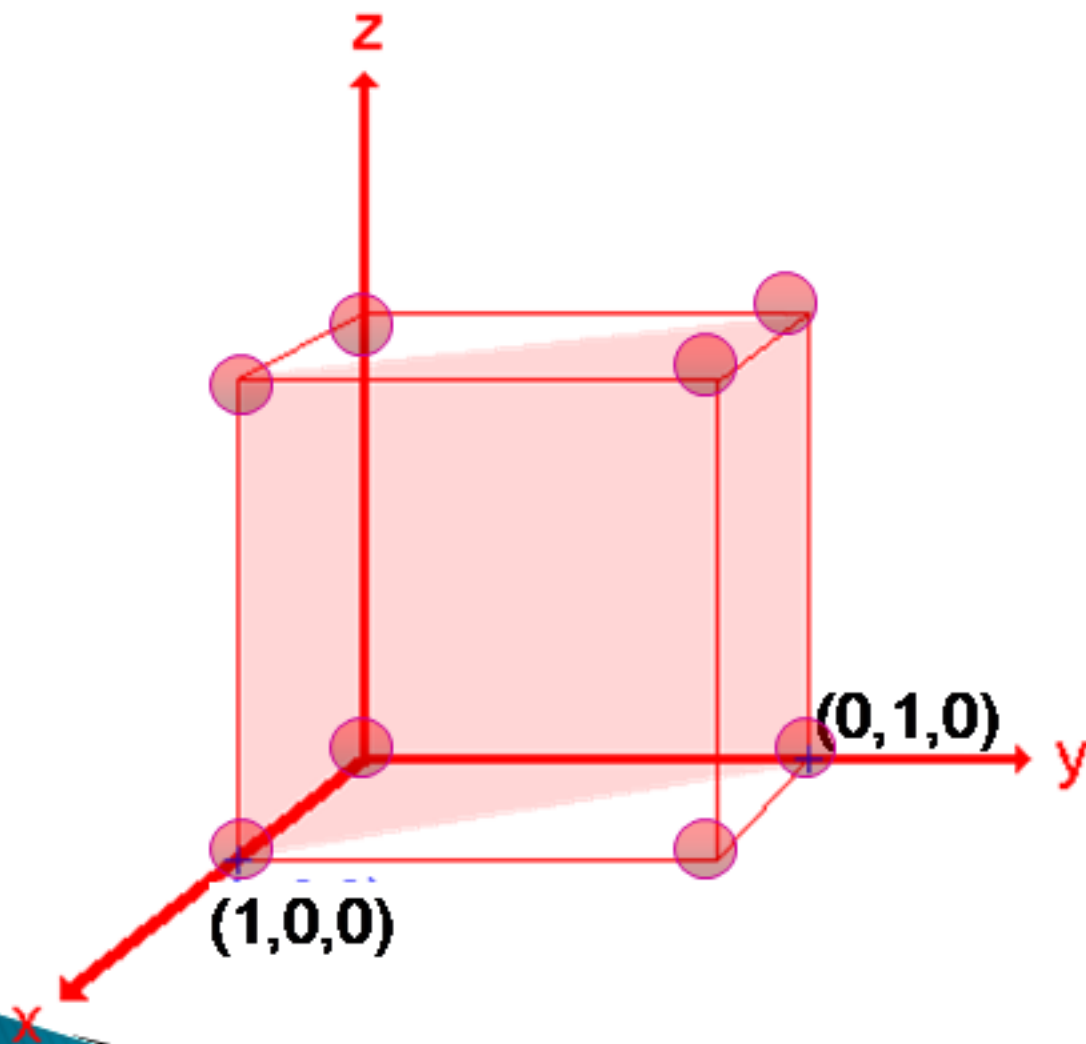
Bidang kristal dan arah bidang

- ▶ Dalam menganalisis struktur kristal, suatu titik tertentu pada kristal akan memiliki seperangkat identitas untuk menspesifikasi atom-atom yang menduduki titik tersebut.
- ▶ Identitas suatu atom dinyatakan dalam koordinat titik dimana atom berada, letak bidang yang ditempati oleh atom dan juga arah bidang yang ditempati atom.

Koordinat titik

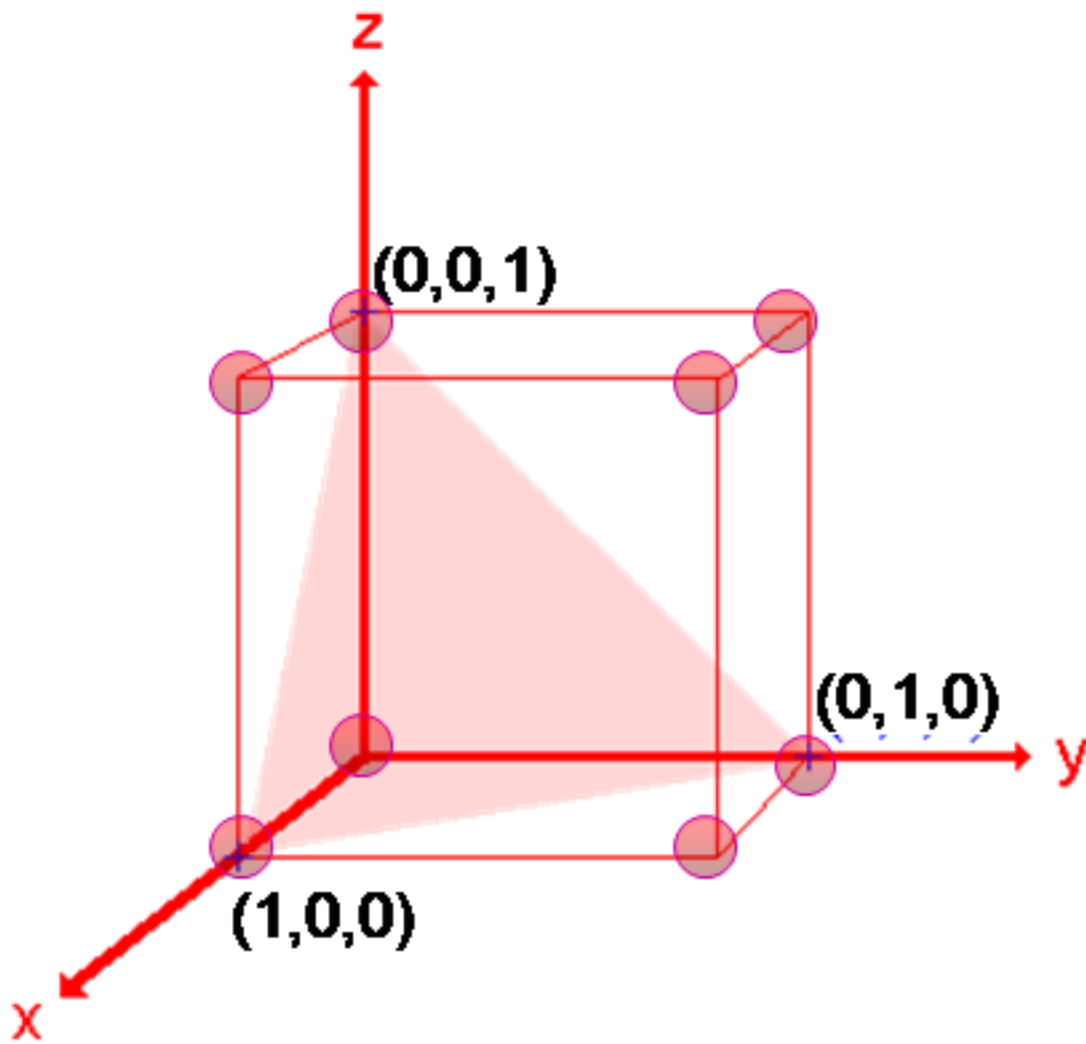
- ▶ Posisi suatu titik pada *unit cell* dapat dinyatakan dalam bentuk vektor satuan dari sumbu-sumbu koordinat penyusun *unit cell*.

Example-2



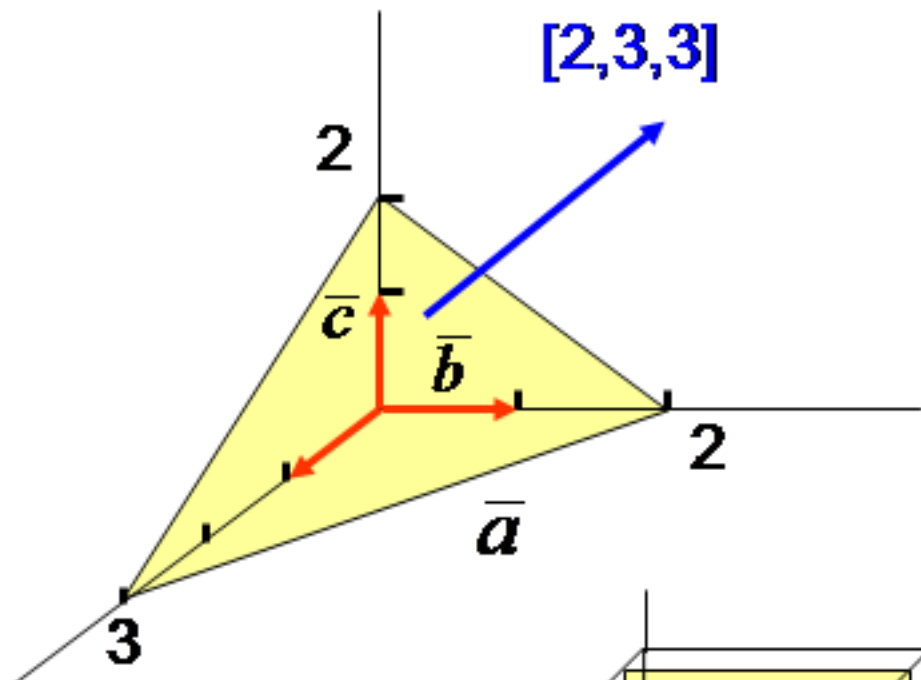
Axis	X	Y	Z
Intercept points	1	1	∞
Reciprocals	1/1	1/1	1/ ∞
Smallest Ratio	1	1	0
Miller indices	(110)		

Example-3



Axis	X	Y	Z
Intercept points	1	1	1
Reciprocals	1/1	1/1	1/1
Smallest Ratio	1	1	1
Miller indices	(111)		

Miller Indices

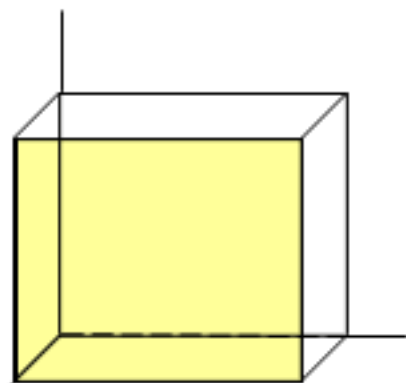


Plane intercepts axes at $3\bar{a}, 2\bar{b}, 2\bar{c}$

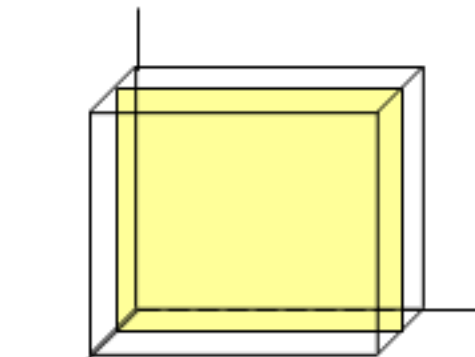
Reciprocal numbers are: $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

Indices of the plane (Miller): $(2,3,3)$

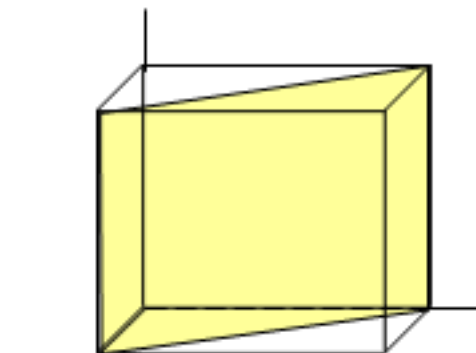
Indices of the direction: $[2,3,3]$



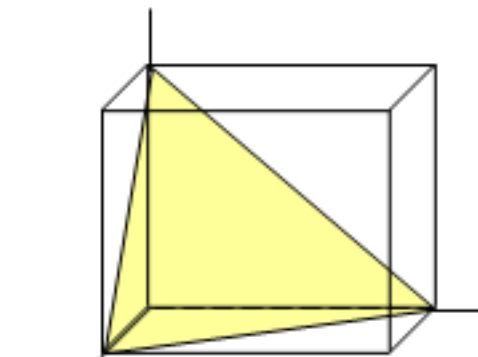
(100)



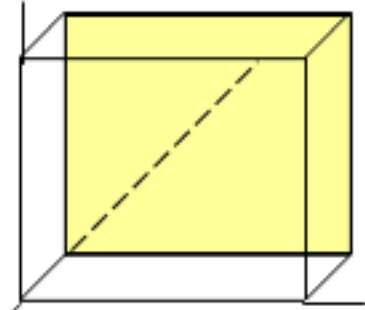
(200)



(110)



(111)

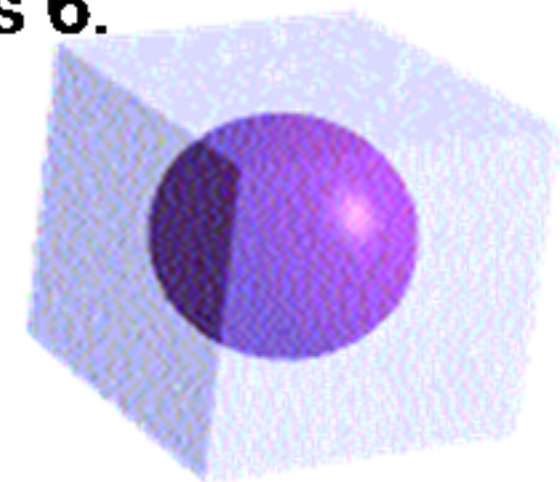
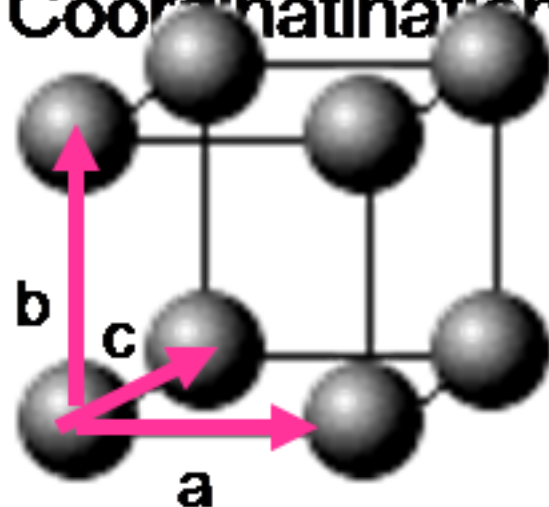


$(\bar{1}00)$

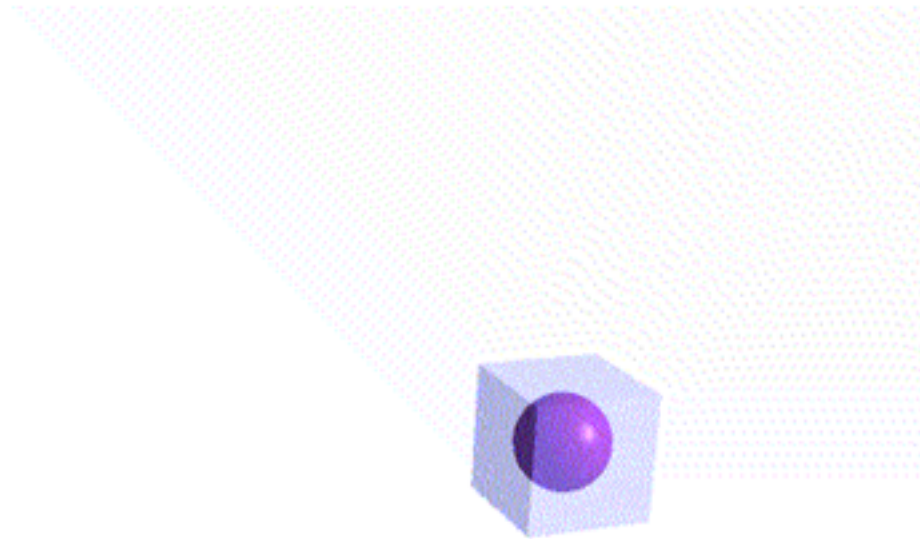
1-CUBIC CRYSTAL SYSTEM

a- Simple Cubic (SC)

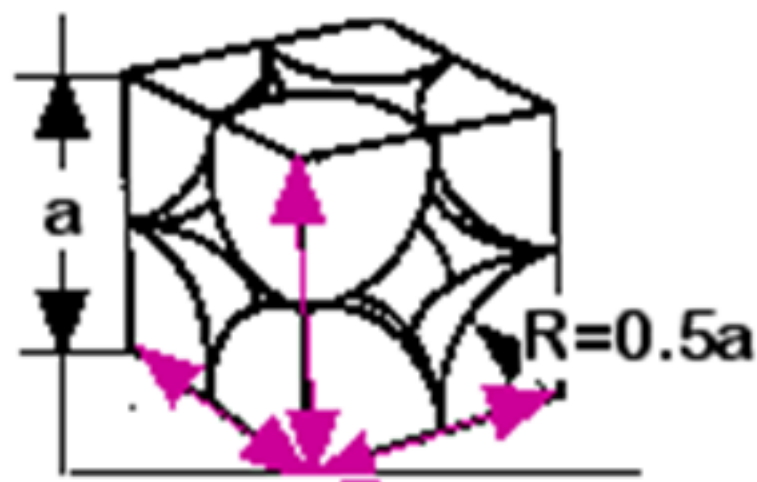
- Simple Cubic has one lattice point so its primitive cell.
- In the unit cell on the left, the atoms at the corners are cut because only a portion (in this case 1/8) belongs to that cell. The rest of the atom belongs to neighboring cells.
- Coordination number of simple cubic is 6.



a- Simple Cubic (SC)



Atomic Packing Factor of SC



contains $8 \times 1/8 =$
1 atom/unit cell

APF = 0.52 for simple cubic

$$\text{APF} = \frac{\text{atom/unit cell} \times \frac{4}{3} \pi (0.5a)^3}{a^3} = \frac{1 \times \frac{4}{3} \pi (0.5a)^3}{a^3}$$

The diagram shows the calculation of the Atomic Packing Factor (APF) for a simple cubic unit cell. The numerator is the volume of the atoms in the unit cell, and the denominator is the volume of the unit cell.

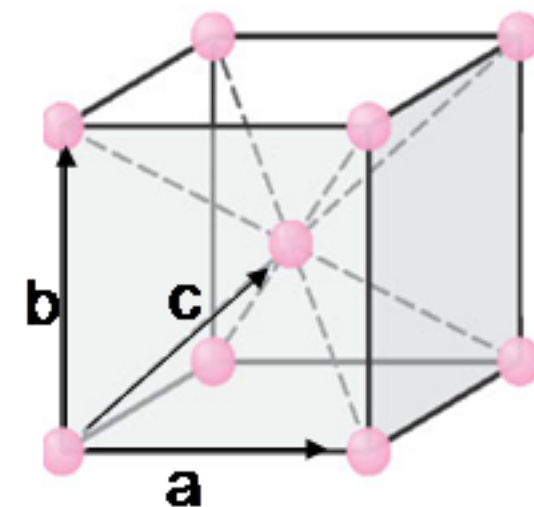
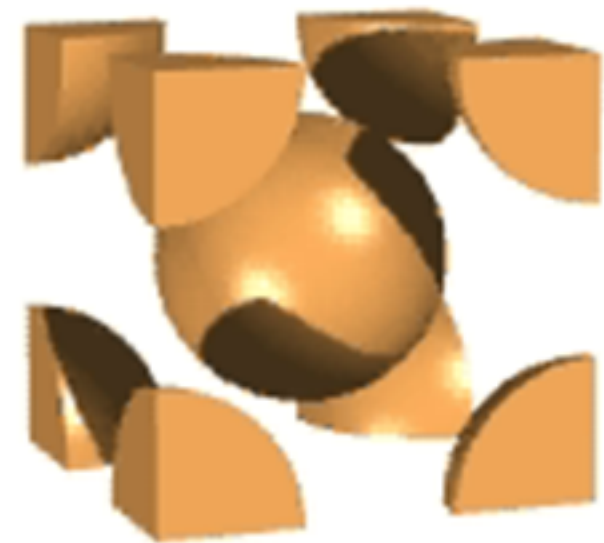
atom/unit cell (green text) points to the '1' in the numerator.

volume/atom (brown text) points to the $\frac{4}{3} \pi (0.5a)^3$ term in the numerator.

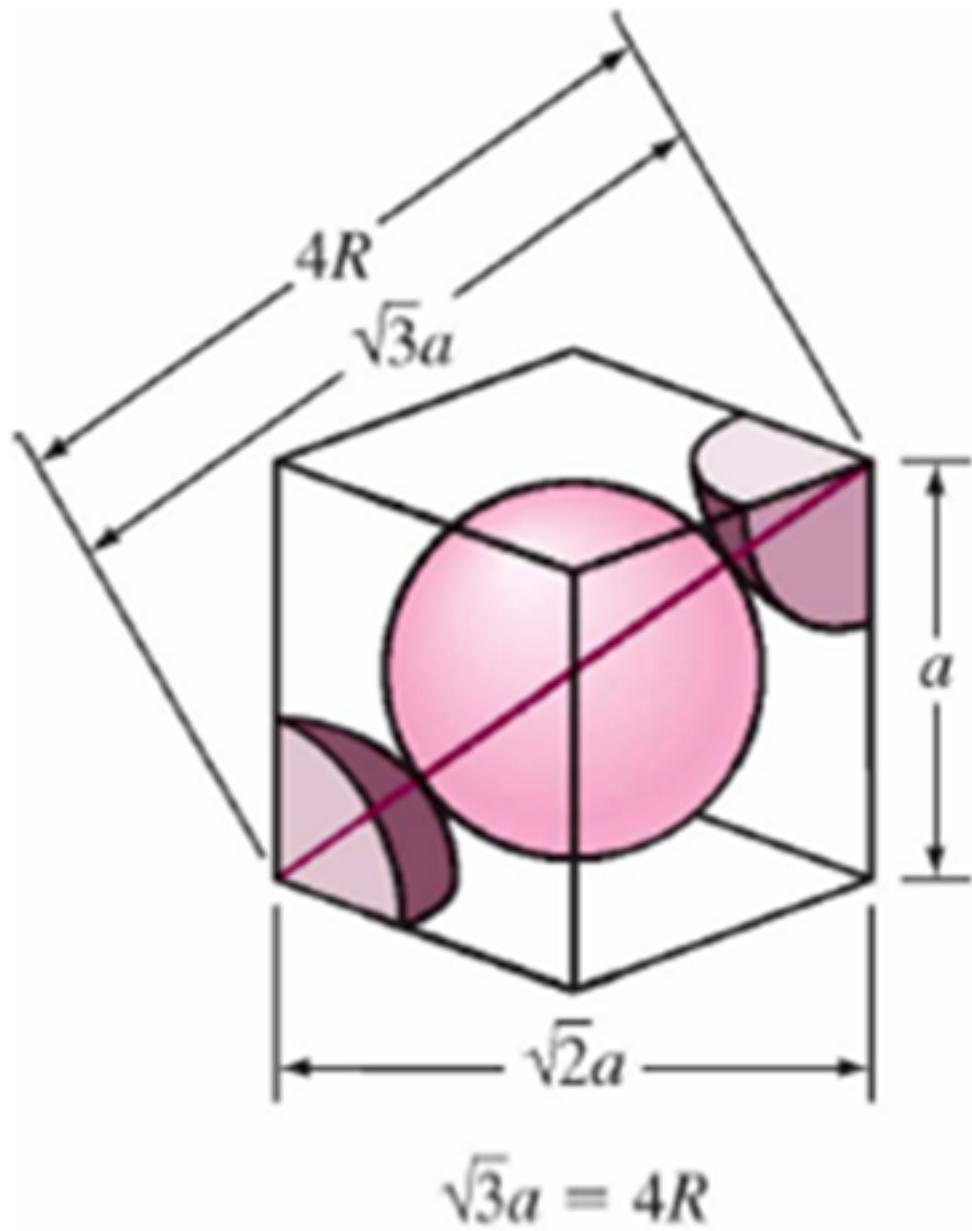
volume/unit cell (blue text) points to the a^3 term in the denominator.

b-Body Centered Cubic (BCC)

- BCC has two lattice points so BCC is a non-primitive cell.
- BCC has eight nearest neighbors. Each atom is in contact with its neighbors only along the body-diagonal directions.
- Many metals (Fe, Li, Na..etc), including the alkalis and several transition elements choose the BCC structure.



Atomic Packing Factor of BCC



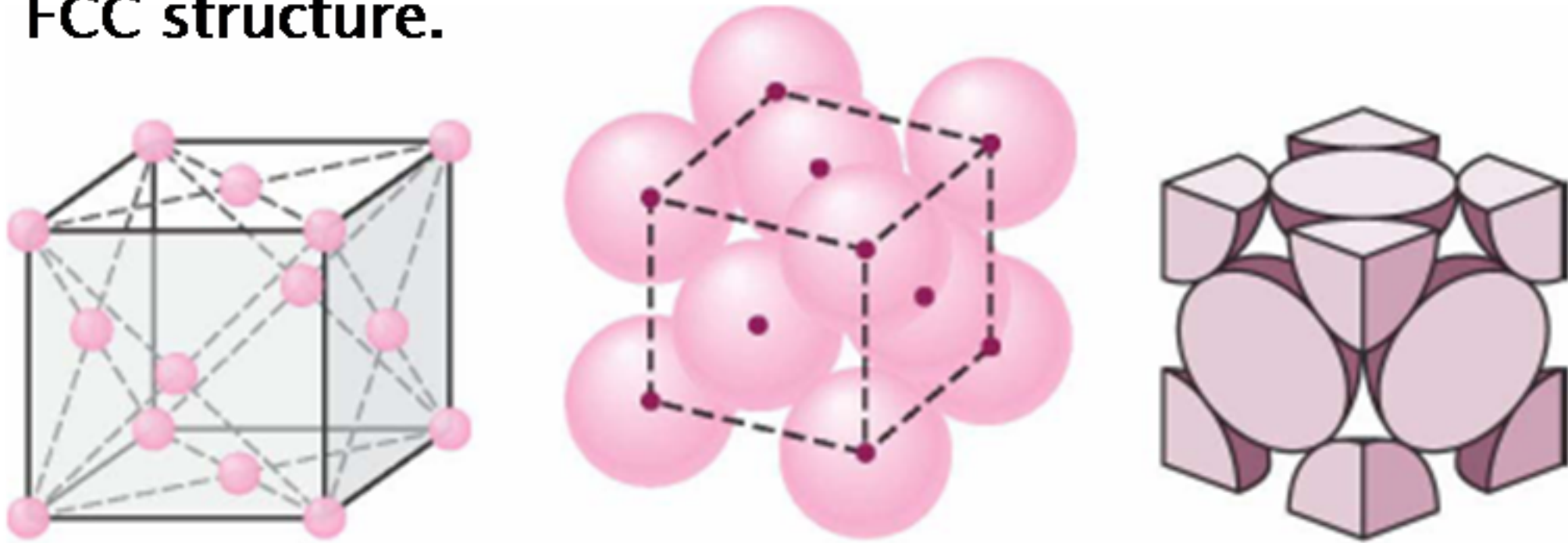
$$APF_{BCC} = \frac{V_{atoms}}{V_{unit\ cell}} = 0.68$$

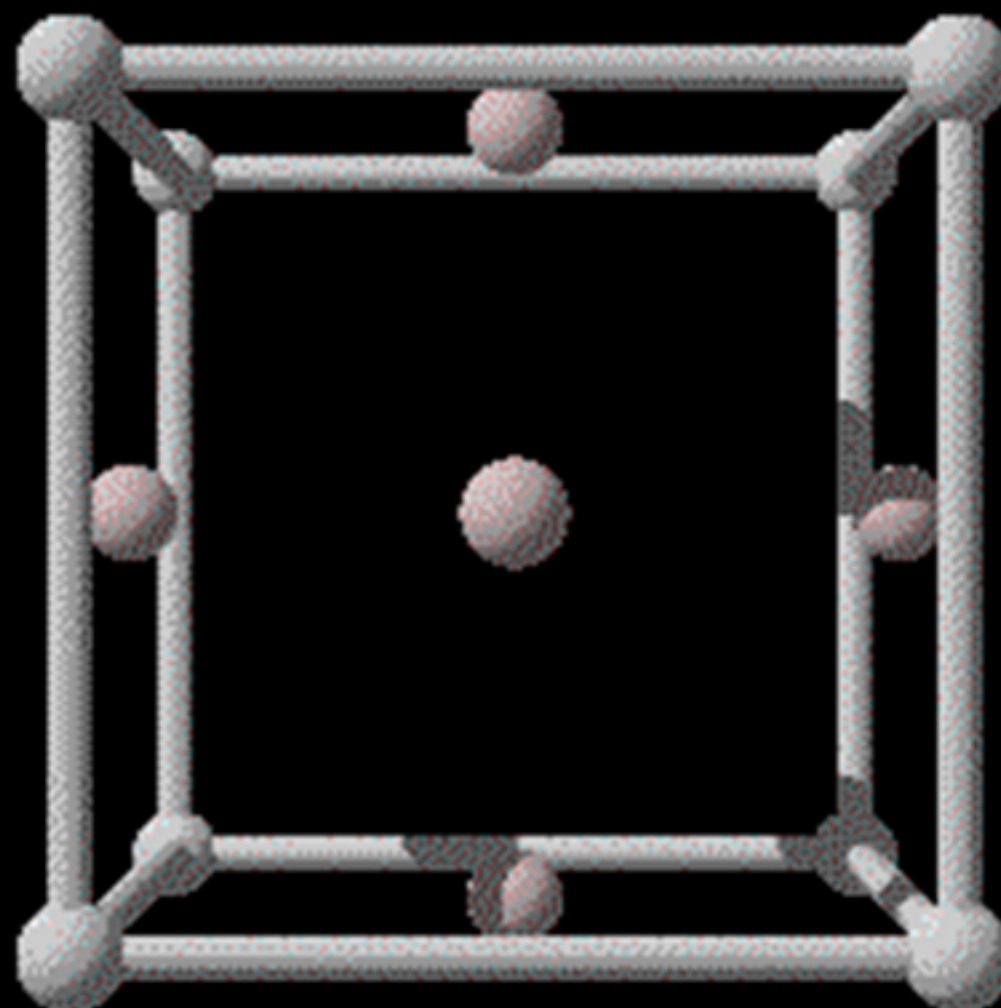
$$APF = \frac{\text{atom unit cell} \left[2 \cdot \frac{4}{3} \cdot (0.433a)^3 \right]}{a^3} = \frac{\text{volume atom}}{\text{volume unit cell}}$$

The diagram shows the calculation of the Atomic Packing Factor (APF) for BCC. The numerator represents the total volume of atoms in the unit cell, calculated as 2 atoms per unit cell multiplied by the volume of one atom, $\frac{4}{3} \pi (0.433a)^3$. The denominator represents the volume of the unit cell, a^3 . The final result is 0.68.

c- Face Centered Cubic (FCC)

- ▶ There are atoms at the corners of the unit cell and at the center of each face.
- ▶ Face centered cubic has 4 atoms so its non primitive cell.
- ▶ Many of common metals (Cu,Ni,Pb..etc) crystallize in FCC structure.



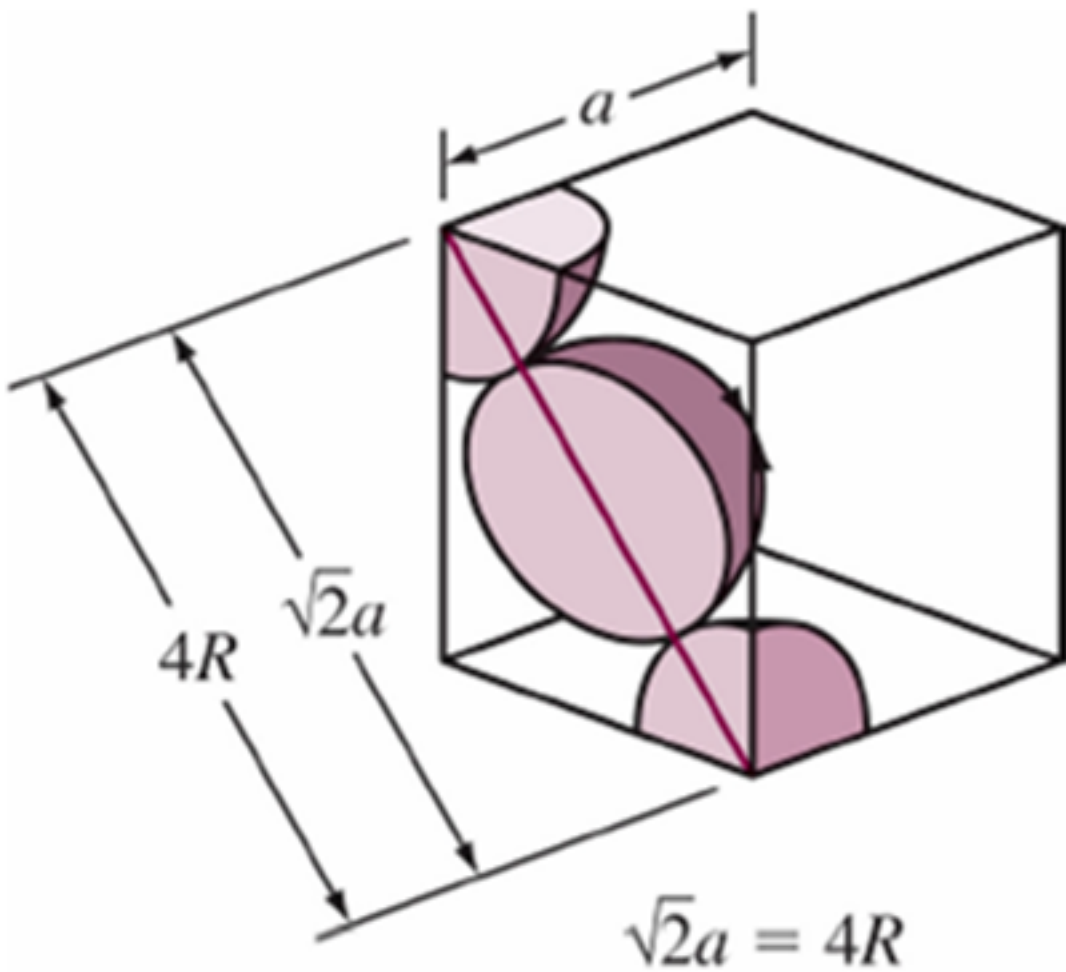


Face centered cubic unit cell

CRYSTALLOGRAPHIC POINTS, DIRECTIONS & PLANES

- ▶ In crystalline materials, often necessary to specify points, directions and planes within unit cell and in crystal lattice
- ▶ Three numbers (or indices) used to designate points, directions (lines) or planes, based on basic geometric notions
- ▶ The three indices are determined by placing the origin at one of the corners of the unit cell, and the coordinate axes along the unit cell edges

Atomic Packing Factor of FCC



$$APF_{\text{FCC}} = \frac{V_{\text{atoms}}}{V_{\text{unit cell}}} = 0,74$$

$$APF = \frac{\text{atom unit cell} \cdot \frac{4}{3} \pi (0,353a)^3}{a^3} \cdot \frac{\text{volume atom}}{\text{unit cell}}$$

The diagram shows the calculation of the Atomic Packing Factor (APF) for FCC. The numerator is $4 \cdot \frac{4}{3} \pi (0,353a)^3$, where 4 is the number of atoms per unit cell, $\frac{4}{3} \pi (0,353a)^3$ is the volume of one atom, and a^3 is the volume of the unit cell. The denominator is a^3 .

Unit cell contents

Counting the number of atoms within the unit cell

Atoms	Shared Between:	Each atom counts:
corner	8 cells	1/8
face centre	2 cells	1/2
body centre	1 cell	1
edge centre	2 cells	1/2

lattice type	cell contents
P	1 [=8 x 1/8]
I	2 [(8 x 1/8) + (1 x 1)]
F	4 [(8 x 1/8) + (6 x 1/2)]
C	2 [(8 x 1/8) + (2 x 1/2)]

Example; Atomic Packing Factor

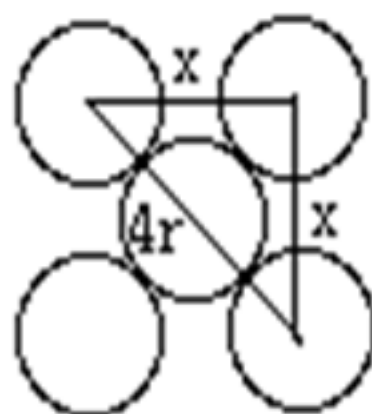
It is very easy to show that the filling of space by spheres is 74%
e.g. for the fcc unit cell of cubic close packing (CCP) with an ABC layer repeat

For spheres of radius, r , touching along the **face diagonal**, the cubic unit cell parameter is calculated as $x = 2\sqrt{2}r$

$$\begin{aligned} \text{total unit cell volume} &= x^3 \\ &= 16\sqrt{2}r^3 \end{aligned}$$

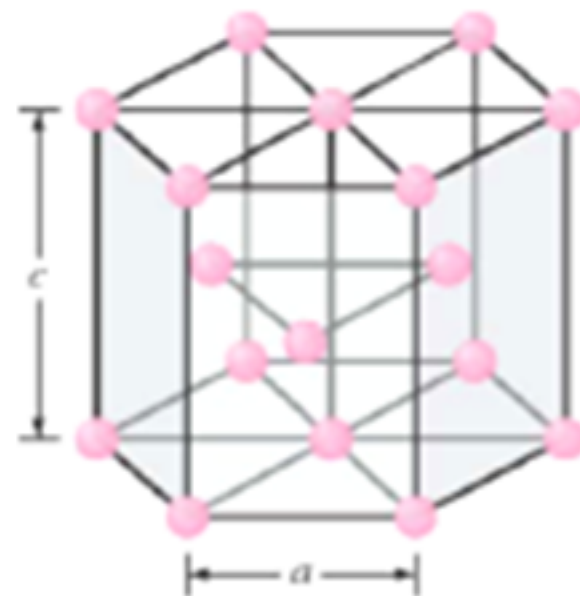
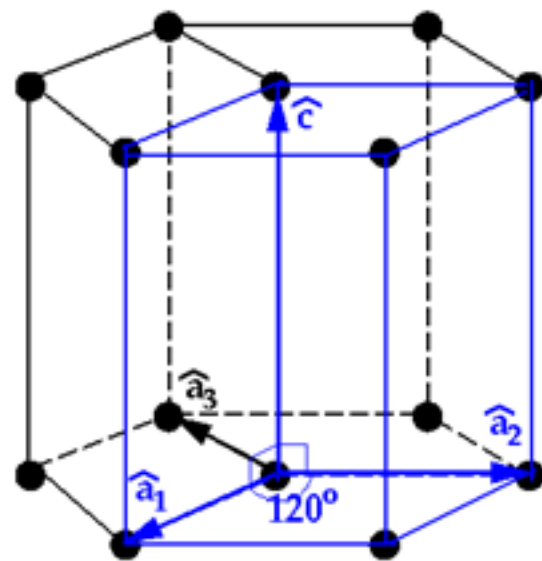
$$\begin{aligned} \text{occupied volume} &= 4 \text{ spheres} \\ &= \frac{16\pi r^3}{3} \end{aligned}$$

$$\text{space filling} = \frac{\pi}{3\sqrt{2}} = 74.05\%$$

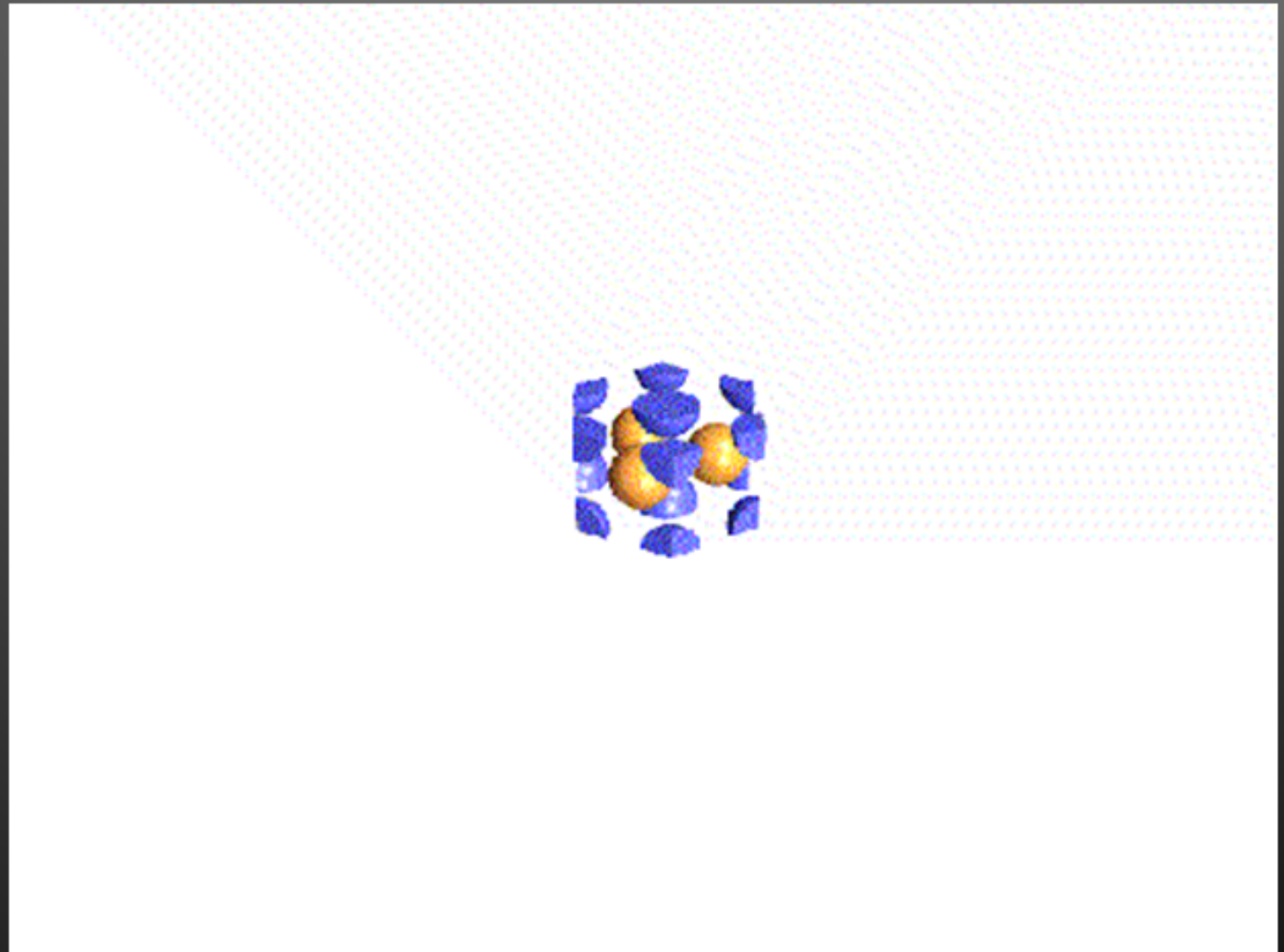


2 - HEXAGONAL SYSTEM

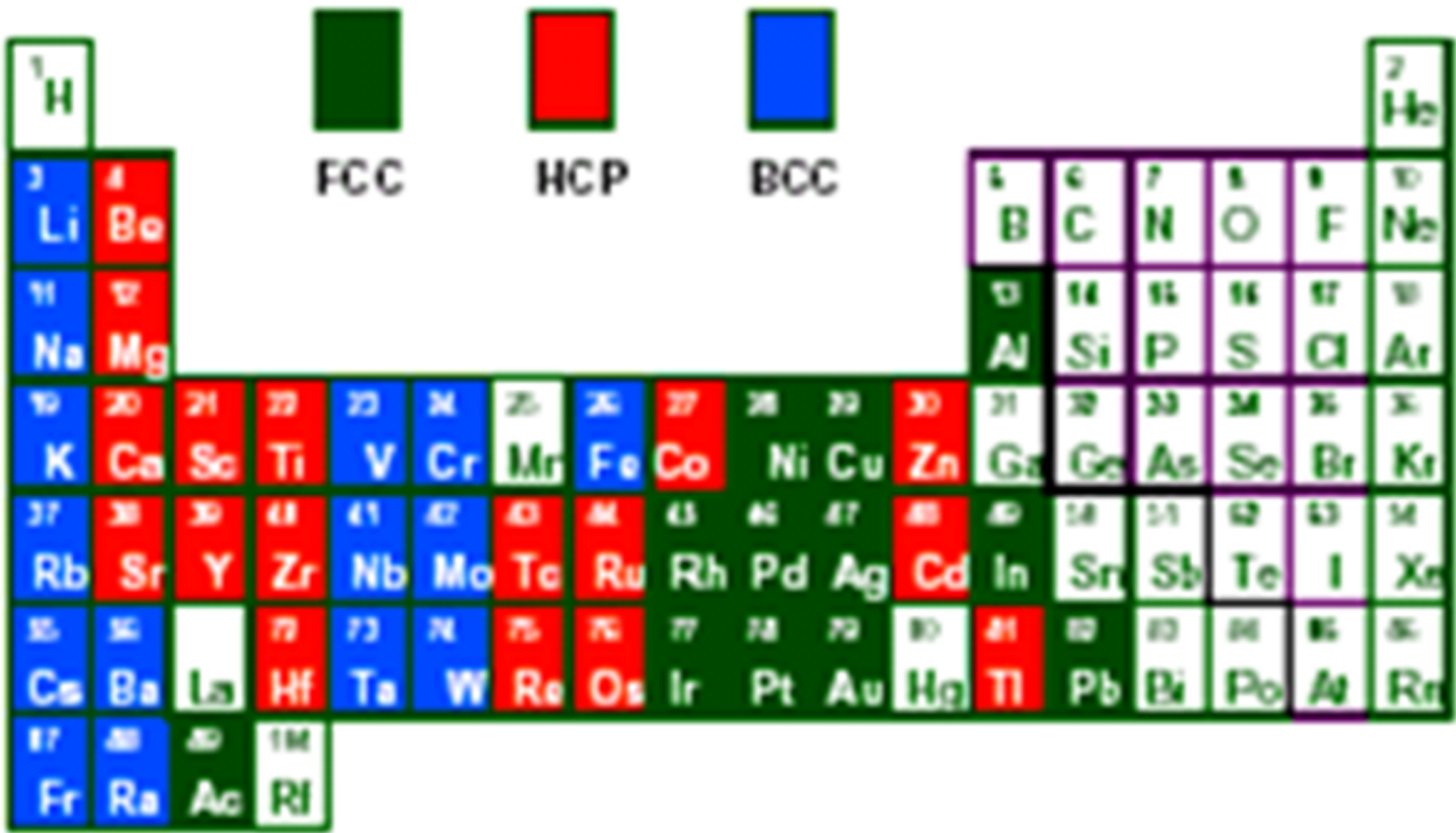
- A crystal system in which three equal coplanar axes intersect at an angle of 60° , and a perpendicular to the others, is of a different length.



2 - HEXAGONAL SYSTEM



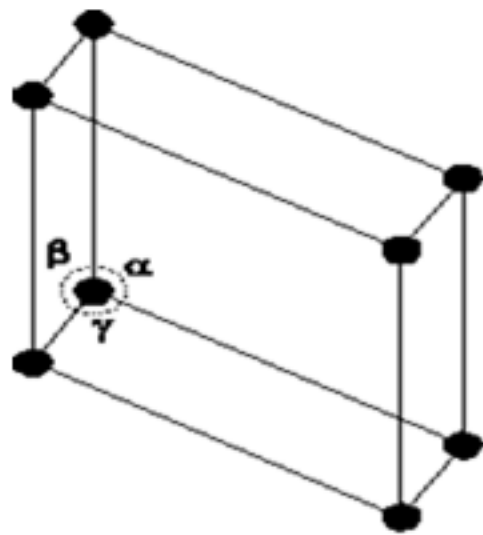
Atoms are all same.



3 - TRICLINIC

4 - MONOCLINIC CRYSTAL SYSTEM

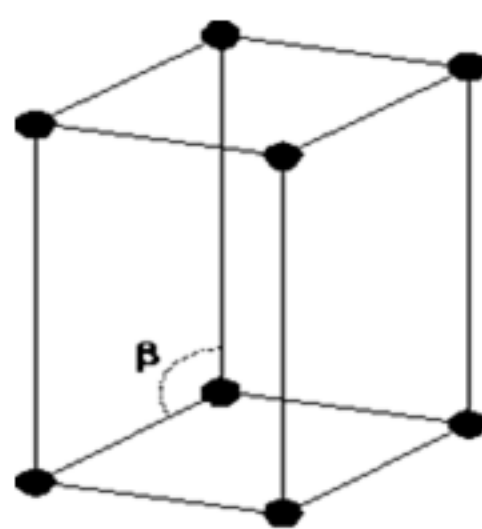
- ▶ Triclinic minerals are the least symmetrical. Their three axes are all different lengths and none of them are perpendicular to each other. These minerals are the most difficult to recognize.



Triclinic (Simple)

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

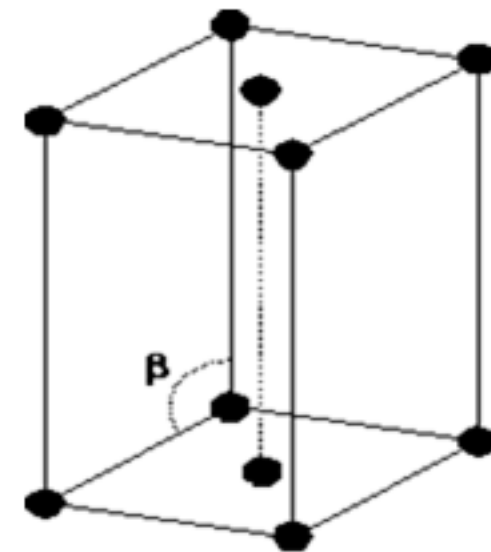
$$a \neq b \neq c$$



Monoclinic (Simple)

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

$$a \neq b \neq c$$

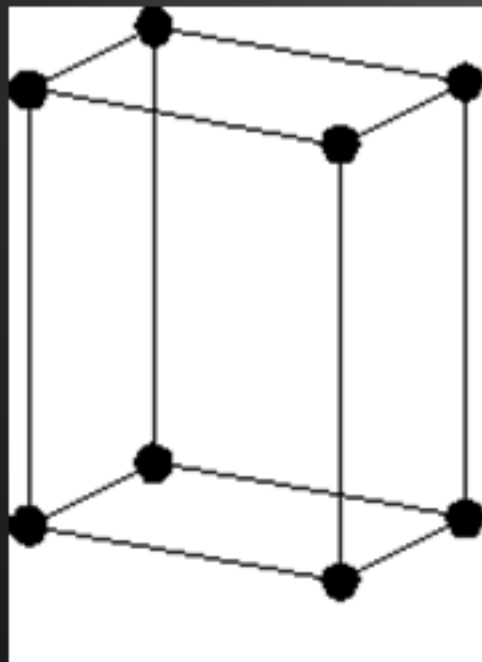


Monoclinic (Base Centered)

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

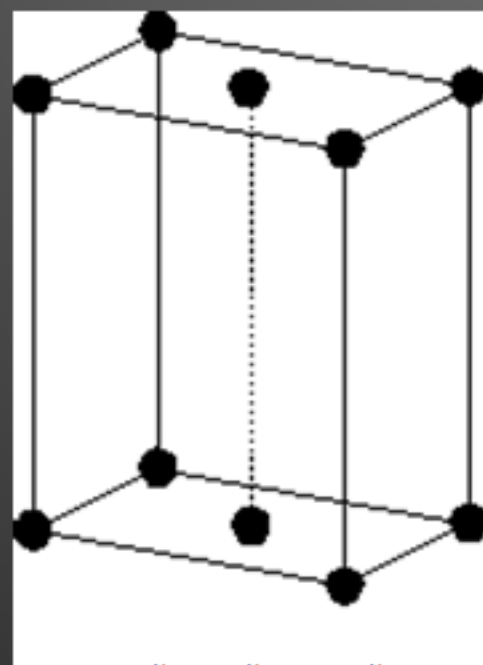
$$a \neq b \neq c,$$

5 - ORTHORHOMBIC SYSTEM



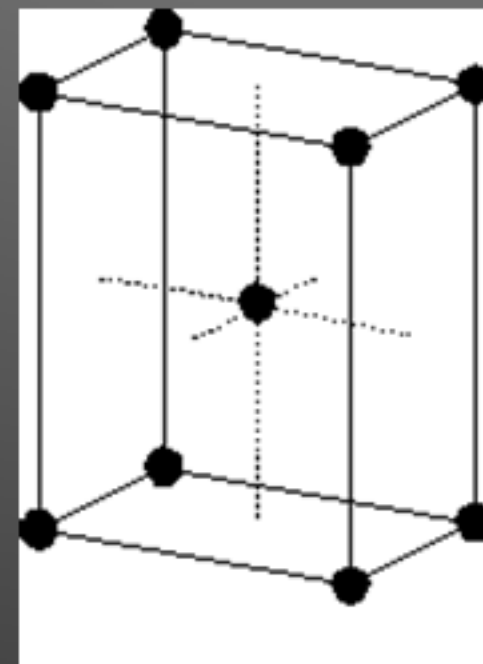
Orthorhombic
(Simple)

$$\alpha = \beta = \gamma = 90^\circ$$
$$a \neq b \neq c$$



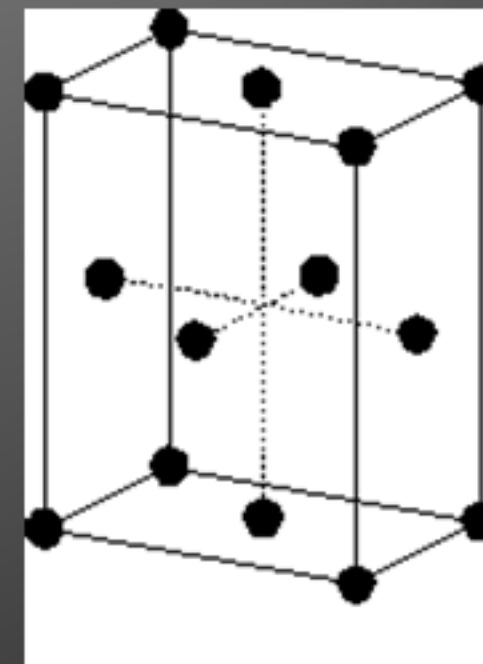
Orthorhombic
(Base-centred)

$$\alpha = \beta = \gamma = 90^\circ$$
$$a \neq b \neq c$$



Orthorhombic (BC)

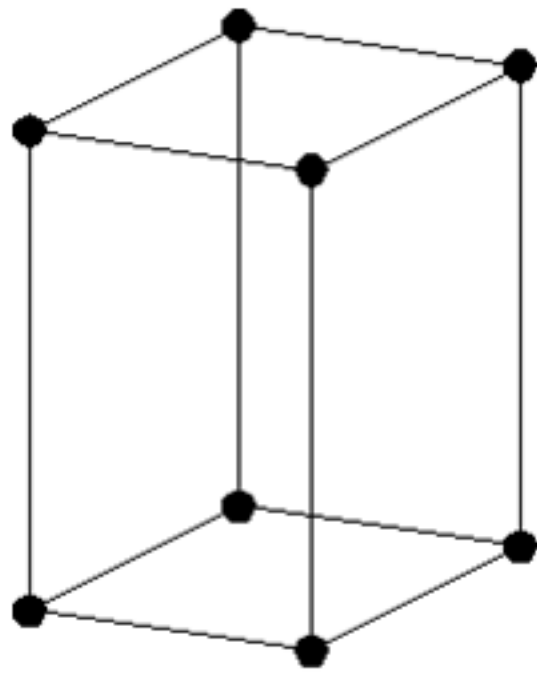
$$\alpha = \beta = \gamma = 90^\circ$$
$$a \neq b \neq c$$



Orthorhombic (FC)

$$\alpha = \beta = \gamma = 90^\circ$$
$$a \neq b \neq c$$

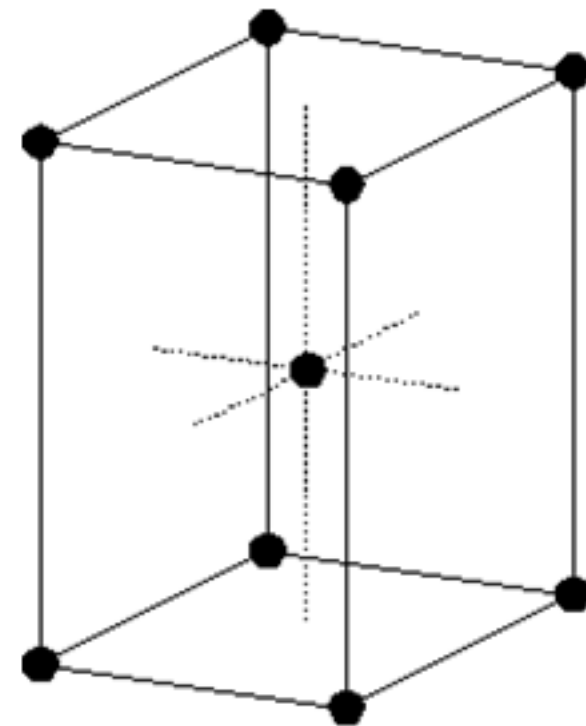
6 – TETRAGONAL SYSTEM



Tetragonal (P)

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

$$a = b \neq c$$

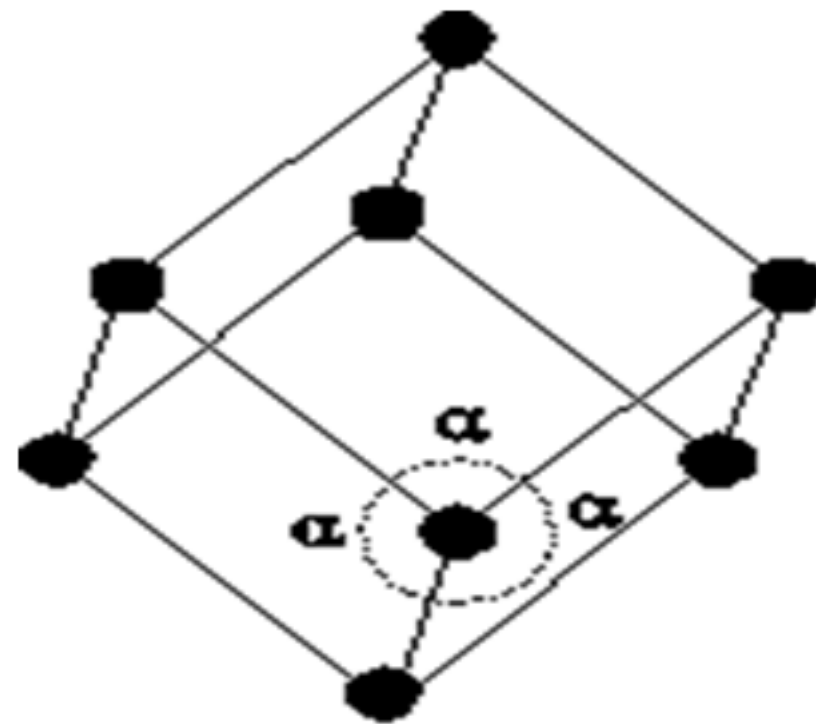


Tetragonal (BC)

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

$$a = b \neq c$$

7 - Rhombohedral (R) or Trigonal



Rhombohedral (R) or Trigonal
(S)

$$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$$

Posisi titik (*crystallographic direction*)

Langkah-langkah untuk menentukan *crystallographic direction*

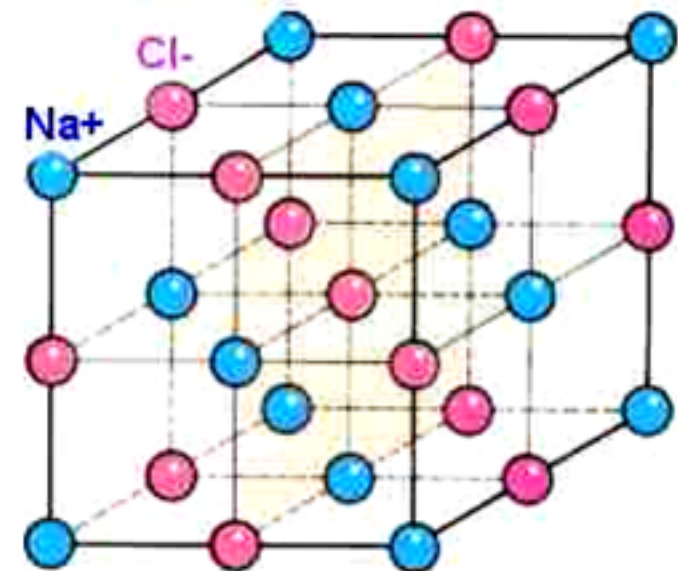
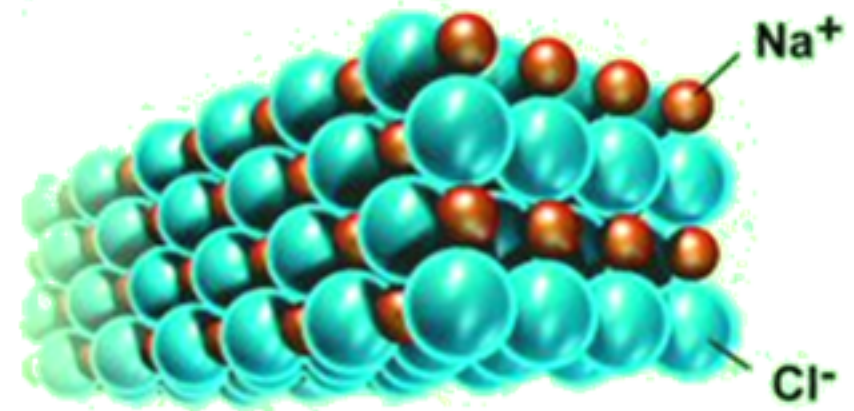
1. Menarik suatu vektor dari titik yang diinginkan dan pusat sumbu koordinat acuan. Vektor satuan selalu berarah dari pusat sumbu koordinat menuju titik yang dimaksud.
2. Menentukan panjang proyeksi vektor pada ketiga sumbu unit cell.
3. Mencari kelipatan bulat terkecil untuk ketiga proyeksi vektor dengan membagi atau mengalikan dengan faktor yang sama untuk ketiga sumbu
4. *Crystallographic direction* dinyatakan dalam ketiga bilangan yang didapatkan pada Langkah 3 dan dituliskan dalam kurung siku tanpa dipisahkan dengan tanda koma. Sehingga *crystallographic direction* $[u\ v\ w]$ menyatakan vektor satuan dari titik pada suatu *unit cell*.

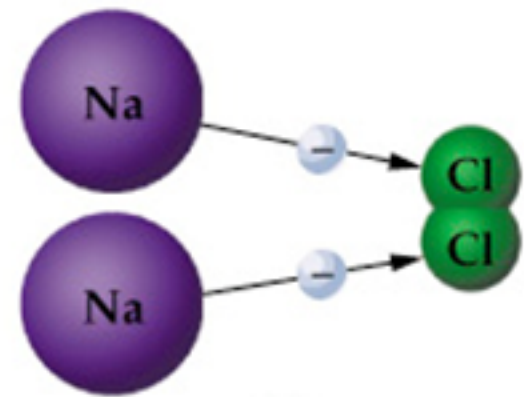
THE MOST IMPORTANT CRYSTAL STRUCTURES

- ▶ Sodium Chloride Structure Na^+Cl^-
- ▶ Cesium Chloride Structure Cs^+Cl^-
- ▶ Hexagonal Closed-Packed Structure
- ▶ Diamond Structure
- ▶ Zinc Blende

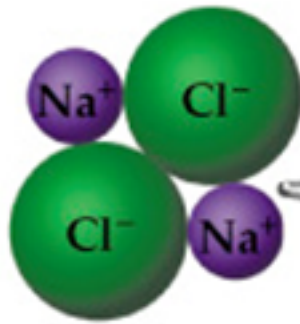
1 – Sodium Chloride Structure

- ▶ Sodium chloride also crystallizes in a cubic lattice, but with a different unit cell.
- ▶ Sodium chloride structure consists of equal numbers of sodium and chlorine ions placed at alternate points of a simple cubic lattice.
- ▶ Each ion has six of the other kind of ions as its nearest neighbours.

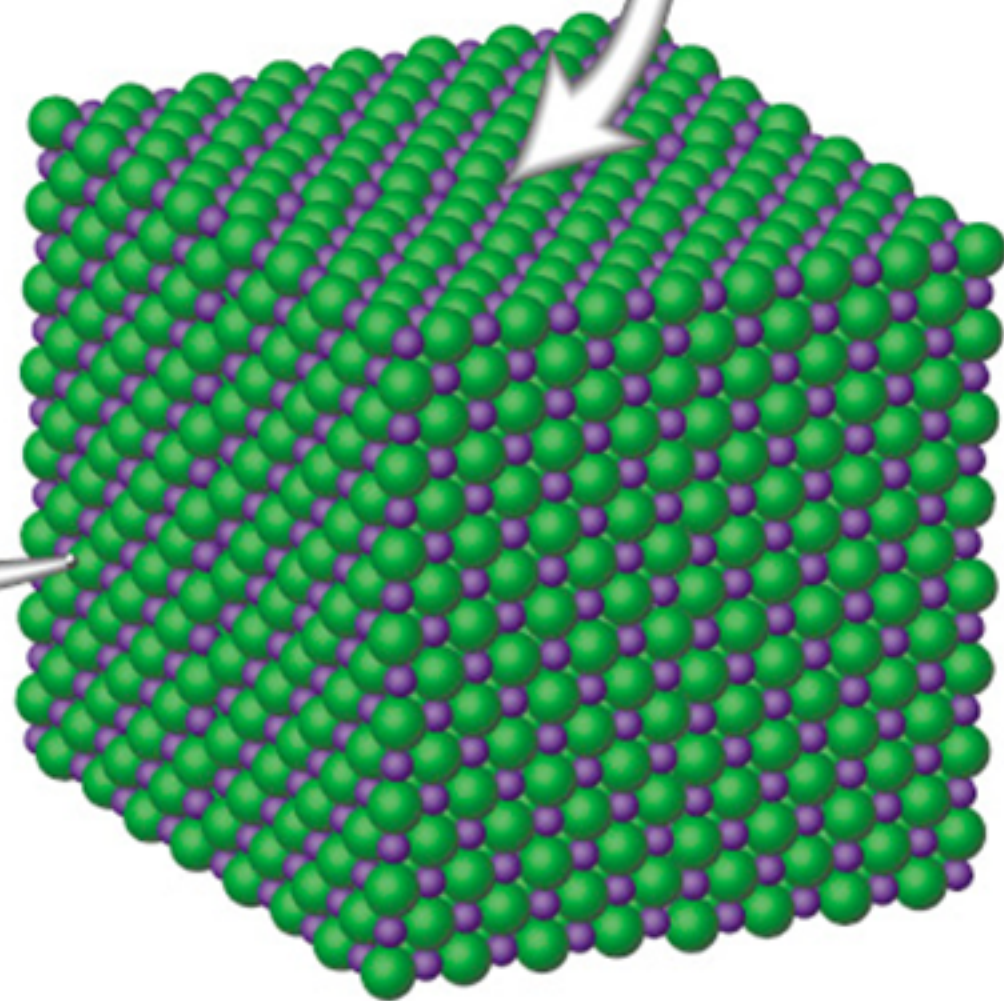
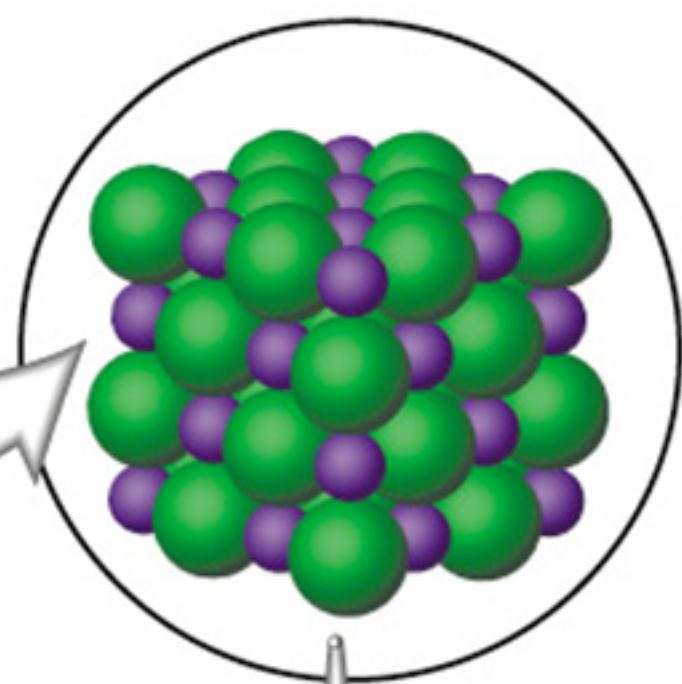




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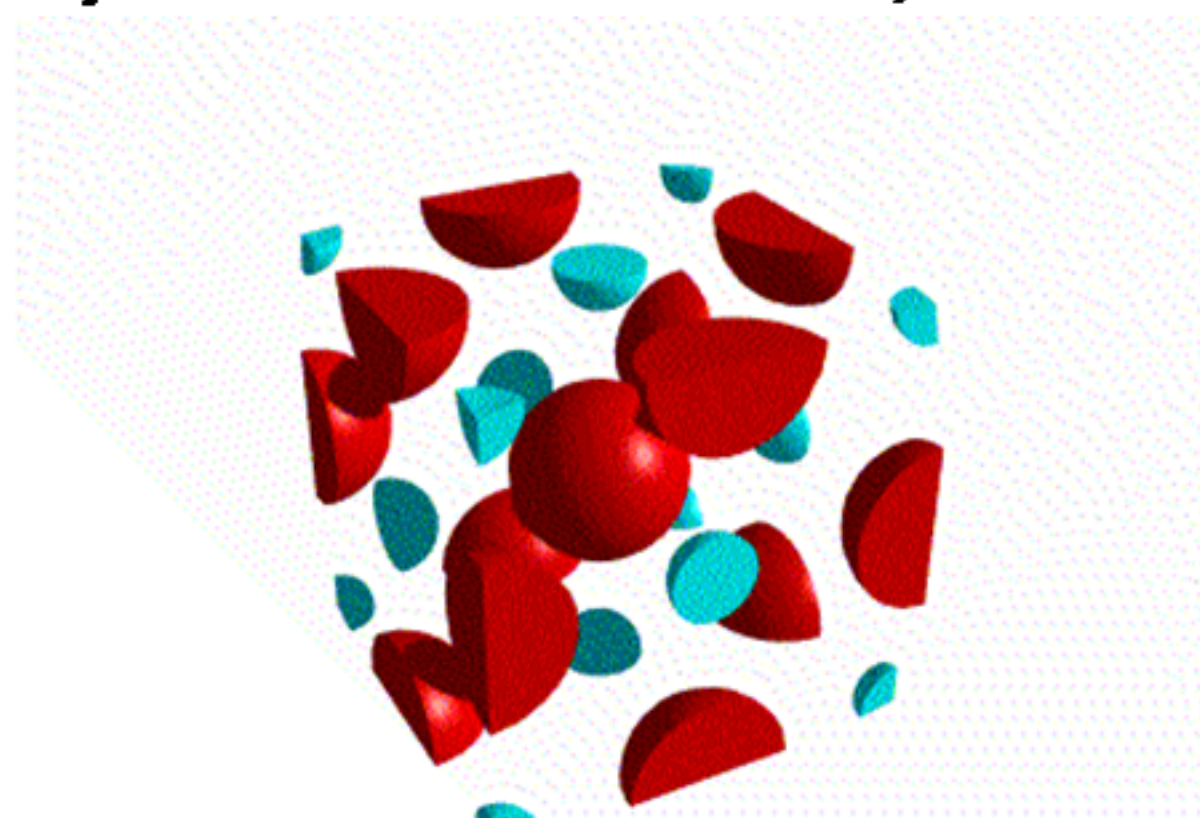
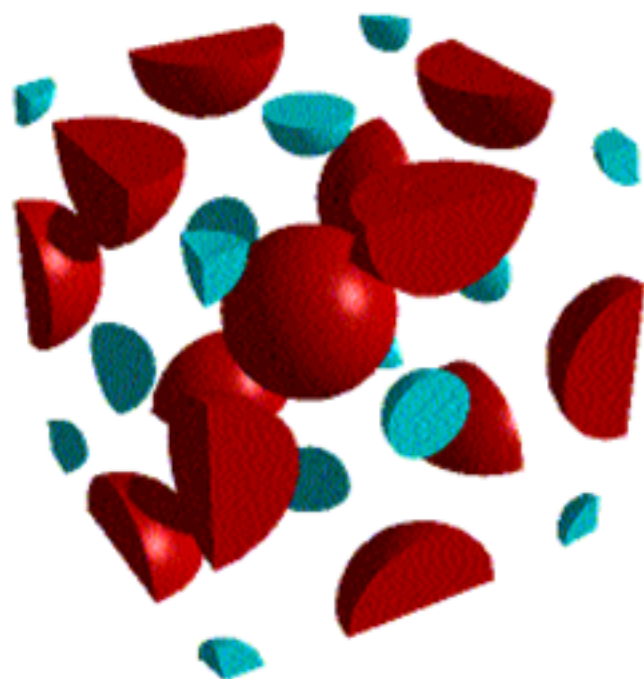


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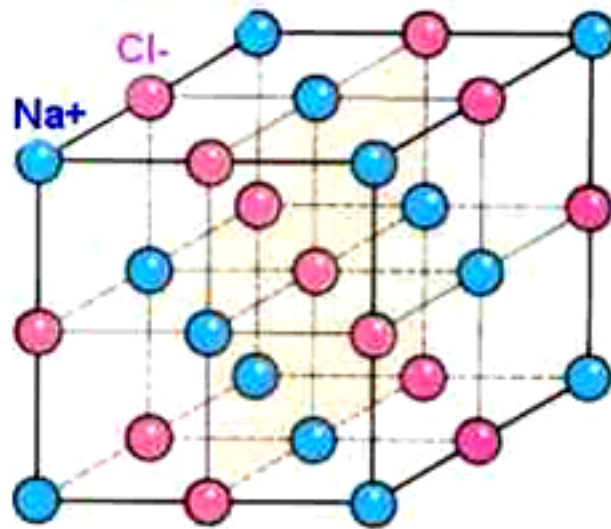


Sodium Chloride Structure

- ▶ **If we take the NaCl unit cell and remove all the red Cl ions, we are left with only the blue Na. If we compare this with the fcc / ccp unit cell, it is clear that they are identical. Thus, the Na is in a fcc sublattice.**



Sodium Chloride Structure



- ▶ This structure can be considered as a face-centered-cubic Bravais lattice with a basis consisting of a sodium ion at 0 and a chlorine ion at the center of the conventional cell,

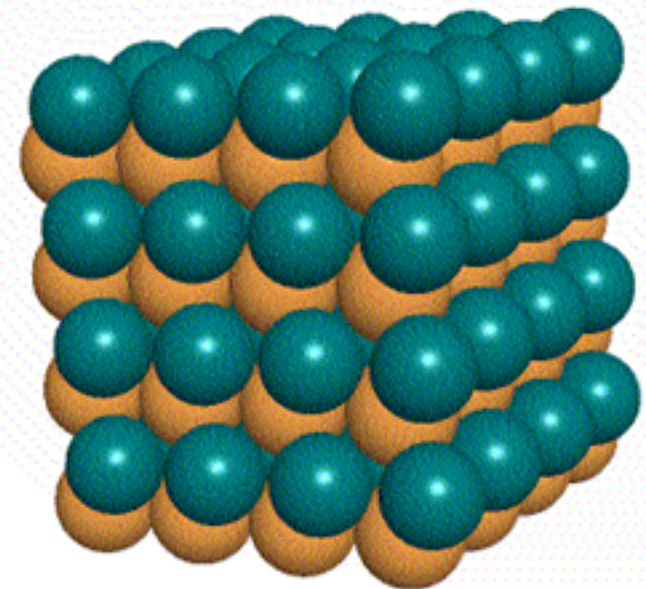
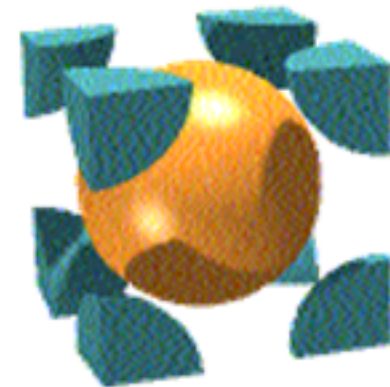
$$a / 2 (\vec{x} + \vec{y} + \vec{z})$$

- ▶ LiF, NaBr, KCl, LiI, etc
- ▶ The lattice constants are in the order of 4–7 angstroms.

2-Cesium Chloride Structure

Cs^+Cl^-

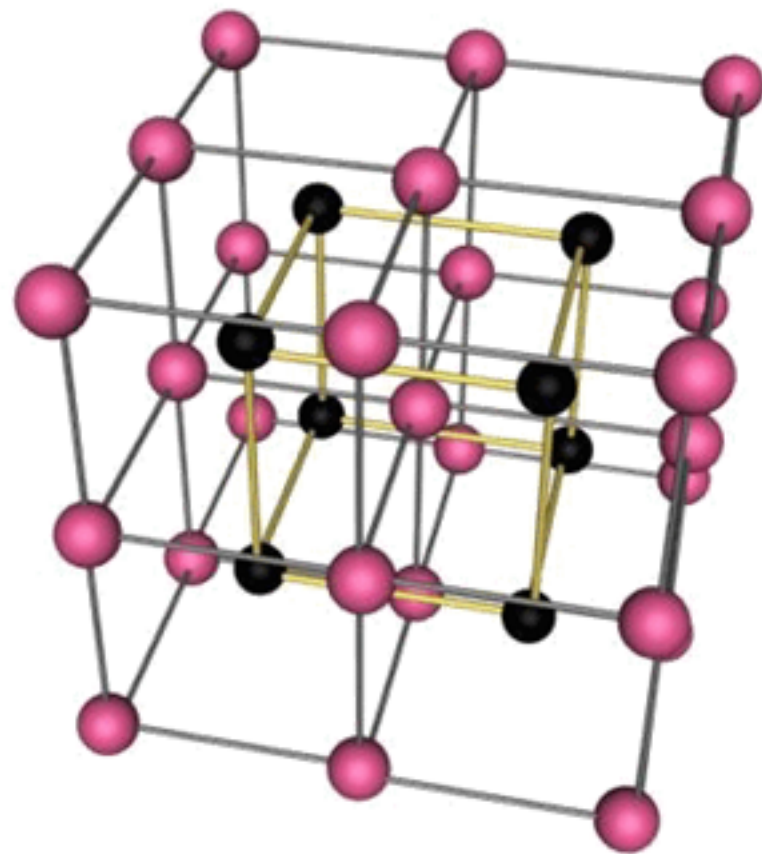
- ▶ Cesium chloride crystallizes in a cubic lattice. The unit cell may be depicted as shown. (Cs^+ is teal, Cl^- is gold).
- ▶ *Cesium chloride consists of equal numbers of cesium and chlorine ions, placed at the points of a body-centered cubic lattice so that each ion has eight of the other kind as its nearest neighbors.*



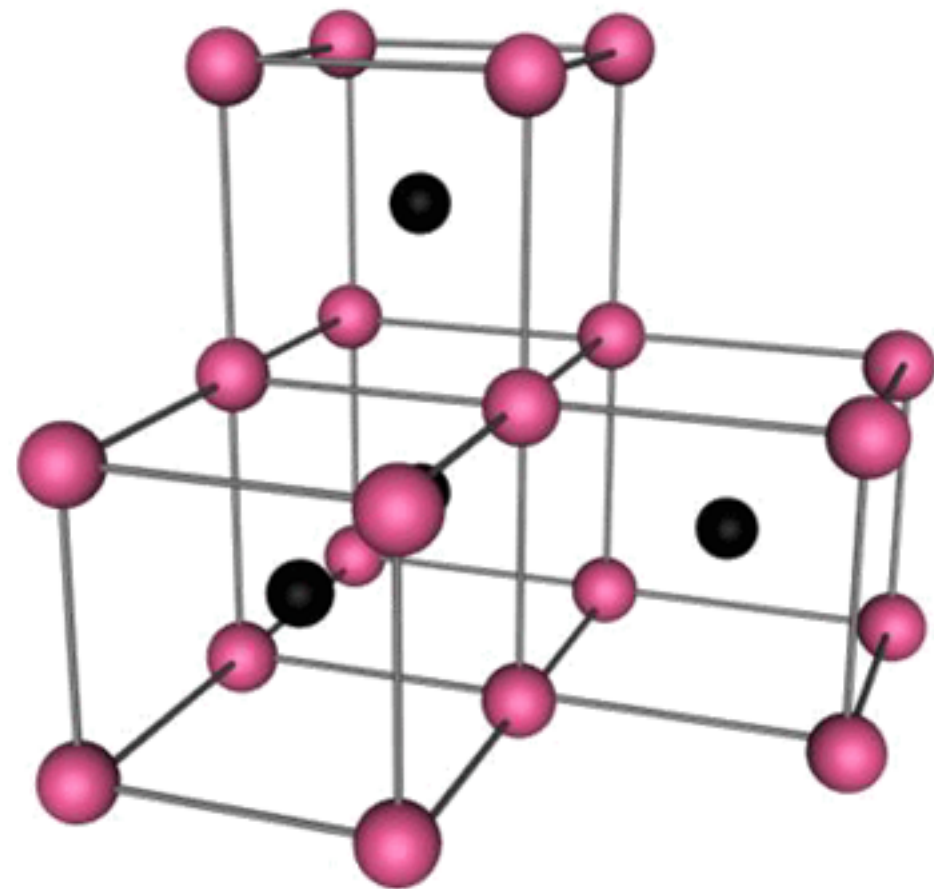
Cesium Chloride Structure Cs^+Cl^-

- ▶ The translational symmetry of this structure is that of the simple cubic Bravais lattice, and is described as a simple cubic lattice with a basis consisting of a cesium ion at the origin 0 and a chlorine ion at the cube center
- ▶ CsBr , CsI crystallize in this structure. The lattice constants are in the order of 4 angstroms.

Cesium Chloride Cs^+Cl^-

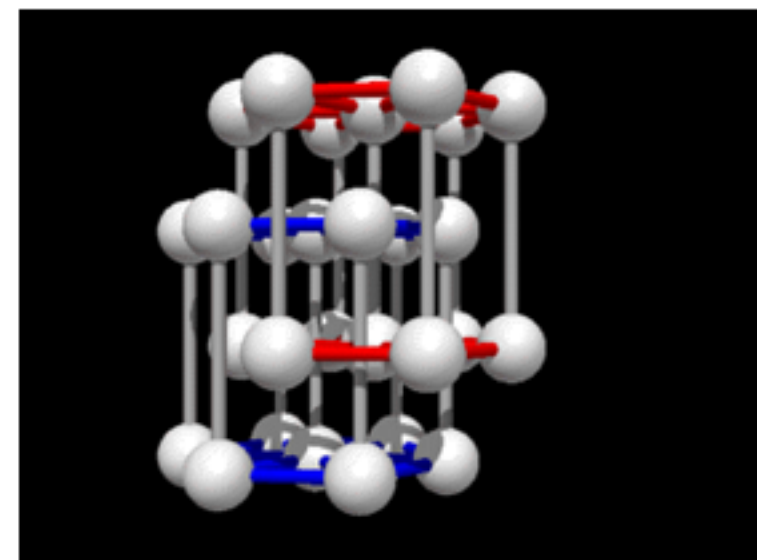
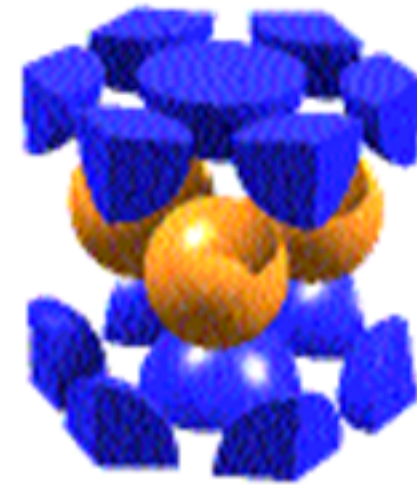


8 cell



3-Hexagonal Close-Packed Str.

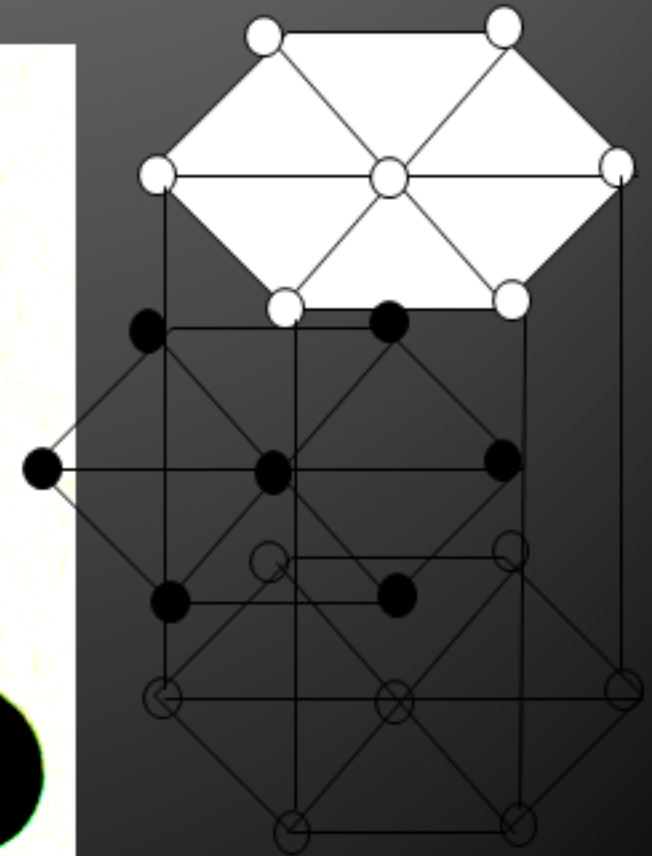
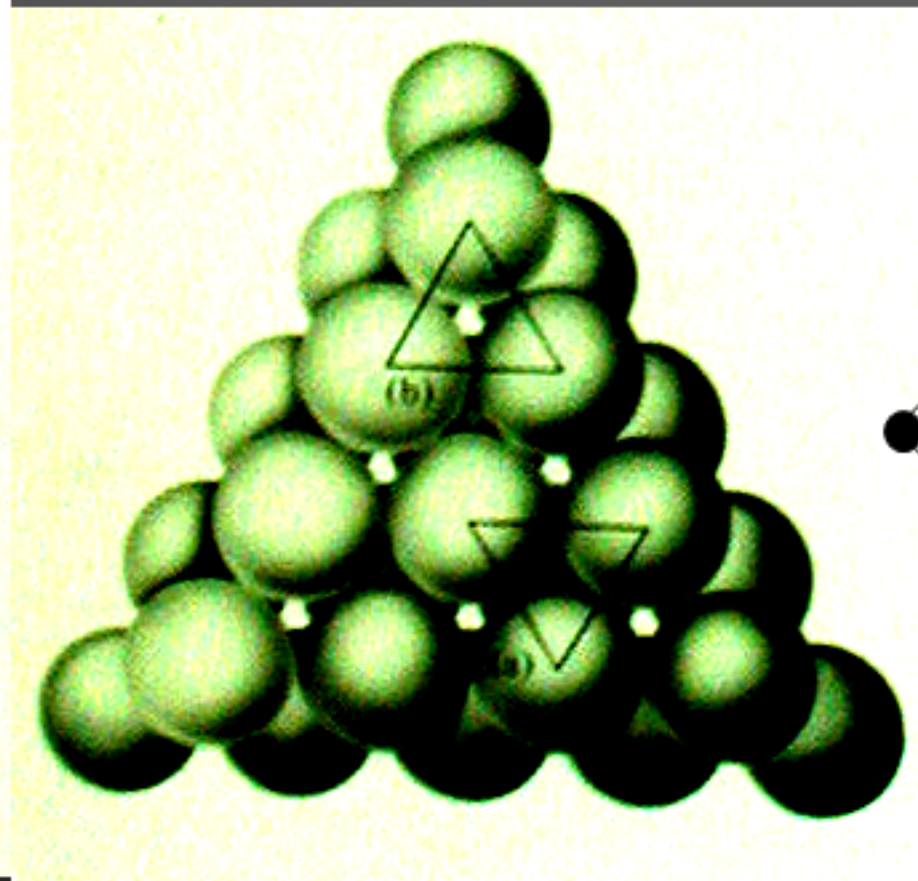
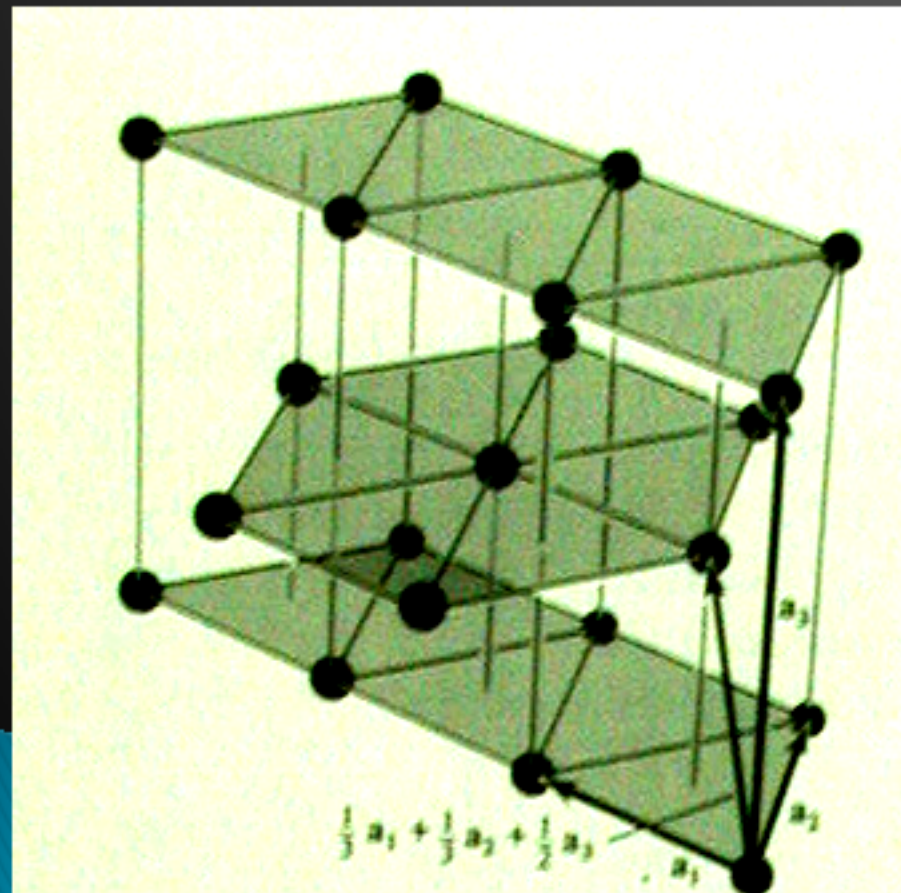
- ▶ This is another structure that is common, particularly in metals. In addition to the two layers of atoms which form the base and the upper face of the hexagon, there is also an intervening layer of atoms arranged such that each of these atoms rest over a depression between three atoms in the base.



Hexagonal Close-packed Structure

Bravais Lattice : Hexagonal Lattice
He, Be, Mg, Hf, Re (Group II elements)
ABABAB Type of Stacking

$a=b$, $\alpha=120^\circ$, $c=1.633a$,
basis : $(0,0,0)$ $(\frac{2}{3}a, \frac{1}{3}a, \frac{1}{2}c)$



POINT COORDINATES

- ▶ Any point within a unit cell specified as fractional multiples of the unit cell edge lengths
- ▶ Position P specified as $q r s$; convention: coordinates not separated by commas or punctuation marks

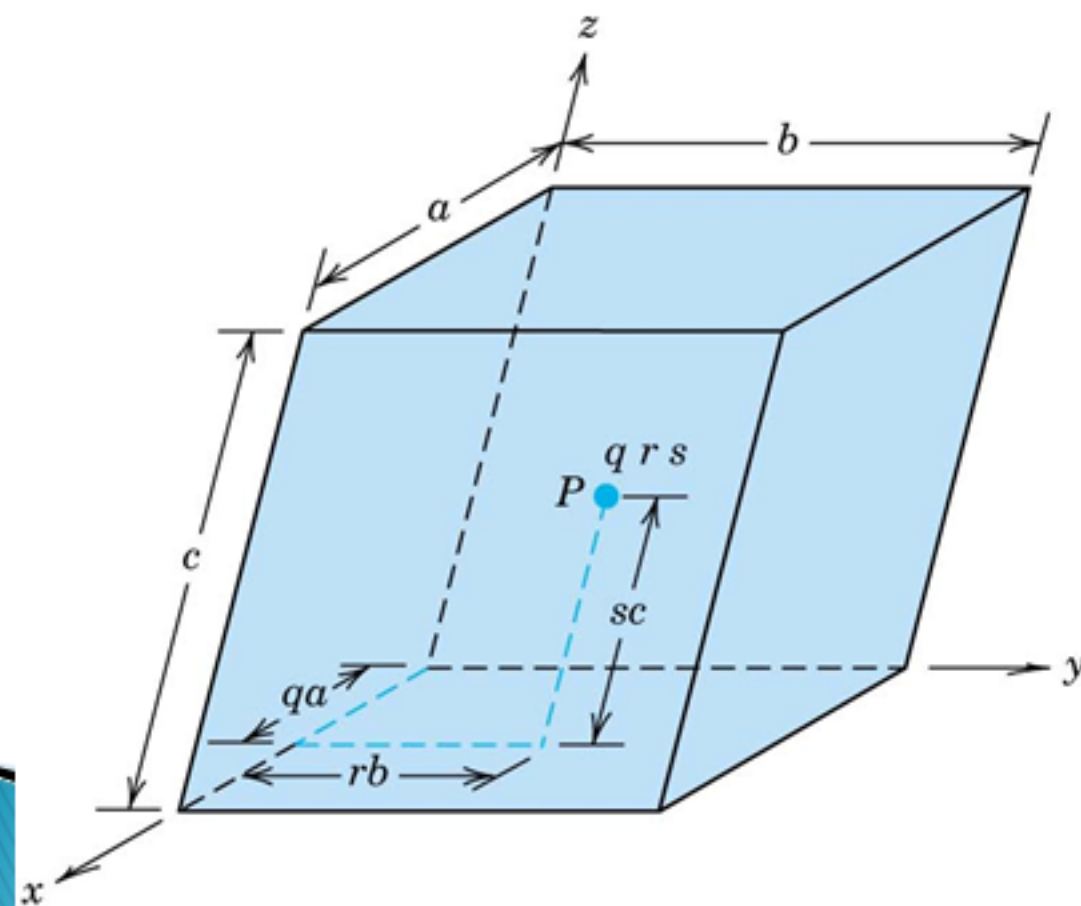
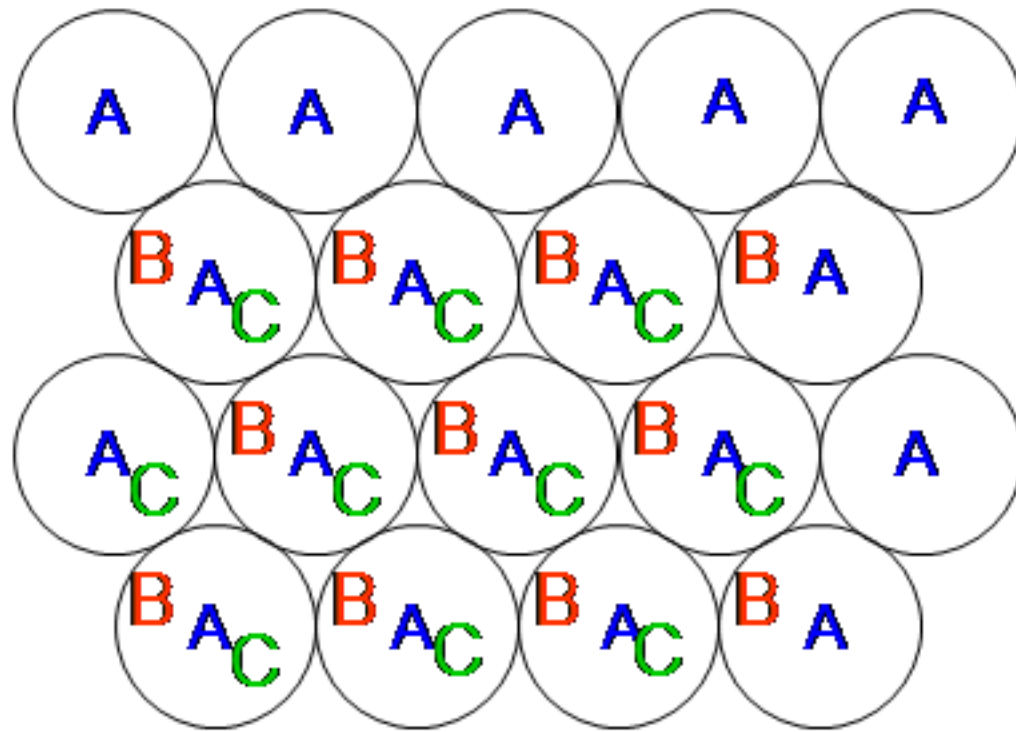


FIGURE 3.5 The manner in which the q , r , and s coordinates at point P within the unit cell are determined. The q coordinate (which is a fraction) corresponds to the distance qa along the x axis, where a is the unit cell edge length. The respective r and s coordinates for the y and z axes are determined similarly.

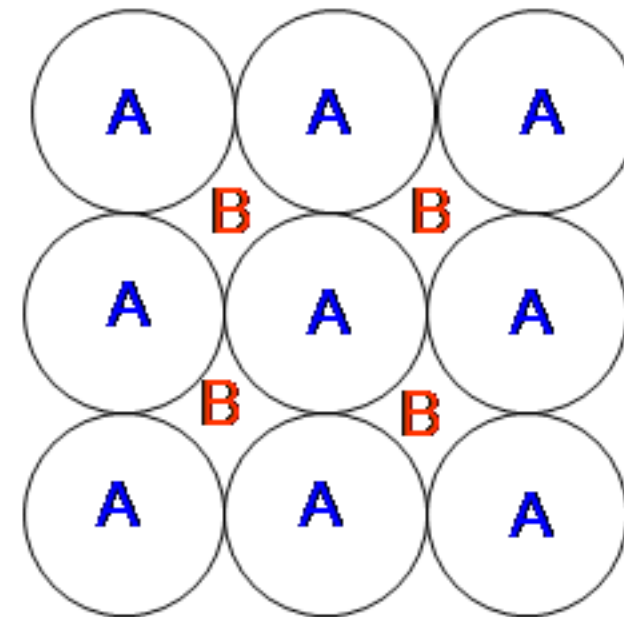
Packing

Close pack



Sequence ABABAB..
- hexagonal close pack

Sequence ABCABCAB..
- face centered cubic close pack



Sequence AAAA...
- simple cubic

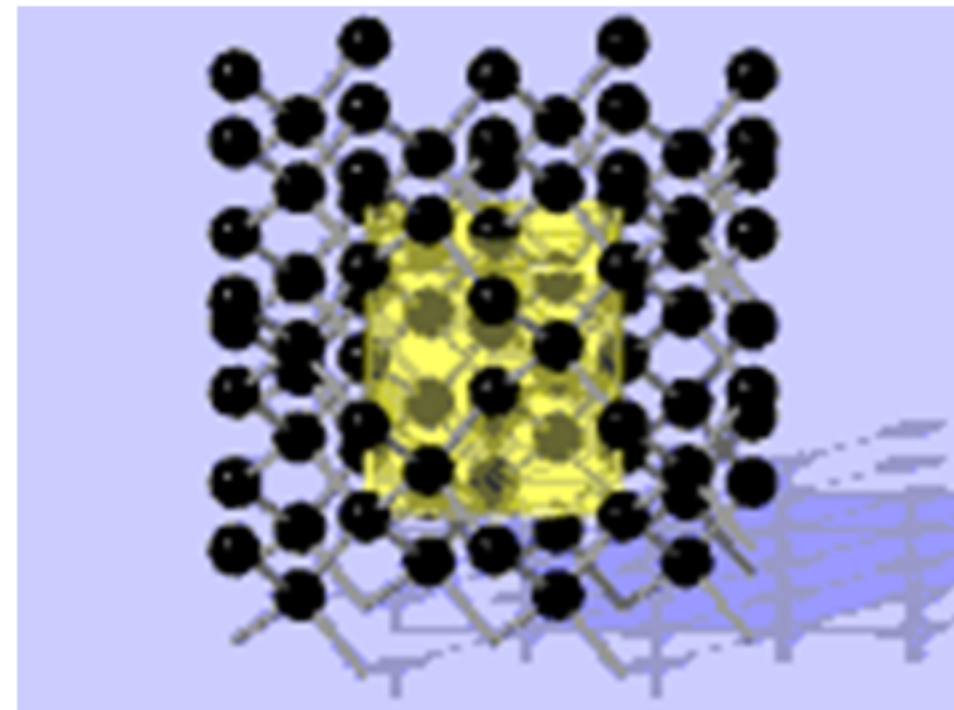
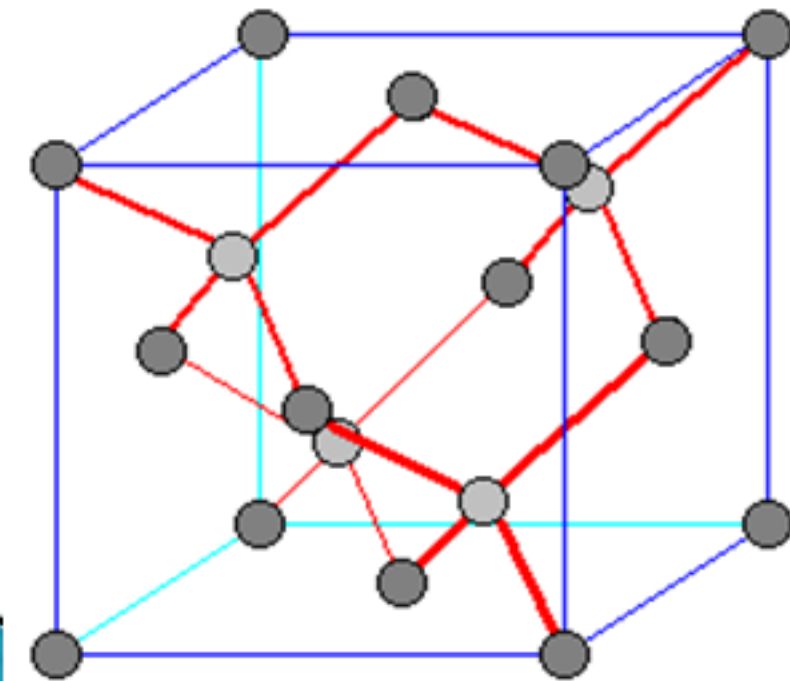
Sequence ABAB...
- body centered cubic



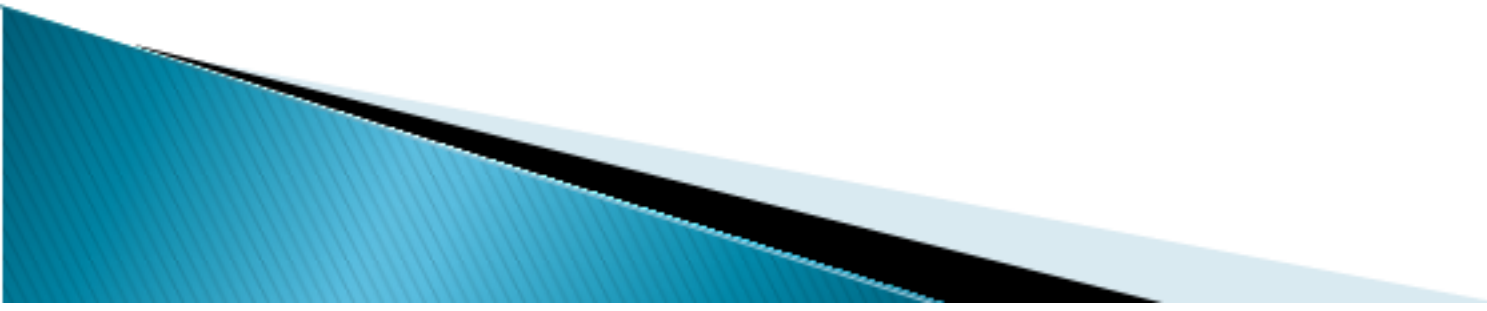
To pack spheres as close as possible
we start with a single row.

4 - Diamond Structure

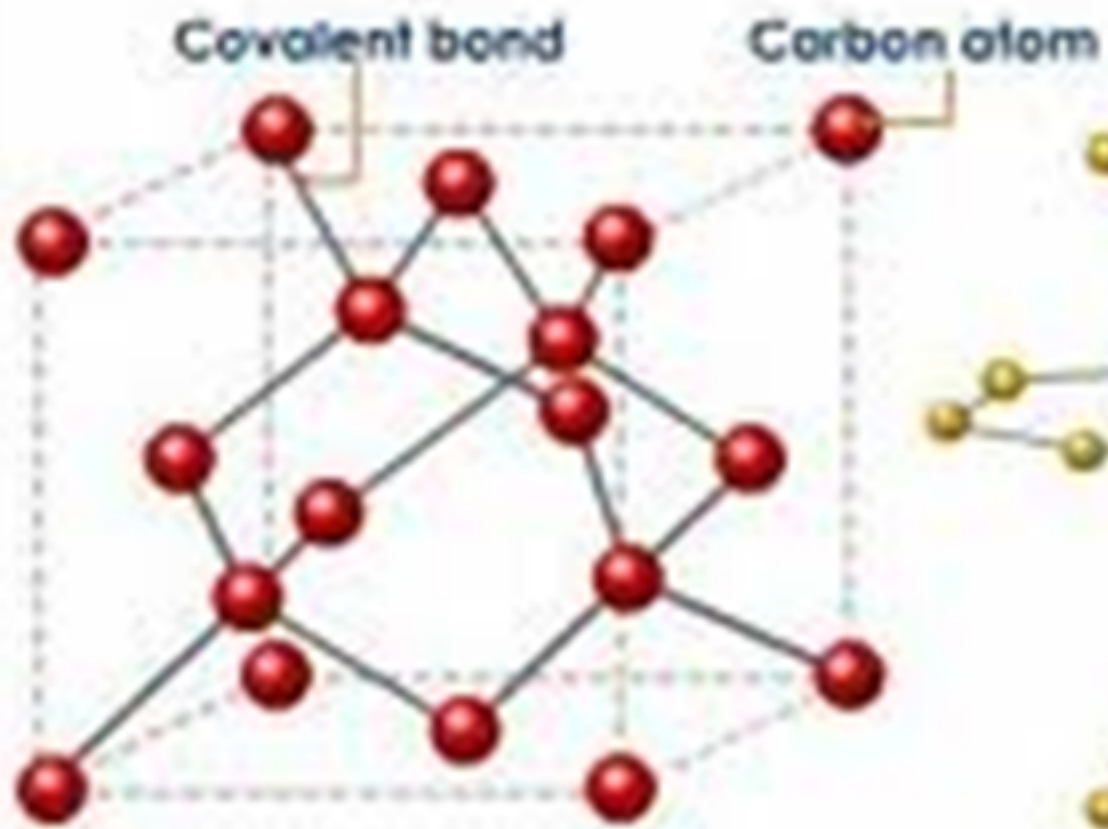
- ▶ **The diamond lattice is consist of two interpenetrating face centered bravais lattices.**
- ▶ **There are eight atom in the structure of diamond.**
- ▶ **Each atom bonds covalently to 4 others equally spread about atom in 3d.**



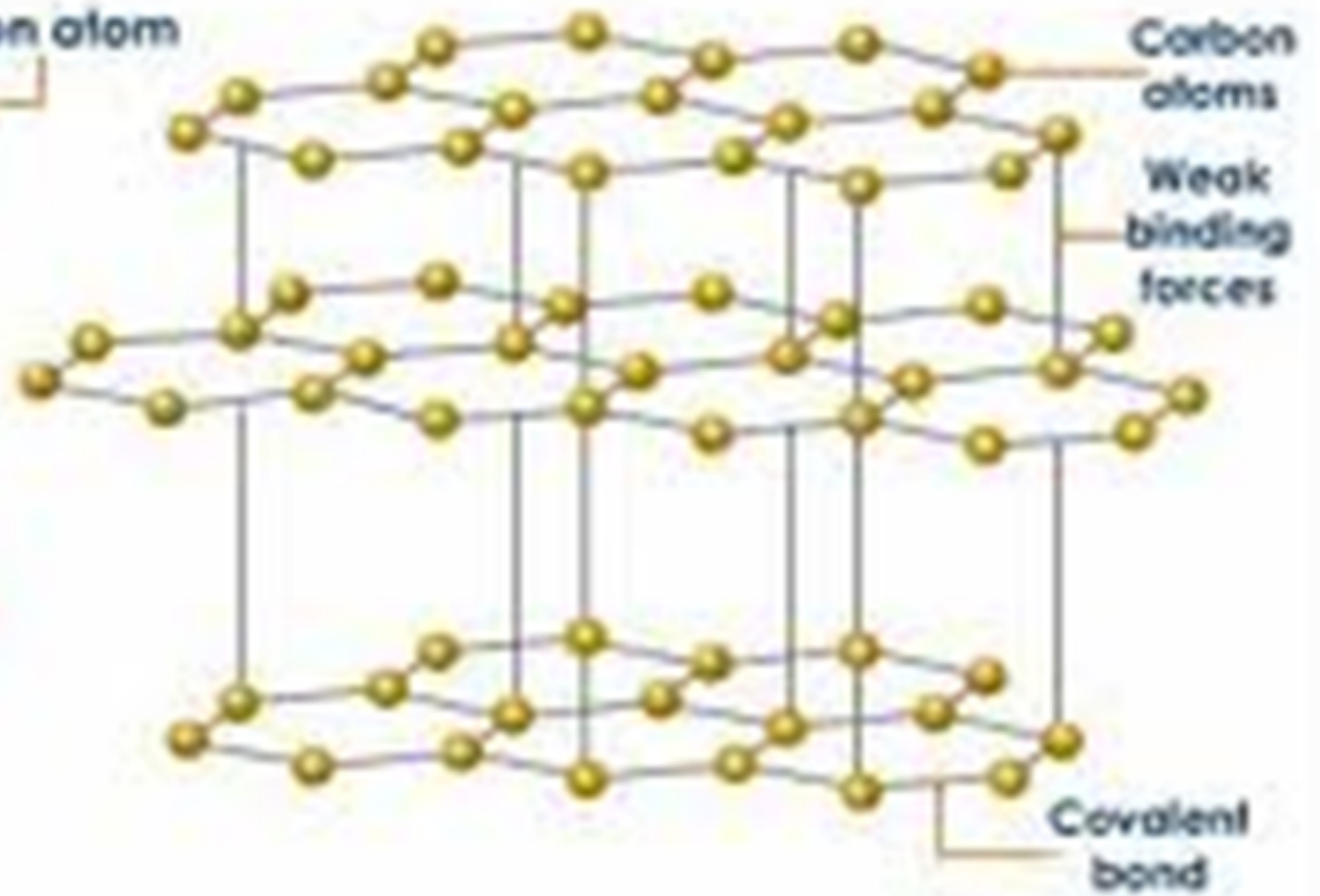
4 - Diamond Structure

- ▶ The coordination number of diamond structure is 4.
 - ▶ The diamond lattice is not a Bravais lattice.
 - ▶ Si, Ge and C crystallizes in diamond structure.
- 





Structure of Diamond

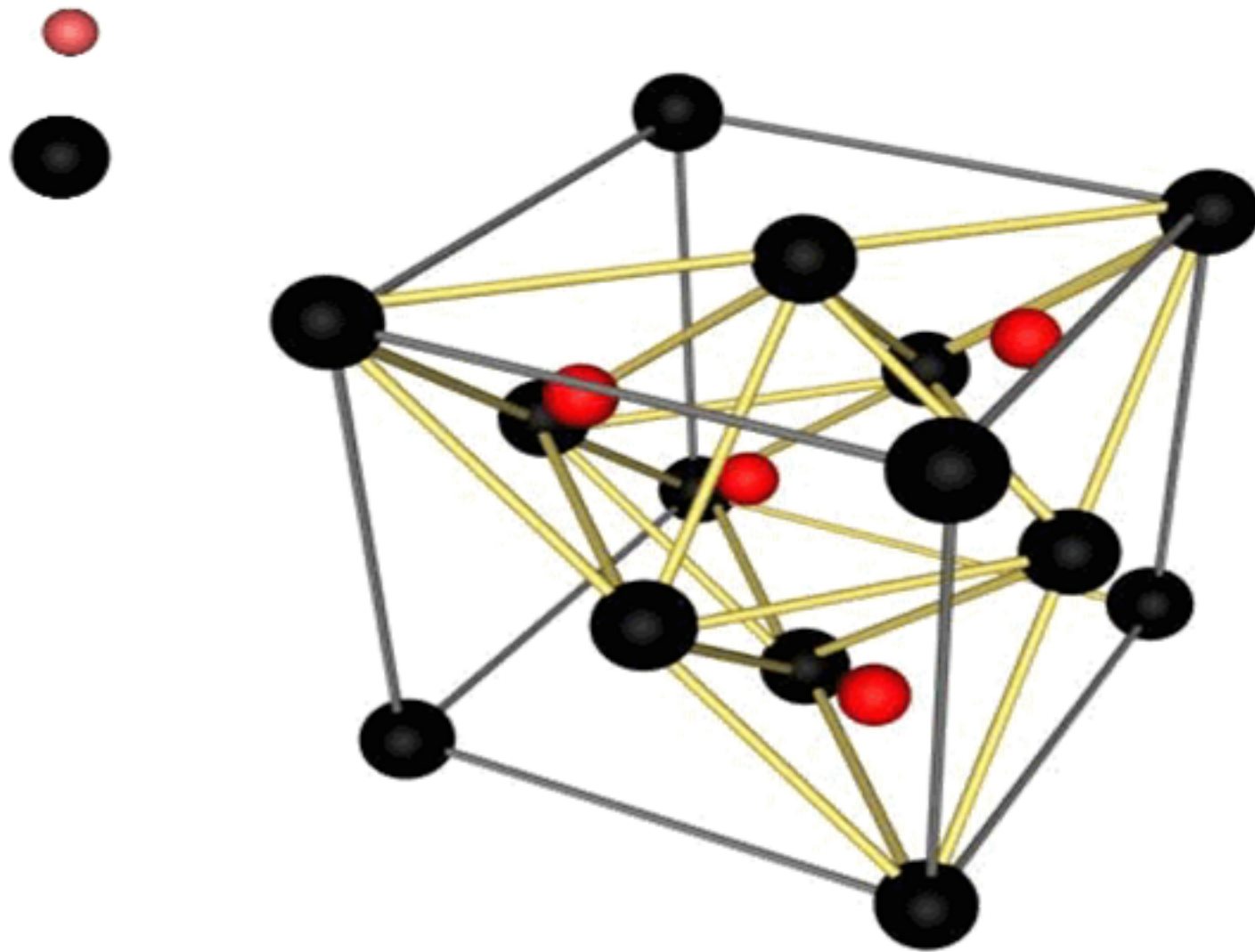


Structure of Graphite

5- Zinc Blende

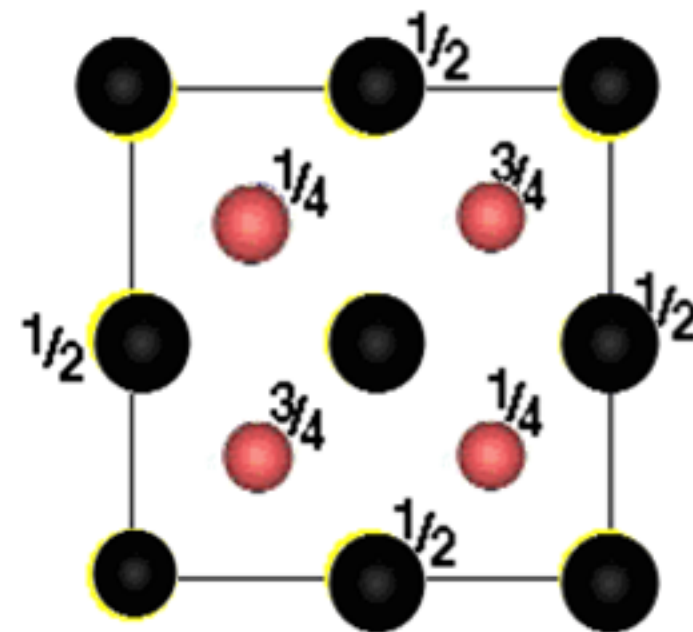
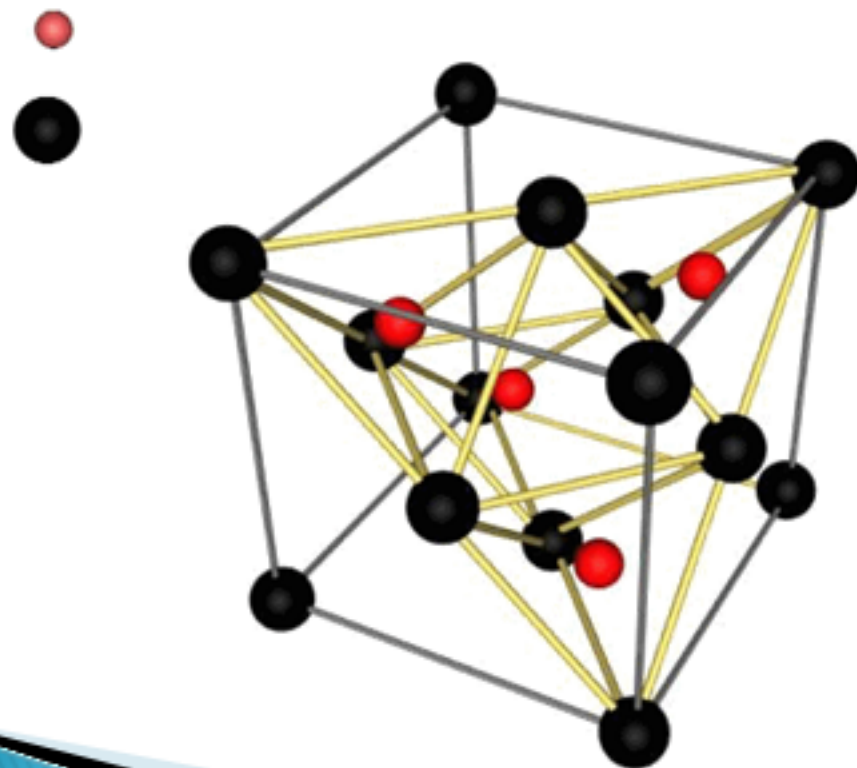
- ▶ Zincblende has equal numbers of zinc and sulfur ions distributed on a diamond lattice so that each has four of the opposite kind as nearest neighbors. This structure is an example of a lattice with a basis, which must so described both because of the geometrical position of the ions and because two types of ions occur.
- ▶ AgI, GaAs, GaSb, InAs,

5- Zinc Blende



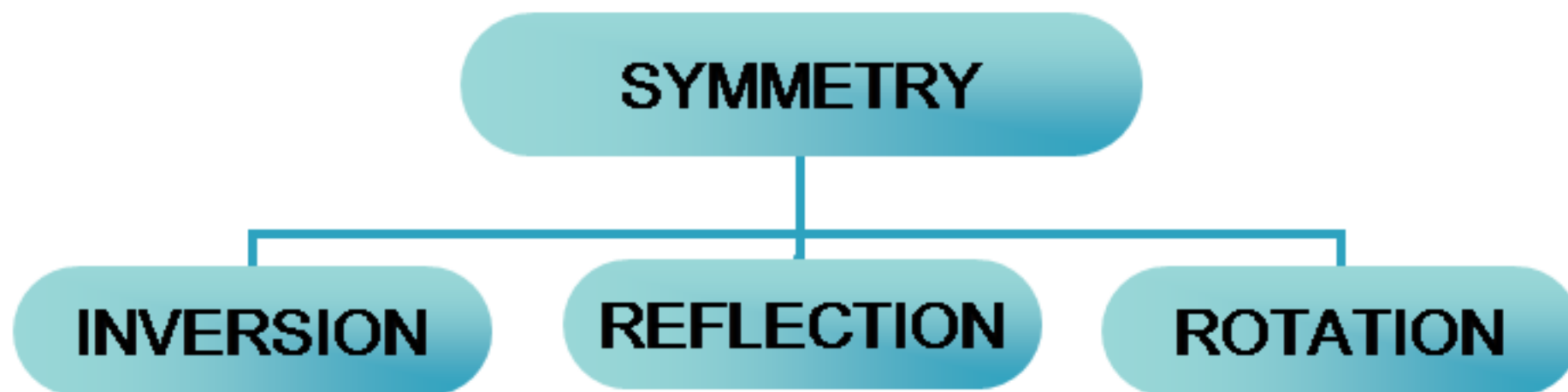
5- Zinc Blende

Zinc Blende is the name given to the mineral ZnS. It has a cubic close packed (face centred) array of S and the Zn(II) sit in tetrahedral ($1/2$ occupied) sites in the lattice.



ELEMENTS OF SYMMETRY

- ▶ Each of the unit cells of the 14 Bravais lattices has one or more types of symmetry properties, such as inversion, reflection or rotation, etc.



Crystal Directions

- ▶ We choose one lattice point on the line as an origin, say the point O . Choice of origin is completely arbitrary, since every lattice point is identical.
- ▶ Then we choose the lattice vector joining O to any point on the line, say point T . This vector can be written as;

$$\mathbf{R} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}$$

- ▶ To distinguish a lattice direction from a lattice point, the triple is enclosed in square brackets $[...]$ is used. $[n_1 n_2 n_3]$
- ▶ $[n_1 n_2 n_3]$ is the smallest integer of the same relative ratios.

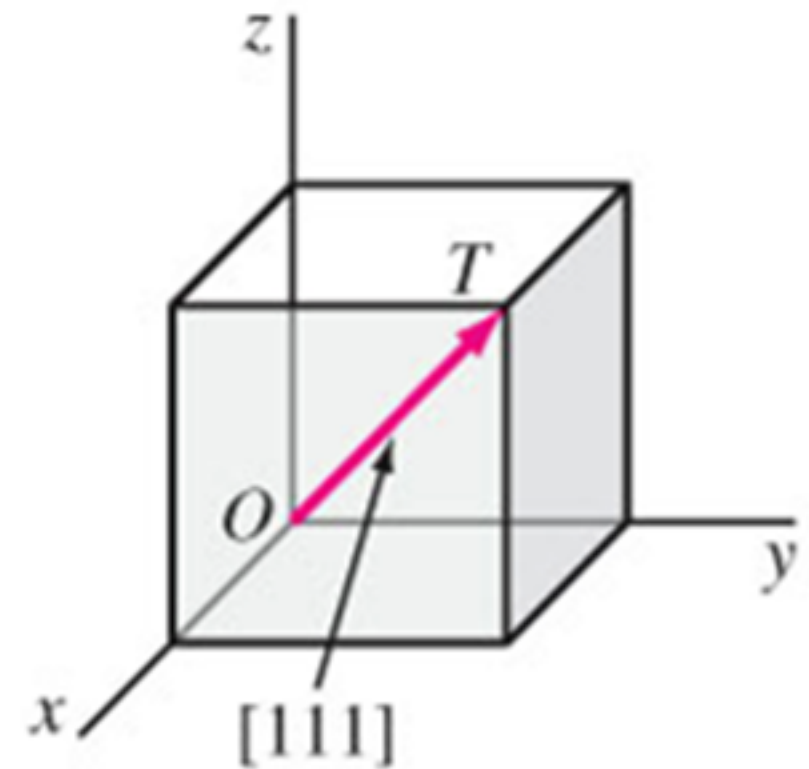


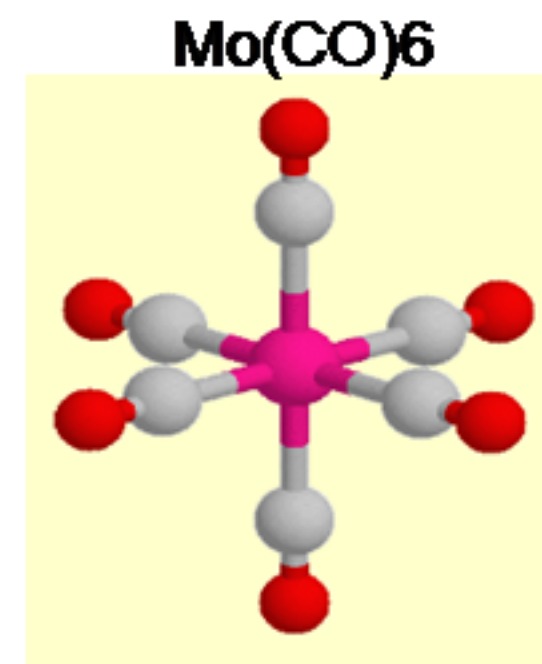
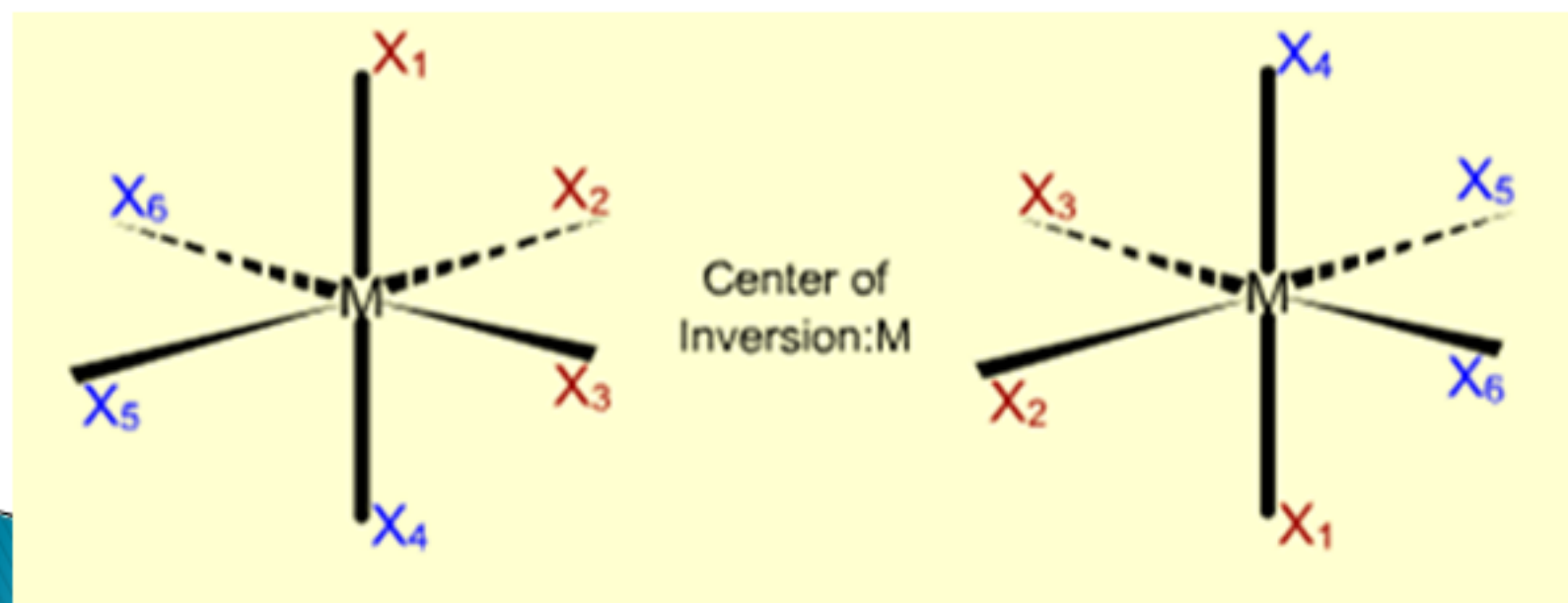
Fig. Shows
[111] direction

Lattice goes into itself through Symmetry without translation

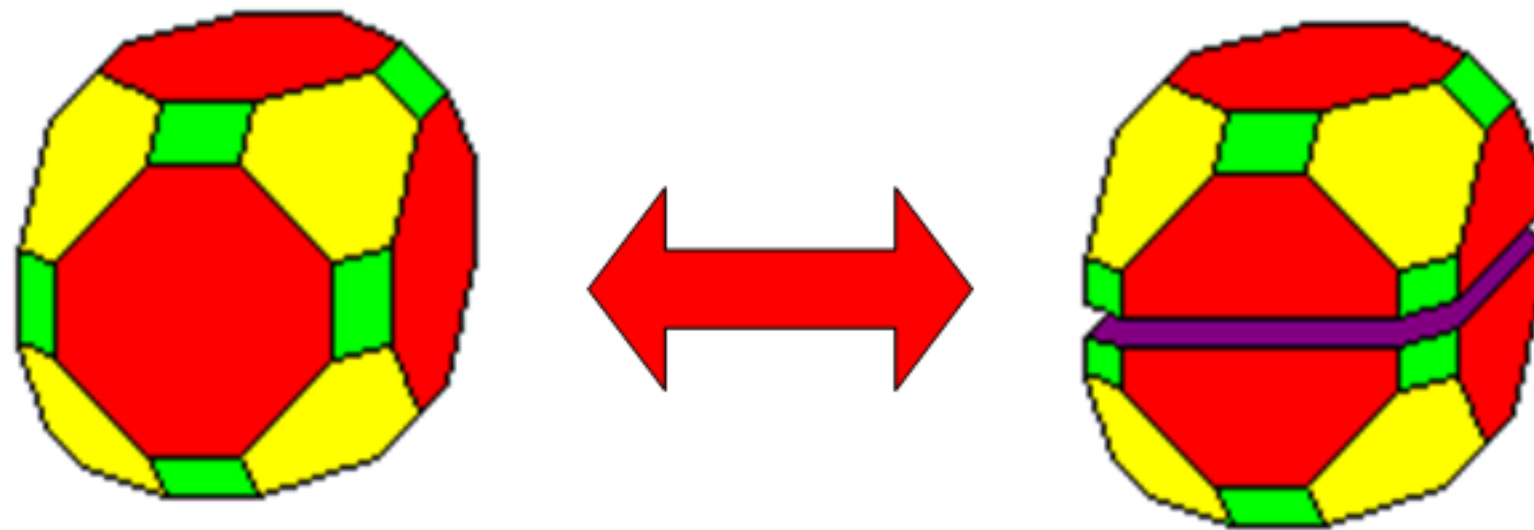
Operation	Element
Inversion	Point
Reflection	Plane
Rotation	Axis
Rotoinversion	Axes

Inversion Center

- ▶ A center of symmetry: A point at the center of the molecule.
 $(x,y,z) \rightarrow (-x,-y,-z)$
- ▶ Center of inversion can only be in a molecule. It is not necessary to have an atom in the center (benzene, ethane). Tetrahedral, triangles, pentagons don't have a center of inversion symmetry. All Bravais lattices are inversion symmetric.

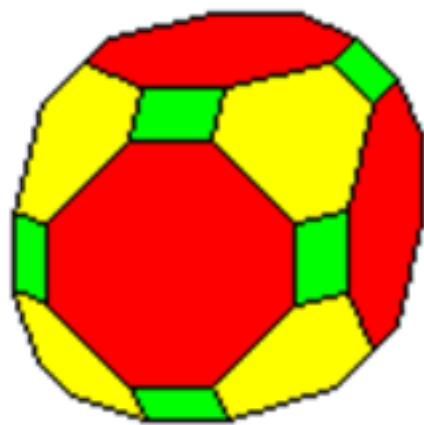


Reflection Plane

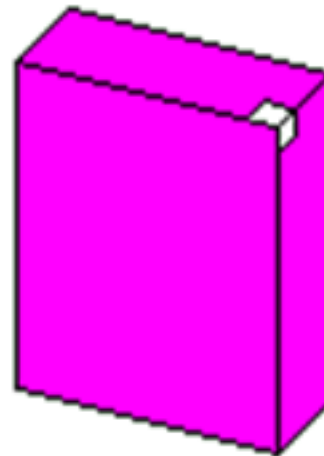


- ▶ A plane in a cell such that, when a mirror reflection in this plane is performed, the cell remains invariant.

Examples



Monoclinic



Triclinic



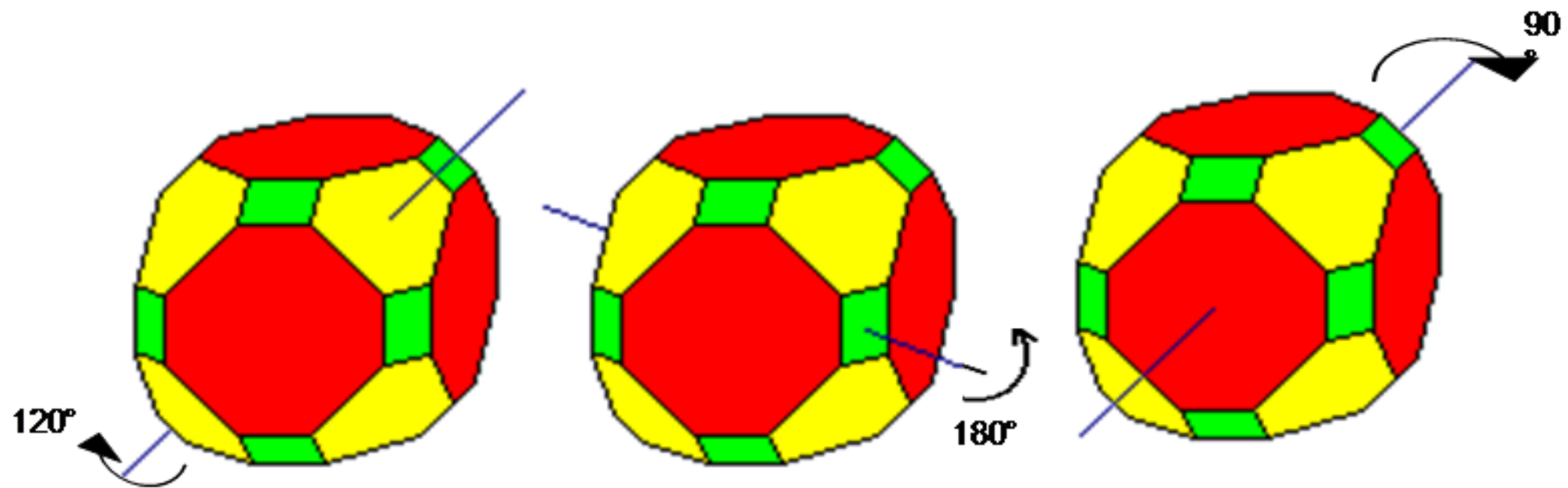
- ▶ Triclinic has no reflection plane.
- ▶ Monoclinic has one plane midway between and parallel to the bases, and so forth.

Rotation Symmetry

We can not find a lattice that goes into itself under other rotations

- A single molecule can have any degree of rotational symmetry, but an infinite periodic lattice – can not.

Rotation Axis






- This is an axis such that, if the cell is rotated around it through some angles, the cell remains invariant.
- The axis is called n-fold if the angle of rotation is $2\pi/n$.

Axis of Rotation



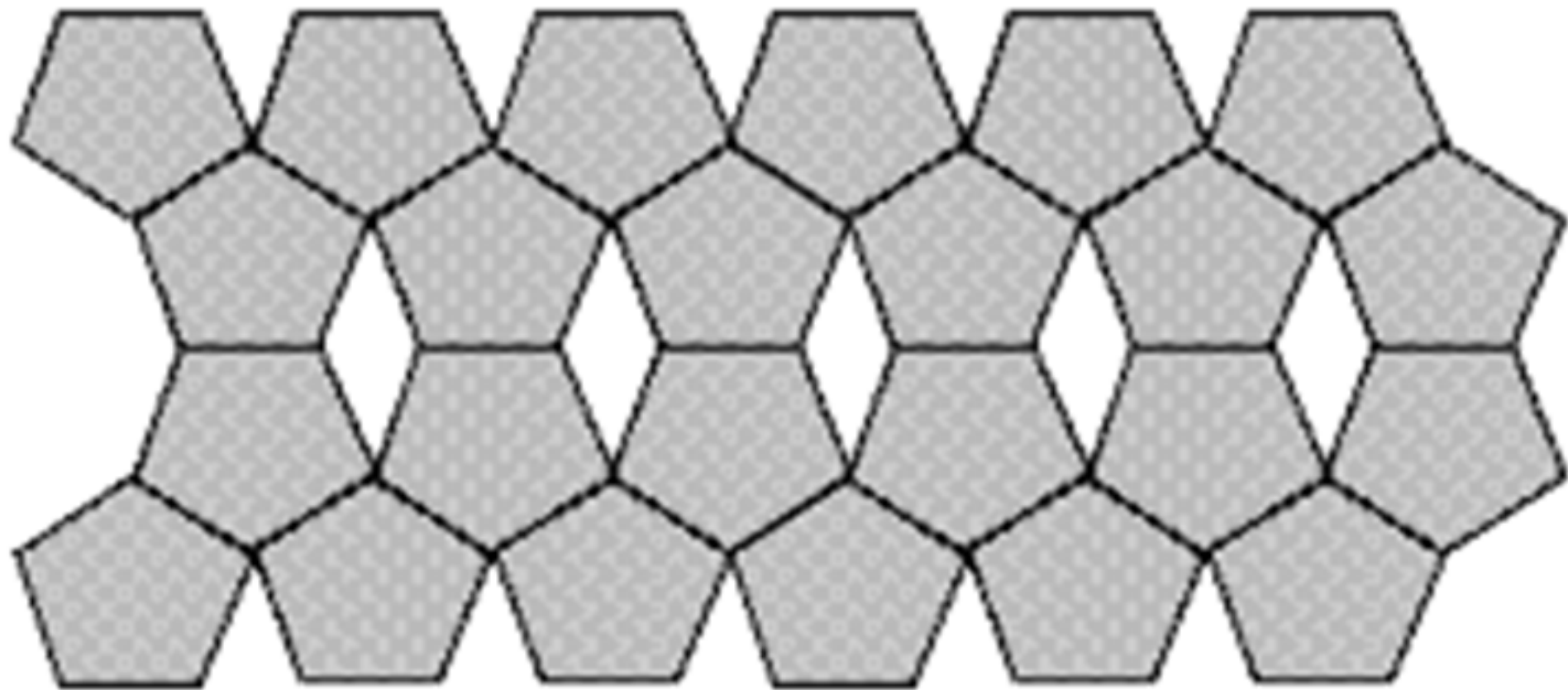
Fold (n)	1	2	3	4	6
Angles	360	180	120	90	60

Axis of Rotation

6 1-fold	6 2-fold	6 3-fold	6 4-fold	6 6-fold
Objects with symmetry: a identity	Z			



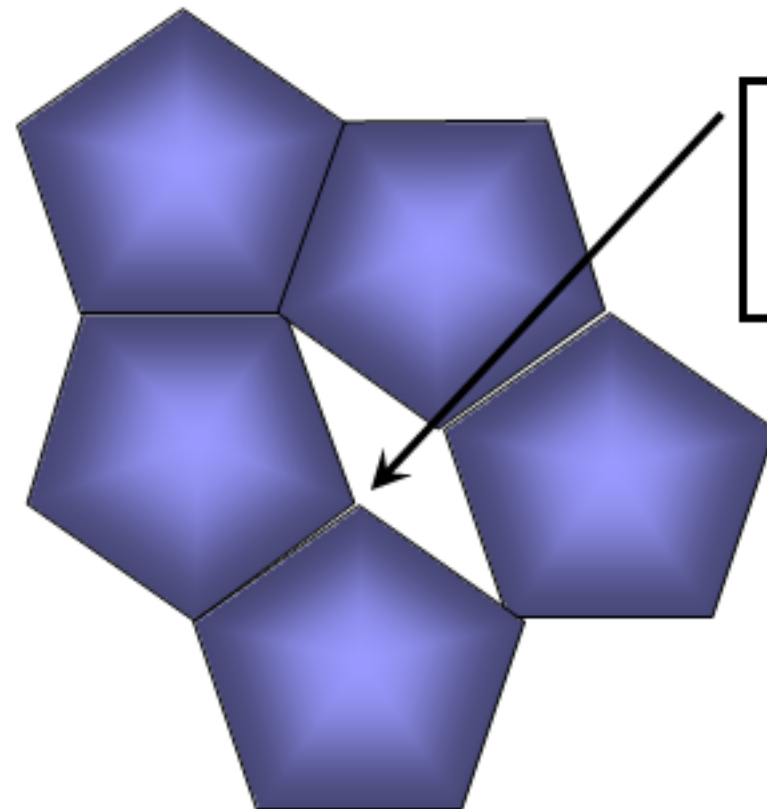
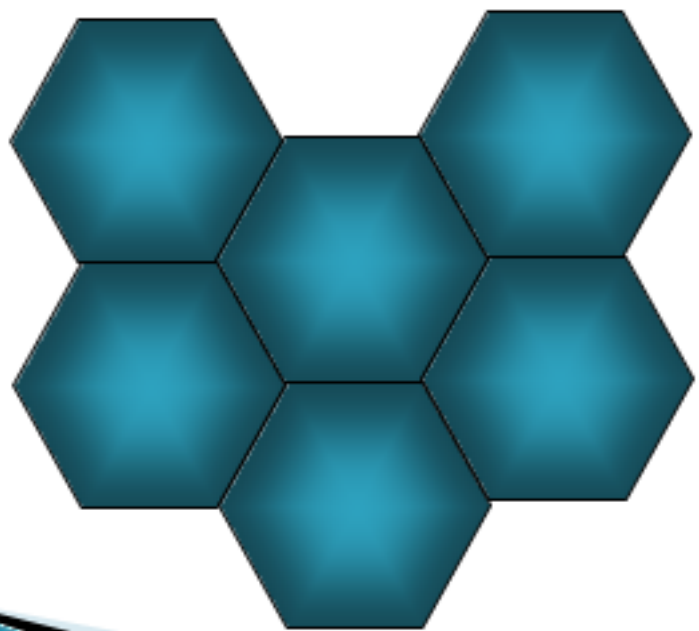
5-fold symmetry



Can not be combined with translational periodicity!

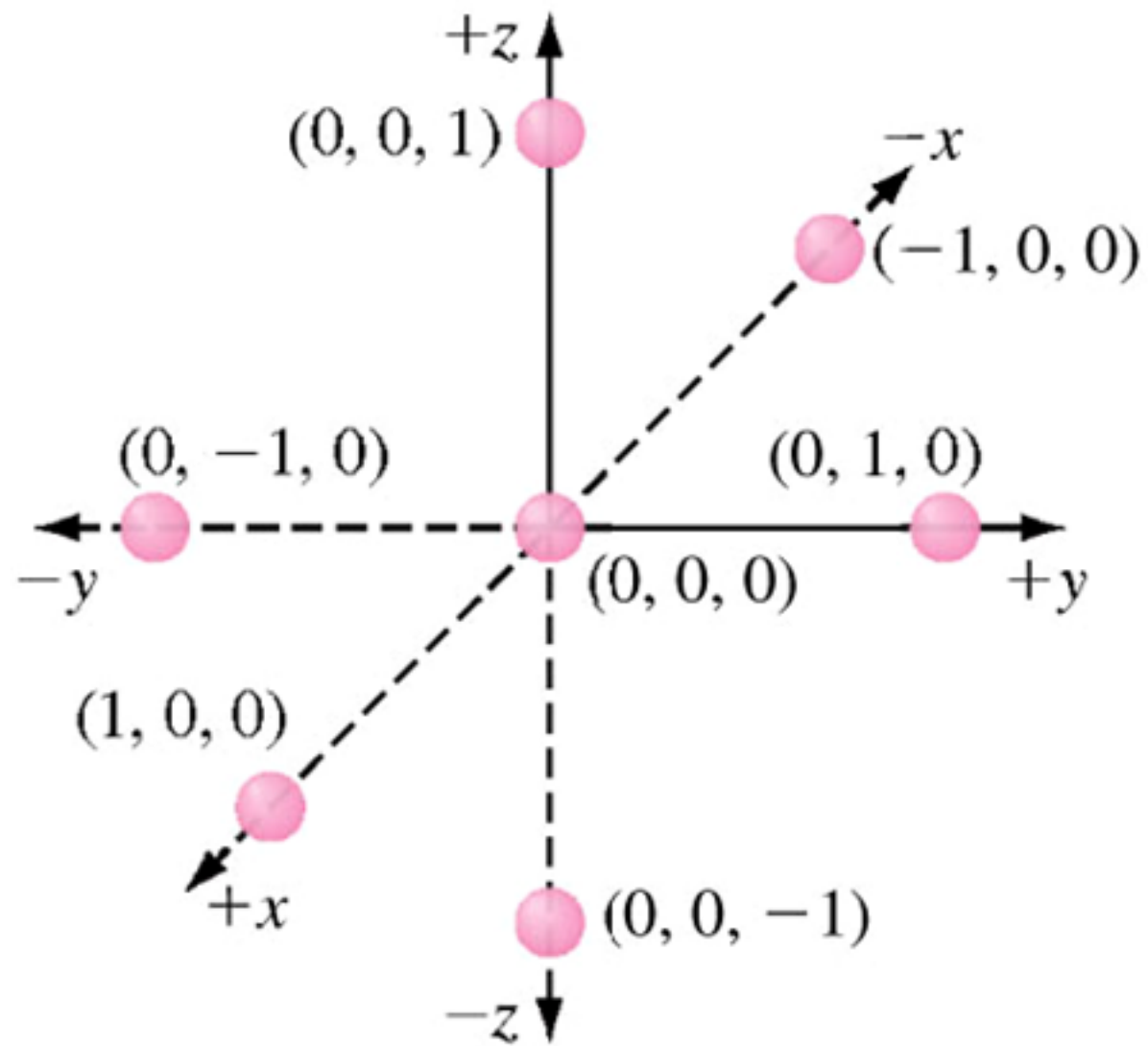
Group discussion

- ▶ Kepler wondered why snowflakes have 6 corners, never 5 or 7. By considering the packing of polygons in 2 dimensions, demonstrate why pentagons and heptagons shouldn't occur.

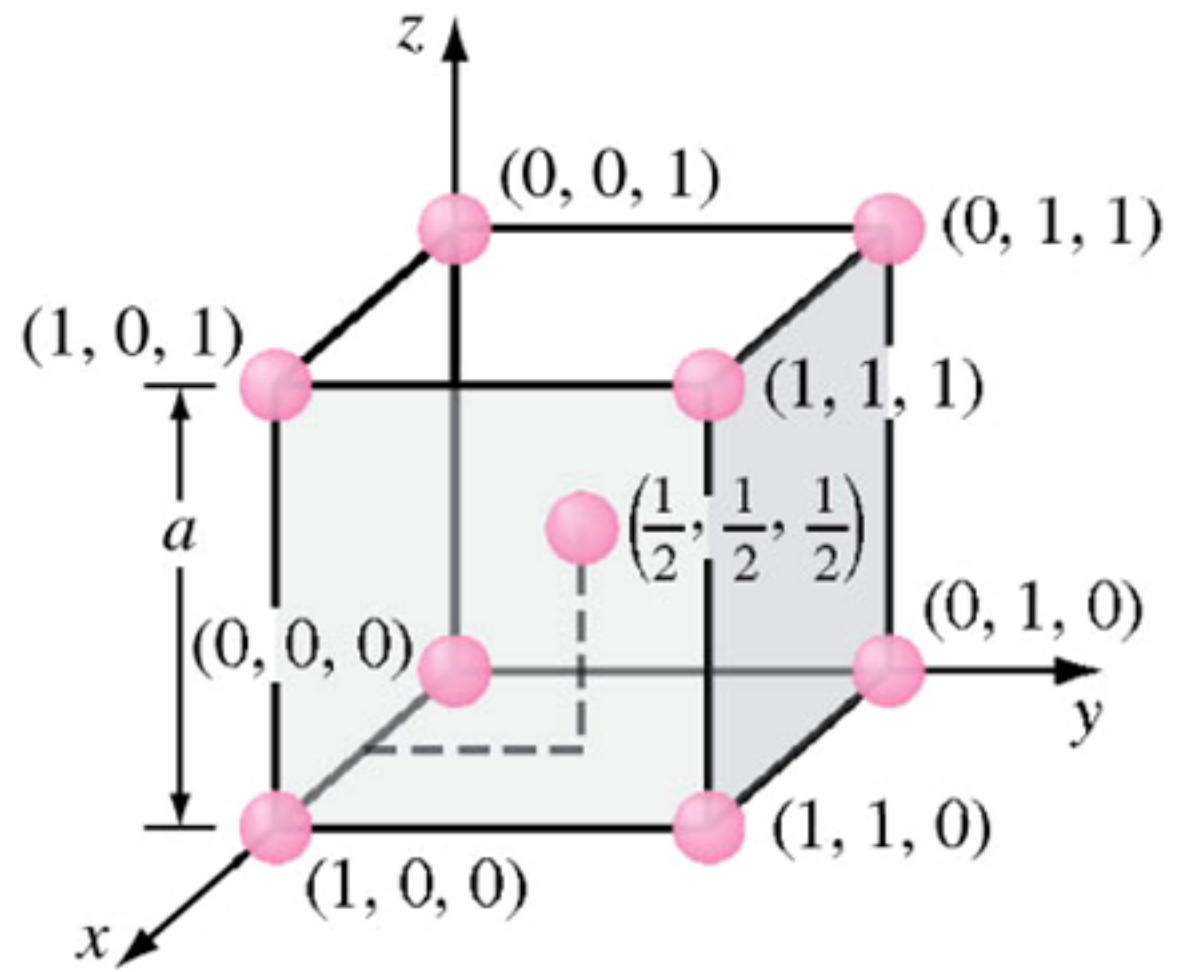


Empty space
not allowed

Lattice Sites in Cubic Unit Cell



(a)

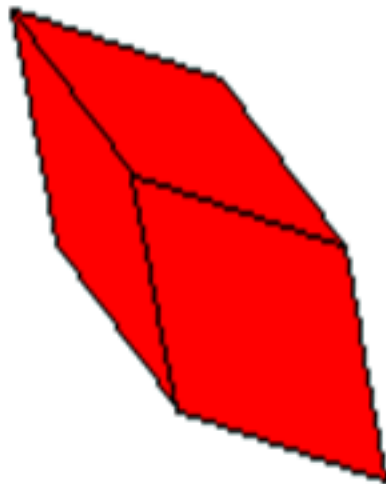


(b)

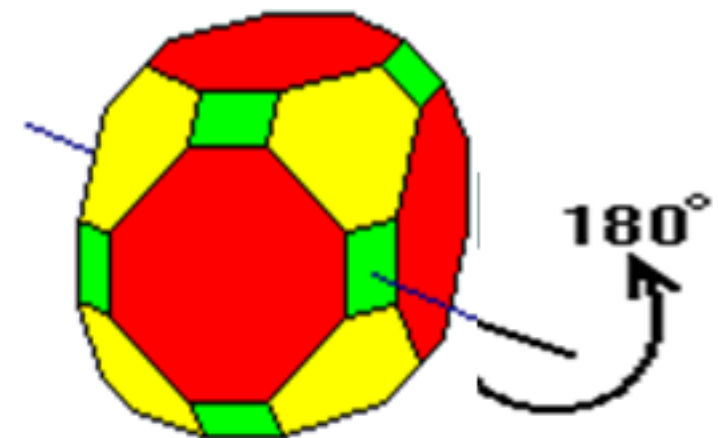
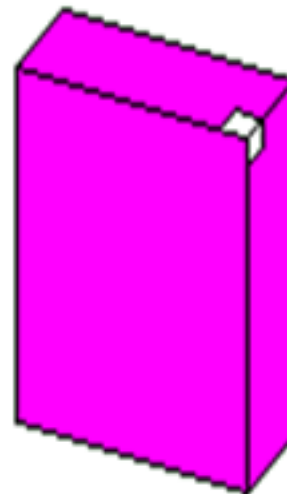
Examples

- ▶ Triclinic has no axis of rotation.
- ▶ Monoclinic has 2-fold axis ($\theta = 2\pi/2 = \pi$) normal to the base.

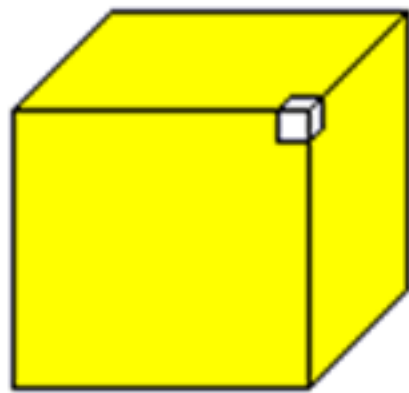
Triclinic



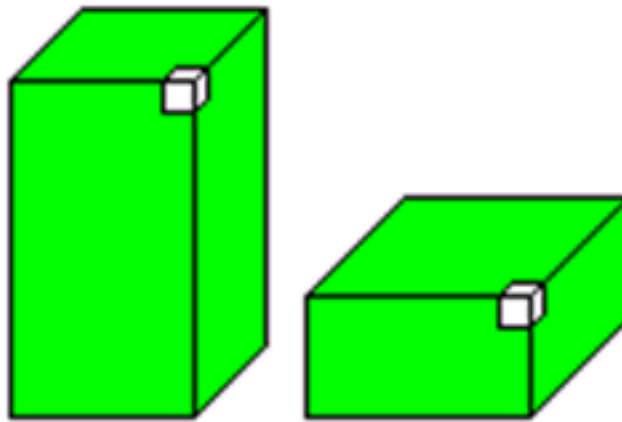
Monoclinic



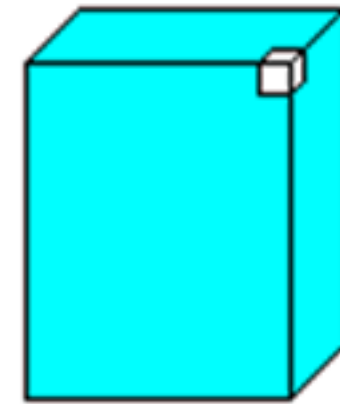
Cubic (Isometric)



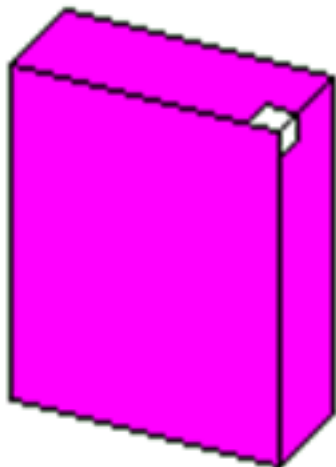
Tetragonal



Orthorhombic



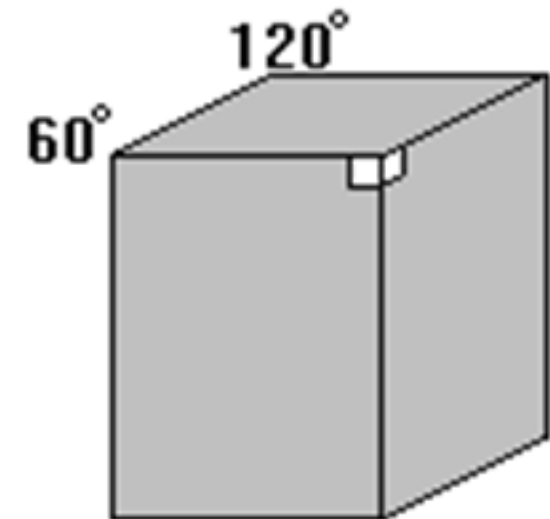
Monoclinic



Triclinic



Hexagonal



Atomic Packing Factor

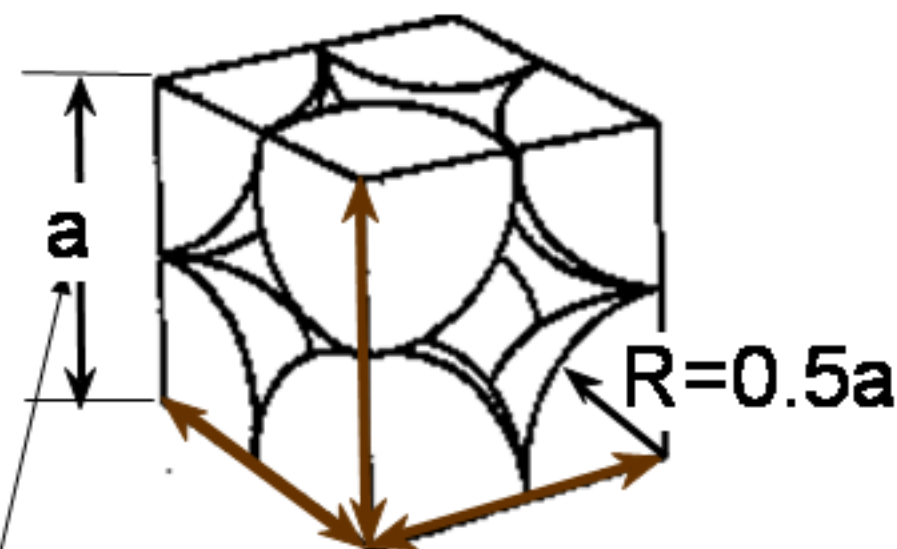
- ▶ Atomic Packing Factor (APF) is defined as the volume of atoms within the unit cell divided by the volume of the unit cell.

$$APF = \frac{\text{Volume of Atoms in Unit Cell}}{\text{Volume of Unit Cell}}$$

ATOMIC PACKING FACTOR

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

*assume hard spheres



close-packed directions

contains $8 \times 1/8 =$

1 atom/unit cell

Adapted from Fig. 3.19,
Callister 6e.

atoms
unit cell

APF =

$$1 + \frac{4}{3} \pi (0.5a)^3$$

volume
atom

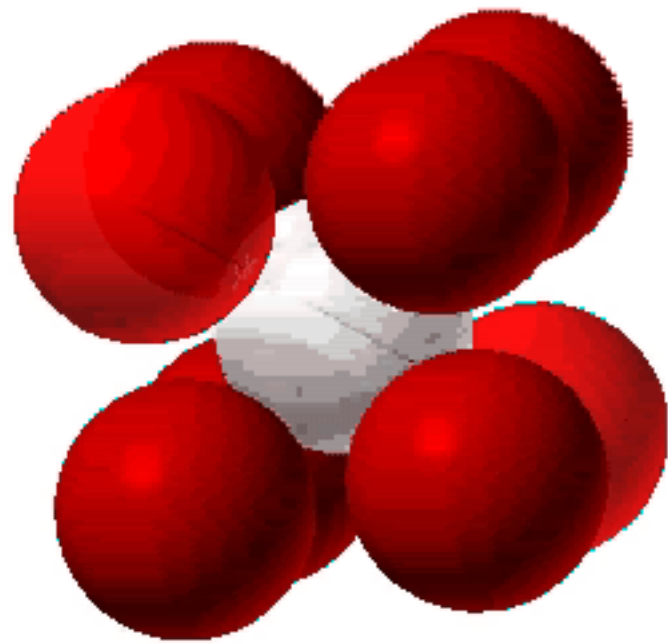
a^3

volume
unit cell

Lattice constant

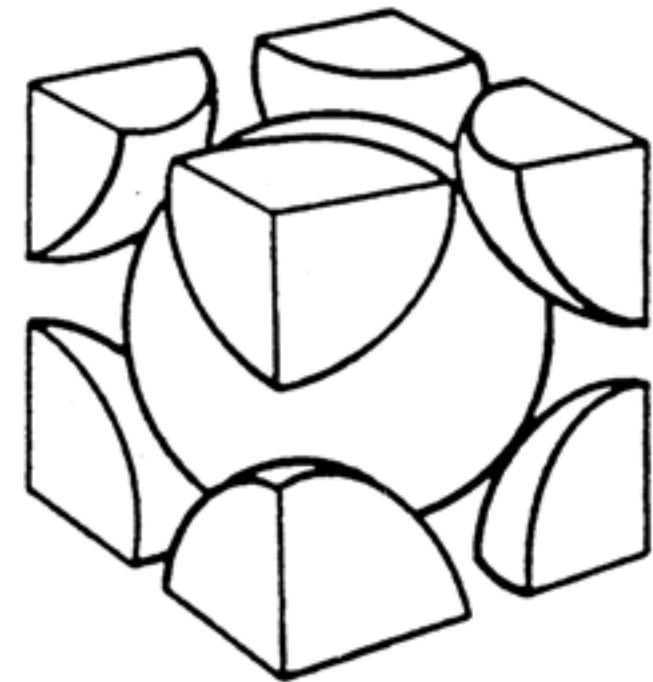
APF for a simple cubic structure = 0.52

BODY CENTERED CUBIC STRUCTURE (BCC)



(Courtesy P.M. Anderson)

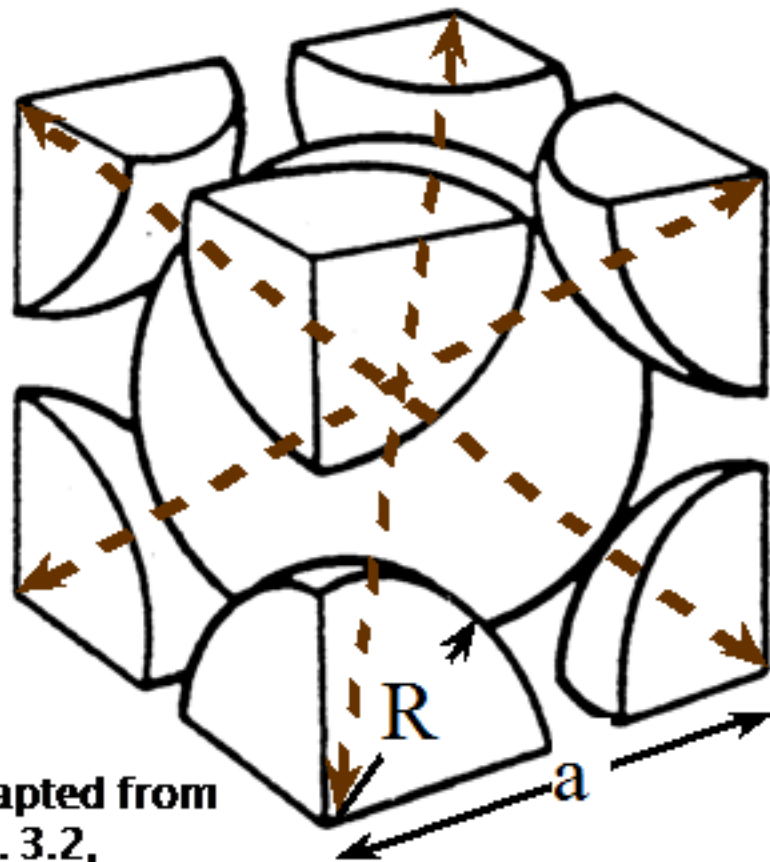
- Coordination # = 8



Adapted from Fig. 3.2,
Callister 6e.

- Close packed directions are cube diagonals.
—Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ATOMIC PACKING FACTOR: BCC



Adapted from Fig. 3.2, Callister 6e.

Close-packed directions:

$$\begin{aligned} \text{length} &= 4R \\ &= \sqrt{3} a \end{aligned}$$

Unit cell contains:

$$\begin{aligned} &1 + 8 \times 1/8 \\ &= \mathbf{2 \text{ atoms/unit cell}} \end{aligned}$$

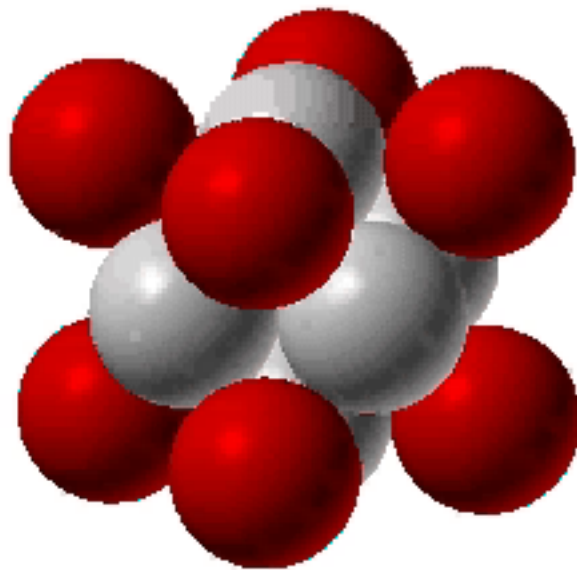
$$\text{APF} = \frac{\text{atoms/unit cell} \times \text{volume/atom}}{\text{volume/unit cell}}$$

$$= \frac{2 \times \frac{4}{3} \pi (\sqrt{3} a/4)^3}{a^3}$$

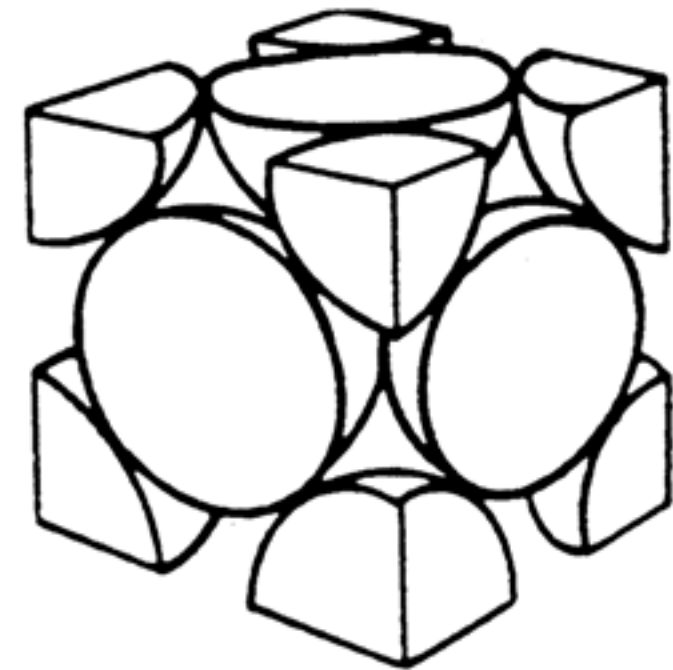
- APF for a body-centered cubic structure = $\pi\sqrt{3}/8 = 0.68$

FACE CENTERED CUBIC STRUCTURE (FCC)

- Coordination # = 12



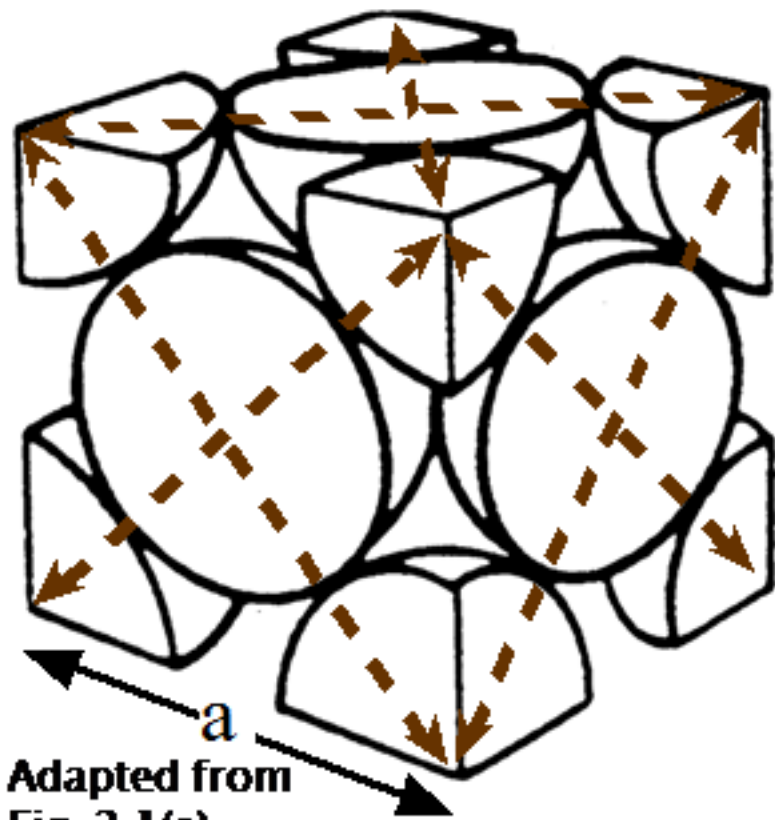
(Courtesy P.M. Anderson)



Adapted from Fig. 3.1(a),
Callister 6e.

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

ATOMIC PACKING FACTOR: FCC



Adapted from
Fig. 3.1(a),
Callister 6e.

Close-packed directions:

$$\begin{aligned} \text{length} &= 4R \\ &= \sqrt{2} a \end{aligned}$$

Unit cell contains:

$$\begin{aligned} &6 \times 1/2 + 8 \times 1/8 \\ &= 4 \text{ atoms/unit cell} \end{aligned}$$

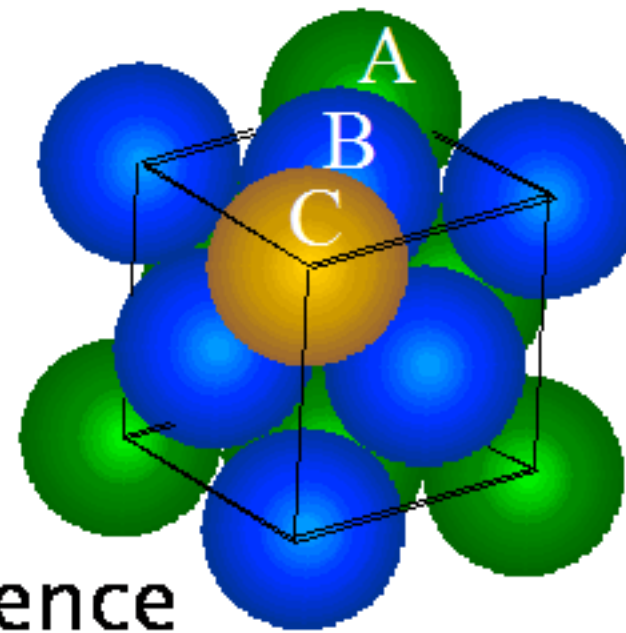
$$\text{APF} = \frac{\text{atoms/unit cell} \times \frac{4}{3} \pi \left(\frac{\sqrt{2} a}{4}\right)^3}{a^3}$$

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

- APF for a body-centered cubic structure = $\pi/(3\sqrt{2}) = 0.74$
(best possible packing of identical spheres)

FCC STACKING SEQUENCE

- FCC Unit Cell

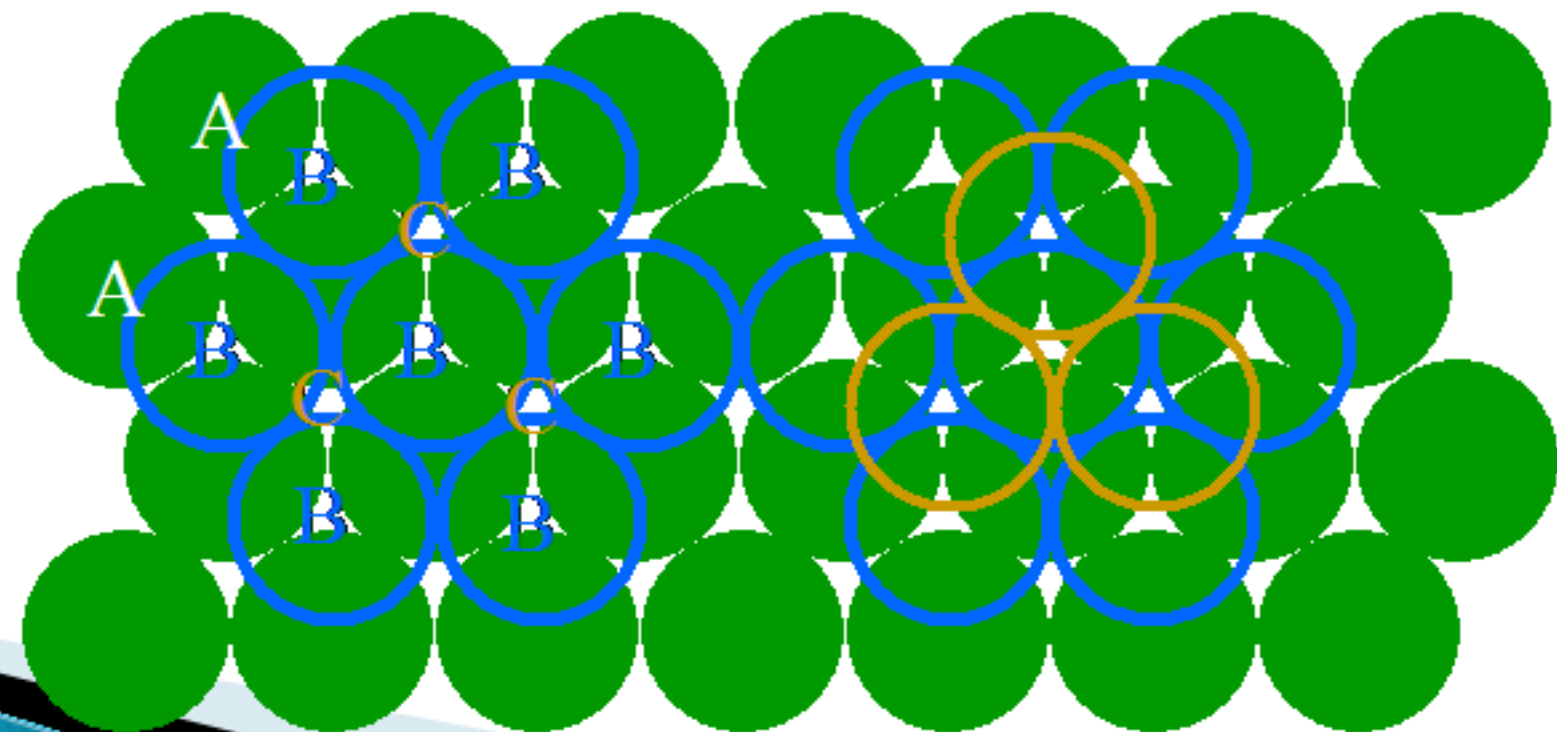


- ABCABC... Stacking Sequence
- 2D Projection

A sites

B sites

C sites



HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

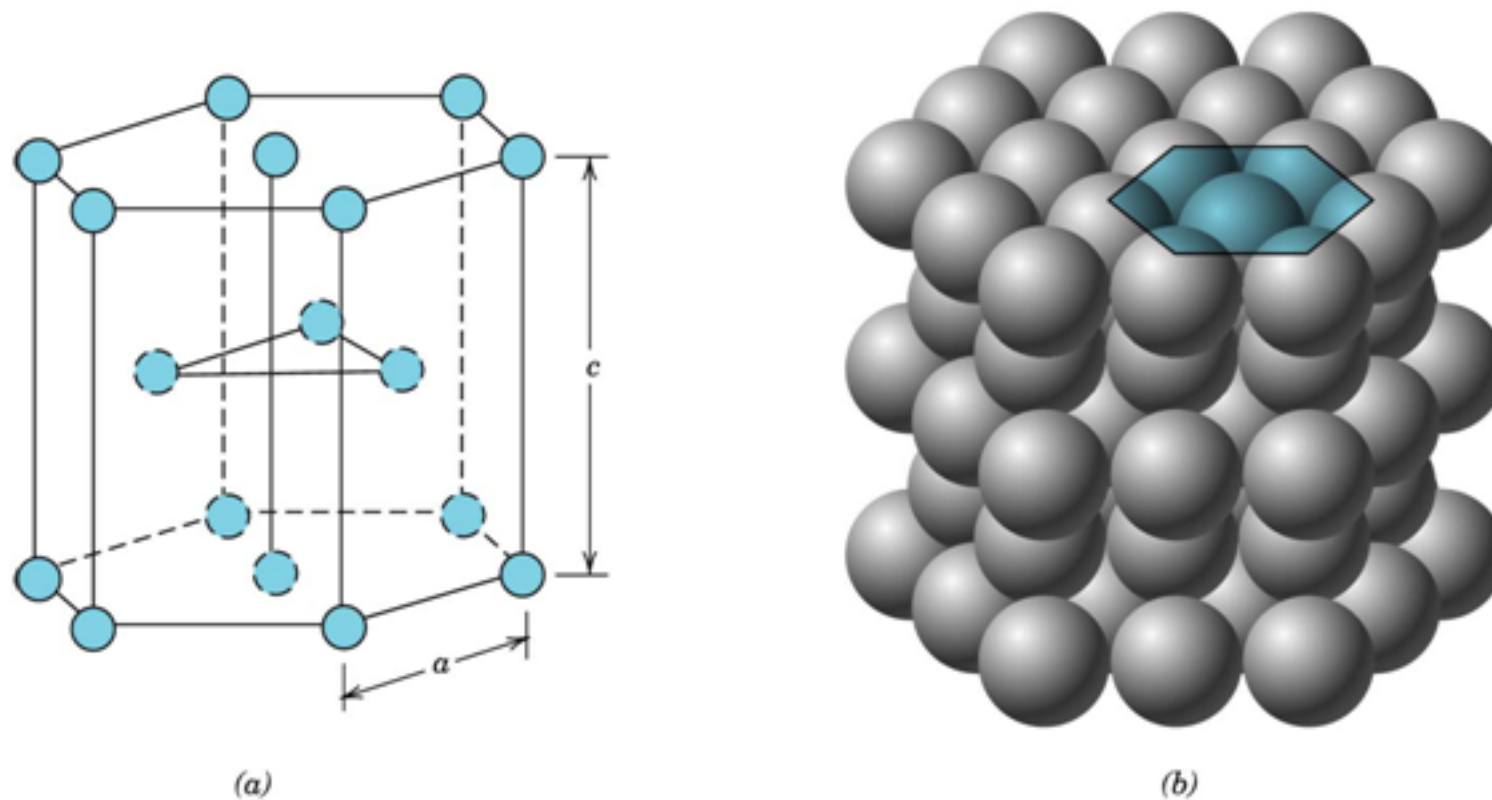


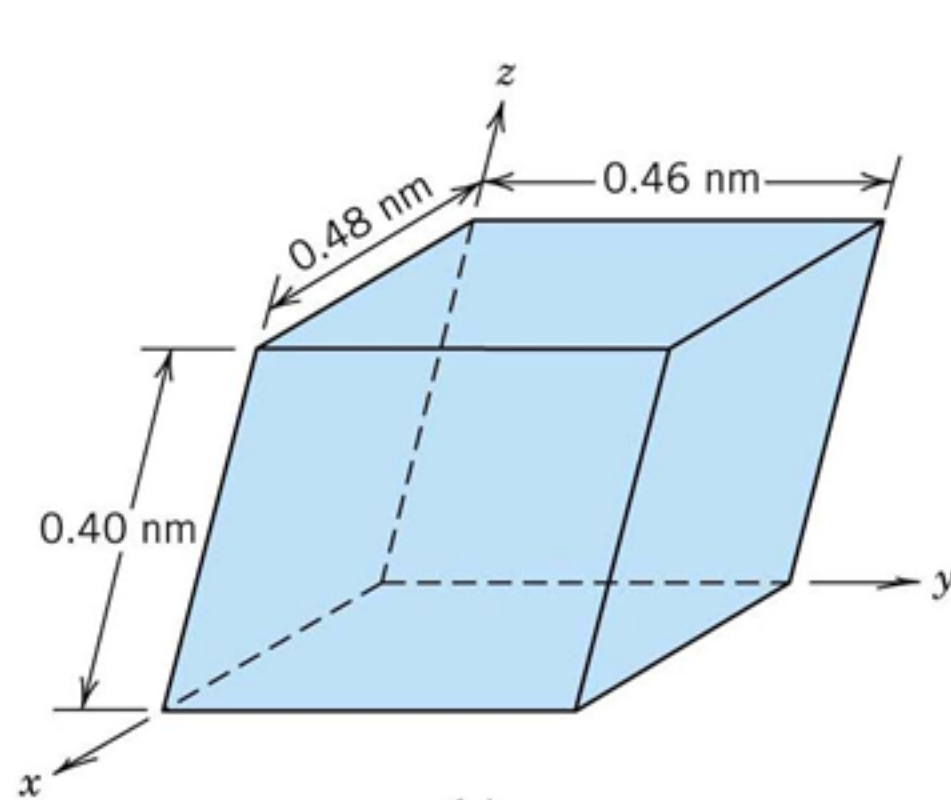
FIGURE 3.3 For the hexagonal close-packed crystal structure, (a) a reduced-sphere unit cell (a and c represent the short and long edge lengths, respectively), and (b) an aggregate of many atoms. (Figure *b* from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

Ideally, $c/a = 1.633$ for close packing

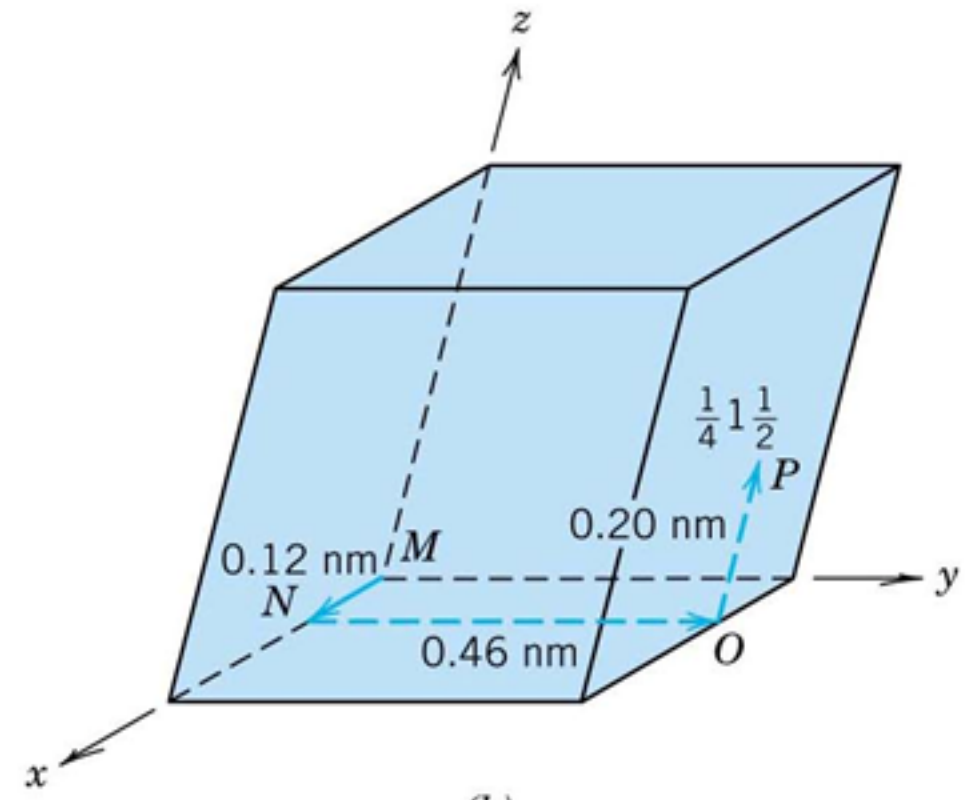
However, in most metals, c/a ratio deviates from this value

EXAMPLE: POINT COORDINATES

- ▶ Locate the point $(\frac{1}{4} \ 1 \ \frac{1}{2})$



(a)

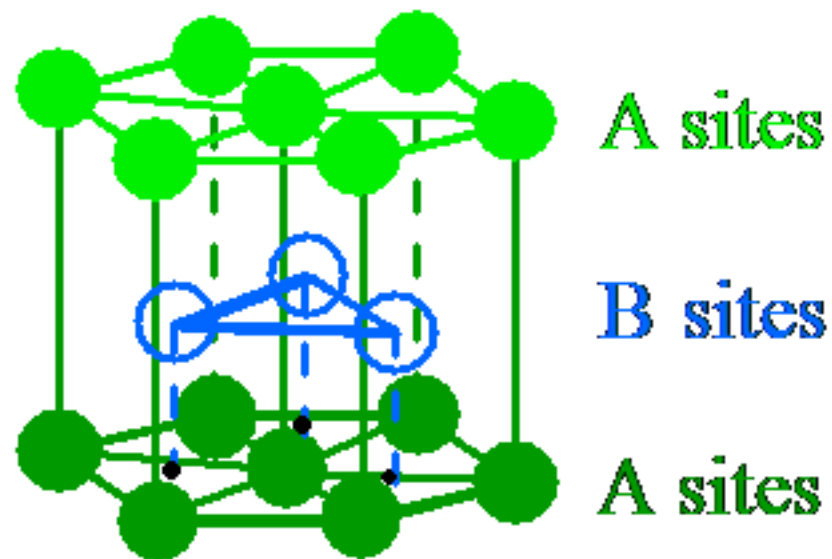


(b)

- Specify point coordinates for all atom positions for a BCC unit cell
 - Answer: $0 \ 0 \ 0$, $1 \ 0 \ 0$, $1 \ 1 \ 0$, $0 \ 1 \ 0$, $\frac{1}{2} \ \frac{1}{2} \ \frac{1}{2}$, $0 \ 0 \ 1$, $1 \ 0 \ 1$, $1 \ 1 \ 1$, $0 \ 1 \ 1$

HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

- ABAB... Stacking Sequence
- 3D Projection



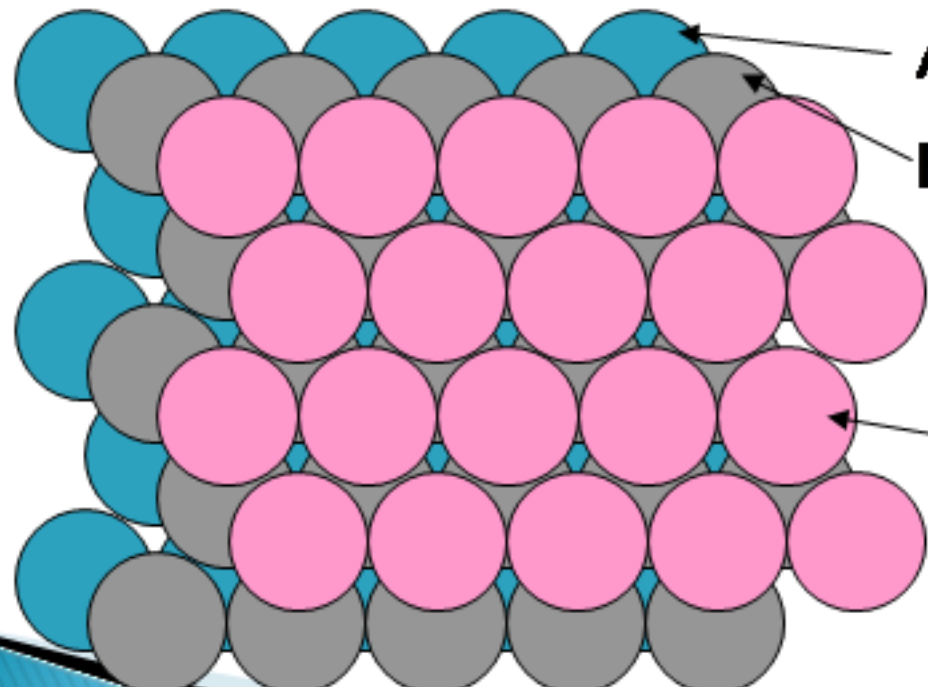
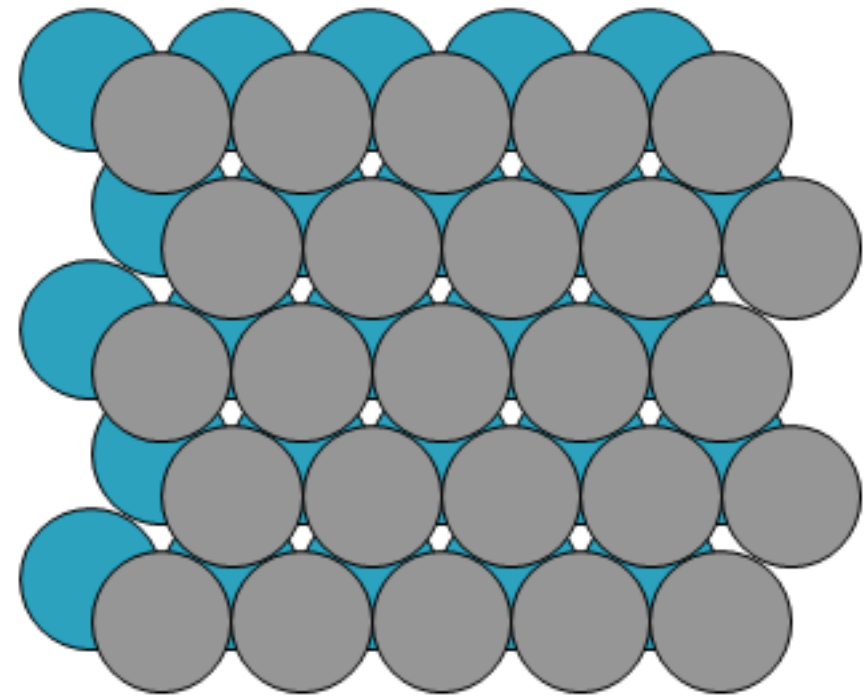
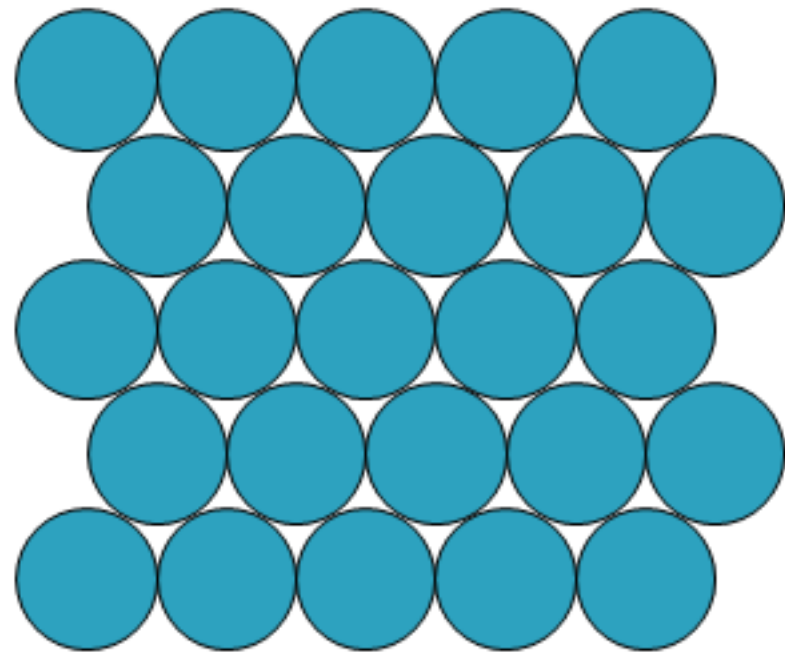
Adapted from Fig. 3.3,
Callister 6e.

- 2D Projection



- Coordination # = 12
- APF = 0.74, for ideal c/a ratio of 1.633

Close packed crystals



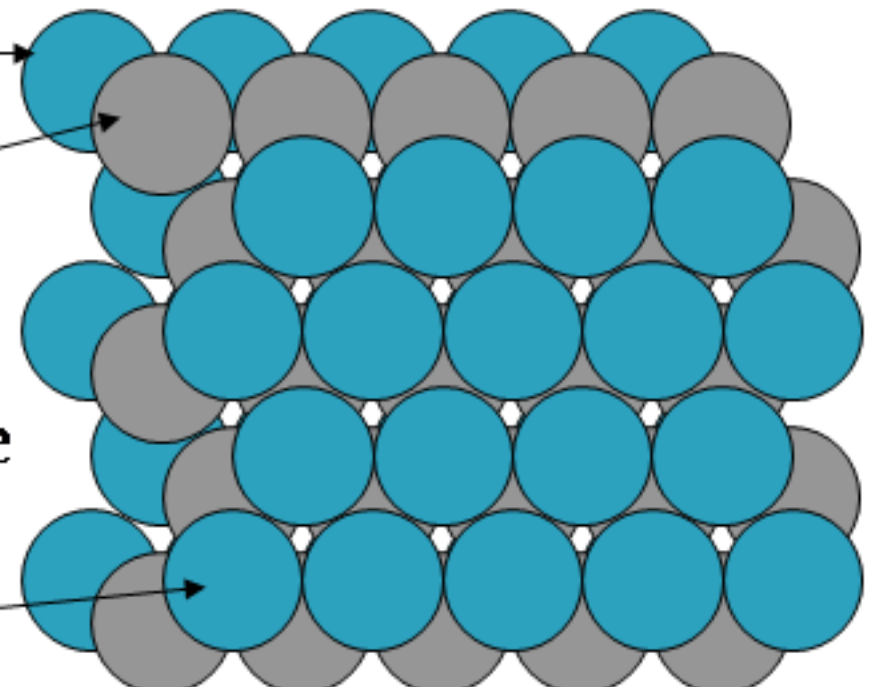
A plane

B plane

C plane

A plane

...ABCABC... packing
[Face Centered Cubic (FCC)]



...ABABAB... packing
[Hexagonal Close Packing (HCP)]

COMPARISON OF CRYSTAL STRUCTURES

Crystal structure coordination #	packing factor	close packed directions
▶ Simple Cubic (SC) edges	6	0.52 cube
▶ Body Centered Cubic (BCC) 8	0.68	body diagonal
▶ Face Centered Cubic (FCC) 12	0.74	face diagonal
▶ Hexagonal Close Pack (HCP) hexagonal side	12	0.74

THEORETICAL DENSITY, ρ

Density = mass/volume

mass = number of atoms per unit cell * mass of each atom

mass of each atom = atomic weight/avogadro's number

atoms/unit cell

Atomic weight (g/mol)

$$\rho = \frac{n A}{V_c N_A}$$

Volume/unit cell
(cm^3 /unit cell)

Avogadro's number

(6.023×10^{23} atoms/mol)

Characteristics of Selected Elements at 20C

Element	Symbol	At. Weight (amu)	Density (g/cm ³)	Crystal Structure	Atomic radius (nm)
Aluminum	Al	26.98	2.71	FCC	0.143
Argon	Ar	39.95	—	—	—
Barium	Ba	137.33	3.5	BCC	0.217
Beryllium	Be	9.012	1.85	HCP	0.114
Boron	B	10.81	2.34	Rhomb	—
Bromine	Br	79.90	—	—	—
Cadmium	Cd	112.41	8.65	HCP	0.149
Calcium	Ca	40.08	1.55	FCC	0.197
Carbon	C	12.011	2.25	Hex	0.071
Cesium	Cs	132.91	1.87	BCC	0.265
Chlorine	Cl	35.45	—	—	—
Chromium	Cr	52.00	7.19	BCC	0.125
Cobalt	Co	58.93	8.9	HCP	0.125
Copper	Cu	63.55	8.94	FCC	0.128
Flourine	F	19.00	—	—	—
Gallium	Ga	69.72	5.90	Ortho.	0.122
Germanium	Ge	72.59	5.32	Dia. cubic	0.122
Gold	Au	196.97	19.32	FCC	0.144
Helium	He	4.003	—	—	—
Hydrogen	H	1.008	—	—	—

Adapted from Table, "Characteristics of Selected Elements", inside front cover, Callister 6e.

THEORETICAL DENSITY, ρ

atoms/unit cell

Atomic weight (g/mol)

$$\rho = \frac{n A}{V_c N_A}$$

Volume/unit cell
(cm³/unit cell)

Avogadro's number

(6.023 x 10²³ atoms/mol)

Example: Copper

Data from Table inside front cover of Callister (see previous slide):

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius R = 0.128 nm (1 nm = 10⁻⁷ cm)

$$V_c = a^3 ; \text{ For FCC, } a = 4R/\sqrt{2}; \quad V_c = 4.75 \times 10^{-23} \text{ cm}^3$$

Result: theoretical

$$\rho_{\text{Cu}} = 8.89 \text{ g/cm}^3$$

Compare to actual:

$$\rho_{\text{Cu}} = 8.94 \text{ g/cm}^3$$

DENSITIES OF MATERIAL CLASSES

$$\rho_{\text{metals}} > \rho_{\text{ceramics}} > \rho_{\text{polymers}}$$

Why?

Metals have...

- close-packing (metallic bonding)
- large atomic mass

Ceramics have...

- less dense packing (covalent bonding)
- often lighter elements

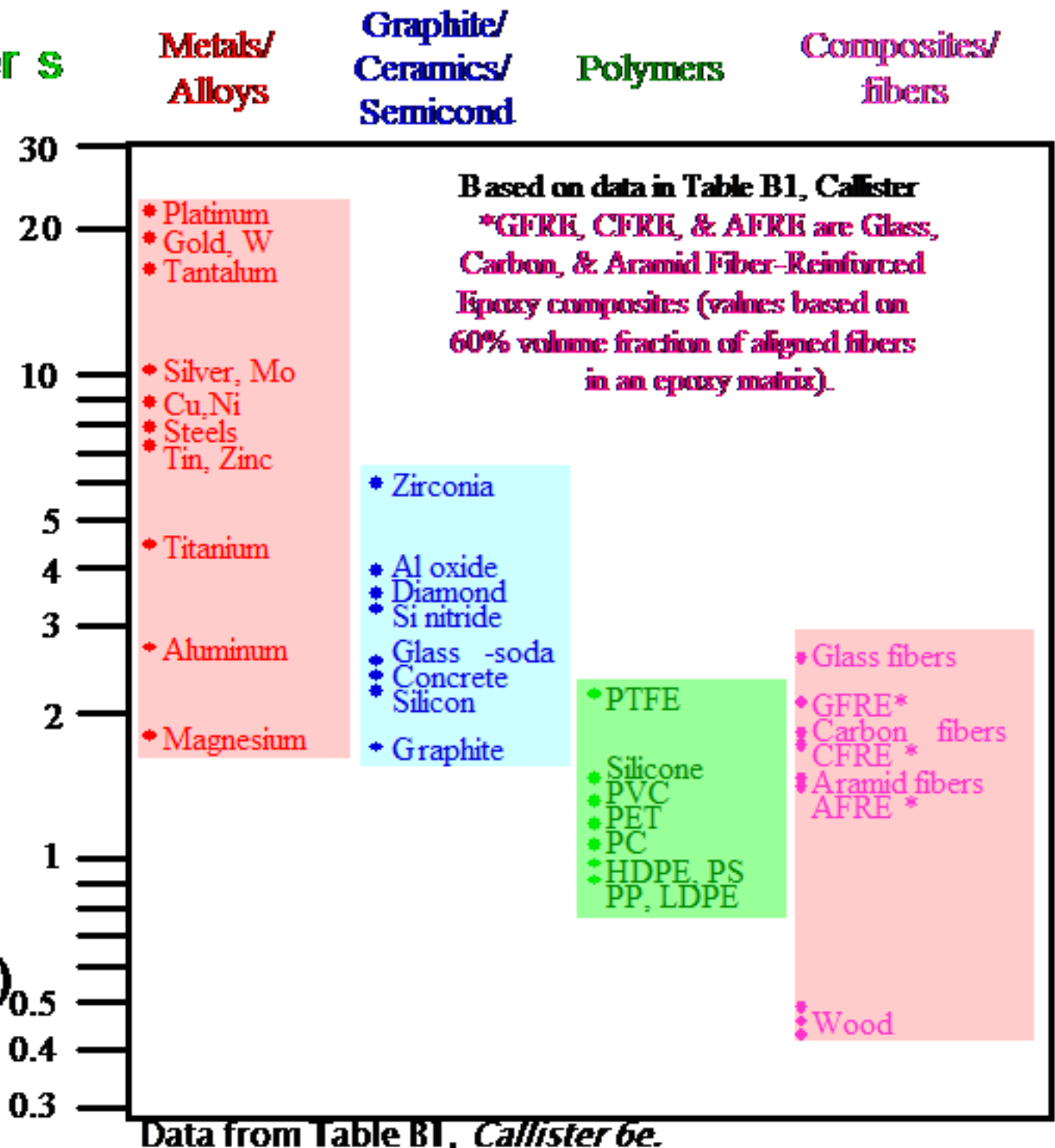
Polymers have...

- poor packing (often amorphous)
- lighter elements (C,H,O)

Composites have...

- intermediate values

ρ (g/cm³)



CRYSTAL SYSTEMS

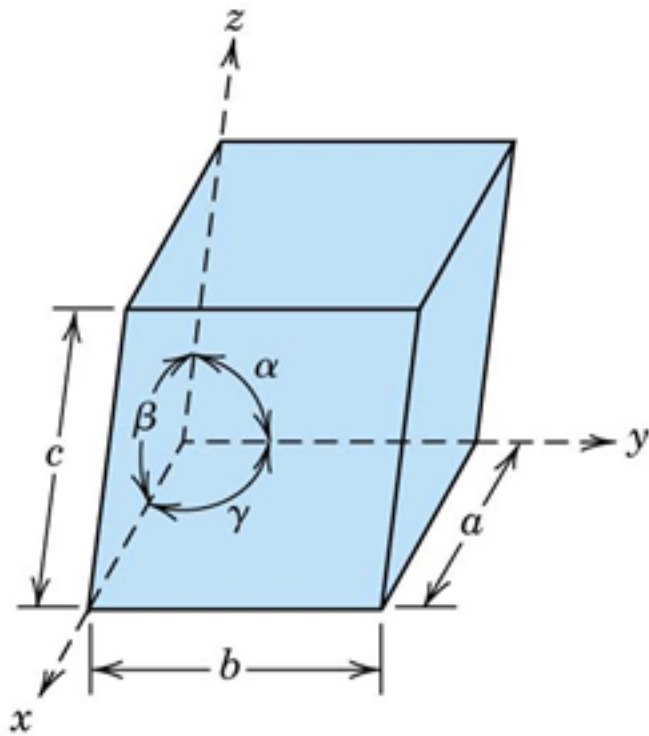


FIGURE 3.4 A unit cell with x , y , and z coordinate axes, showing axial lengths (a , b , and c) and interaxial angles (α , β , and γ).

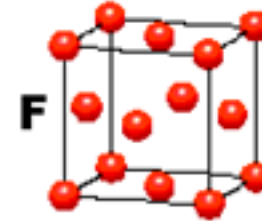
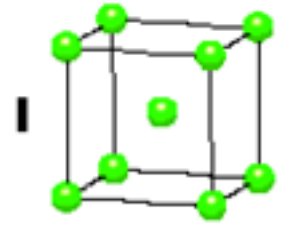
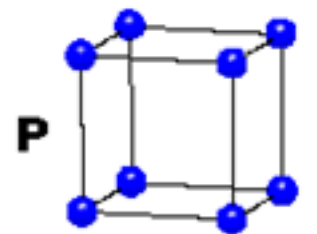
- ▶ Based on shape of unit cell ignoring actual atomic locations
- ▶ Unit cell = 3-dimensional unit that repeats in space
- ▶ Unit cell geometry completely specified by a , b , c & α , β , γ (*lattice parameters or lattice constants*)
- ▶ Seven possible combinations of a , b , c & α , β , γ , resulting in seven crystal systems

CRYSTAL SYSTEMS

CUBIC

$$a = b = c$$

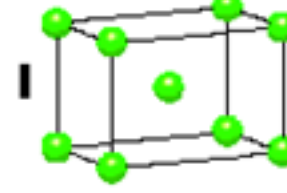
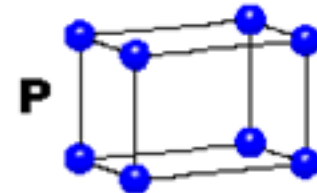
$$\alpha = \beta = \gamma = 90^\circ$$



TETRAGONAL

$$a = b \neq c$$

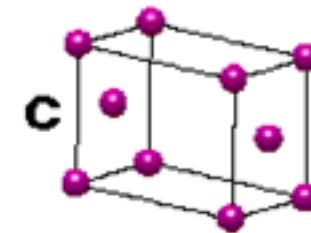
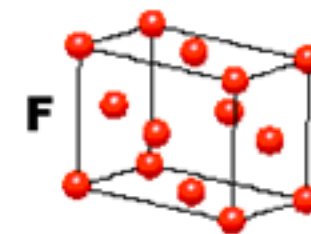
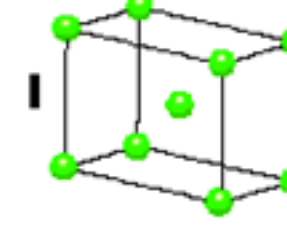
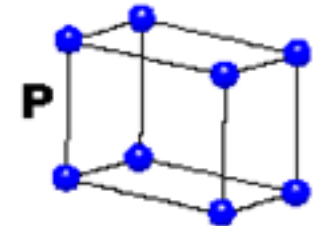
$$\alpha = \beta = \gamma = 90^\circ$$



ORTHORHOMBIC

$$a \neq b \neq c$$

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

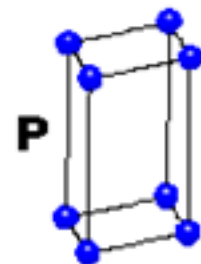


HEXAGONAL

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

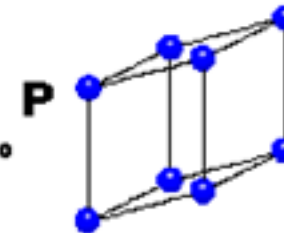
$$\gamma = 120^\circ$$



TRIGONAL

$$a = b = c$$

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

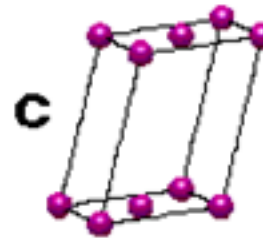
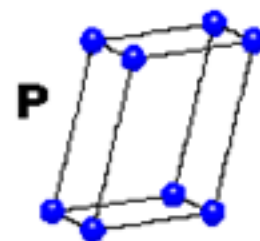


MONOCLINIC

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ$$

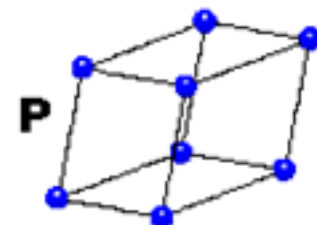
$$\beta \neq 120^\circ$$



TRICLINIC

$$a \neq b \neq c$$

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



4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

+

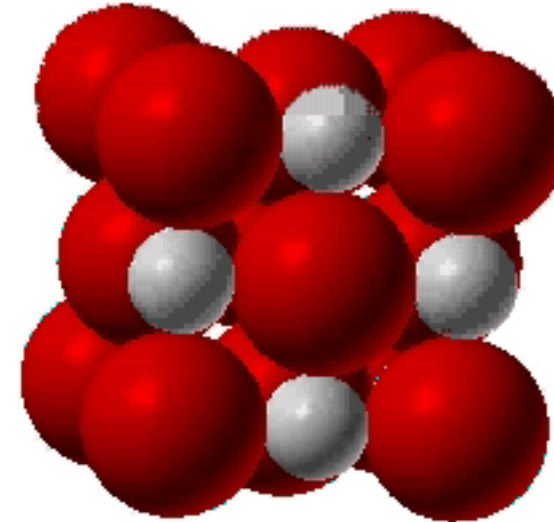
7 Crystal Classes

→ **14 Bravais Lattices**

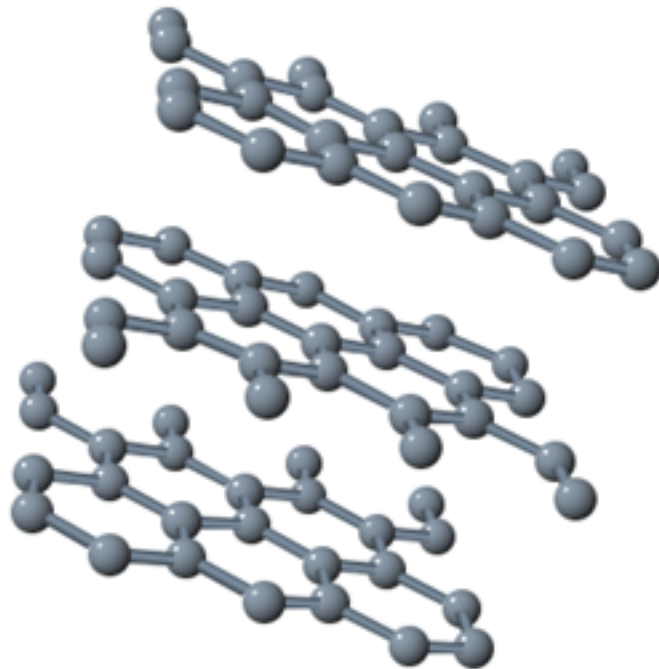
STRUCTURE OF OTHER SYSTEMS

- Structure of NaCl

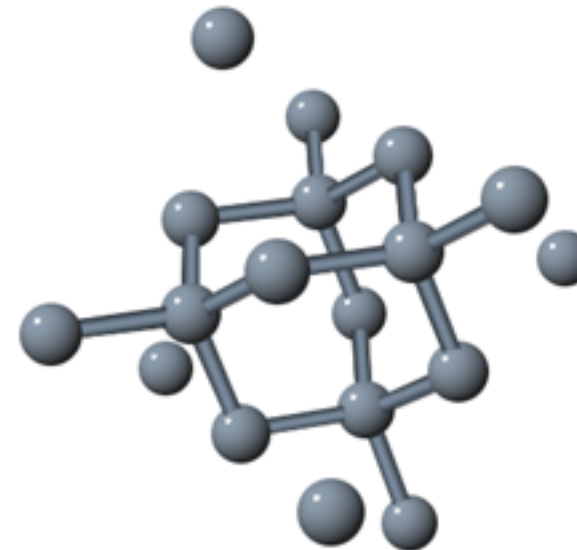
(Courtesy P.M. Anderson)



- Structure of Carbon



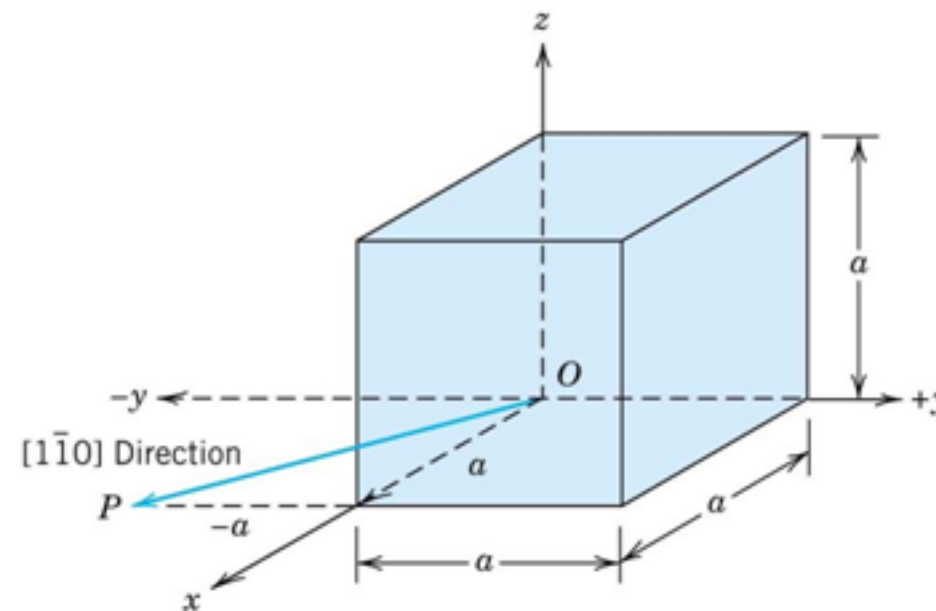
Graphite



Diamond

EXAMPLES: DIRECTIONS

- ▶ Draw a $[1, -1, 0]$ direction within a cubic unit cell



- Determine the indices for this direction
 - Answer: $[1\ 2\ 0]$

