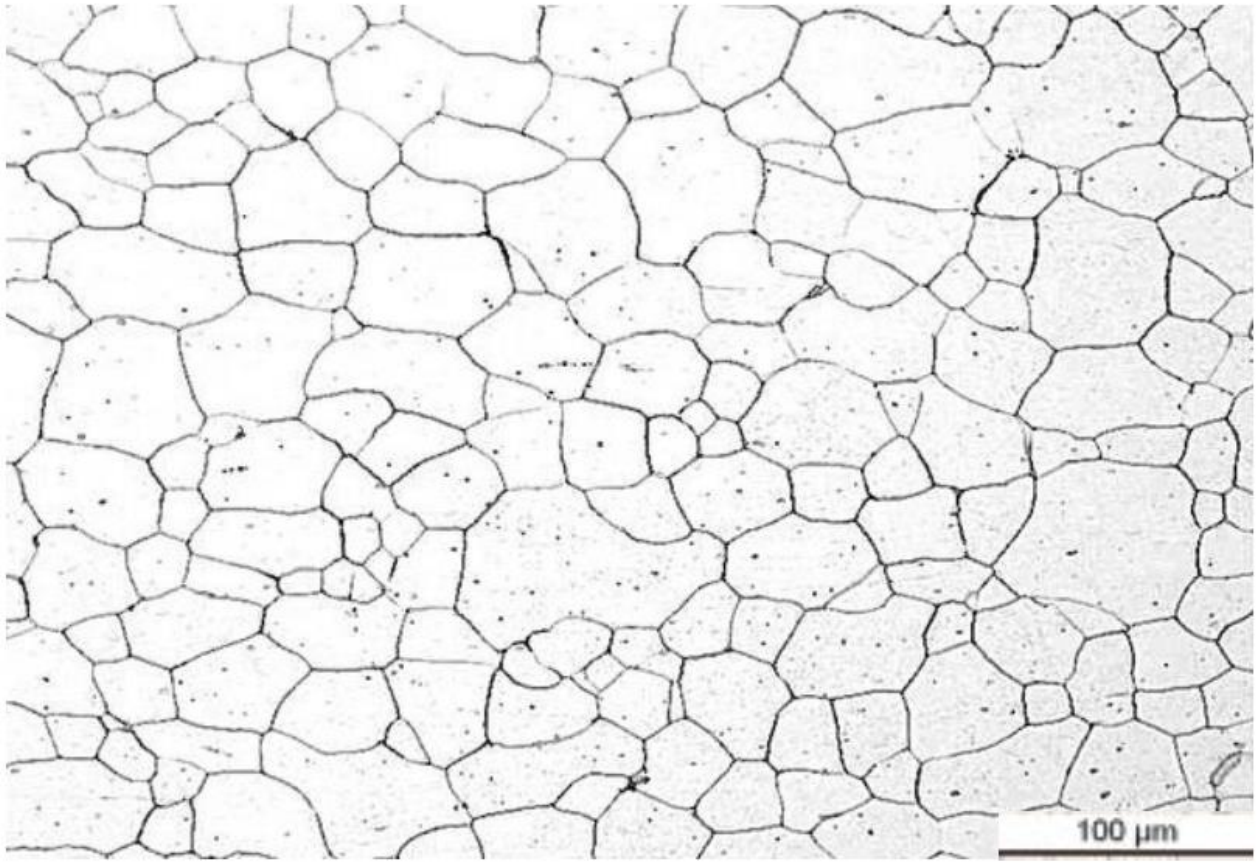
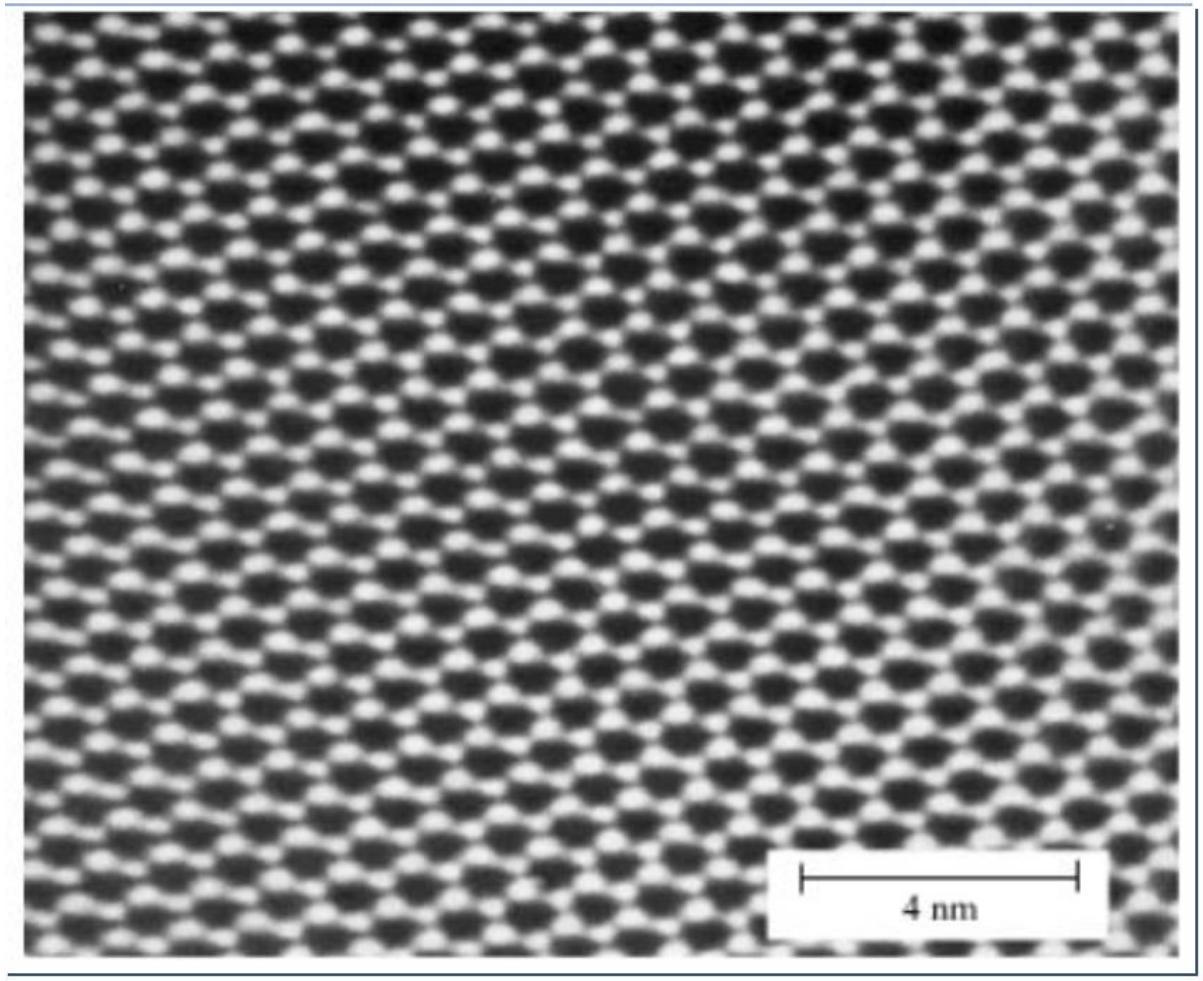
Crystal Systems and Structure of Crystalline Materials

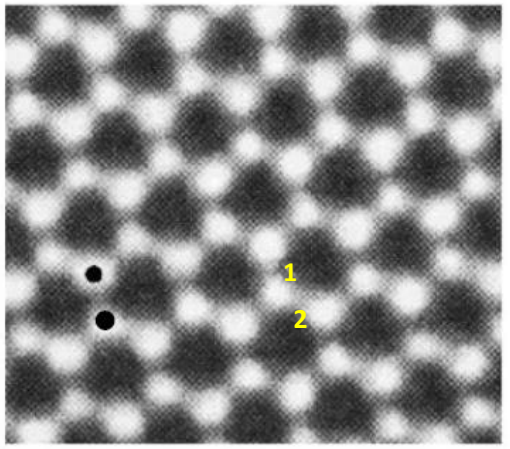
Micro structure

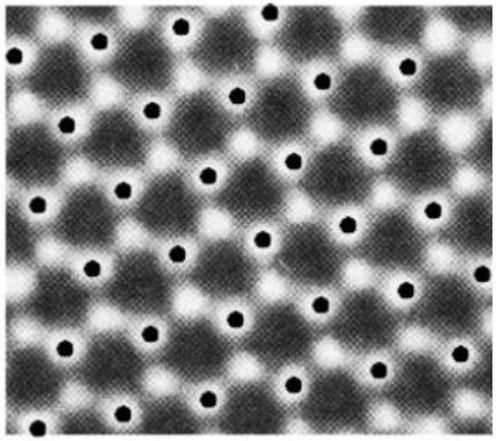


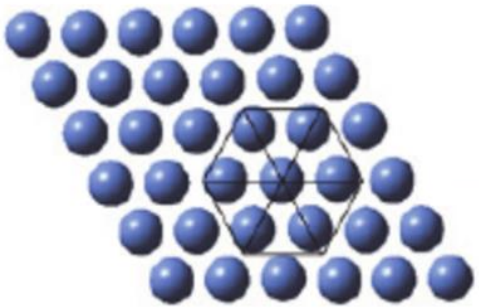
- Microstructure of Poly-crystalline sample consist of several grain, separated by grain boundary.

Periodic arrangement of atoms



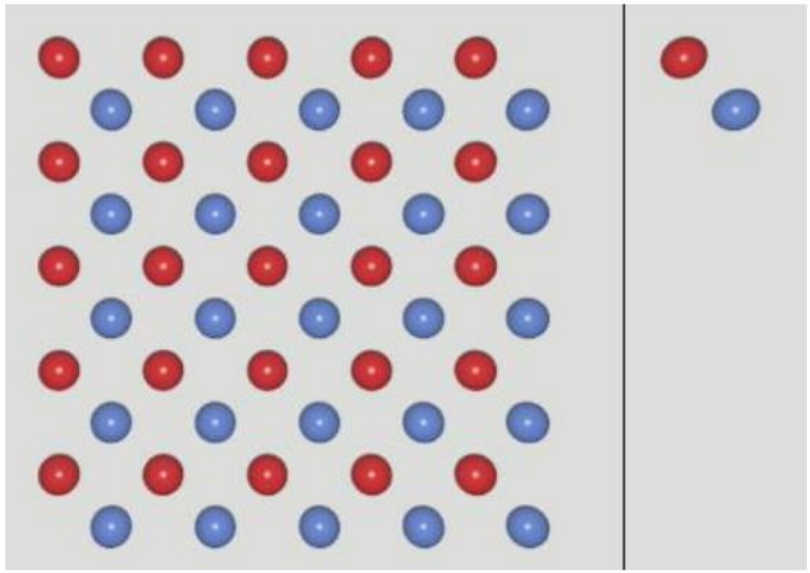


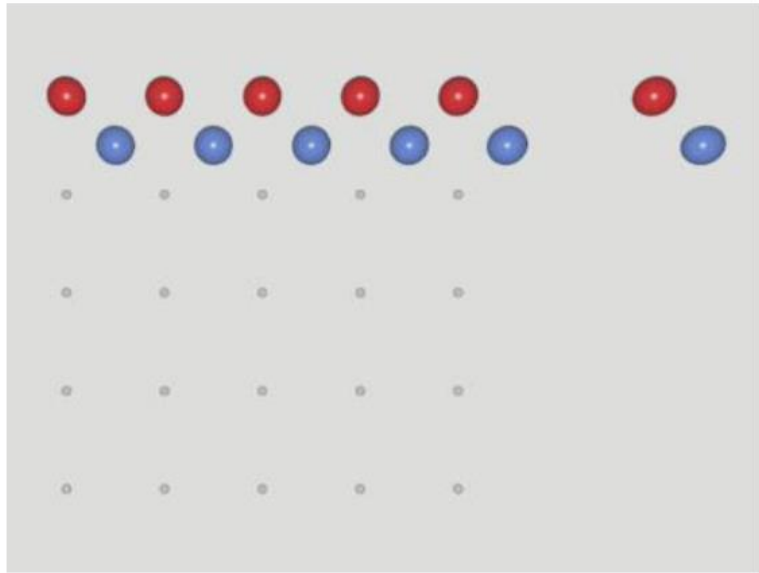




Long range ordering

- Crystalline Solid have long range ordering
- Crystalline materials are characterised by a regular atomic structure that repeats itself in all three dimensions. In other words, the structure displays **translational symmetry**
- The periodic nature of the structure can be represented using a **lattice**. Every lattice point have **identical surrounding**.



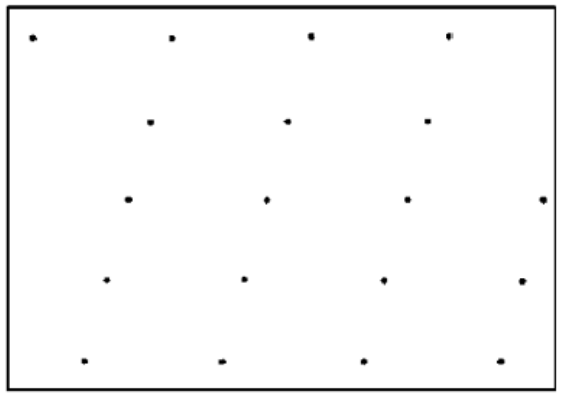


Crystal = Lattice + Motif

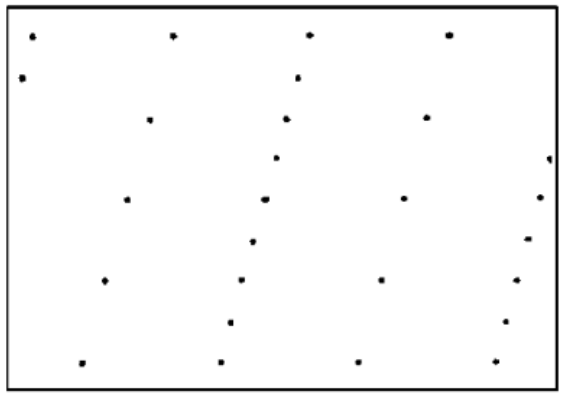
How to repeat

what to repeat

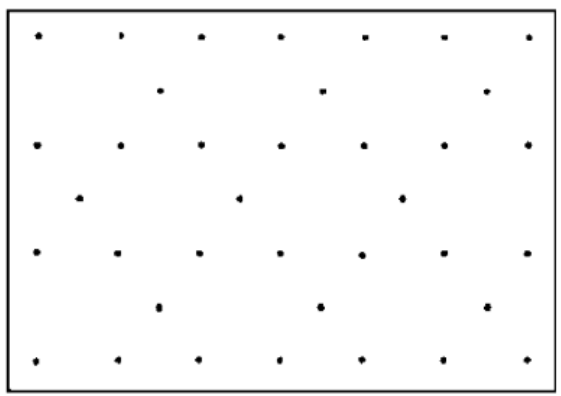
Lattice



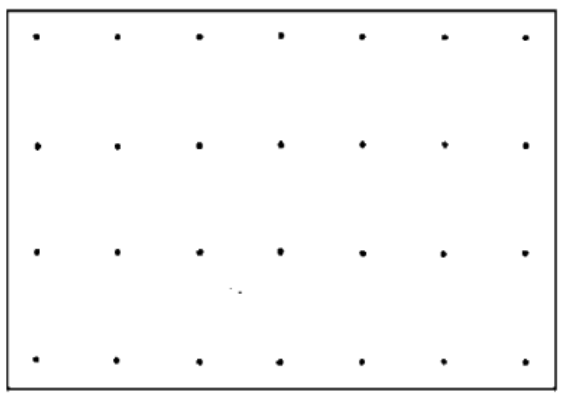
(a)



(b)



(c)

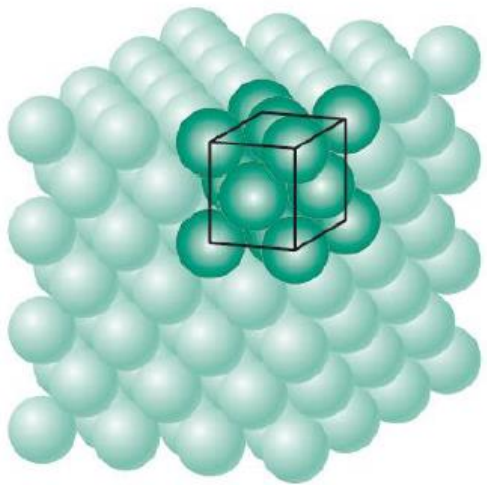


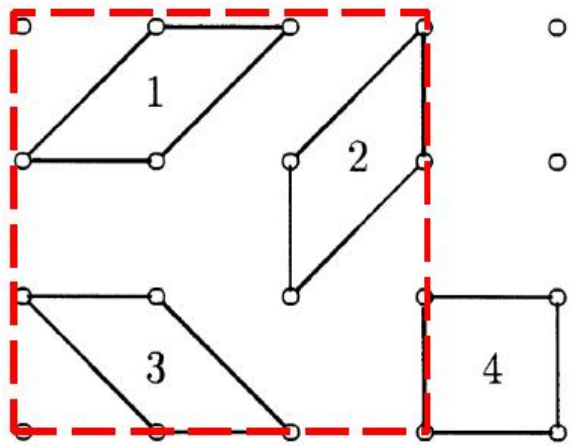
(d)

Here, Only (a) and (d) constitute lattices

Unit cell

- The structure of a crystal can be seen to be composed of a repeated element in three dimensions. This repeated element is known as the unit cell.
- In three dimension the unit cell is any parallelepiped whose vertices are lattice points. In two dimension it is any parallelogram whose vertices are lattice points.
- There are infinite possibilities to chose the unit cell.
- In general, the unit cell is chosen such that it is the **smallest unit** cell that reflects the **symmetry** of the structure.





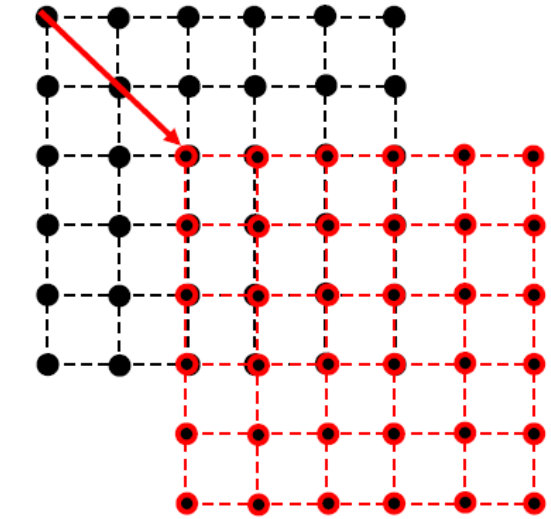
What is symmetry?

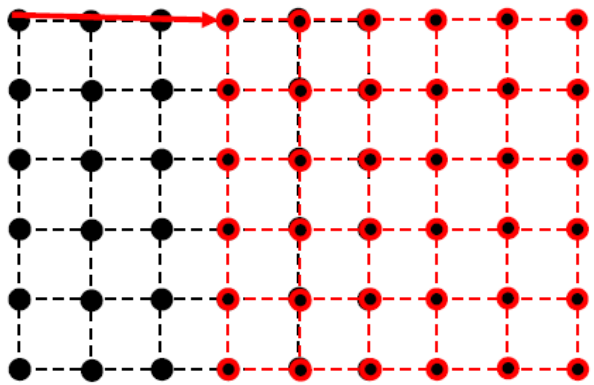
- An object is said to be symmetric with respect to a geometric operation if it can be brought into self coincidence by that operation.

OR

- An object is described as *symmetric* with respect to a *transformation* if the object appears to be in a state that is identical to its initial state, after the transformation.
- There are two main types of symmetries (i.e. symmetry operations): (a) Translation symmetry (b) Point symmetry

Translational symmetry

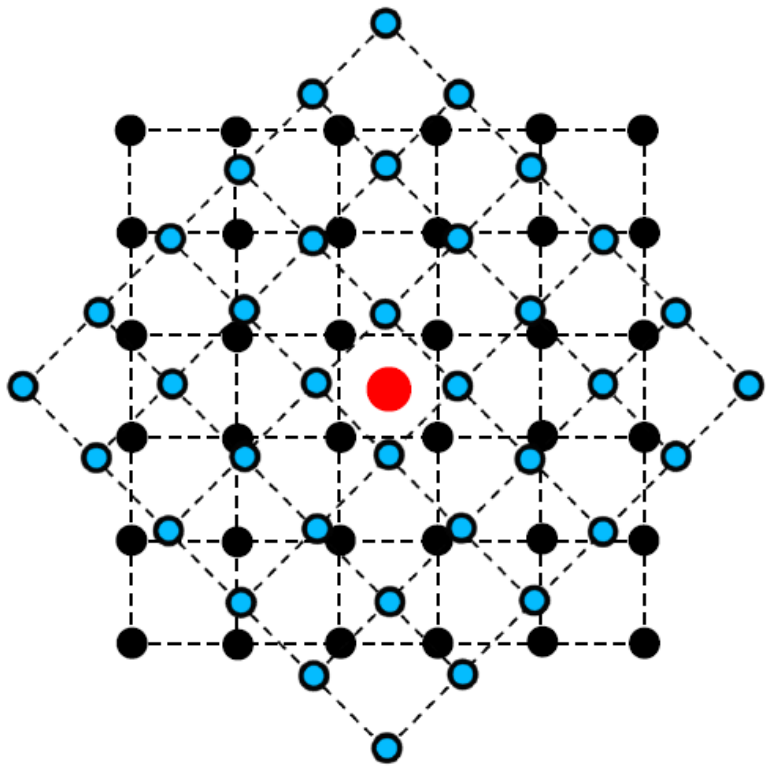




- Translations, i.e. executable shifting movements, proceeding along a straight line and on a certain specified distance, such that the operation does not result in any change of the shifted pattern.
- Lattice considered as infinite array of points
- Translational vector can be any vector joining two points
- Translation symmetry is the defining symmetry of a lattice

Point Symmetries

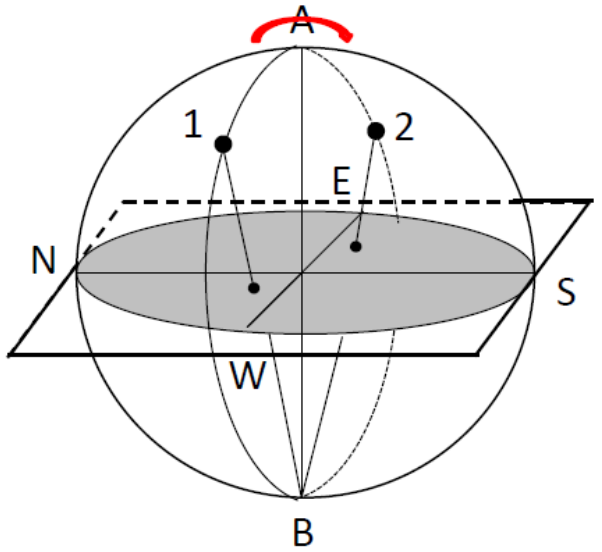
- It is a macroscopically visible symmetry operations: after it has been applied to the crystal at least one point remains where it was !!



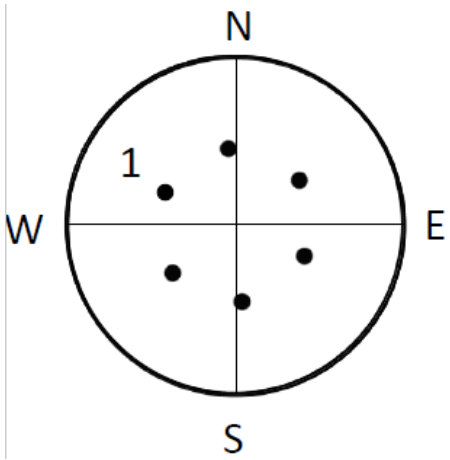
❑ **Different point symmetry operations:**

- Rotation (1,2,..)
- Mirror (m)
- Inversion ($\bar{1}$)
- Roto-inversion ($\bar{2}, \bar{3}, \bar{4}, \ldots$)

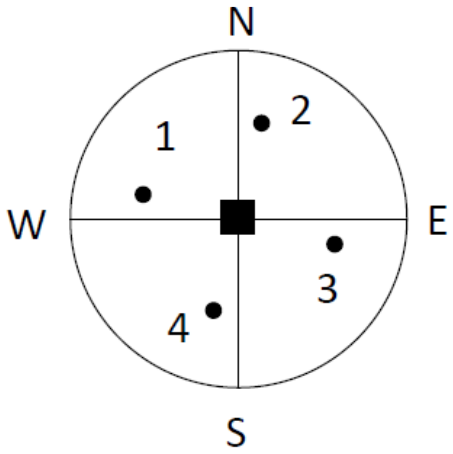
Rotational



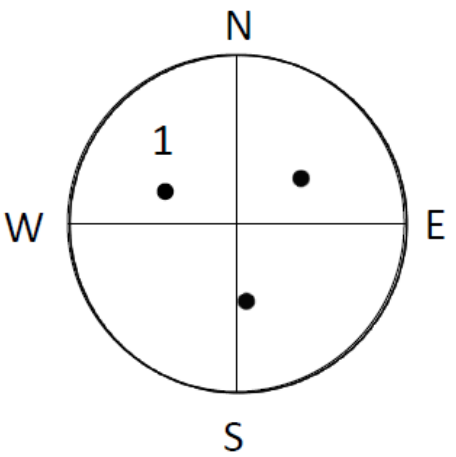
Degree of rotation = (360 degree/order of fold)



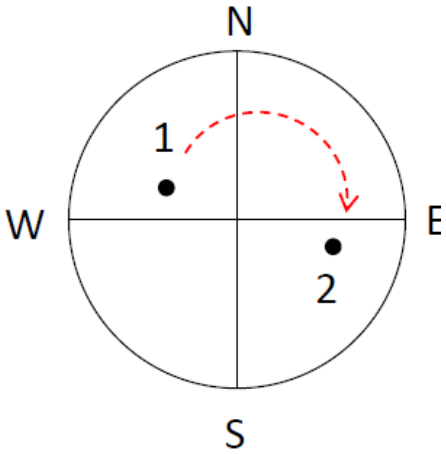
6 fold rotation symmetry



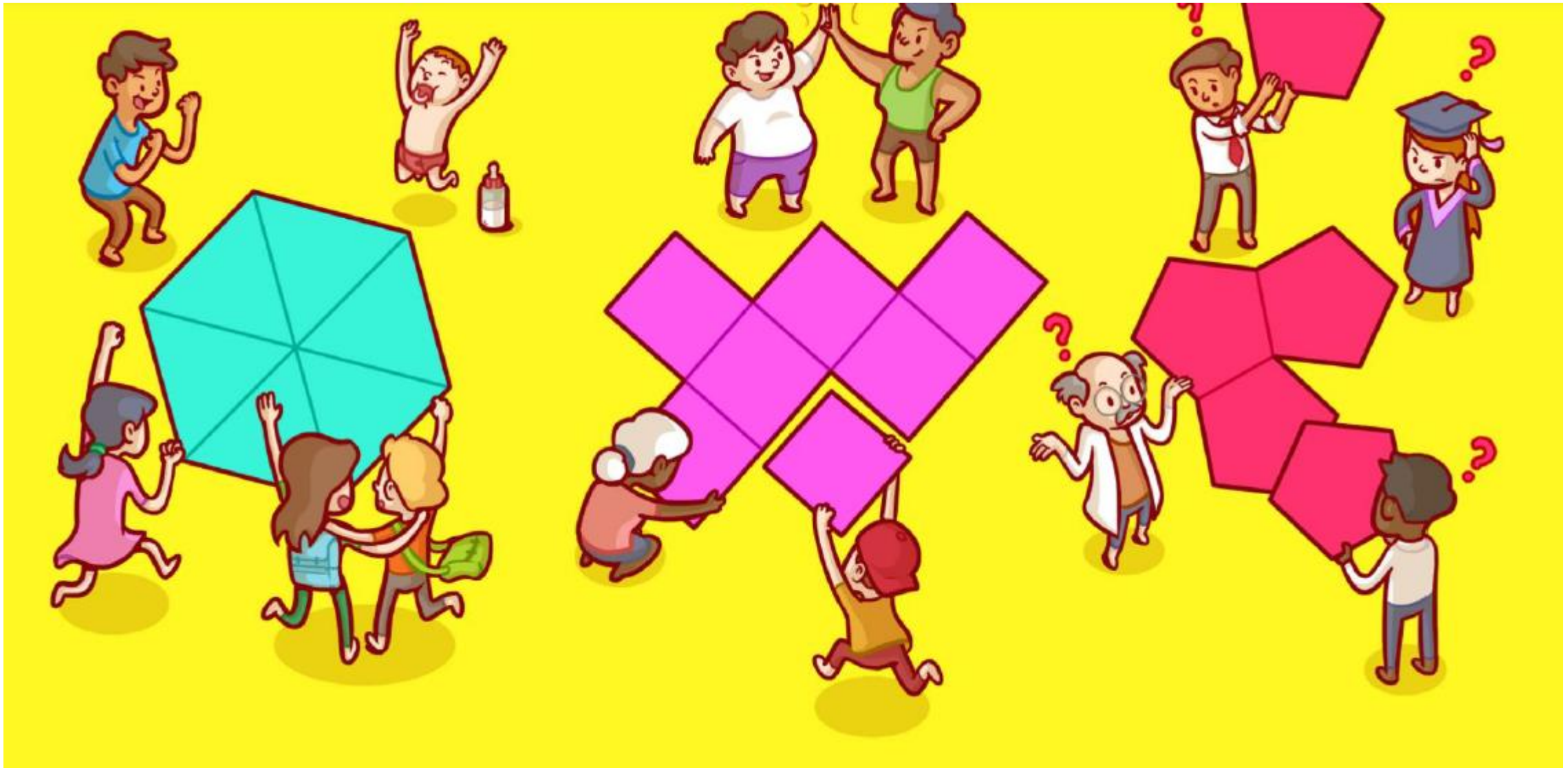
4 fold rotation symmetry



3 fold rotation symmetry



2 fold rotation symmetry

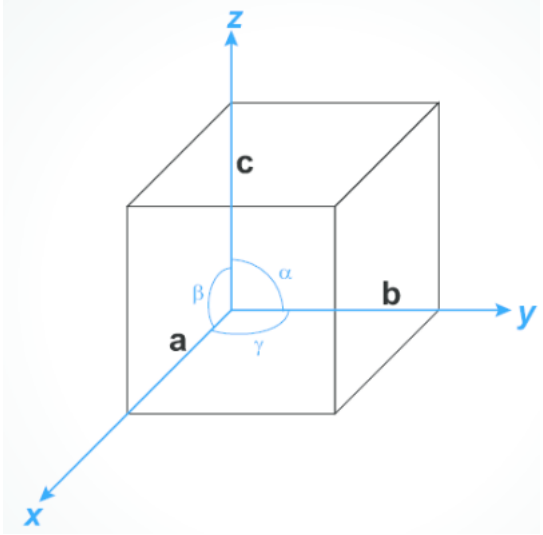


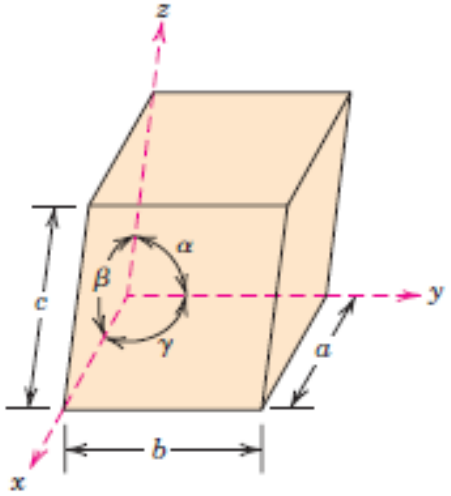
3 Fold symmetry

4 Fold symmetry

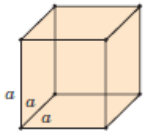
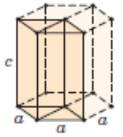
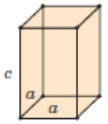
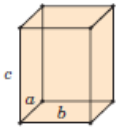
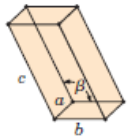
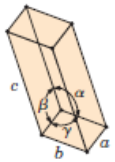
5 Fold symmetry

Crystal Systems





Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

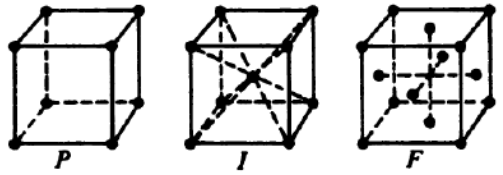
Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

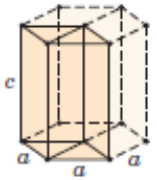
Decreasing symmetry

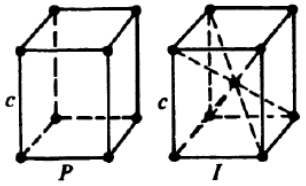
Crystal System	Axial Relationships	Interaxial Angles
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$

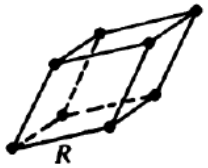
Decreasing symmetry

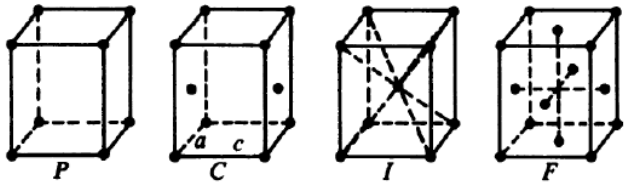
Bravais lattices

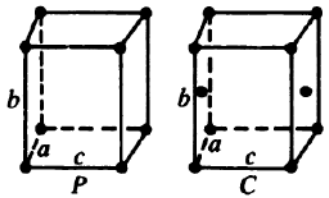










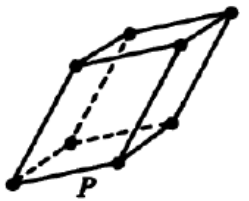


Unit Cell Notation

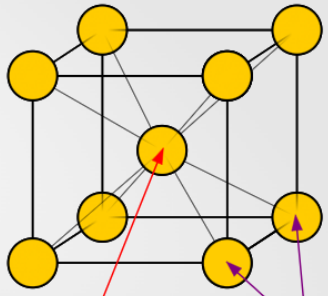
P (or R for rhombohedral): Primitive
I: Body center
F: Face center
C: Edge center or Base center

Crystal System	Axial Relationships	Interaxial Angles
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$

Bravais lattices



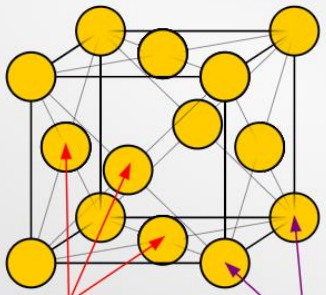
Body-Centered Cubic
BCC



One atom at the **center of the cube**

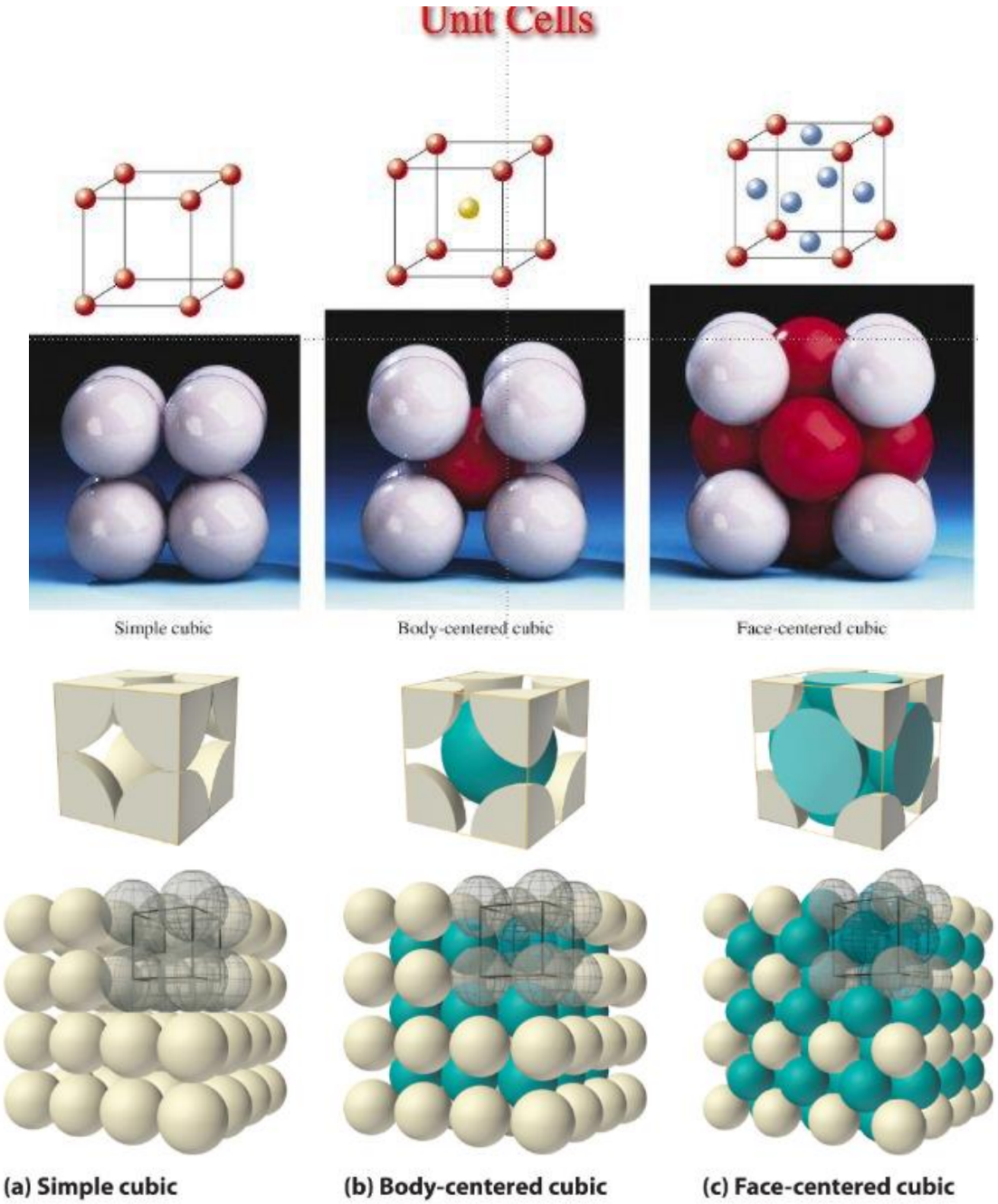
An atom at all **8 corner positions**

Face-Centered Cubic
FCC



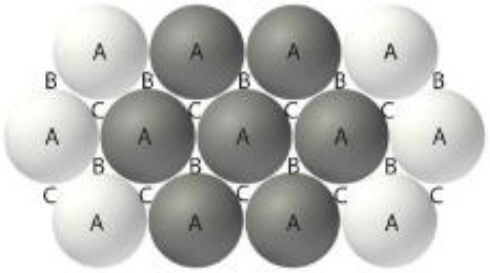
An atom at the **center of all 6 faces**

An atom at all **8 corner positions**

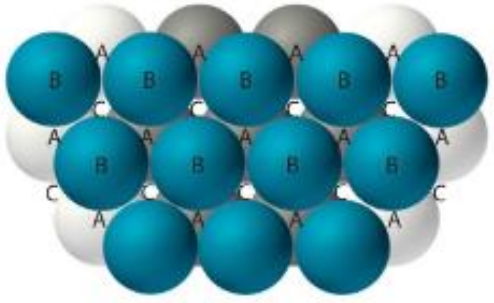


Note: All the atoms belong to the same element, colour difference is shown only to illustrate their respective positions more clearly.

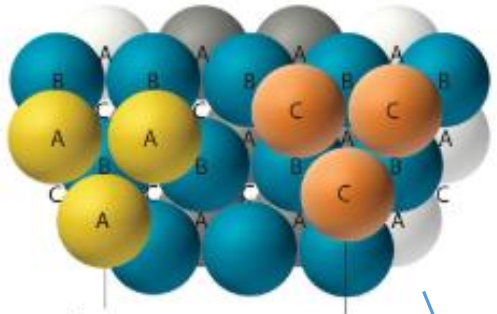
Closed Packed Structures



Single layer

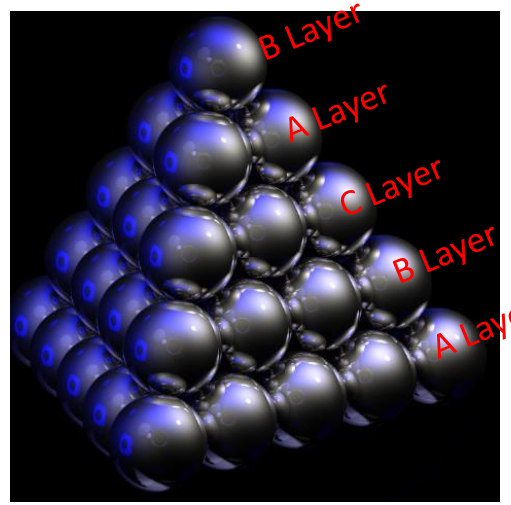


Two layers

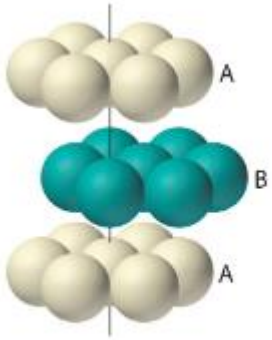


Three layers

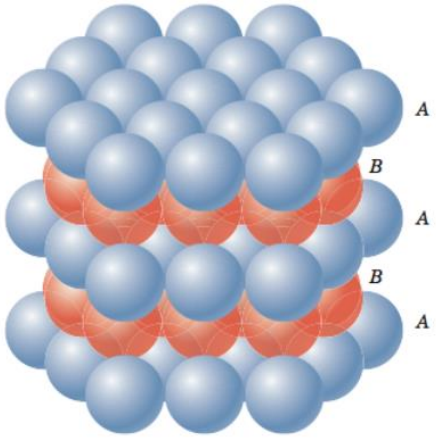
Note: All the different coloured atoms belong to the same element



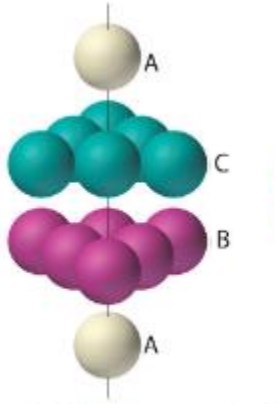
Cubic close-packed (or FCC) structure



(a) Hexagonal close-packed (hcp)

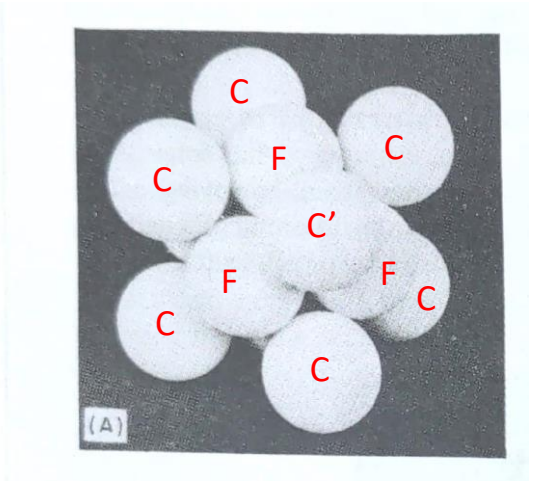


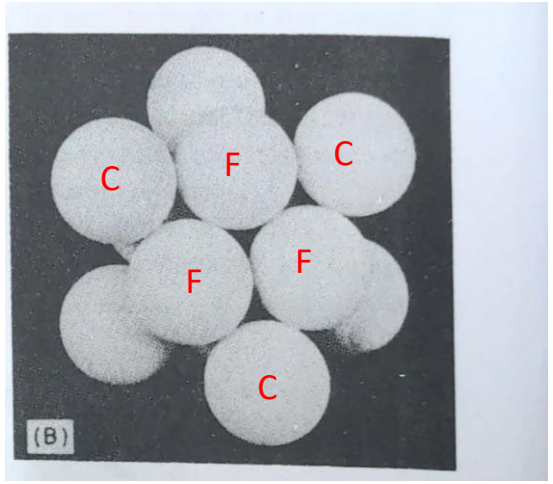
Hexagonal close-packed structure



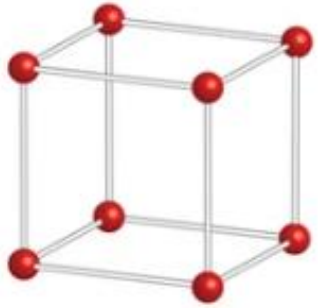
(b) Cubic close-packed (ccp)

Close Packing in FCC Unit Cell

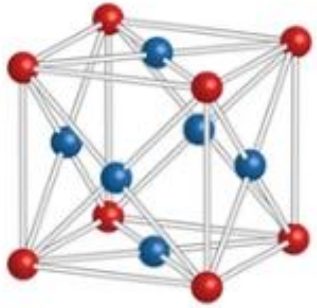




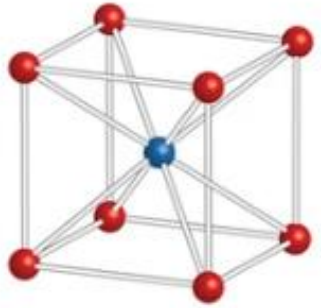
C or C' : corner atoms
F: face centering atom



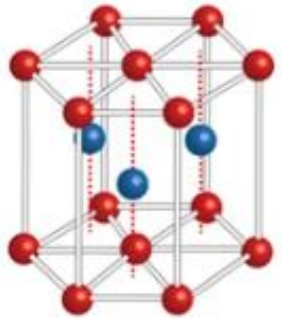
simple cubic
sc



cubic face-centered
fcc or ccp

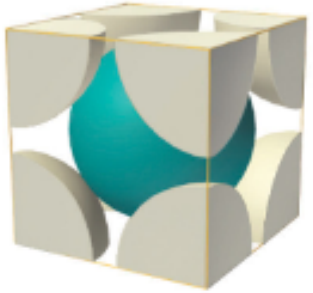


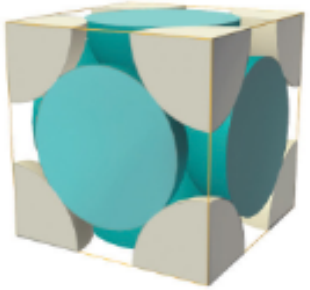
cubic body-centered
bcc



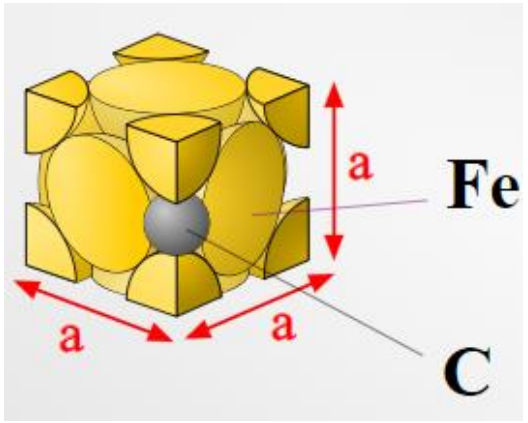
hexagonal
hcp

Alloy

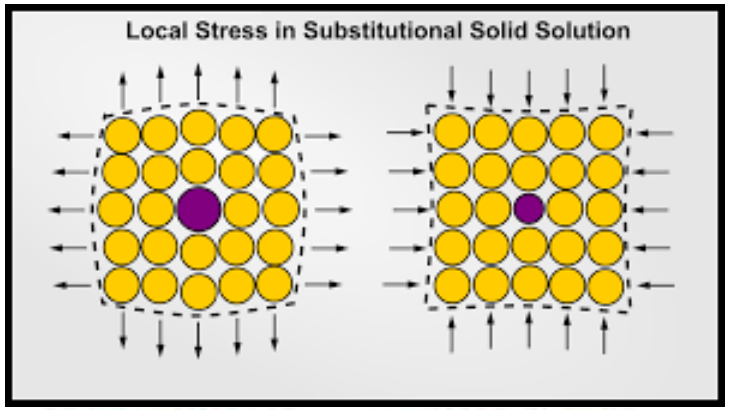


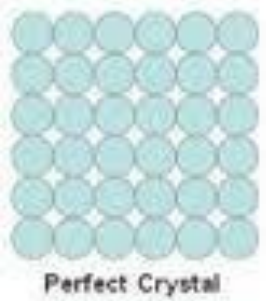


Substitutional alloys

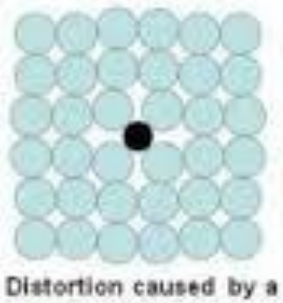


Interstitial alloy





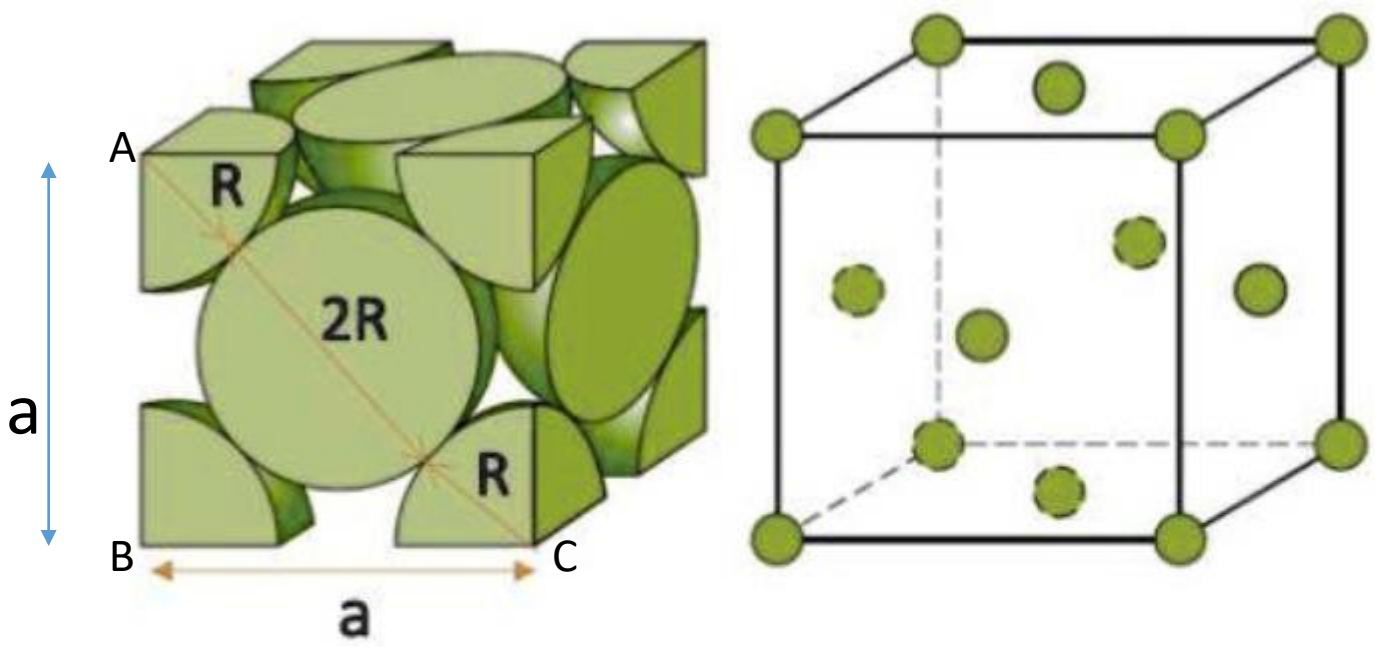
Perfect Crystal



Distortion caused by a
large interstitial atom

Lattice
Distortion

FCC



$$AB^2 + BC^2 = AC^2$$

$a = 2\sqrt{2}R$

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

$$V_S = (4)\tfrac{4}{3}\pi R^3 = \tfrac{16}{3}\pi R^3$$

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

$$\text{APF} = \frac{V_S}{V_C} = \frac{(\frac{16}{3})\pi R^3}{16R^3\sqrt{2}} = 0.74$$

a) Find the relation between R and a.
b) How many atoms are in a face centered cubic (FCC) unit cell?
c) Calculate the atomic packing factor (APF) for a face centered-cubic structure (FCC).
d) Which structure has the highest atomic packing factor: face centered cubic (FCC), body centered cubic (BCC) or simple cubic (SC).

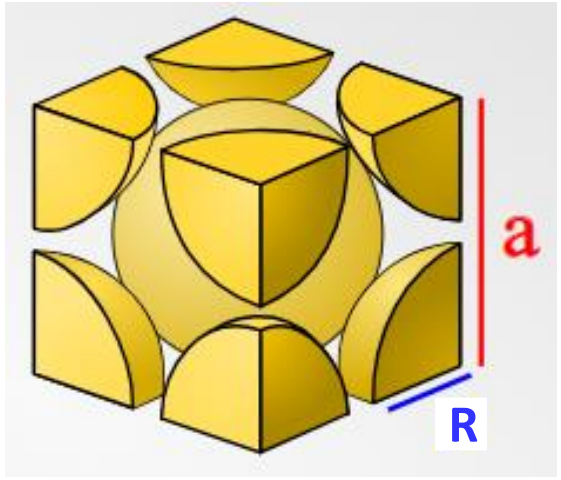
Simple Cubic

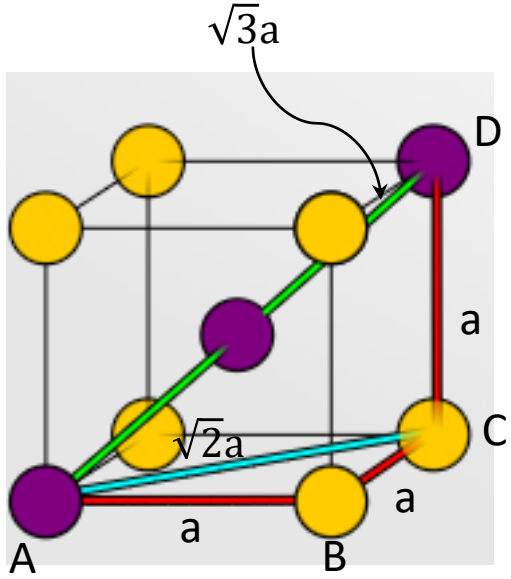
APF= 0.52

$2R = a$

APF = 0.52

BCC



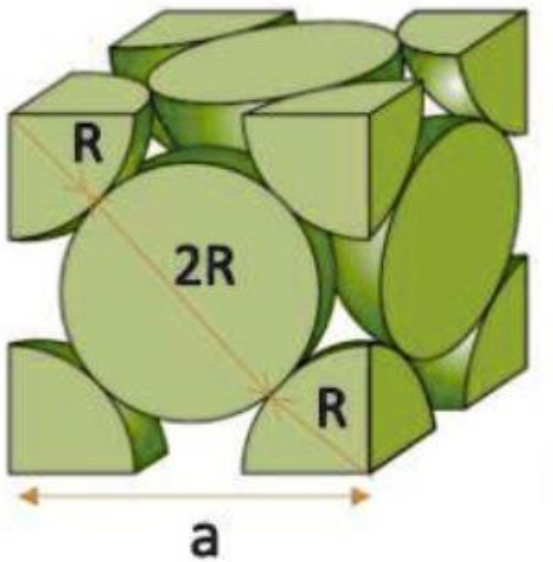


$4R = \sqrt{3}a$

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

$= 0.68$

Theoretical Density (ρ) Calculation

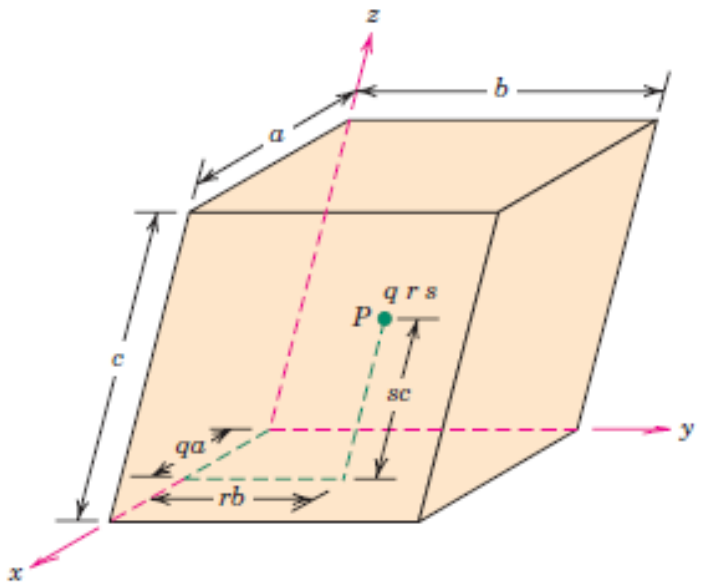


$$\rho = \frac{nA}{V_C N_A}$$

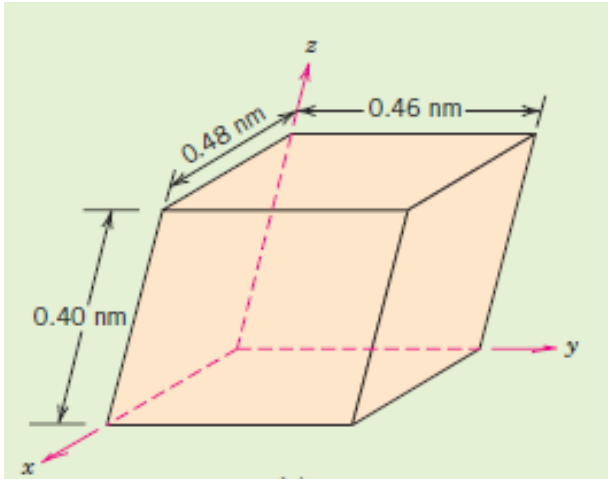
n = number of atoms associated with each unit cell
A = atomic weight
V_C = volume of the unit cell
N_A = Avogadro's number (6.023×10^{23} atoms/mol)

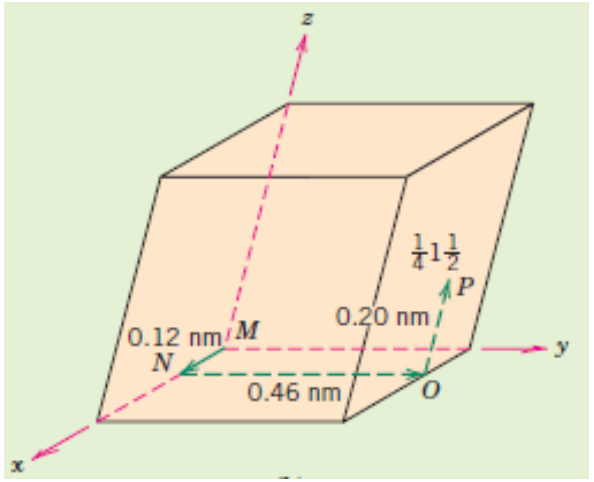
Unit cell	Number of atoms at			No. of atoms per unit cell	Volume occupied by particles (%)
	Corners	Centres	Faces		
Simple cubic	$8 \times \frac{1}{8} = 1$	0	0	1	52.4
Body centred cubic (BCC)	$8 \times \frac{1}{8} = 1$	1	0	2	68
Face centred cubic (FCC)	$8 \times \frac{1}{8} = 1$	0	$6 \times \frac{1}{2} = 3$	4	74

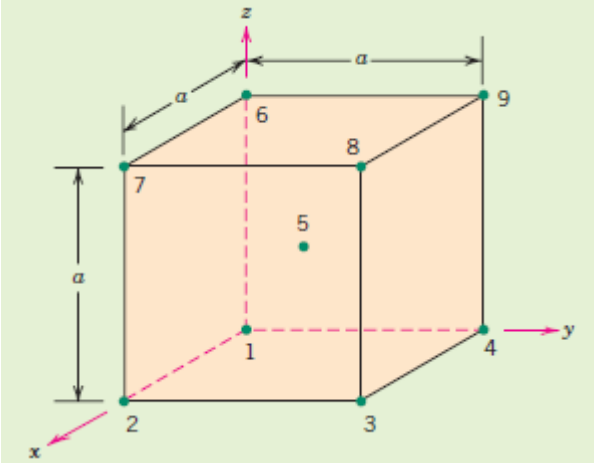
Crystallographic Points



For the unit cell shown in the accompanying sketch (*a*), locate the point having coordinates $\frac{1}{4}\,1\,\frac{1}{2}$.







Point Number	Fractional Lengths			Point Coordinates
	x axis	*y axis*	*z axis*	
1	0	0	0	0 0 0
2	1	0	0	1 0 0
3	1	1	0	1 1 0
4	0	1	0	0 1 0
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$
6	0	0	1	0 0 1
7	1	0	1	1 0 1
8	1	1	1	1 1 1
9	0	1	1	0 1 1