The Role
of
Crystal Structure – II
(Miller Indices)

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Content

- ✓ Significance of crystallographic direction and plane
- ✓ Miller indices
- ✓ Linear & Planar density

Significance of Crystallographic directions and planes

- ✓ **Deformation** under loading (eg. slip) occurs on certain crystalline **planes** and in certain crystallographic **directions**.
- ✓ Helps to predict **modes** of **material failure**.
- ✓ **Other properties** of materials (electrical conductivity, thermal conductivity, elastic modulus, magnetic property, piezoelectric property etc.) can vary in a crystal with **orientation**.

Example

Turbine blade

Image : http://www.swansea.ac.uk/

Efficient strong Ni based single crystal turbine blades withstand high temperature due to absence of grain boundaries because blades are grown on close packed direction [1 1 0] FCC Ni.

GaAs lasers in CD players are grown from GaAs single crystals grown along [1 0 0] direction.

CD player laser

Silicon ingots and wafers in various sizes

Image : http://www.chipsetc.com/

Computer chips come from Si wafers sliced from single crystal Si grown along [1 0 0] direction.

Miller Indices

- Miller Indices are the **designation of the planes and direction** in the unit cell.
- The number of indices will match with the dimension of the lattice or the crystal. Example: In 3-D, unit cell has 3 indices namely **(h k l)**.
- **(h, k, l)** represents a point – but "no comma" is used while representing indices.

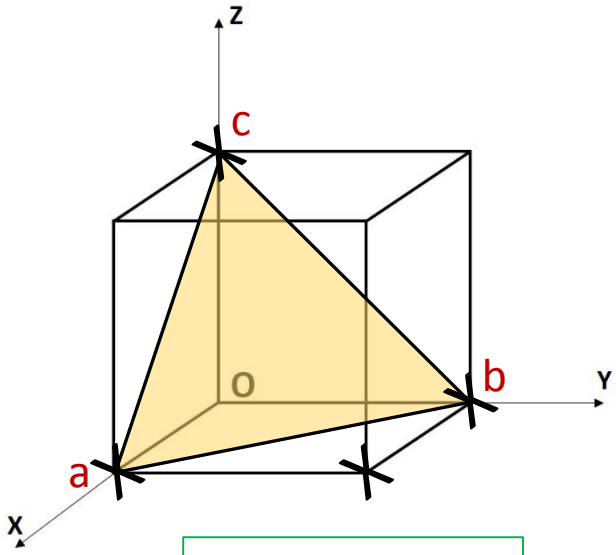
Meaning of the different brackets

Name	Symbol	Meaning
Half-moon Bracket	**( )**	Individual Plane - (1 0 0)
Curly Bracket	**{ }**	Family of Planes {1 0 0} = (1 0 0), (0 1 0), (0 0 1)
Square bracket	**[ ]**	Individual direction - [1 0 0]
Carrot Bracket	**< >**	Family of Directions <1 0 0> = [1 0 0], [0 1 0], [0 0 1]

How to find Miller Indices of a given plane?

Steps involved

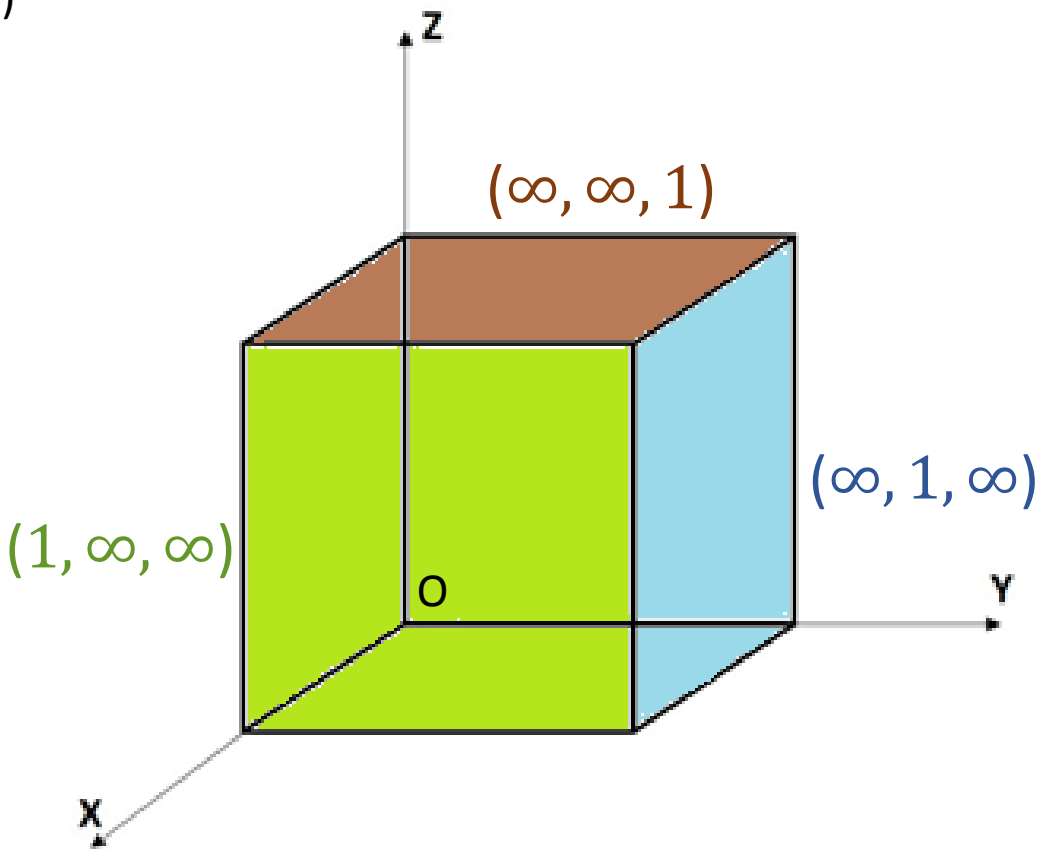
- **Choose origin** O in unit cell such that
  - ✓ Plane does not touch the origin.
  - ✓ Plane is closest to the origin.
- **Mark intercepts** from chosen origin O along X-axis as '**a**', from O along Y-axis as '**b**' and from O along Z-axis as **'c'**.
- **Take reciprocal** of the intercepts, i.e.,1/a, 1/b, 1/c.
- **Modify the reciprocal**
  - ✓ Reduce multiples.
  - ✓ Eliminate fraction
  - ✓ Put bar above the negative integer in indices (if any)
  - ✓ Place round bracket around indices (no commas)



Answer: (1 1 1)

Thus, Miller Indices (h j k) are the reciprocals of the parameters (l, m, n) of each crystal face.

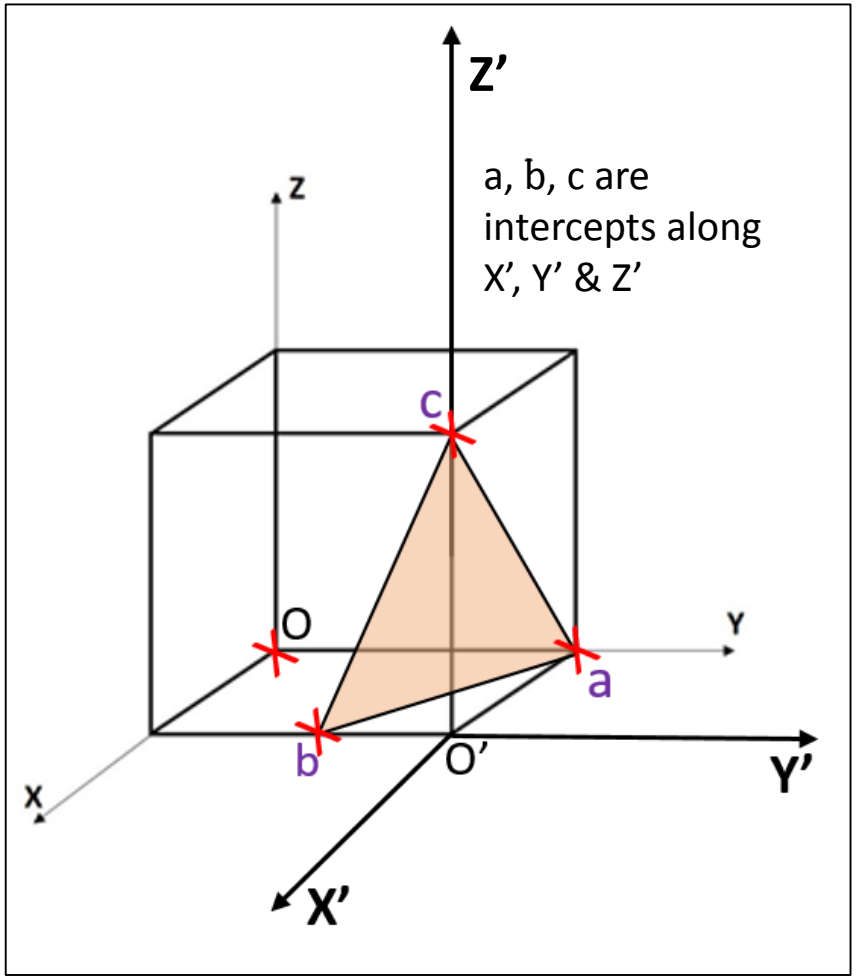
- **Green Face** = (1/1, 1/∞, 1/∞) = (1 0 0)
- **Brown Face** = (1/ ∞, 1/ ∞, 1/1) = (0 0 1)
- **Blue Face** = (1/ ∞, 1/1, 1/ ∞) = (0 1 0)



Determine the indices for the given plane.

- Plane cannot touch origin
- Choose closest origin

1.Choose new Origin (O')	1	1	0
Unit cell intercepts	a	b	c
2. Intercept from origin (O')	-1	$\frac{-1}{2}$	1
3. Reciprocal value	-1	-2	1
4. Miller Indices		$(\bar{1}\ \bar{2}\ 1)$	

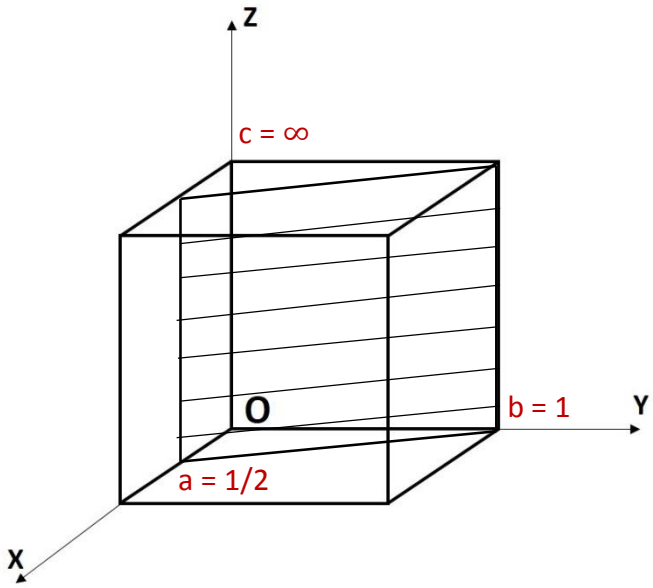


Determine the indices for the given plane.

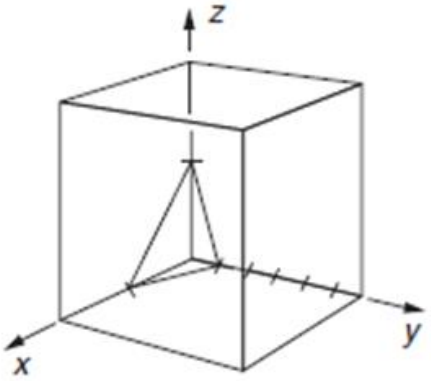
- Plane cannot touch origin
- Choose closest origin

This plane cuts two of the reference axes(X & Y) at intercepts a & b

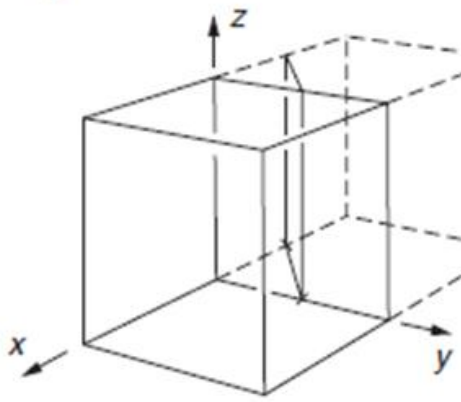
1.Choose Origin (O)	0	0	0
Unit cell intercepts	a	b	c
2. Intercept from origin (O)	$\frac{1}{2}$	1	∞
3. Reciprocal value	2	1	0
4. Miller Indices	(2 1 0)		



Miller indices – more examples (given plane)



	x	y	z
Intercepts	1/2	1/6	1/2
Reciprocals	2	6	2
Lowest integers to give same ratio	1	3	1
Quote	(131)		



x	y	z
1/2	1/2	∞
−2	2	0

$(\bar{1}10)$

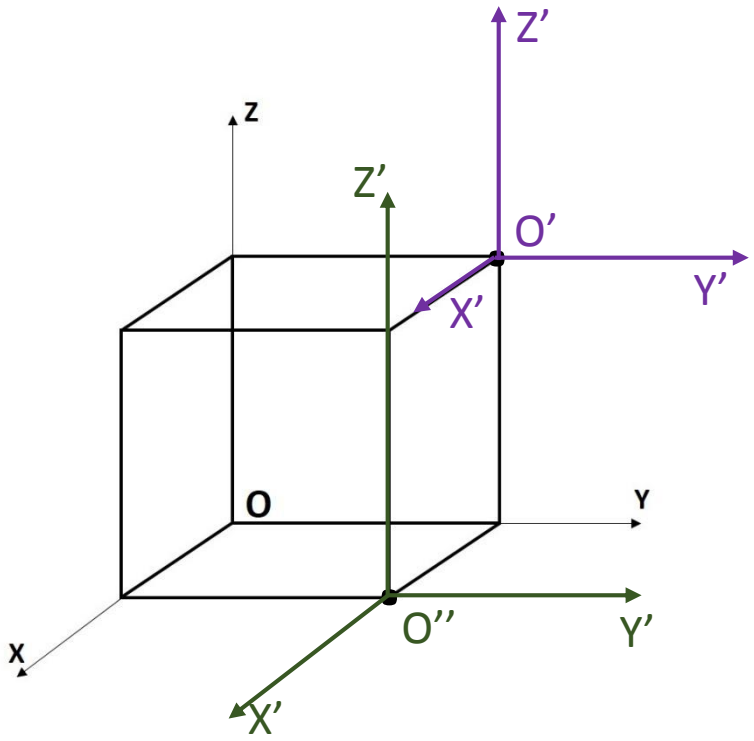
Reference: Engineering Materials 1: Ashby & Jones, 4th Ed.

Selecting the Origin – Indices with bar

- If there is a bar over the number (x, y or z), the new origin O' should have a '1' in the same place as number with a bar.
- If there is not a bar over the number, the new origin O' should have zero '0' in the same place as the non-bar number.

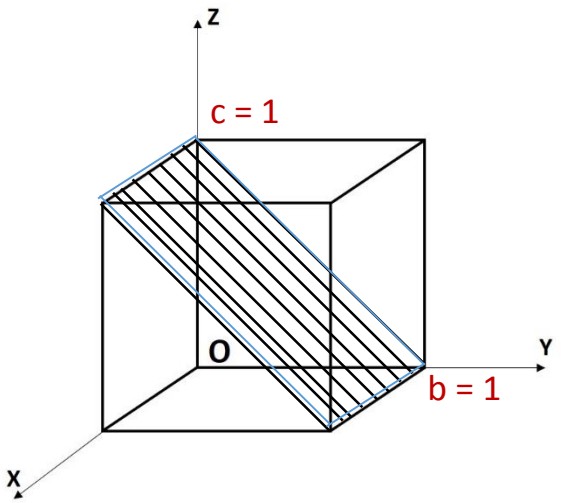
Number with bar, then replace $\bar{N}$ = 1
If no bar over the number, then N = 0

Indices	New Origin
(0 1 2)	X = 0, Y = 0, Z = 0 (No change)
$(0\ \bar{1}\ \bar{1})$	**X'= 0, Y'= 1, Z'= 1**
$(\bar{1}\ \bar{2}\ 2)$	**X''= 1, Y''= 1, Z''= 0**



Given Indices (h k l) > Draw the Plane

- Select origin O at (0,0,0) OR if there are negative indices then origin at O’ in X’, Y’, Z’ frame.
- Take reciprocal of indices to get 1/h, 1/k, 1/l : which will be the intercept.
- Mark intercept along x, y, z axes at a, b, c.
- Draw plane by connecting intercepts (a, b, c).

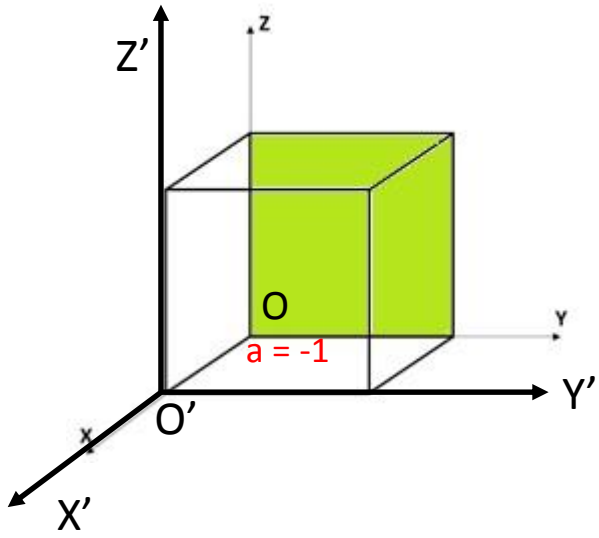


Given Indices (0 1 1) > Draw the Plane

1.Choose Origin (O)	0	0	0
2. Reciprocal value of indices (0 1 1)	∞ (parallel to x-axis)	1	1
Unit cell intercept	a	b	c
3. Mark & connect intercepts	Draw Plane		

Given Indices ($\bar{1}$ 0 0) > Draw the Plane

1.Choose Origin (O’)	1	0	0
2. Reciprocal value of indices ($\bar{1}$ 0 0)	-1	∞ (parallel to Y-axis)	∞ (parallel to Z-axis)
Unit cell intercept	a	b	c
3. Mark & connect intercepts	Draw Plane		



Families of plane – are "Equivalent"

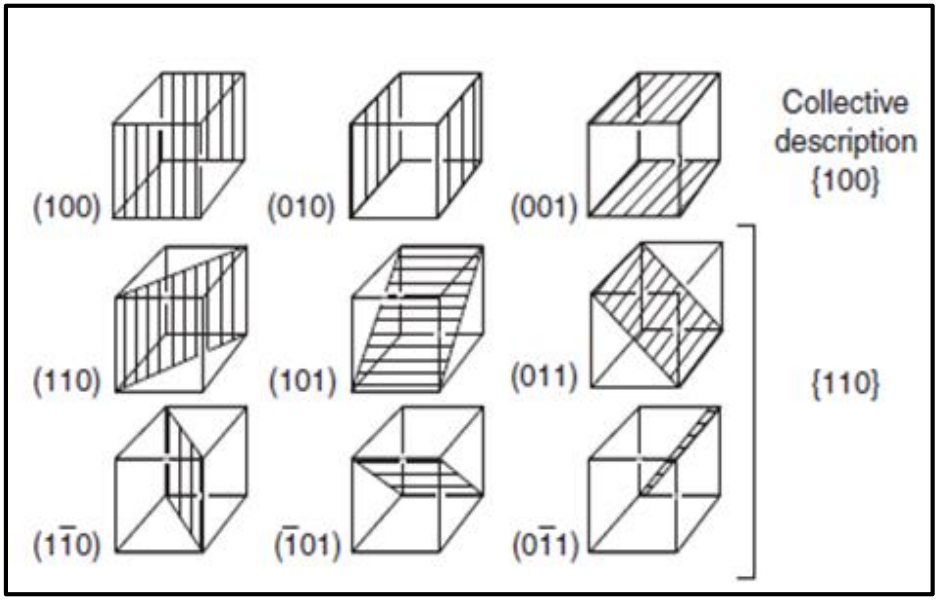
- Different planes having same index in their miller indices (not necessarily in same order) is shown by Miller indices of family of planes.

✓ Same Packing density

✓ Same environment

✓ Denoted by curly bracket {H K L}

For cubic system, indices of a family of plane is given by all permutation(+ & -) of 3 integer indices.

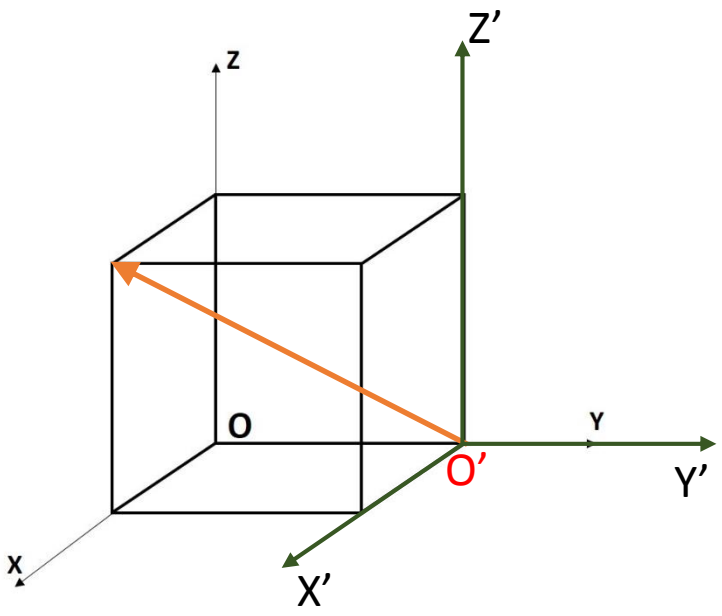


Reference: Engineering Materials 1: Ashby & Jones, 4th Ed.

How to find Miller Indices of a given direction ?

Given direction > determine **indices** [? ? ?].

- Create **new origin** O’ at **tail**, if necessary.
- Label O’ and new axes X’, Y’ & Z’.
- Find coordinates from tail at O’ to the head of direction.
- Reduce multiples, eliminate fractions, use ‘bar’ for negative.
- Place square bracket “[ ]” around integer.



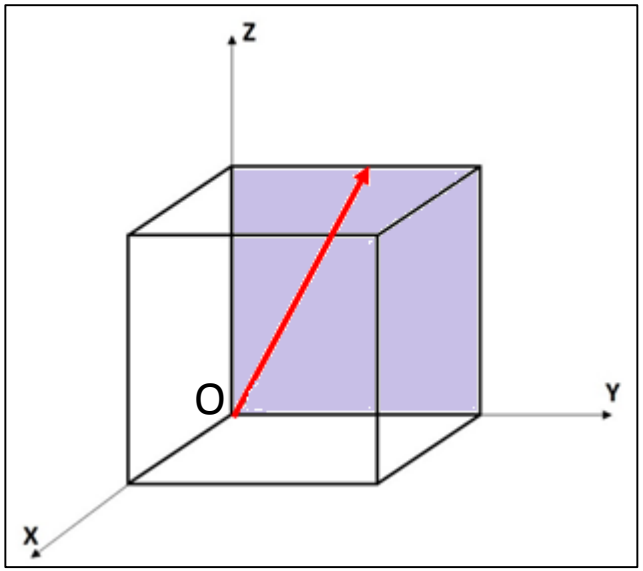
Ans : [1 $\bar{1}$ 1]

Drawing directions from Indices

Example

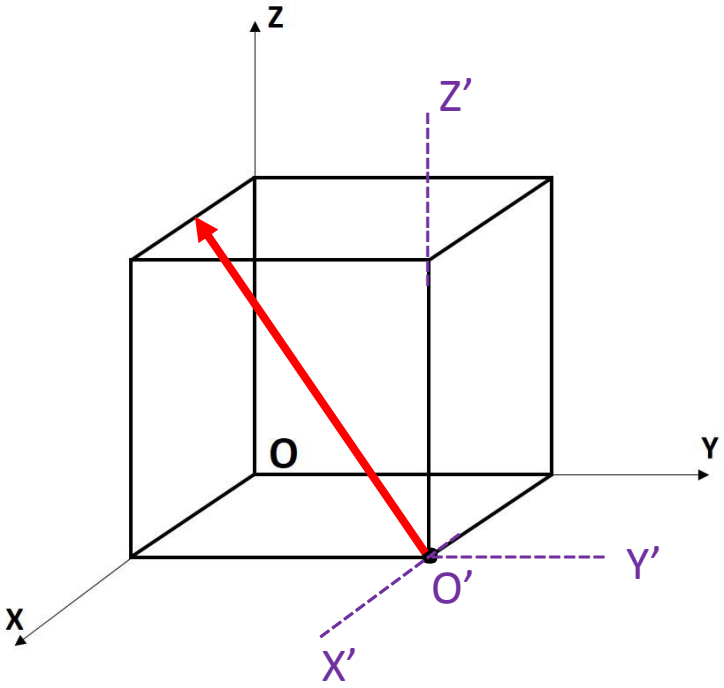
Given indices **[0 1 2]** > draw direction.

- **Select** origin O at (0,0,0) OR choose new O' if there are negative indices.
- **Reduce** indices to keep direction within unit cell (in this case divide by 2).
- **Locate** from origin at (0,0,0) to a position (0, ½ ,1) in the unit cell.
- **Draw** direction from tail (0,0,0) to arrow tip at (0, ½ ,1)



Draw the **specified direction** in the unit cell with **indices given** as **$[\bar{1}\ \bar{2}\ 2]$.**

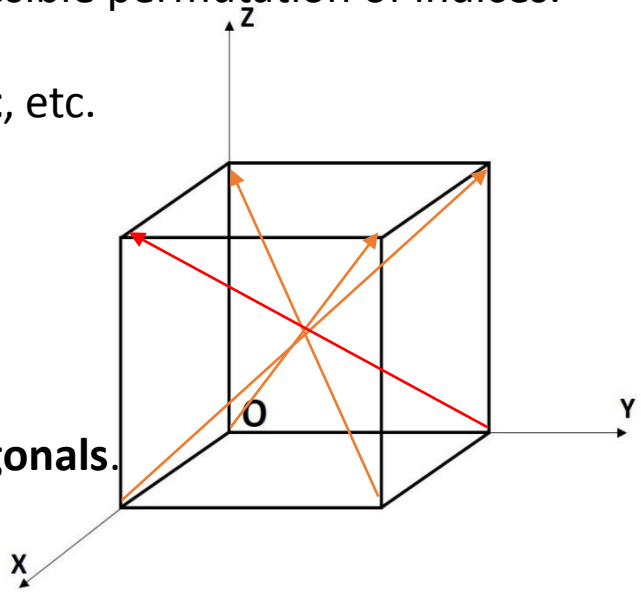
- Select new origin O’ as (1,1,0)
- Reduce $[\bar{1}\ \bar{2}\ 2]$ to -1/2, -1, 1 with in the unit cell
- Locate the coordinates.
- Draw direction from origin to the coordinates.



Unit Cell families of Direction

- Composed of unique unit cell direction that are "**equivalent**".
- In cubic system members of a family are given by all possible permutation of indices.
- **Same properties, packing densities, same environment**, etc.
- Denoted by integers in a "**Carrot Bracket**", <U V W>
- Example : Specify all unique direction in family <1 1 1>

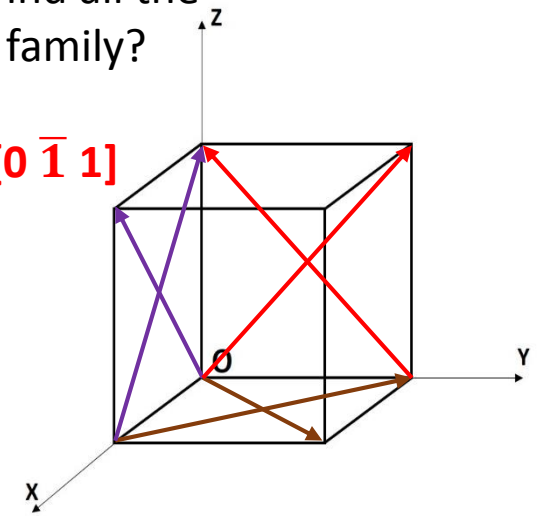
<1 1 1> : [1 1 1], [$\bar{1}$ 1 1], [1 1 $\bar{1}$], [1 $\bar{1}$ 1] called **Body Diagonals**.



Identify and draw unit cell families of direction

Find all of the unique direction for the given family. Find all the indices, draw the direction and give the name of the family?

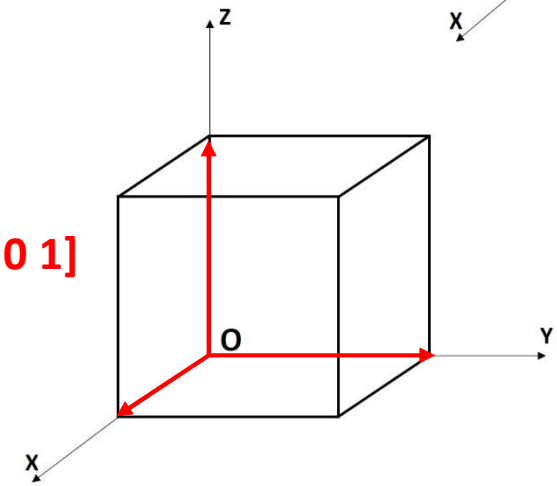
A) <1 1 0> = **[1 1 0], [$\bar{1}$ 1 0], [$\bar{1}$ 0 1], [1 0 1], [0 1 1], [0 $\bar{1}$ 1]**



Face diagonals

(parallel directions are not unique)

B) < 1 0 0> = **[1 0 0], [0 1 0], [0 0 1]**



Cube Edges

Always remember

What do the different brackets mean?

Name	Symbol	Meaning
Half-moon Bracket	**( )**	Individual Plane (1 0 0)
Curly Bracket	**{ }**	Family of Planes {1 0 0} = (1 0 0), (0 1 0), (0 0 1)
Square bracket	**[ ]**	Individual direction [1 0 0]
Carrot Bracket	**< >**	Family of Directions <1 0 0> = [1 0 0], [0 1 0], [0 0 1]

Properties of Miller Indices

- **Miller indices** of **equally spaced** parallel planes are the **same**.
- Miller indices of a **plane passing** through the ***origin*** is shown by a miller indices of a **plane parallel** to it.
- If two planes having miller indices as (h_1 k_1 l_1) and (h_2 k_2 l_2) are **perpendicular** to each other.

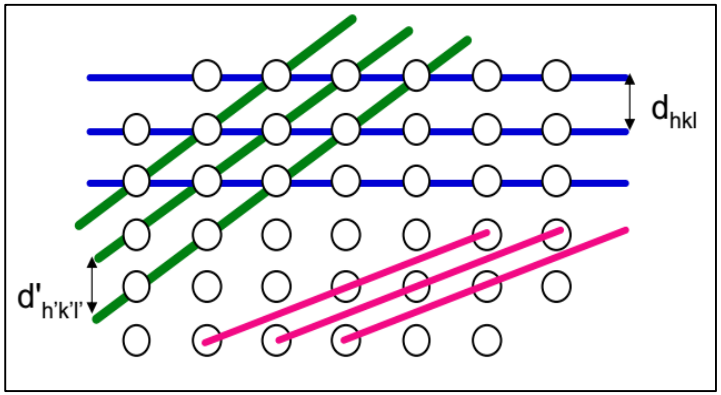
  then, $h_1h_2 + k_1k_2 + l_1l_2 = 0$
- All **members** of **family of planes** or **directions** are **not necessarily parallel** to one another.

Inter Planer Spacing (d_{hkl})

- Distances between planes defined by the same set of Miller indices.
- Members of family of planes have the same inter planer spacing.

Inter planer spacing (**cubic only**), $d_{hkl} = \frac{(cube\ side\ length)}{\sqrt{h^2+k^2+l^2}}$

Inter planer angle (**cubic only**), $\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2+k_1^2+l_1^2}\sqrt{h_2^2+k_2^2+l_2^2}}$



Ref: http://www.uio.no/studier/emner/matnat/fys/FYS3410/v09/undervisningsmateriale/Lecture2AK_1.pdf

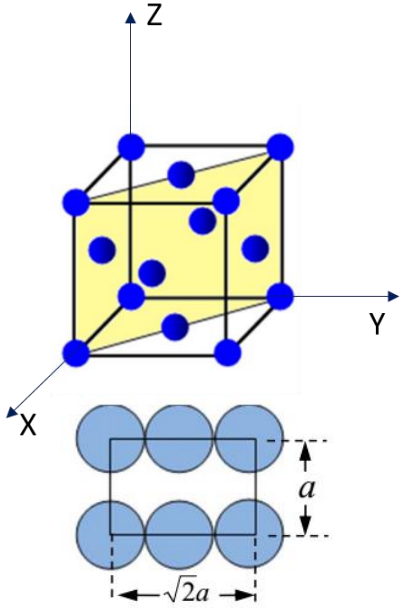
Planar density

Planar density , PD = $\frac{\text{No. of effective atoms per unit area}}{\text{Area of plane}}$

Planar density of (110) plane in the FCC crystal

No. of effective atoms per unit area = $\frac{1}{4}$ x 4 corner atoms + $\frac{1}{2}$ x 2 side atoms = 2

$$PD_{(110)} = \frac{2}{a\sqrt{2}a} = \frac{\sqrt{2}}{a^2}$$



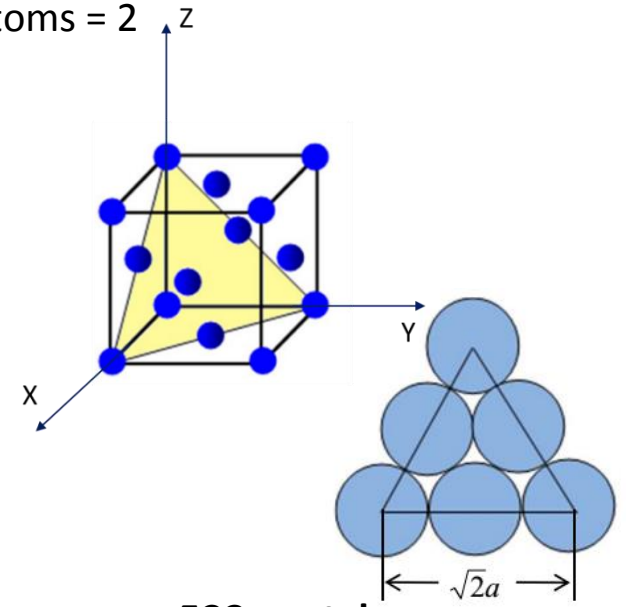
FCC crystal

Planar density of (111) plane in the FCC crystal

No. of effective atoms per unit area = $\frac{1}{6}$ x 3 corner atoms + $\frac{1}{2}$ x 3 side atoms = 2

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

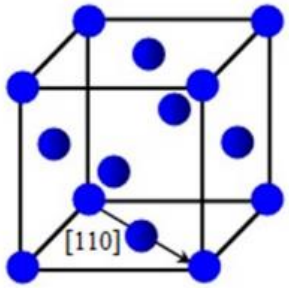
This is higher than [110} and any other plane. Therefore, **(111) plane** is the **most densely packed plane** in the **FCC** crystal



FCC crystal

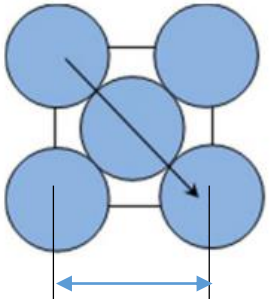
Linear density

$$\text{Linear density , LD} = \frac{\text{No. of effective atoms on a line}}{\text{Length of direction vector}}$$



Linear density in [110] direction in the FCC crystal

$$LD_{[110]} = \frac{\text{No. of effective atoms on a line}}{\text{Length of direction vector}} = \frac{\frac{1}{2}+1+\frac{1}{2}}{\sqrt{2}\,a} = \frac{2}{\sqrt{2}\,a}$$



FCC crystal

This is the most densely packed direction in the FCC lattice.

Similarly for BCC crystal
Highest atomic density plane: (110)
Highest atomic density direction: [111]

- ✓ Deformation in metals depends on linear and planar density.
- ✓ **Slip occurs** on most **densely packed** crystallographic **planes** and along **directions** having the **greatest atomic packing** due to **lower shear stress/energy requirement**.

The Role of Crystal Structure – III

(Crystal defects)

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

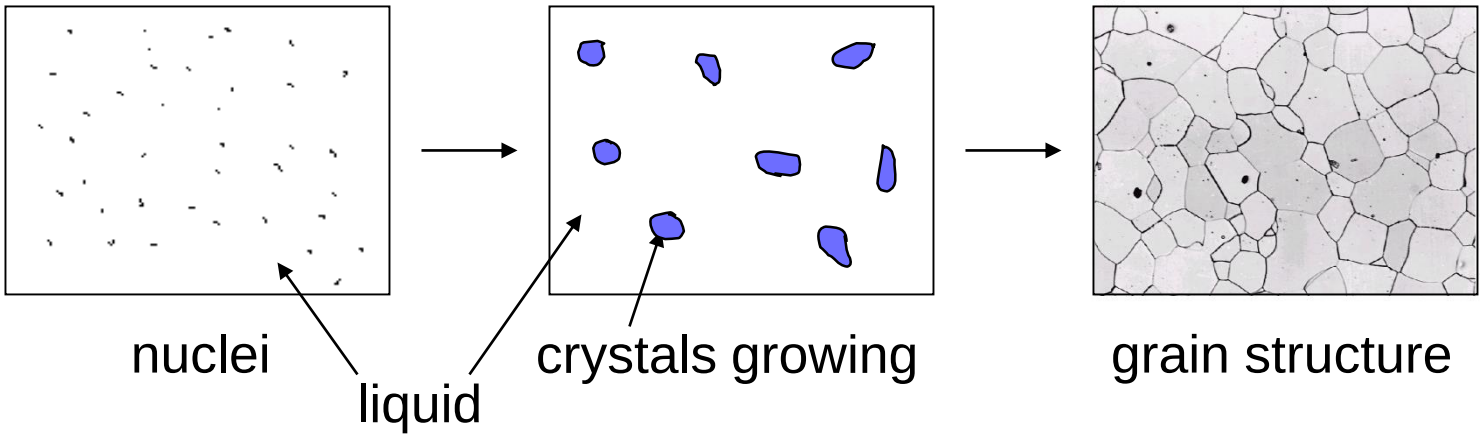
Contents

Crystal Defects

- ✓ Introduction
- ✓ Point defects
- ✓ Line defects
- ✓ Plane defects
- ✓ Volume defects

Solidification

- Result of casting of molten material.
  - ❖ 2 steps
    - ✓ Nucleation (site of new thermodynamic phase)
    - ✓ Nuclei grow to form crystals – grain structure
  - ➢ Start with a molten material – all liquid.
  - ➢ Crystals grow until they meet each other.



Crystal Defects

- Any **deviation** from completely **ordered arrangement** of constituent particles in a crystal is called a "**Defect or Imperfection**".
- **Properties** of material are **influenced** by the **presence** of **imperfections**.
- **Mechanical properties** of pure metal **change significantly** when metals are alloyed.

  Yield strength of **Pure Copper** (Cu) : 117 MPa
  Yield strength of **Brass** (70% Cu + 30% Zinc) : 200 MPa
- Thus, it is important to have knowledge about the types of imperfections that exist and the roles they play in affecting the behavior of materials.

Classification

Based on shape and size of defects :

- **Point defects** (zero dimensional)
  - ✓ Vacancy defect
  - ✓ Interstitial defect
  - ✓ Substitutional defect
  - ✓ Frenkel defect
  - ✓ Schottky defect
- **Line defects / Dislocations** (One dimensional)
  - ✓ Edge dislocation
  - ✓ Screw dislocation
  - ✓ Mixed dislocation
- **Plane defects** (Two dimensional)
  - ✓ Grain boundaries
  - ✓ Twin boundaries
- **Volume defects** (Three dimensional)
  - ✓ Pores
  - ✓ Cracks, etc.

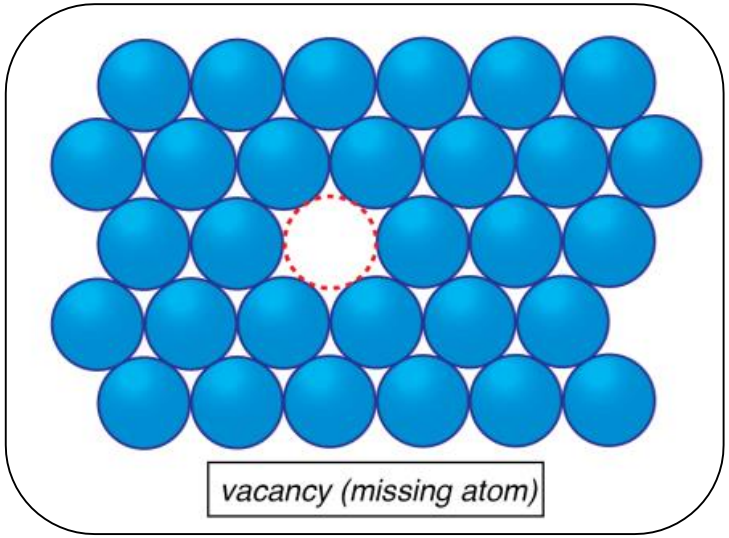
Extended defects

Point defects

(associated with atomic sites)

Vacancy defect

- When an **atom** is **missing** from its **regular lattice site**, it is called a Vacancy.
- Impossible to create a material free from vacancy defects.
- Presence of vacancies increases the entropy/disorderness in the crystal.
- Decreases the density of substance.
- The concentration of vacancies increases with
  - Increasing temperature.
  - Decreasing activation energy (Q_v) - **energy** required for the **formation of vacancies**



$$No.\ of\ vacancies, Nv = N\ exp\left(\frac{-Q_v}{kT}\right)$$

Where, **N** is the total no. of potential defect sites (each lattice site is potential defect site),
Q_v is the activation energy ,
k is Boltzmann constant = 1.38×10^{-23} J/atom-K or 8.62×10^{-5} eV/atom-K
T is absolute temperature in Kelvin

Reference: W.D Callister, 7 Ed.

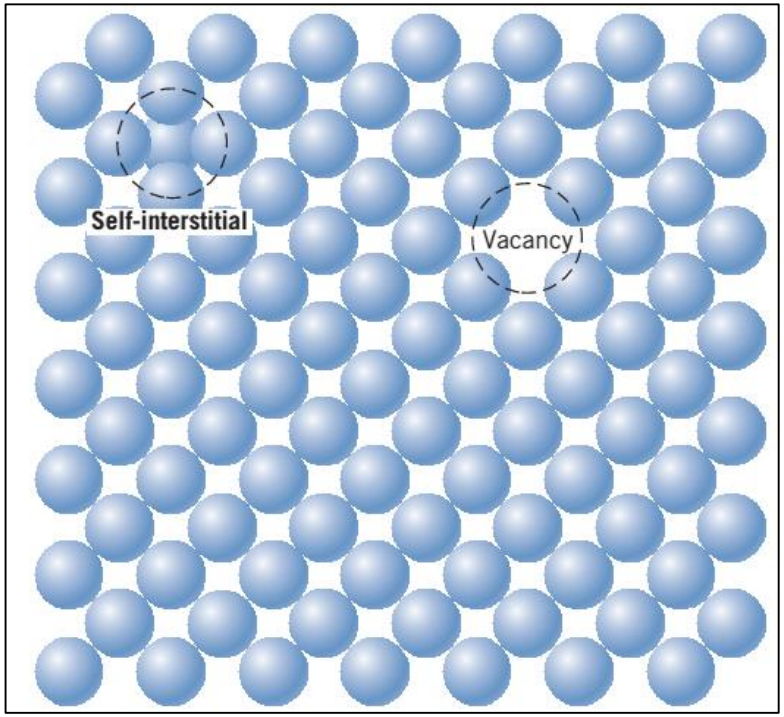
Self-interstitial defect

- **Atom from the crystal** occupies a position in between the **atomic sites** called as **self-interstitial defect.**
- **Vacancies** and **Self-Interstitial** are **inverse phenomenon**.
- In metals, it introduces relatively large distortions (strain) in the surrounding lattice since the atom is substantially larger than the interstitial site.
- When a **foreign atom** occupies an **interstitial site** called an **Interstitial defect**.
- **Interstitial defect** increases the density of the substance.

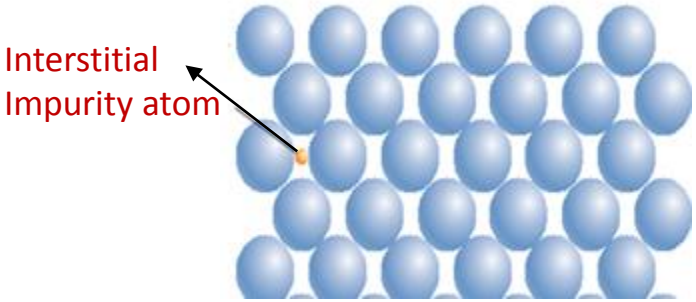
Example:

✓ Carbon forms an interstitial solid solution when added to iron.

✓ The atomic radius of the carbon (0.071 nm) atom is much less than that for iron (0.124 nm)



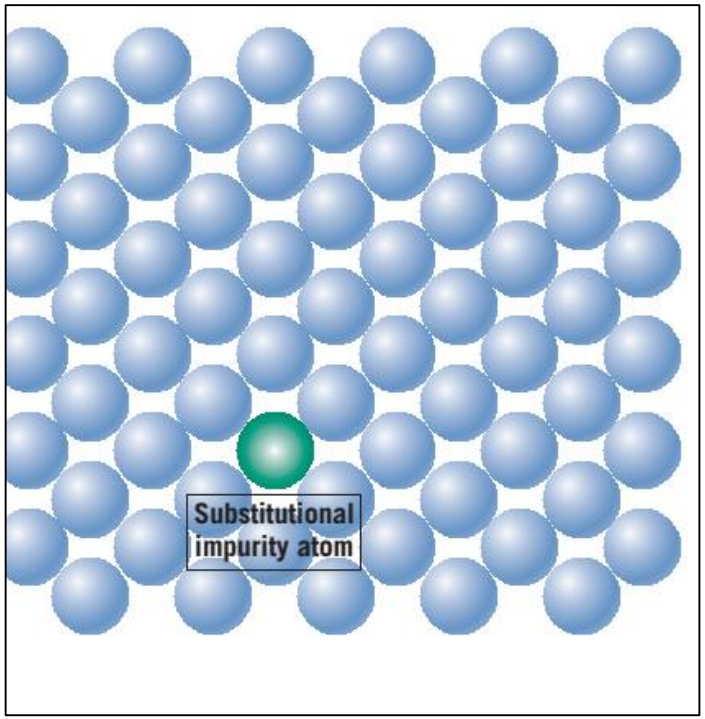
Vacancy and a self-interstitial



Reference: W.D Callister, 7 Ed.

Substitutional defect

- A Substitutional defect is introduced when one atom replaced by a different type of atom.
- **Crystal structures** of both atom types must be the **same** and almost equal electronegativity's.
- The **substitutional** atom **occupy** the **normal lattice** site.
- The substitutional defects can be introduced either as an impurity or as alloy addition.
- **Example**: Cu (0.128 nm) & Ni (0.125 nm) form substitutional solid solution (both FCC) and are completely soluble at all proportions.

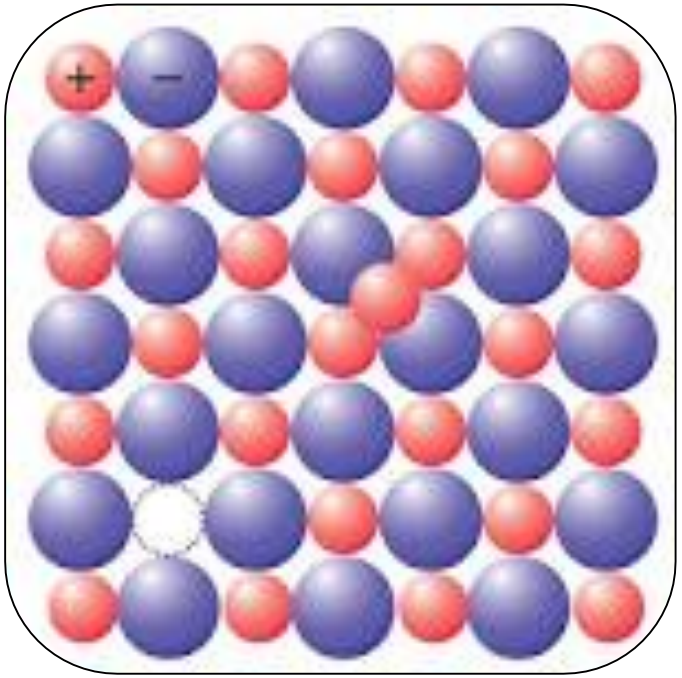


Substitutional defect

Reference: W.D Callister, 7 Ed.

Frenkel defect

- It is a **combination** of **Vacancy** and **Interstitial defect**.
- Occurs when an atom or ion **leaves** its **regular site** and **occupies** an **interstitial site**, it is known as **Frenkel defect**.
- Cations being smaller in size gets displaced to interstitial voids.
- **No change** in the **density** occurs.
- Found in ionic compounds with **low coordination numbers.**
- Example : AgI, CaF_2



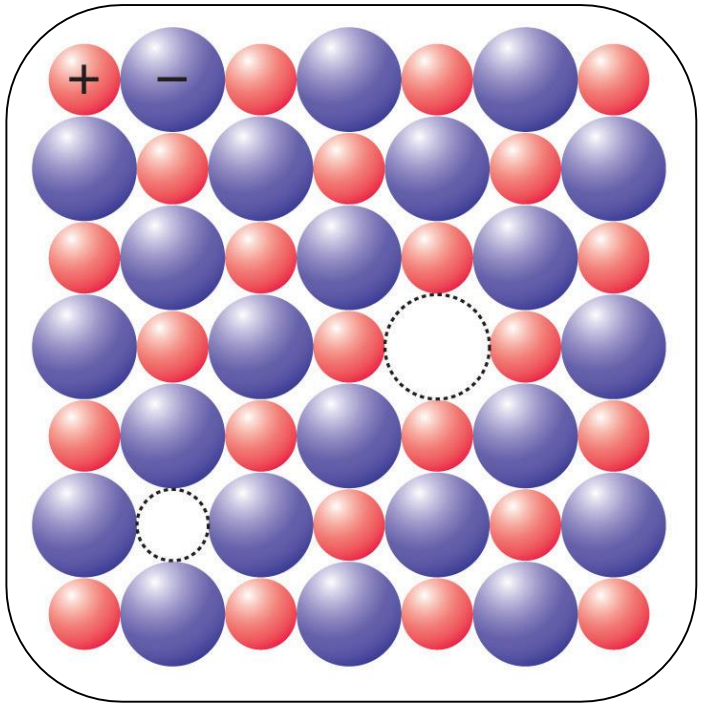
Frenkel defect

Image courtesy: http://www.majordifferences.com/

Schottky defect

- Associated with a **paired set** of cation and anion vacancies.
- **Density** of the solid **decreases**.
- Found in ionic compounds with **high coordination numbers.**
- In order to maintain electrical neutrality, the number of **missing cations** and **anions** are **equal**.
- Example : Alkali halides such as NaCl, KF, etc.

In both Frenkel and Schottky – No change in **electrical neutrality** of the crystal



Schottky defect

Image courtesy: http://www.majordifferences.com/