The Role

of

Crystal Structure – III

(Crystal defects)

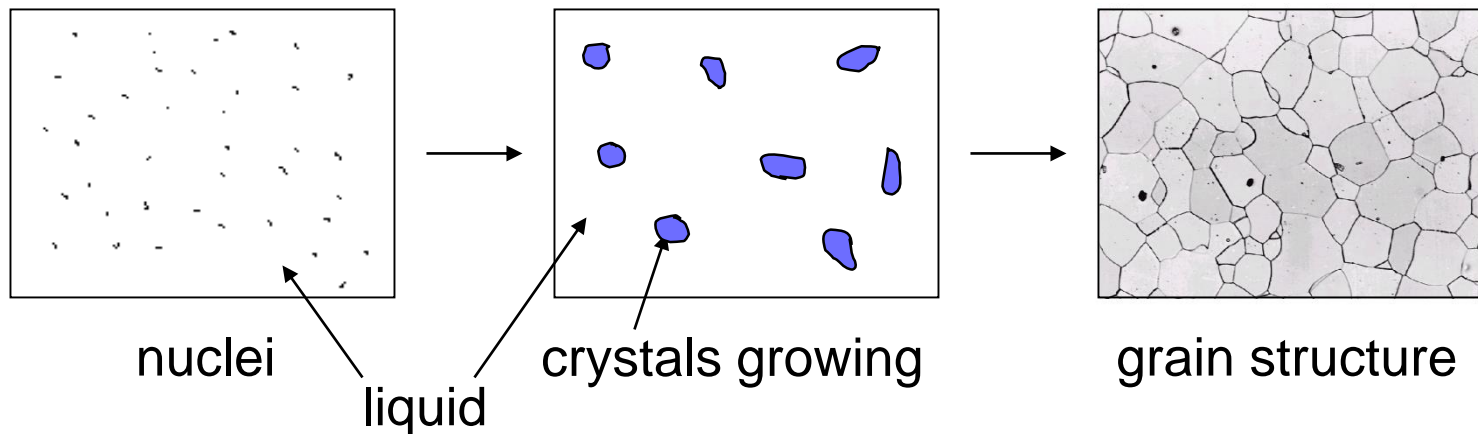# Contents

Crystal Defects

✓ **Introduction**

✓ **Point defects**

✓ **Line defects**

✓ **Plane defects**

✓ **Volume defects**

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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.

nuclei   crystals growing   grain structure

liquid

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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**

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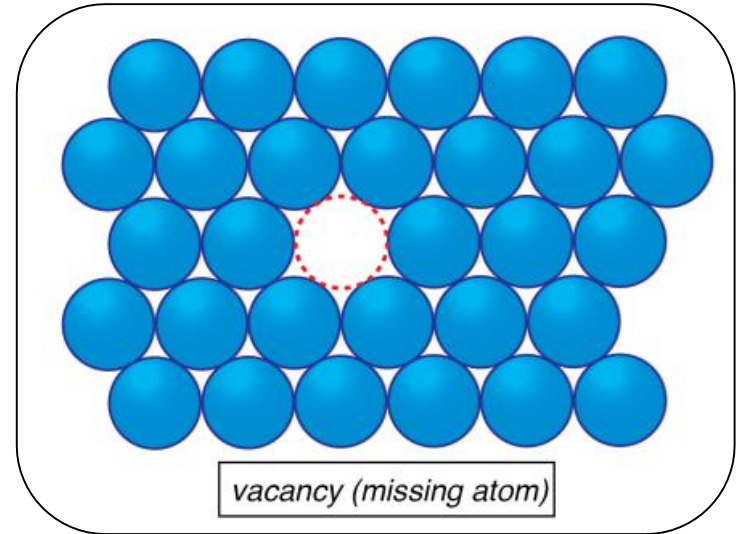
$$No. of\ vacancies, Nv = N\ exp\left(\frac{-Q_v}{kT}\right)$$

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 = 1.38x10^{-23} J/atom-K or 8.62x10^{-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)
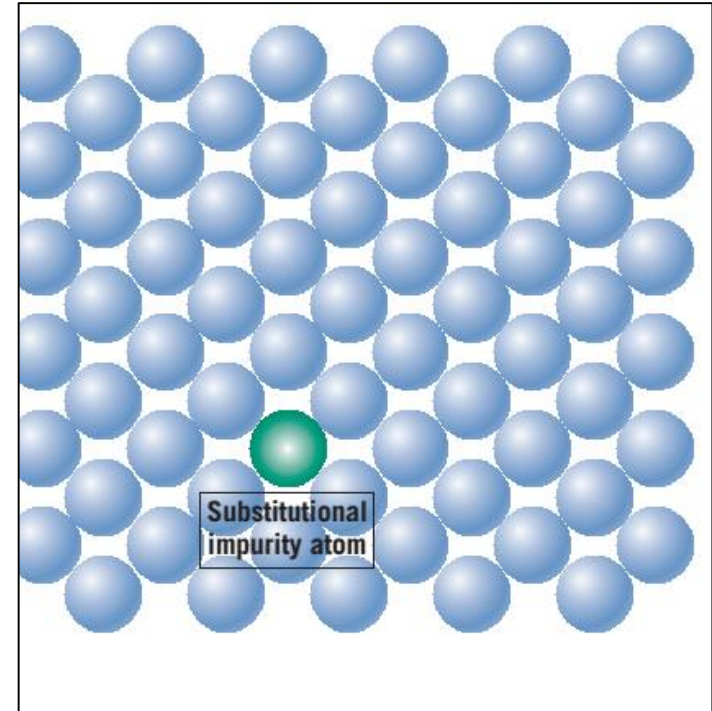

Self-interstitial
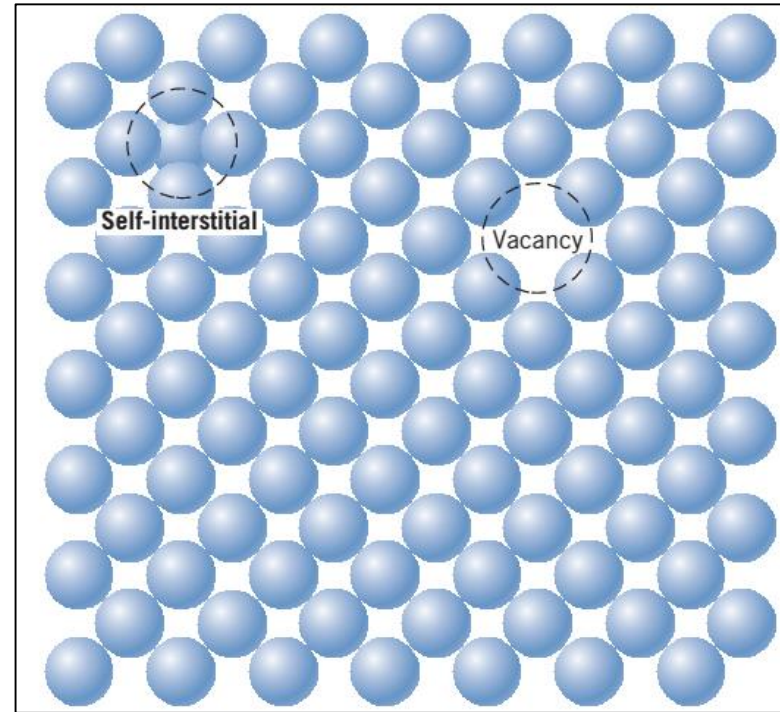
Vacancy

Vacancy and a self-interstitial

Interstitial Impurity atom
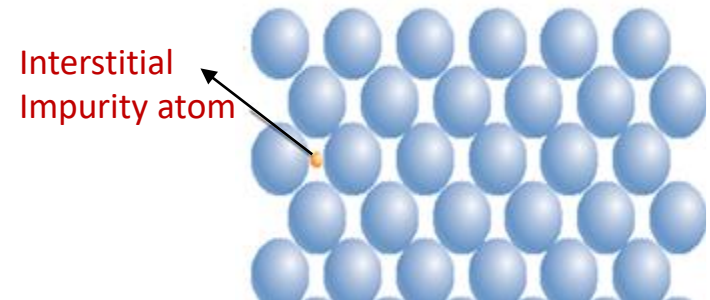
Substitutional defect

- 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

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
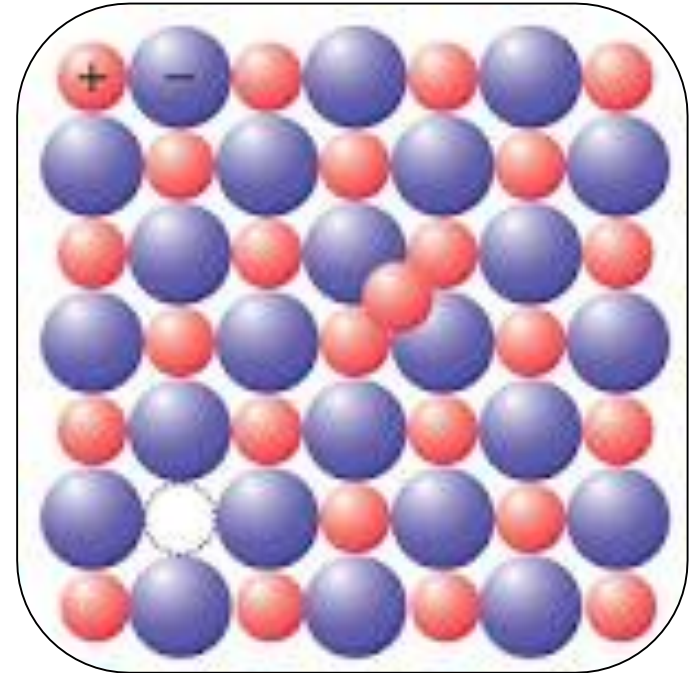
Frenkel defect

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

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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
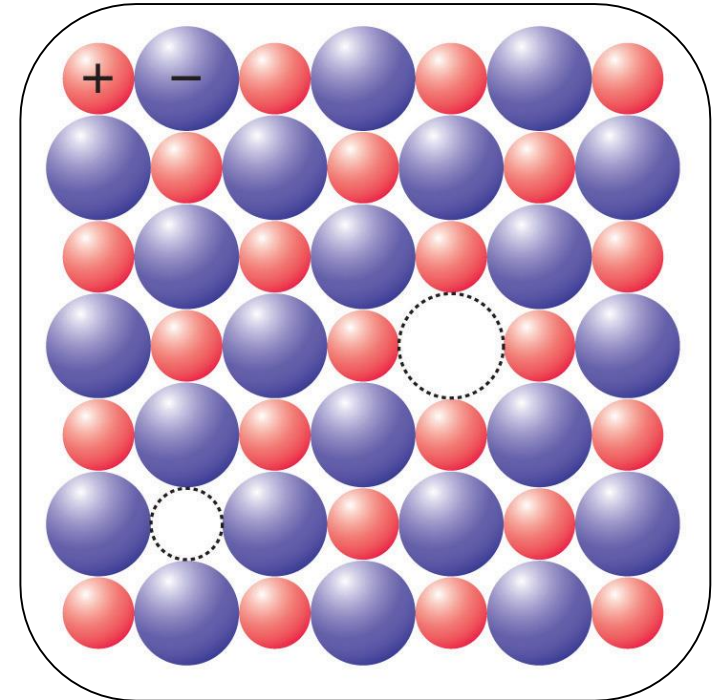
Schottky defect

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

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Line defects / Dislocations
## (leads to plastic deformation)
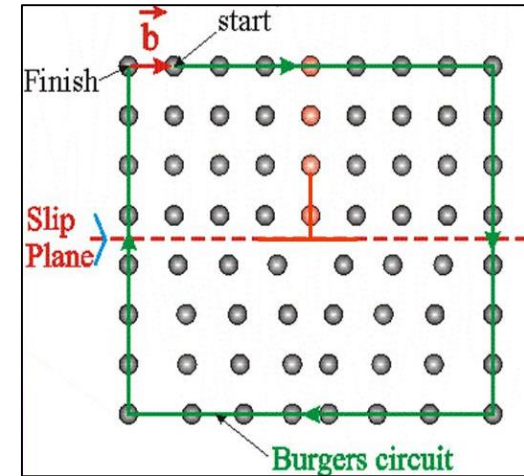
Edge dislocation

- Introduction of an **extra half-plane of atoms** in mid way, distorts nearby planes of atoms.

- Atoms above dislocation line are 'squeezed' while below are pulled 'apart'.

- **Dislocation line** is **perpendicular** to plane of page.

- The direction & magnitude of edge dislocation is shown by **Burger vector**.

- **Move around the dislocation line** (Clockwise) making equal steps in each direction. (e.g. 7 hz. and 7 vt.). The **vector** that goes from **finish to start** is the Burger vector.

- An **edge dislocation** lies **perpendicular** to its **Burgers vector**.

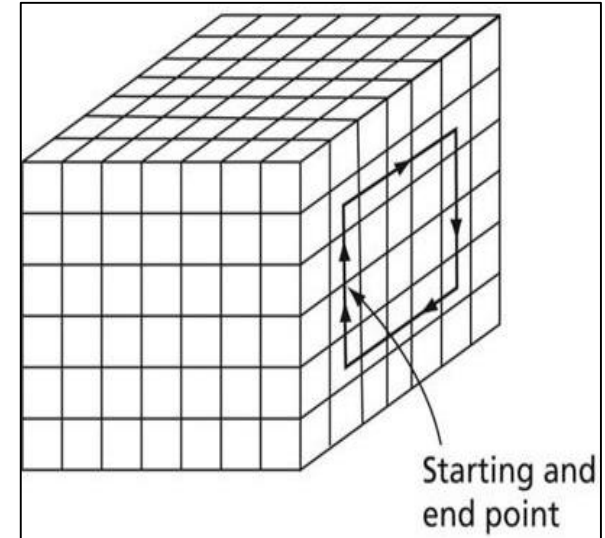- This dislocation creates normal stress and strain in the crystal.
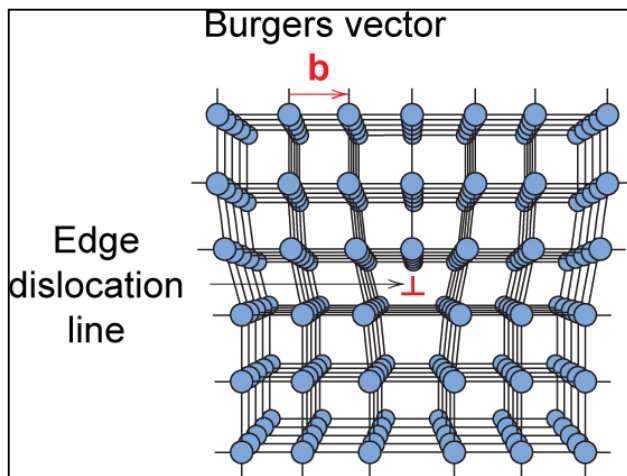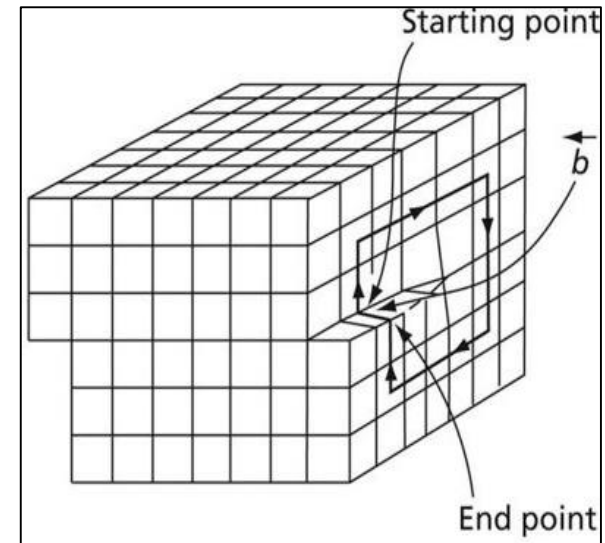

Edge dislocation
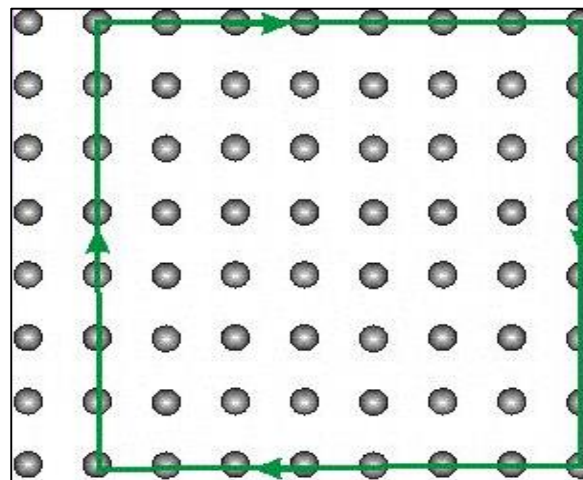
Perfect crystal

Crystal with dislocation

Reference: W.D Callister, 7 Ed.

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Screw dislocation

- A screw dislocation results from shear distortion.

- Move around the dislocation line (Clockwise) making equal steps in each direction. The vector that goes from finish to start is the Burger vector.

- A screw dislocation lies parallel to its Burgers vector.

- A screw dislocation moves in a direction perpendicular to the Burgers vector.

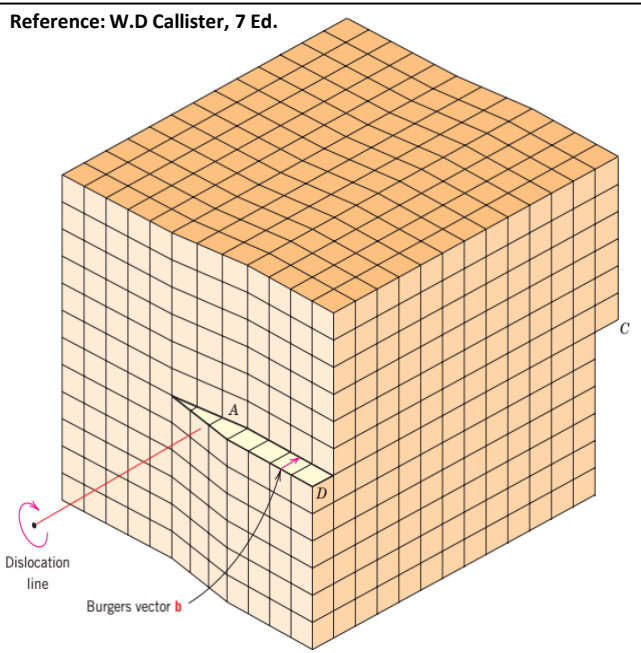Starting and end point

Perfect crystal

Reference: W.D Callister, 7 Ed.

A

C

D

Dislocation line

Burgers vector **b**

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Starting point

b

End point

Crystal with dislocation

Ways to avoid Dislocation

➢ **Use single crystals** (but expensive – used especially with large items like turbine blades).

➢ **Work hardening** (strengthening by plastic deformation of the metal) - this moves all dislocations to grain boundaries (the dislocation essentially becomes part of the grain boundary).

➢ **Introduce impurity** atoms (that is alloying elements) or impurity phases that "pin" the motion of defects. An impurity atom stops the motion because it is of different size, or makes stronger bonds.

Dislocations may be good or bad, depending on whether plastic deformation is desirable or not.

Surface/Planar defects

(associated with grain boundaries)

Grain Boundaries

- **Boundary separating** the two grains or **crystals** having **different crystallographic orientations** in polycrystalline materials.

- The atoms near the boundaries are slightly disordered & have higher energy than those within the grains.

- In general, a **grain boundary has five degrees of freedom**.

- We need **three DOF** to specify the **orientation of one grain with respect to the other & two DOF** to specify **the orientation of the boundary** with respect to one of the grains.

Grain Boundaries

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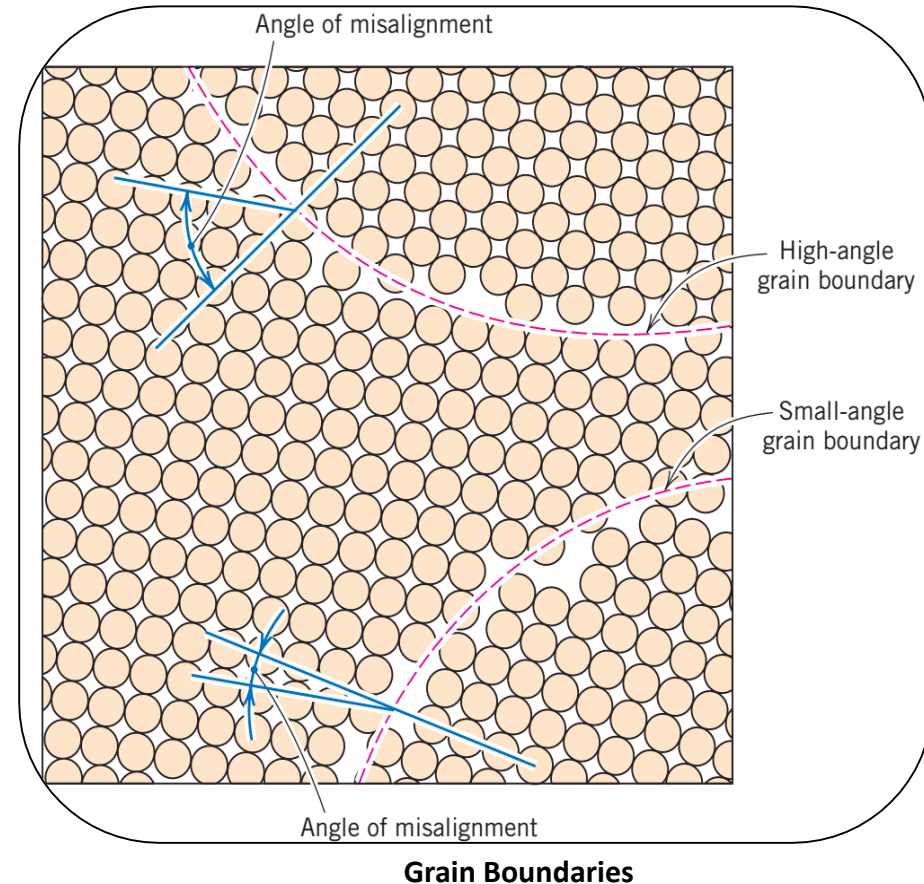
Role of Grain boundaries

- At temperatures (T < 0.5T_m, where T_m is the melting point), the **grain boundaries** act as strong **obstacles to dislocation** motion giving **strength** to a material.

- At higher temperatures, they tend to **weaken** a material as **grain boundary sliding** may occur, leading to **plastic flow** and/or **opening** up of **voids** along the boundaries.

- In general, **fine grained materials** are **stronger** than coarse grained ones because they have **more grain boundaries per unit volume**.

Grain size determination

American Society of testing material (ASTM E 112) method

$$N = 2^{n-1}$$

where,
n: grain size number (1- 10), which is then compared with standard charts as per ASTM E 112.
N: average number of grains per square inch at a magnification of 100X

1). **Determine the ASTM grain size number of a metal specimen if 45 grains per square inch are measured at a magnification of 100X ?**

Answer: Using ASTM method $N = 2^{n-1}$, n= grain size no., N = grains/inch²

Taking logarithm both sides and on simplifying, we get

$$n = \frac{logN}{Log2} + 1$$

Therefore, $\qquad n = \frac{log45}{Log2} + 1 = 6.5$

2). **For same specimen, how many grains per square inch will there be at a magnification of 85X?**

Answer: Use equation, $N_M \left(\frac{M}{100}\right) = 2^{n-1}$, N_M = grains/inch² at magnification M.

Substituting n = 6.5 & M = 85, we get

$$N_M = 62.6 \text{ grains/inch}^2 \text{ at 85X}$$

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Slip System

Slip system = Slip plane + Slip direction

- Slip plane is generally taken as the closest packed plane in the system
- Slip direction is taken as the direction on the slip plane with the highest linear density.

- ✓ In **FCC** the four **{1 1 1}** family planes are the **slip planes**, and as each plane contains **three** of the family of **<1 0 0> directions** , there are altogether, 3 x 4 = **12 slip systems**.

- ✓ Similarly in **BCC**, there are **six {110} planes** with **two** of the **<1 1 0>** directions in each, giving 6 x 2 = **12 slip system.**

- ✓ Thus, **FCC and BCC** materials have **large numbers** of **slip systems** (at least 12) and are considered **ductile**.

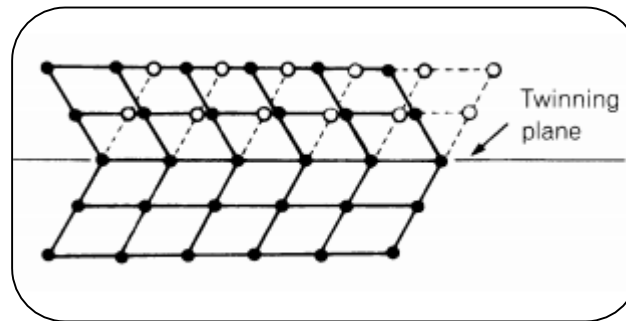- ✓ **HCP** systems have **3 slip systems** and are quite **brittle**.
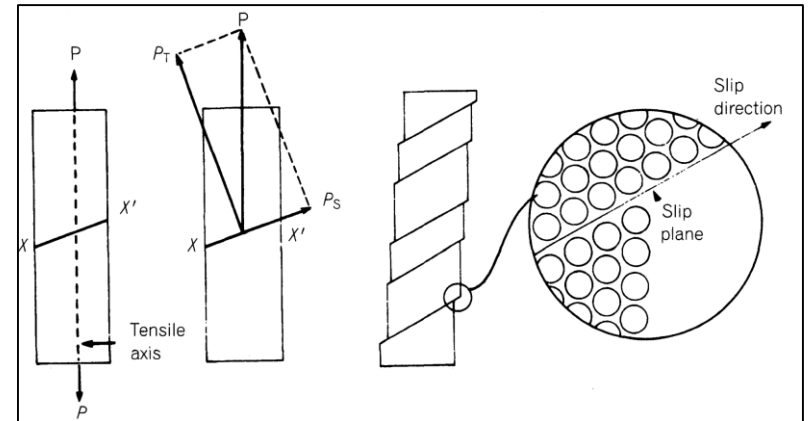
Slip mechanism for plastic deformation

Image courtesy: Material science for Engineers, Anderson, 5th Ed.

Twinning

- Special type of grain boundary – mirror lattice symmetry.

- Occurs on definite crystallographic plane &
  in specific direction – crystal structure dependent.

- Produced by
  a) **Mechanical twin** (Shear forces)
     ✓ Occurs in metals with BCC & HCP crystal structure.

  b) **Annealing twin** (Deformation due to annealing)
     {Annealing - heating material followed by slow cooling to remove internal stresses and toughen it}

     ✓ Occurs in metals with FCC crystal structure.

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Properties of Twinning

- Of the three common crystal structures BCC, FCC and HCP, the **HCP structure** is the **most** likely to **twin**.

- **FCC, BCC** structures will not usually twin because **slip is more** energetically favorable.

- Twinning occurs at **low temperatures** and high rates of shear loading (**shock loading**) conditions where there are **few slip systems present** .

- **Small** amount of **deformation** when compared with slip.

Volume/Bulk defects
(Large & undesirable)

Volume or Bulk Defects

- These are introduced during **processing and fabrication**.

- **Examples**

  ✓ Pores – gases trapped during solidification.

  ✓ Cracks – improper shrinkage during solidification.

  ✓ Foreign inclusions and other phases.

- They are **always undesirable.**

- **Decreases** mechanical strength and **promote** fracture.

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Summary

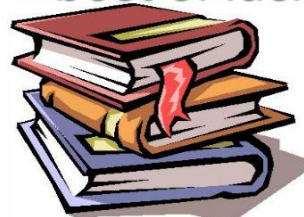| S. No.	Type of defect	Properties affected	Applications
1	Vacancies	Solid-state diffusion	Annealing
		Mechanical creep	
2	Substitutional	Electrical conductivity	Semiconductor diodes and transistors
		Mechanical strength	Solute hardening of alloys
3	Interstitial	Magnetic coercivity	Strong permanent magnets
		Dielectric strength	Capacitors
		Optical transparency	Coloring of glasses & plastics
4	Dislocations, Twin boundaries	Plastic deformation (ductility)	Strain hardening
5	Grain boundaries	Dislocation movement	Mechanical hardening
		Electrical resistance	
		Magnetic coercivity	Strong permanent magnets
		Optical transparency	
6	Stacking faults (interruption in stacking sequence)	Mechanical strength	
		Electrical resistance	

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In the **next lecture**, we will learn:

- **Metals (Ferrous alloys)**

  ✓ Properties

  ✓ Classification

best of luck