Crystal Imperfections

Ideal crystal → Lattice + basis

Real crystal → Deviation from ideality → Defects/ imperfections → Controls the physical and mechanical properties

Classification of defect

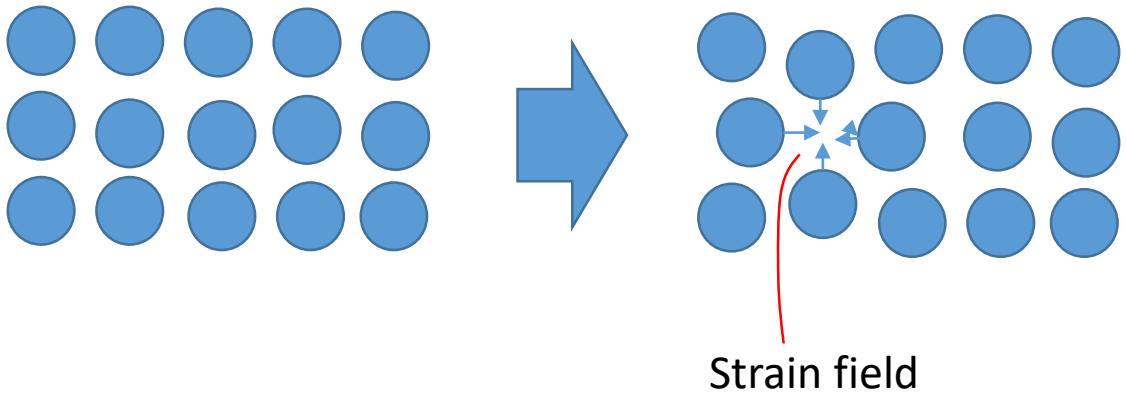
1) Zero dimension : point defect, Ex: vacancy/ interstitial
2) One dimension : line defect Ex: dislocation
3) Two dimensional: Surface defect, Ex: Free surface, grain boundary, twin boundary, stacking fault.
4) Three dimensional defect: Volume defect, Ex: precipitate, voids, blow holes, pores

1) Point defect

A point defect is a very localized disruption in the regularity of a lattice. It is a defect of Dimensions just like a point (zero dimensions). The size of defect could be an atom, or two atomic diameters. Which is just like a point.

Various types of point defects are given below……

a) Vacancy or Schottky defect in metal



Vacancies (Point defect)

When an atom is missing from its lattice site in a crystal structure of a metal, it is called vacancy.

- There must be some vacant sites in a crystal which provides equilibrium in crystal lattice.
- A crystal with vacancy Exhibits lower free energy that a perfect crystal.

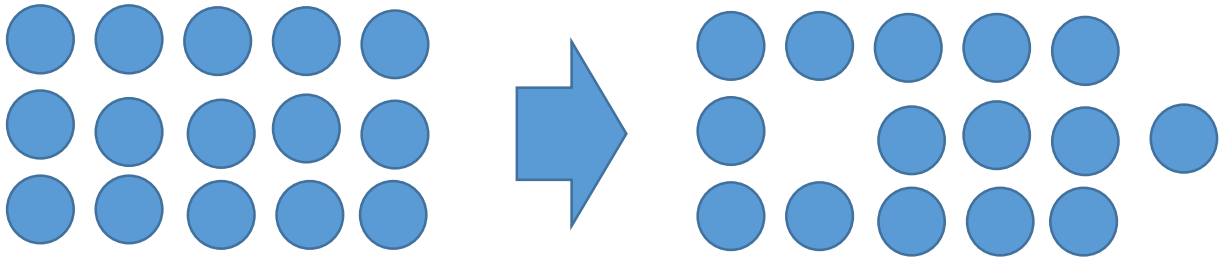
Equilibrium concentration of vacancy can be expressed as

$$\frac{n_{eq}}{N} = \text{Exp}\left[-\frac{H_f}{RT}\right]$$

H_f = Enthalpy of formation of a 1 mole of vacancies

R= Gas constant

Thermal expansion occurs due to vacancy …..



Volume of crystal increases.

Thermal expansion

↓

Lattice parameter expansion

+

Increase in volume due to vacancy

b) Interstitialcy (self interstitial)

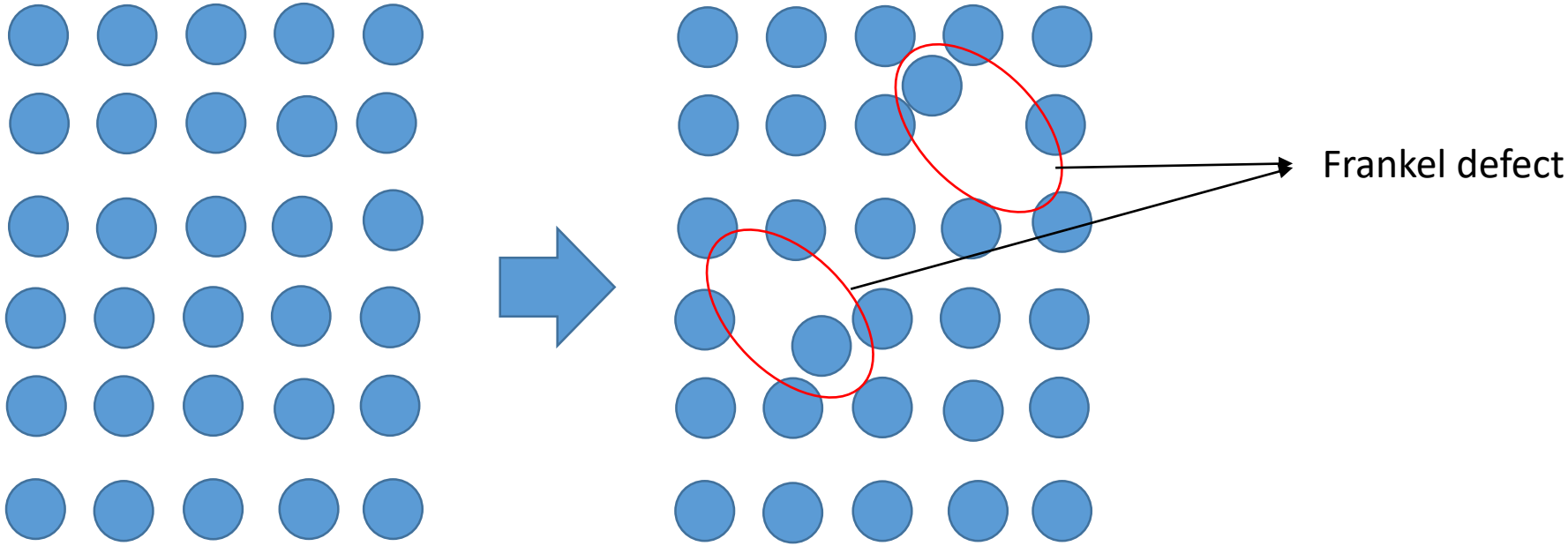
When an atom of the metal occupies an interstitial site (which is not its normal sites).
It is called Interstitialcy.

- Interstitialcy – An atom trapped in the interstitial point (a point intermediate between regular lattice points) is called an interstitialcy.
- An impurity atom at the regular or interstitial position in the lattice is another type of point defect.

B, C, N, H O is present in the interstitial sites

c) Frenkel defect :

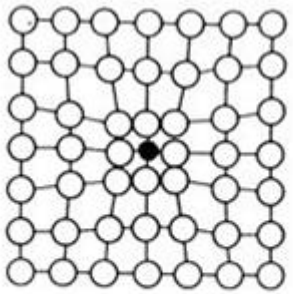
When an atom shifted from a normal lattice site (thus creating vacancy) an is forced into interstitial position. The resulting pair of point defects (a vacancy as well as interstitialcy) together is called Frenkel defect.



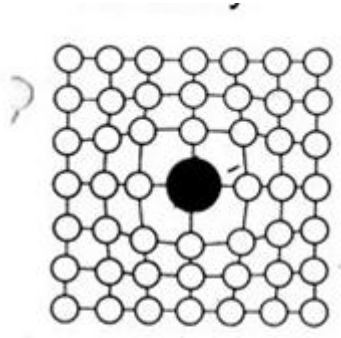
d) Impurity atom substitutional or interstitial type

(impurity atom substitutional or interstitial type)

- An impurity atom if present on the lattice by substituting the lattice site atom,
- substitutional impurity atom is point defect.
- Impurity atom either larger or smaller than the normal lattice atom.
- They create elastic strain field in lattice



small substitutional atom



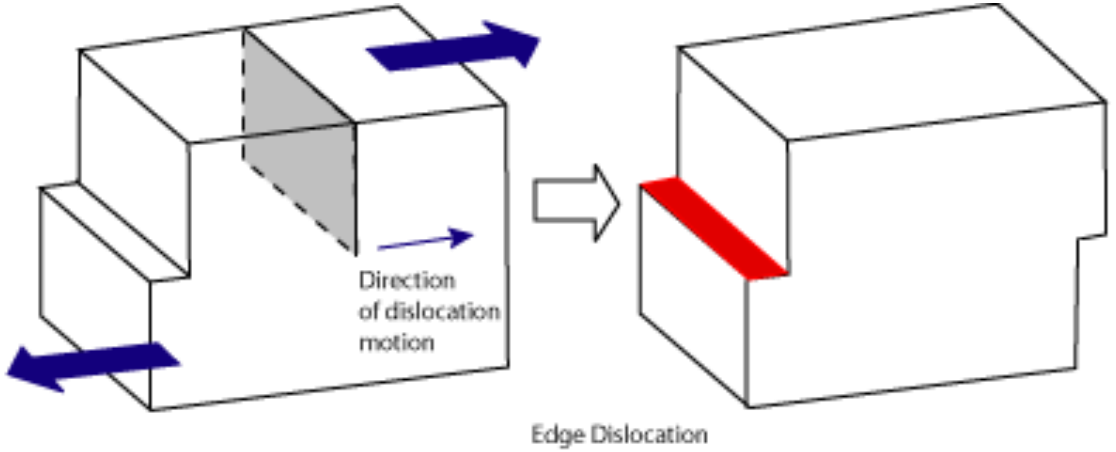
large substitutional atom

Dislocation : Line defect: 1D defect

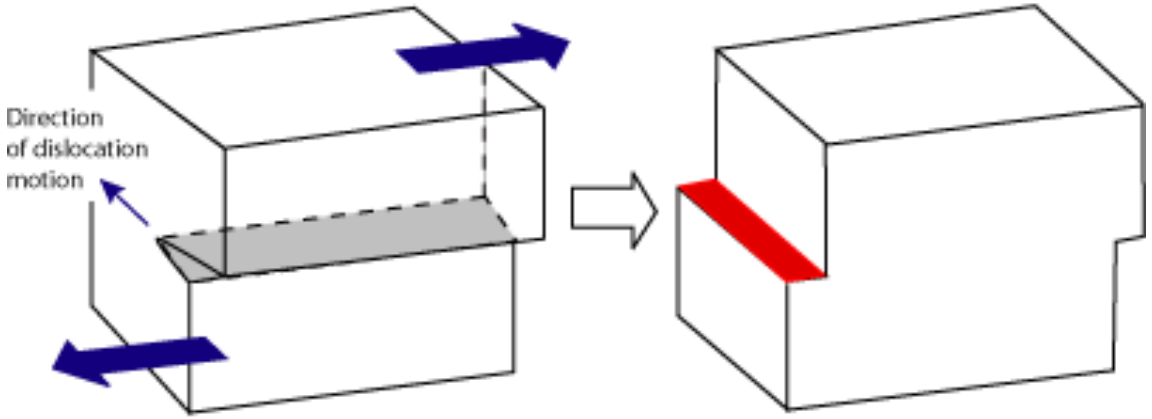
Crystal imperfection in one dimension is called dislocation.

Based on the angular relation between burgers vector and tangent vector

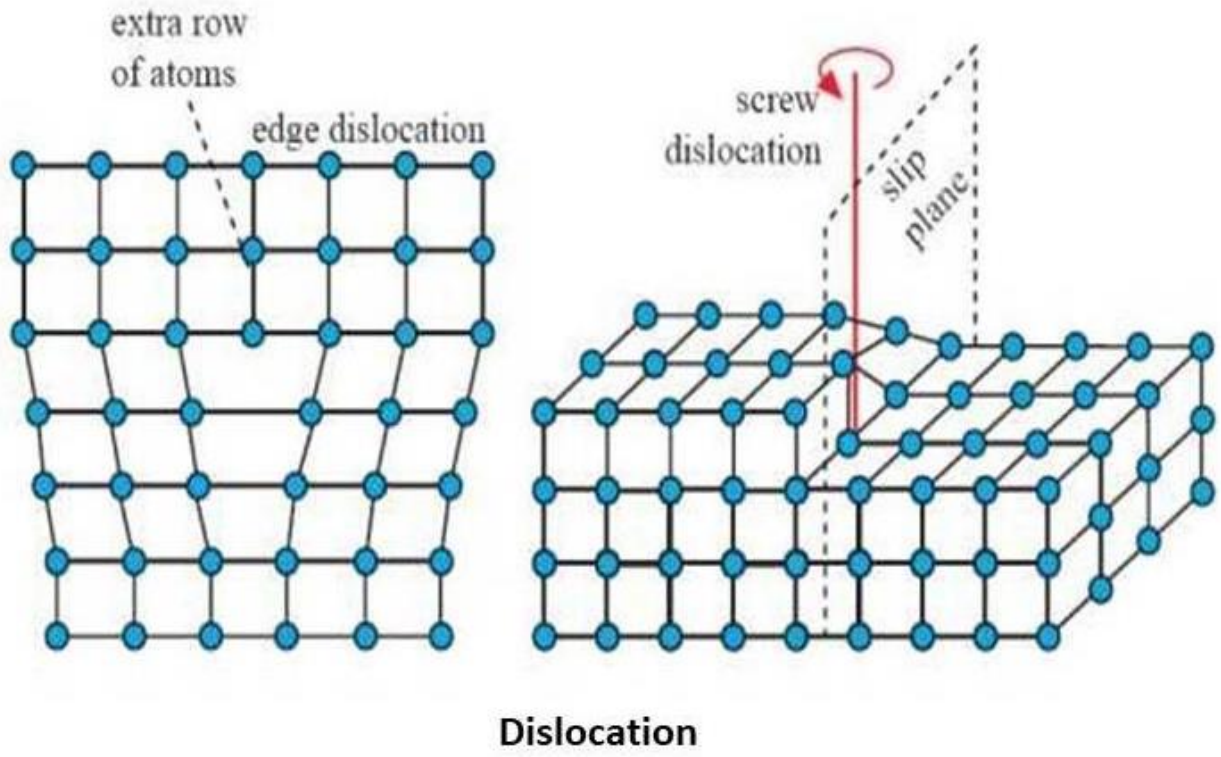
1) Edge dislocation
2) Screw dislocation
3) Mixed dislocation



Edge Dislocation

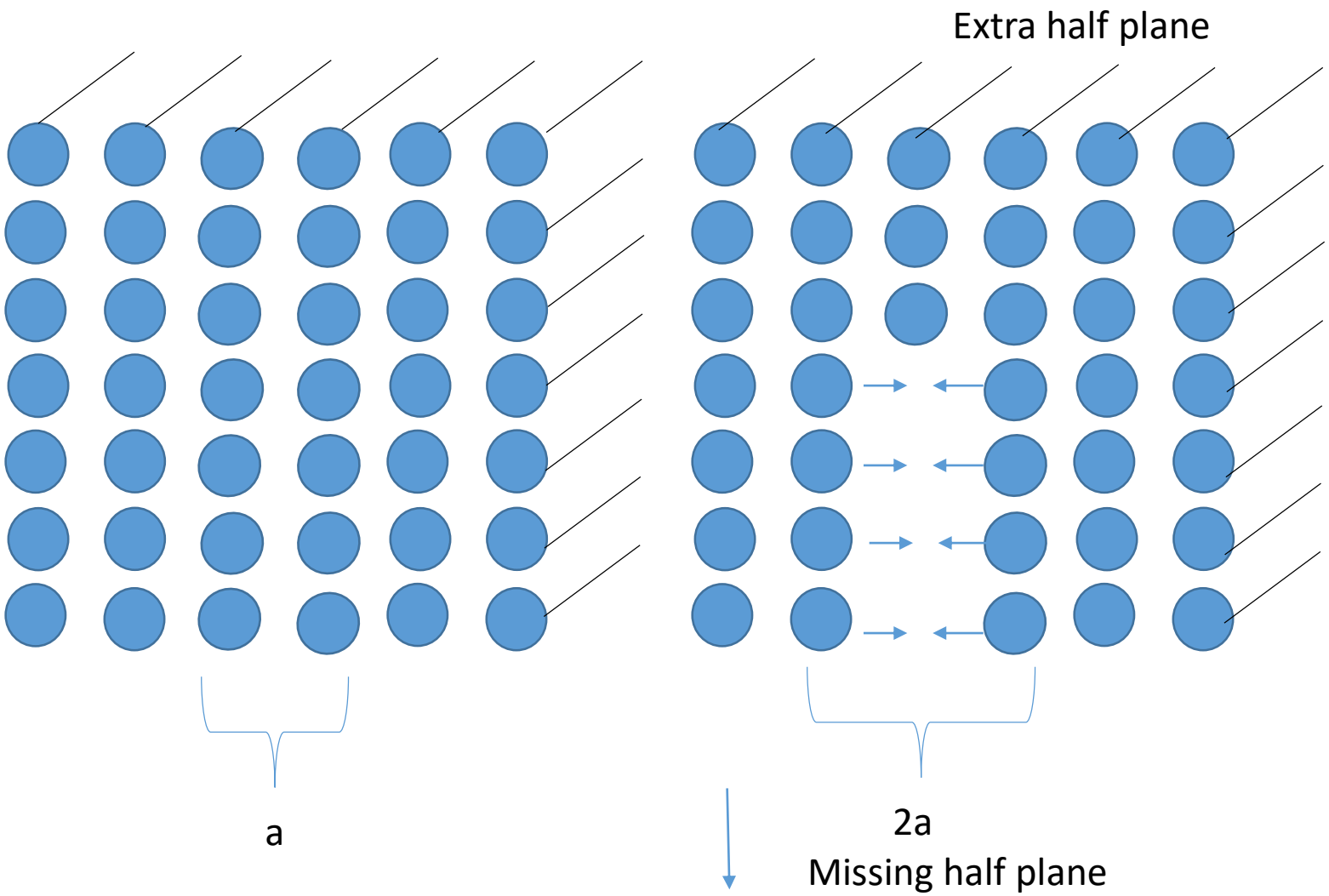


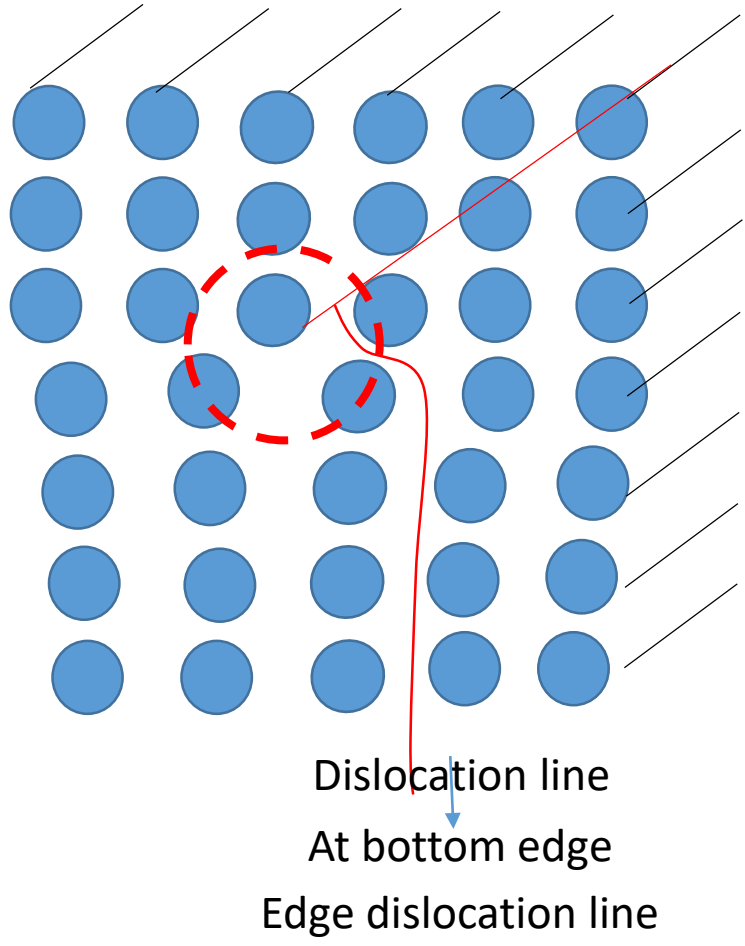
Screw Dislocation



Dislocation

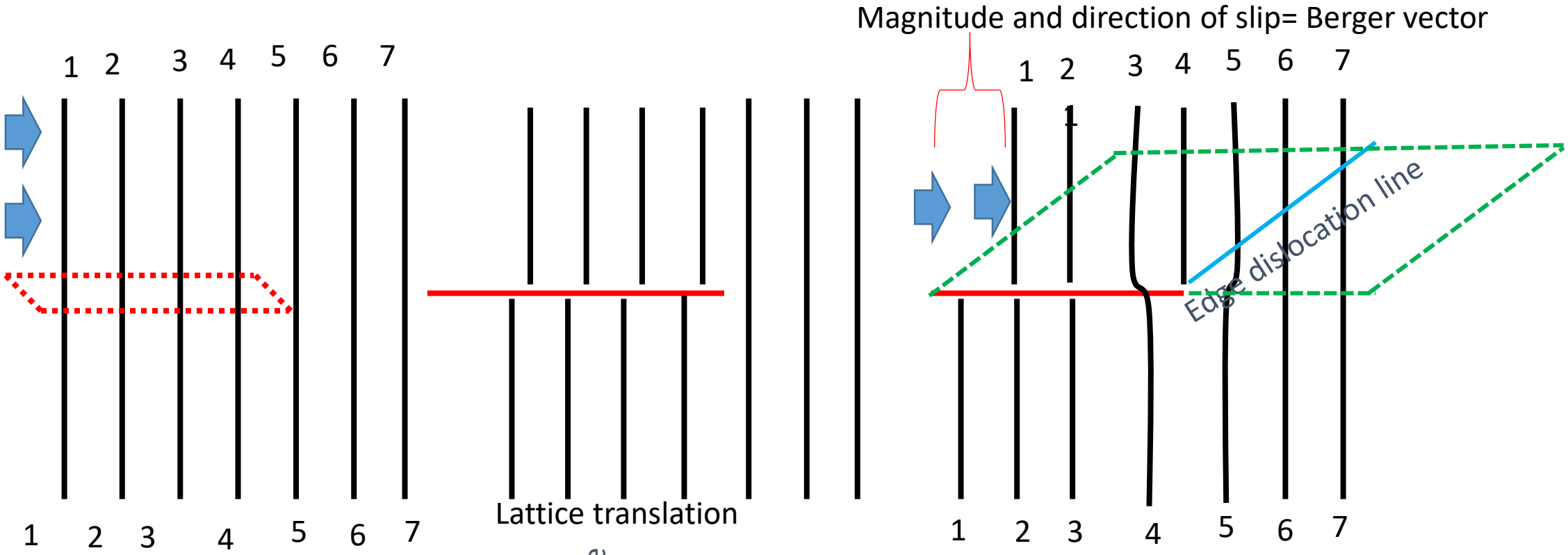
Dislocation : Line defect: 1D defect

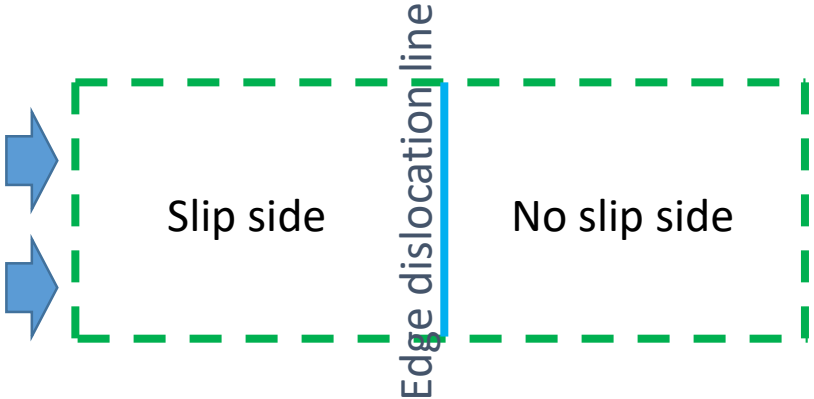




Only bottom edge of the half plane is defect not the entire half plane

Slip approach

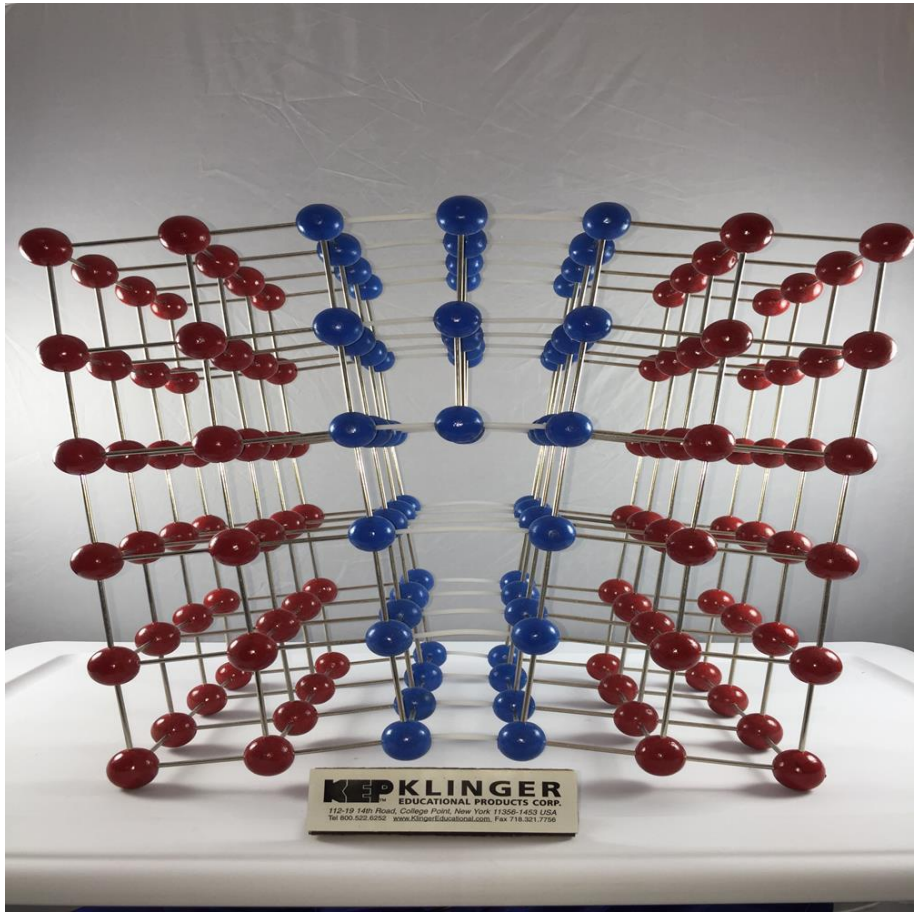




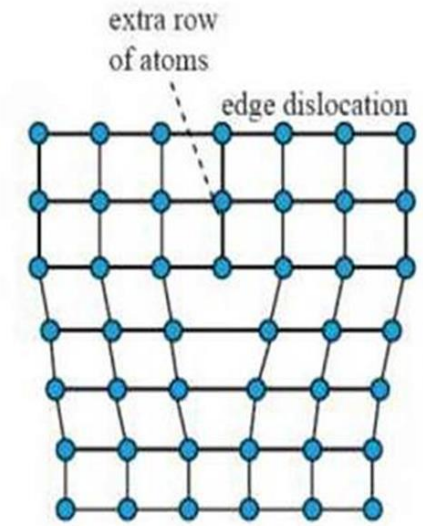
Dislocation line is a boundary between slip and no slip region

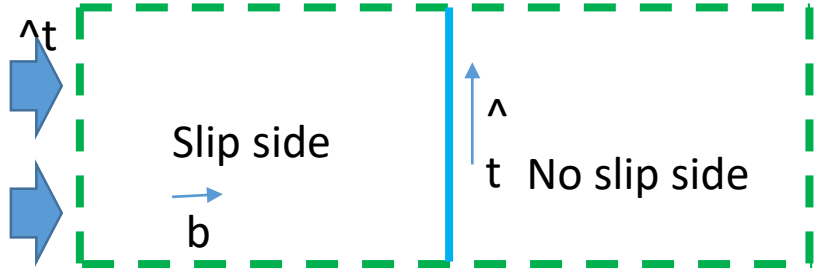
Characteristics vector of dislocation

Berger vector : -->b,
magnitude and direction of slip



Tangent/ unit vector : ^t = orientation of dislocation line,
Parallel or tangent to the dislocation line

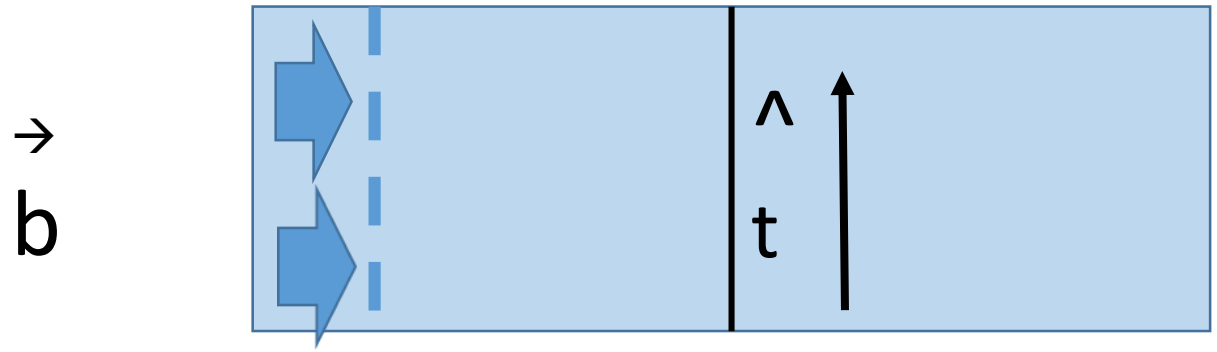




Edge dislocation line

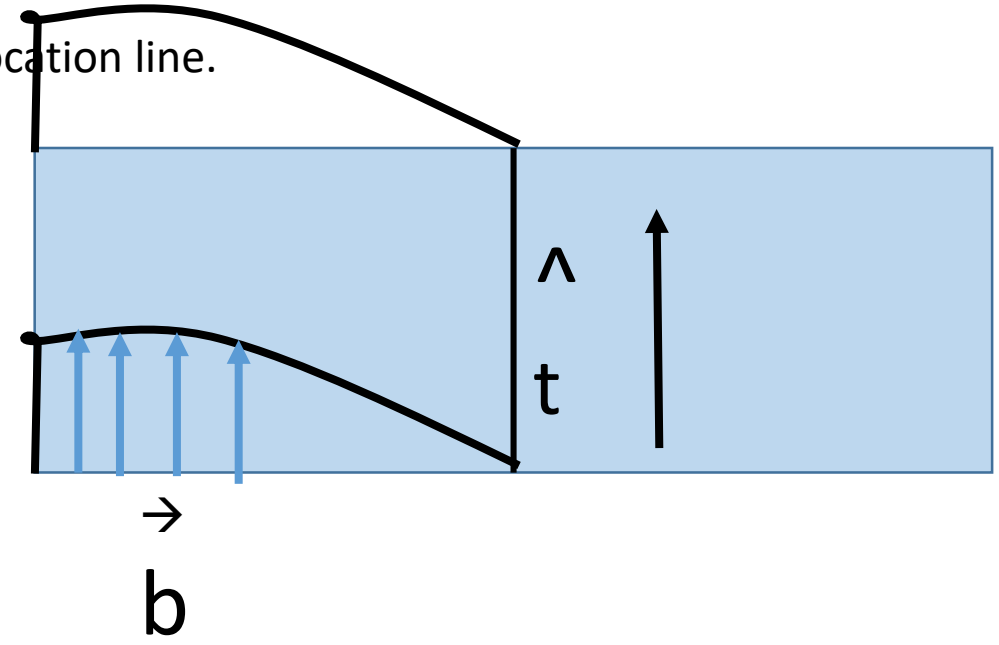
If b, burger vector is perpendicular to tangent vector (t) called, edge dislocation.

Slip direction is perpendicular to dislocation line.

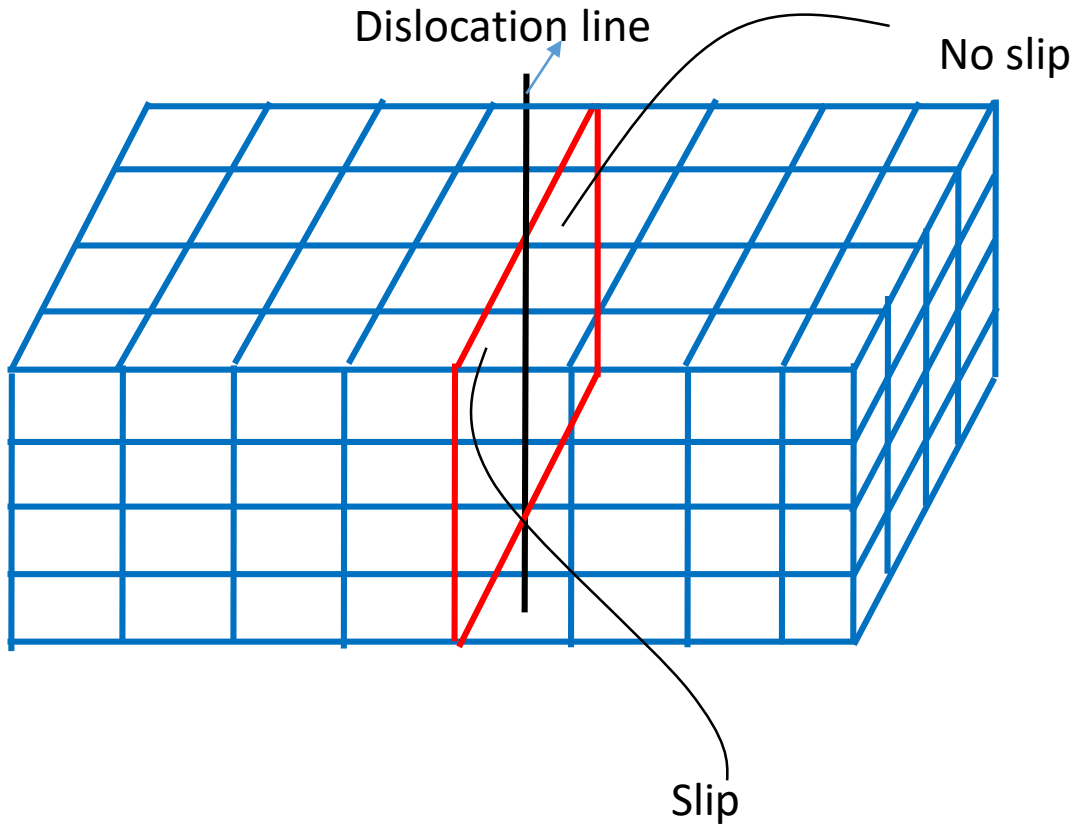


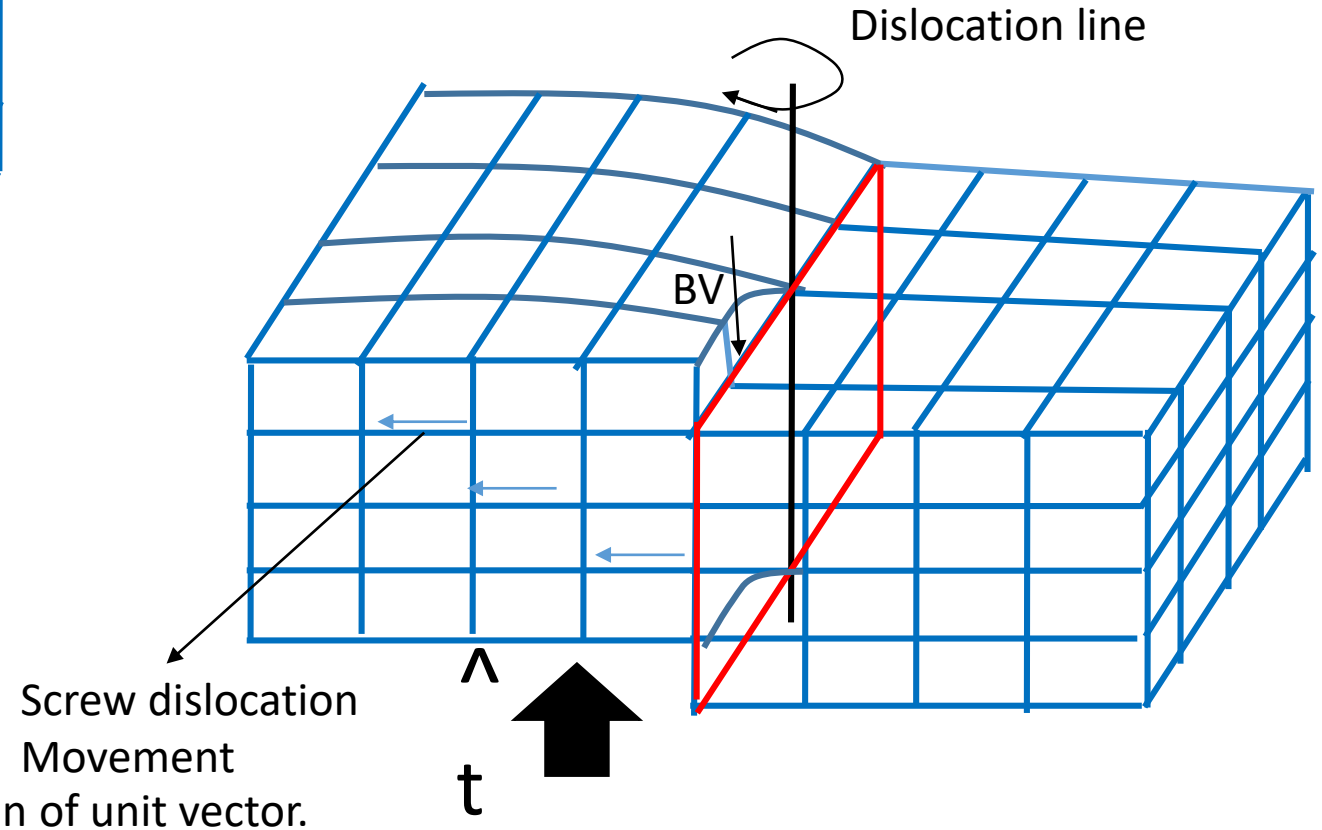
If b, burger vector is parallel to tangent vector (t) called, screw dislocation.

Slip direction is parallel to dislocation line.



Screw dislocation

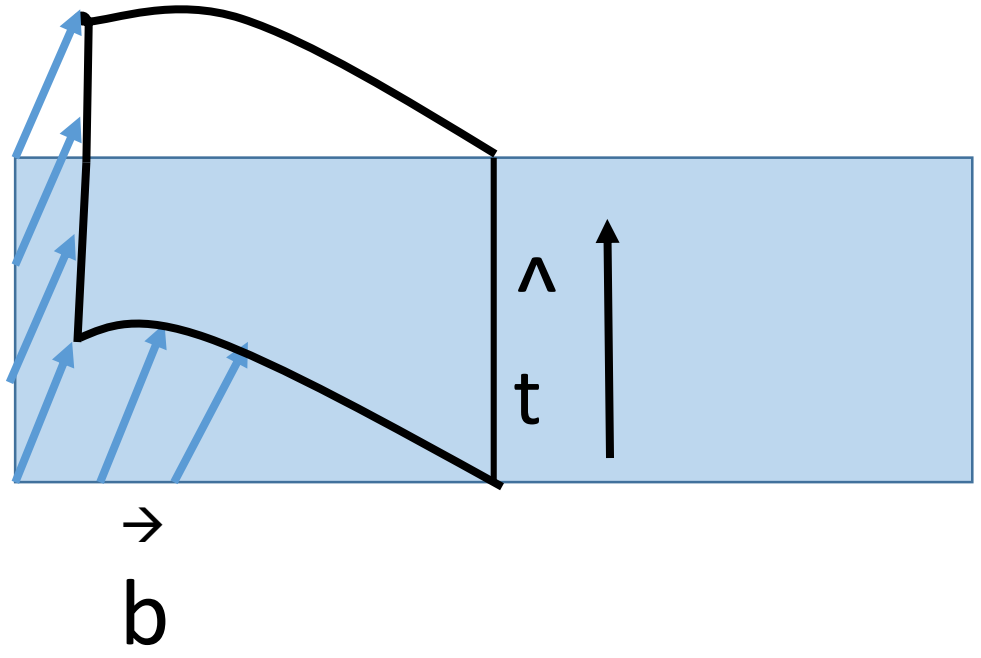




Right handed circuit with thumb pointing in the direction of unit vector.

Mixed dislocation:

Burger vector neither perpendicular nor parallel to tangent vector

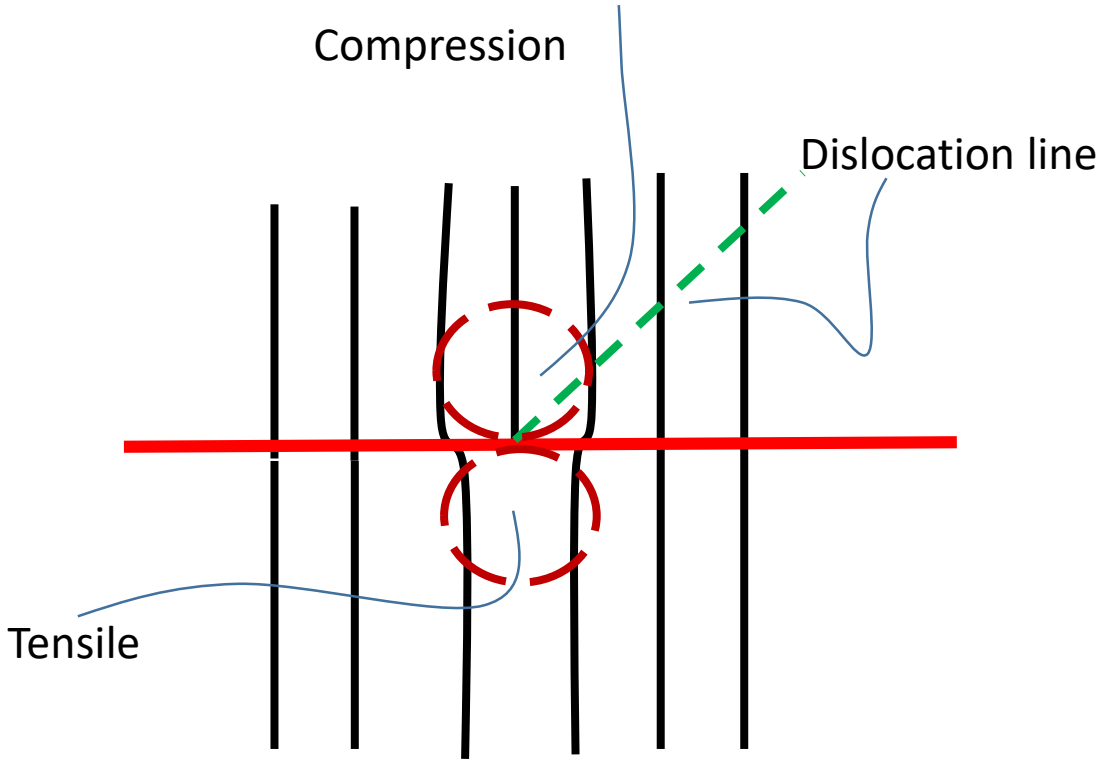


Difference between edge and screw dislocation

Table 4.6. Difference Between The Two Main Types of Dislocations

	Property	*Edge dislocation*	*Screw dislocation*
1.	Burgers Vector	Is perpendicular to edge dislocation line	Is parallel to the screw dislocation line
2.	Dislocation movement relative to Burgers Vector	Dislocation moves parallel to Burgers Vector	Dislocation moves perpendicular to the Burgers vector
3.	Slip direction	Atoms move parallel to Burgers Vector	Atoms move parallel to Burgers vector
4.	Movement of dislocation relative to slip direction	Atoms move parallel to motion of dislocation	Atoms move perpendicular to motion of dislocation
5.	Method of leaving the slip plane	By climb up or down	By cross-slip
6.	Velocity of motion	Faster than screw dislocation	Slower than edge dislocation
7.	Strain energy of dislocation	It has more strain energy than a screw dislocation	It has less strain energy then edge dislocation

Elastic energy of a dislocation line



Strain field around the dislocation line called elastic strain energy

Its depends on:

1) Burger vector magnitude
2) Shear modulus of materials

Elastic strain energy per unit length = $\frac{1}{2}$ G b^2

Mechanism of edge and screw dislocation

Burgers vectors at different crystals

The smallest distance between two atomic sites lies along the close packed directions. Accordingly, the burgers vector of full dislocations lies along close packed directions in typical crystals as listed below.

Crystal	BCC	FCC	SC	HCP
Burgers vector	½ <111>	½ <110>	<100>	$<11\bar{2}1>$

Dislocation density of annealed crystal 10^6 - 10^{10} m/m^3

Movement of dislocation or slip lies at close packed plane which contained close packed direction.

Motion of dislocation on slip plane containing dislocation line → Glide motion,

Edge dislocation have unique defined slip plane, not for screw dislocation.
Screw dislocation can cross-glide or cross-slip from one slip plane to another.

Cross-Slip Mechanism

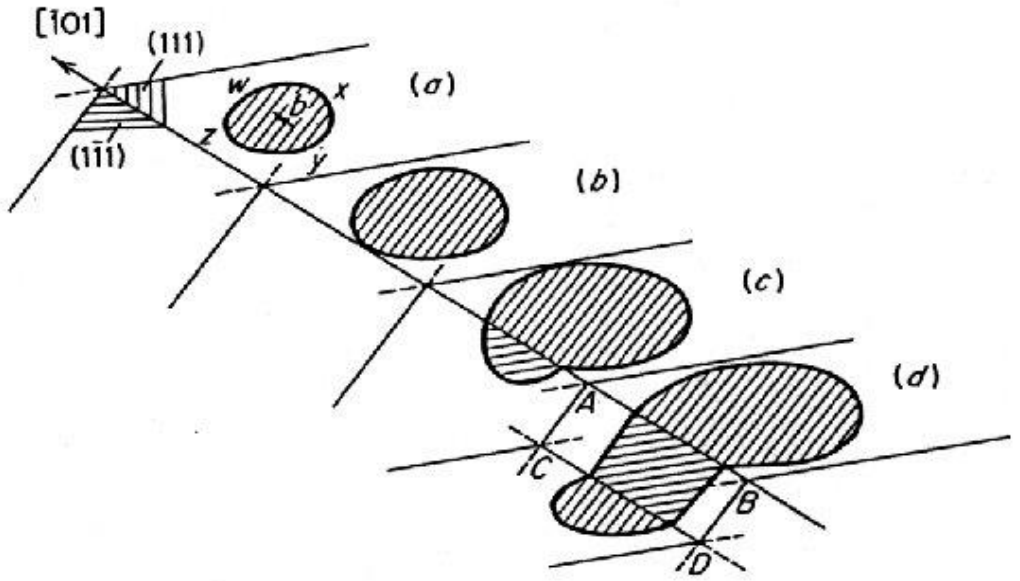


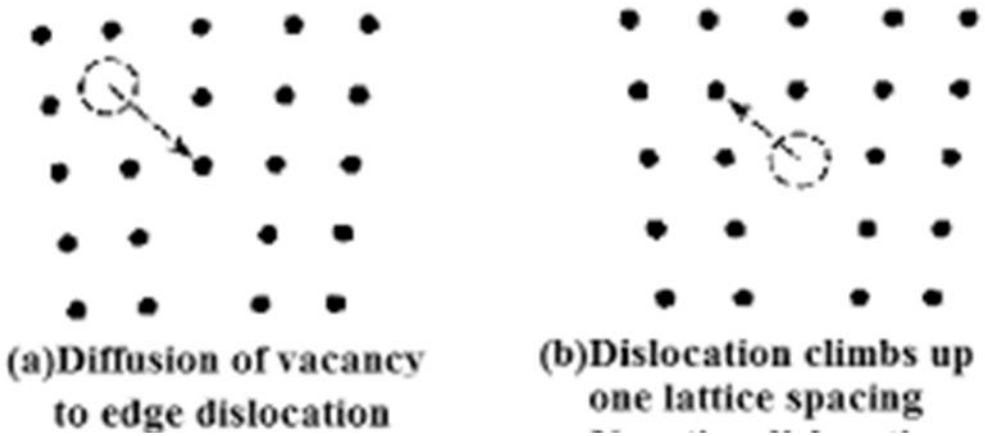
Figure 12-2. Cross slip in a face-centered cubic crystal.

Edge and screw dislocations are full dislocation and integral lattice translation.

Edge dislocation

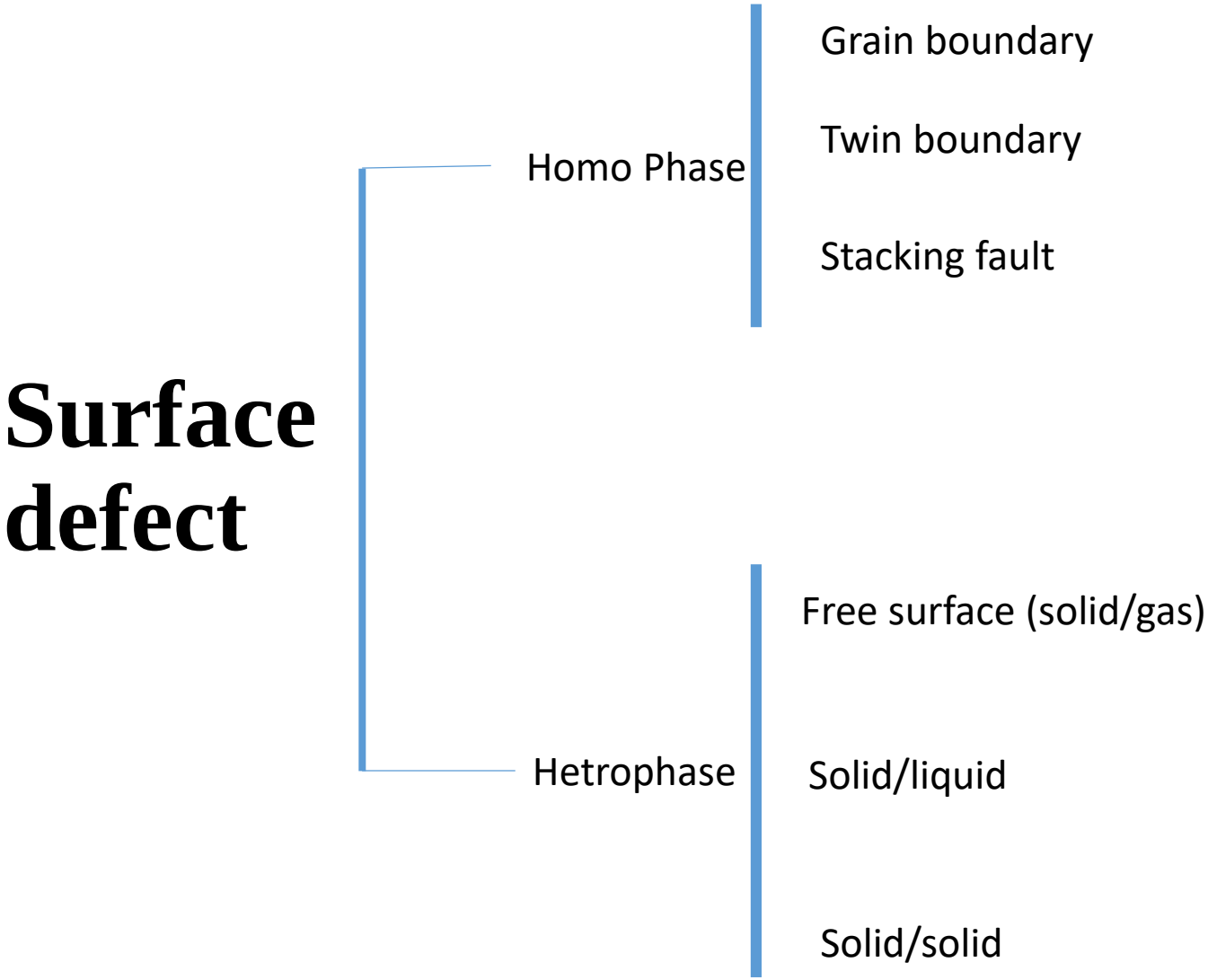
It can not cross slip, they move on the plane other than the slip plane, the motion involves addition or subtraction Of atoms to the edge, called climb motion.
Edge dislocation climb up or climb down depending on weather the incomplete plane shrinks or increase in extent.

Addition of atoms is required for climb down.
Subtraction of atoms is required for climb up.
Climb process requires thermal energy.



Edge and screw dislocations are full dislocation and integral lattice translation.

Two dimensional defect



Close packed plane and direction of crystals

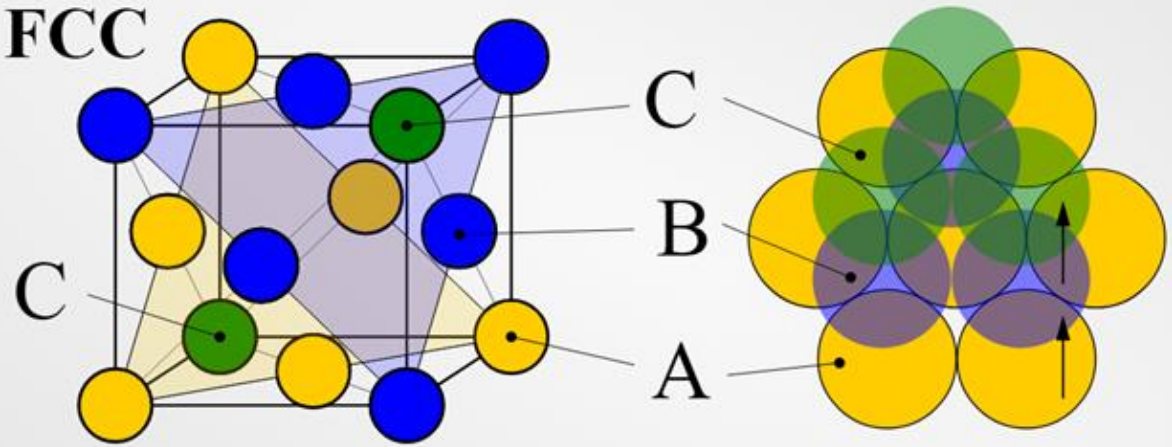
Table 6.5. Slip Plane and Directions in Common Metallic Crystals.

Crystal Structure	*Prominence*	*Slip planes*	*Slip directions*	*No. of slip systems*	*Examples*
FCC	All	{111}	<110>	12	Cu, Al, Au, Ag, Ni, Pb, γ-Fe
BCC	More common	{110}	<111>	12	Fe, W, Mo, brass, Nb, Ta
	Less common	{112}	<111>	12	Fe, Mo, W, Na
		{321}	<111>	24	Fe, K
HCP	More common	(0001)	$<11\bar{2}0>$	3	Cd, Zn, Mg, Ti, Be, Co
	Less common	$\{10\bar{1}0\}$	$<11\bar{2}0>$	3	Ti, Mg, Zr, Be
		$\{10\bar{1}1\}$	$<11\bar{2}0>$	6	Ti, Mg

Movement of dislocation occurs in close-packed plane which contained close-packed direction.

HCP vs FCC Stacking: ABABAB vs ABCABC

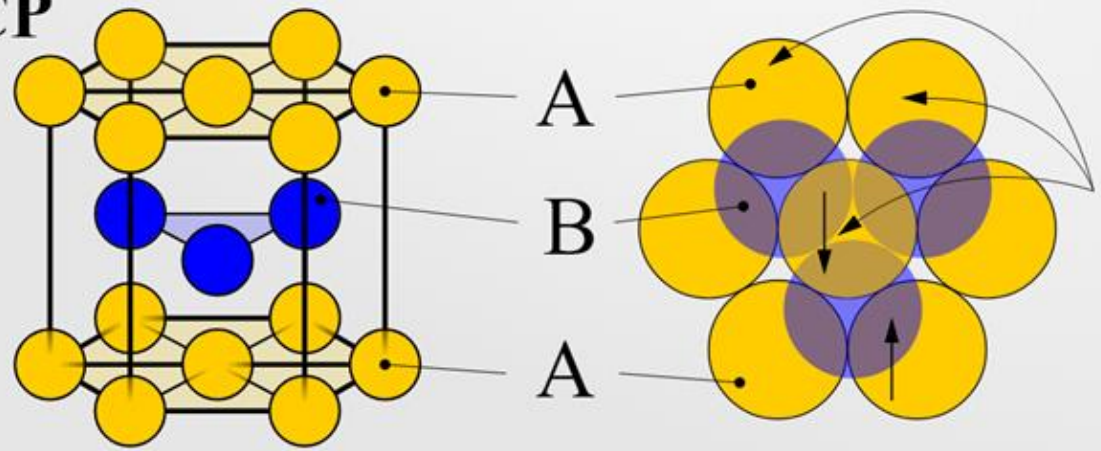
FCC



Sequence: ABCABC

There are **3 possible positions** for a close-packed layer. If **all 3** positions are used in ABC pattern, this makes an **FCC** crystal. This is hard to see because the close-packed planes are along the body diagonal.

HCP



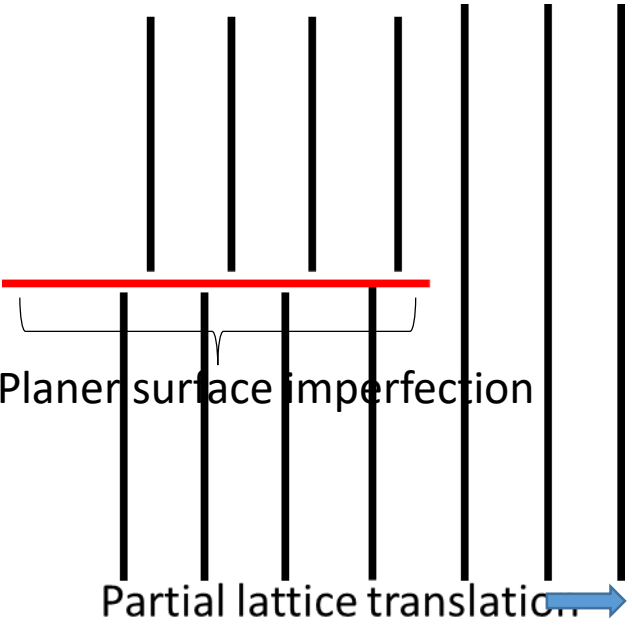
Sequence: ABABAB

The stacking is easier to see in HCP because the layers stack within the unit cell. For an HCP crystal, **only 2** of the 3 possible positions are used, so the third layer is a repeat of the first layer.

Stacking fault
(fault in a stacking sequence of a crystal)

- In crystallography, a stacking fault is a planar defect that can occur in crystalline materials. Crystalline materials form repeating patterns of layers of atoms. Errors can occur in the sequence of these layers and are known as stacking faults.
- Stacking faults are in a higher energy state which is quantified by the formation enthalpy per unit area called the stacking-fault energy.
- Stacking faults can arise during crystal growth or from plastic deformation.
- Dislocations in low stacking-fault energy materials typically dissociate into an extended dislocation, which is a stacking fault bounded by partial dislocations.

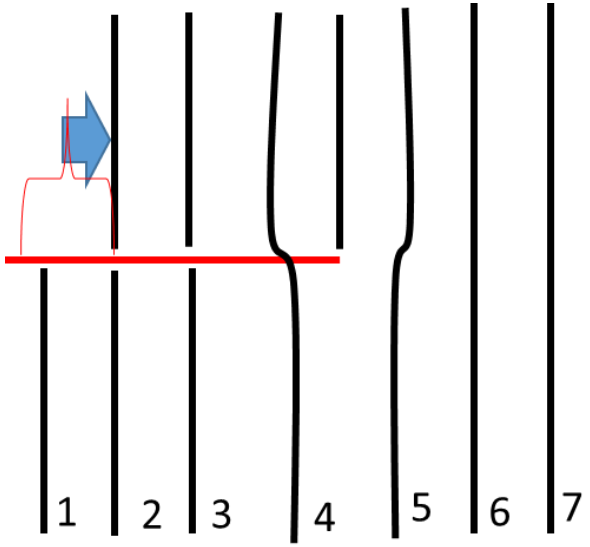
Partials dislocation and stacking faults



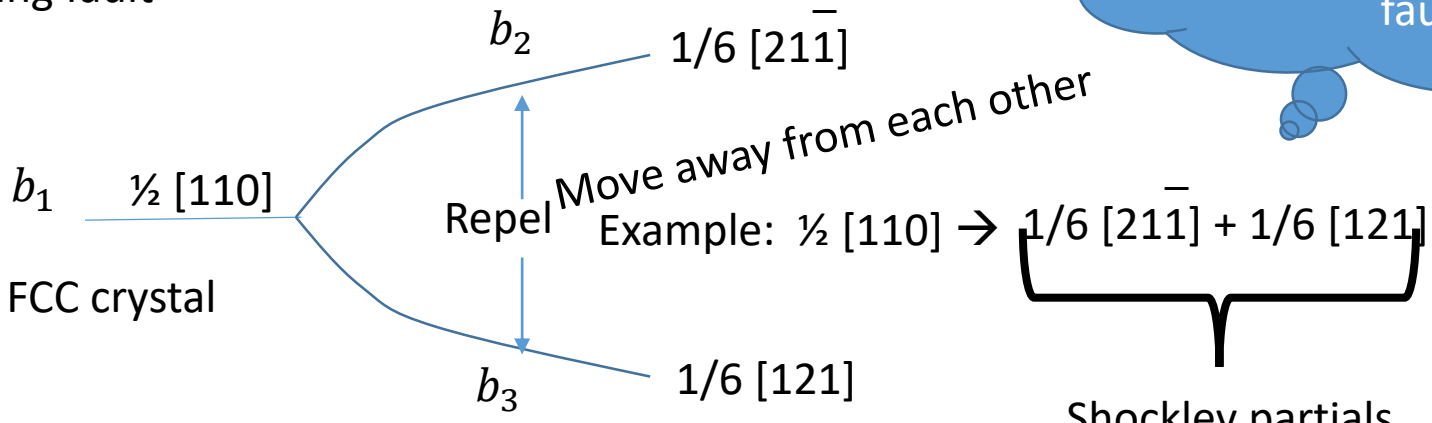
Partials dislocation, burgers vector is a fraction of an interatomic distance. (not a full interatomic distance)
The splitting of a full dislocation b_1 into to partials b_2 and b_3.
Elastic strain energy is proportional to square of burgers vector.

Stacking fault

Region becomes a planer surface imperfection : stacking fault



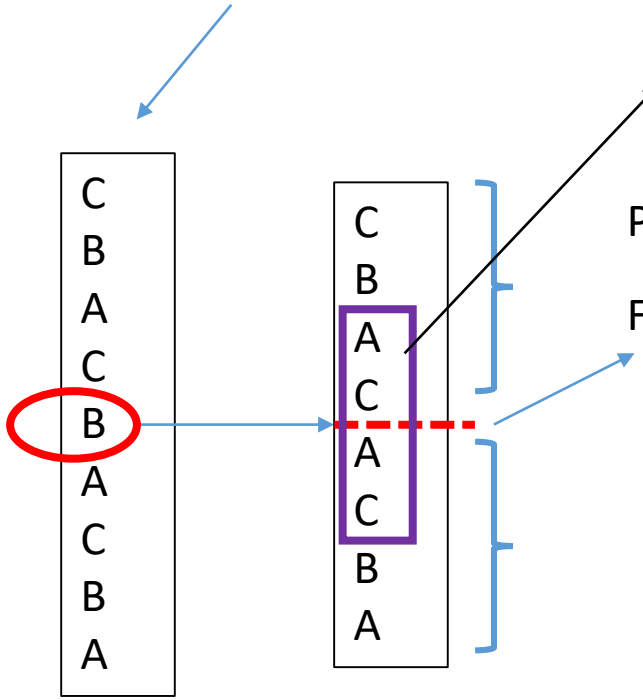
Full lattice translation



Elastic strain energy is favorable if $b_1{}^2 > b_2{}^2 + b_3{}^2$

Stacking fault

Stacking sequence of FCC



Stacking fault in FCC crystal

The stacking sequence across the slip plane in the region between the two partials becomes AB*CACA*BC, HCP stacking sequence in FCC crystal.
Stacking is improper or faulty, called stacking fault.

HCP like plane

Perfect planes above and below the fault

Fault/ missing plane B

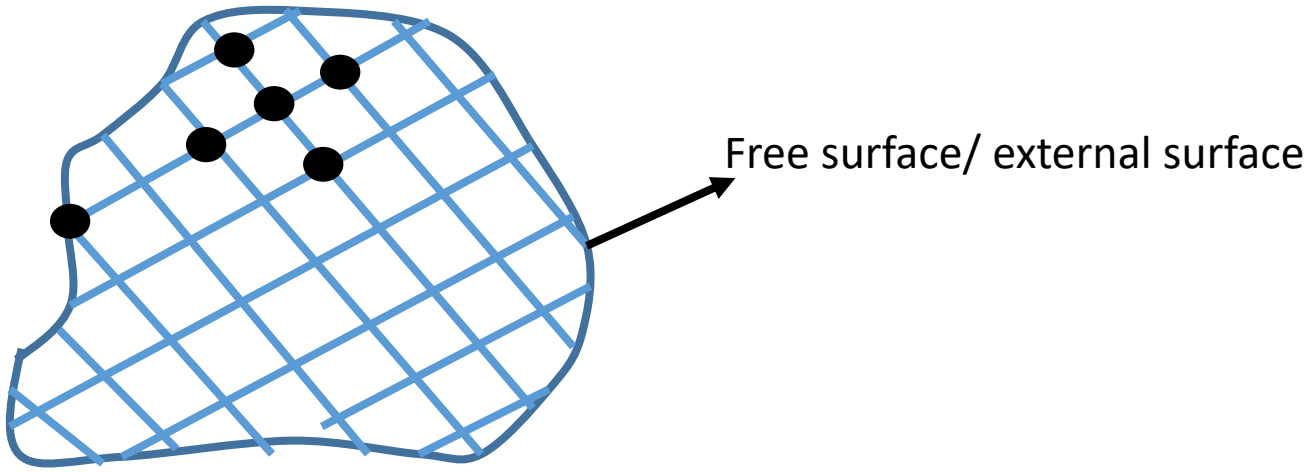
Stacking fault→ surface energy→ minimize area of fault region

FCC materials show high Stacking fault energy, chances of slip easier

- ❑ Orientation above and below the fault plane is same, Unlike grain boundary.
- ❑ Crystal on one side of the fault is shifted by Non- lattice translation w.r.t other side.

Free surface

Free surfaces (external surfaces) of materials are surface defects in the sense that **growth of crystal has stopped abruptly at the surface**. The atoms in the free surface of a solid (or, even liquid) have no neighbors.



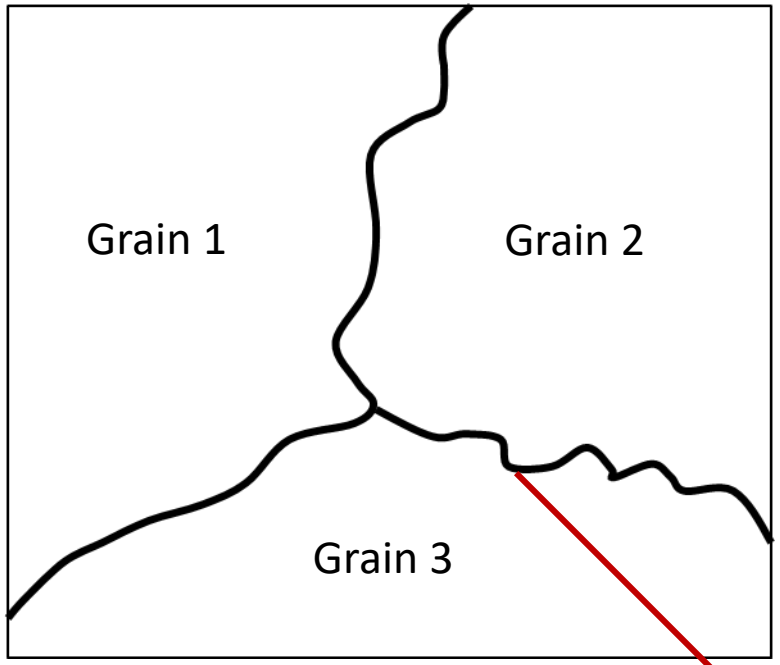
Atom lost certain number of bonds, it requires energy to break the bond, this broken bond energy provided to the external surface, called surface energy per unit area.

Surface energy per unit area (γ)= $\frac{A * n_A * n_B * \varepsilon}{2A} = \frac{n_A * n_B * \varepsilon}{2}$

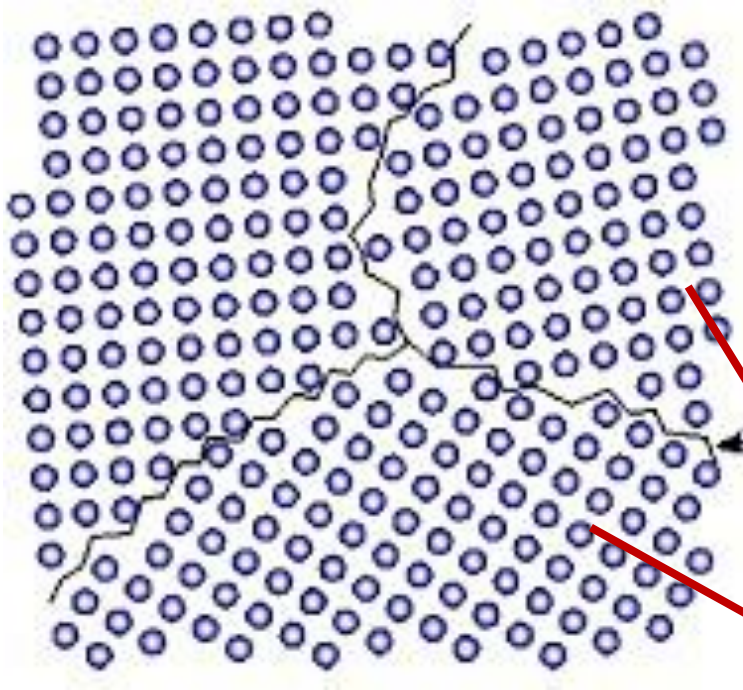
No. of atoms per unit area on the surface = n_A
No. of broken bond/atom = n_B
Bond energy per bond = ε

Grain boundary

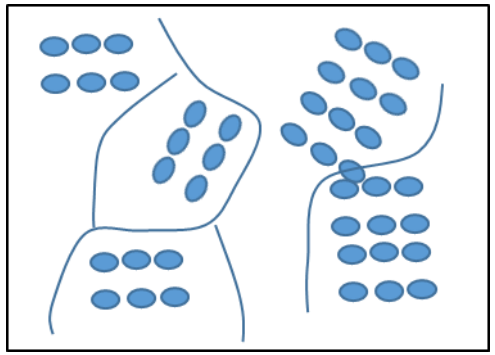
- A grain boundary is a two dimensional planar/ surface defect, that occurs where two such crystallites meet.
- Internal boundary of a polycrystalline.
- The same crystal structure and chemical composition exists on each side but the orientation differs.
- Movement of dislocation hindered due to presence of grain boundary



Polycrystalline



Grain boundary



Different orientation of unit cell

Grain boundaries are rotation boundary : grain on one side of boundary rotated (rotation axis and rotation angle) w.r.t. the other side.

Classification of grain boundary based on:--

Magnitude of angle of rotation:

- **Sub-boundaries :** boundaries existing within the grain, small difference in orientation les than 1°
- **low angle grain boundaries :** are boundaries between two adjacent grains differing in orientation less than 15°
- **High angle grain boundaries :** large difference in orientation 15° -65° between grains.

Rotation axis w.r.t. the boundary plane :

- **Tilt boundary :** boundaries between adjacent grains having misorientation in such a way that lattice appear to be Tilted w.r.t. another (Rotation axis parallel to boundary plane).
- **Twist boundary:** lattice appear to be rotated (twisted) w.r.t. one another (Rotation axis perpendicular to boundary plane).
- **Coincidence boundary :** in which atomic positions common to both the adjacent grains form some fraction of the total boundary area.

Twin boundary

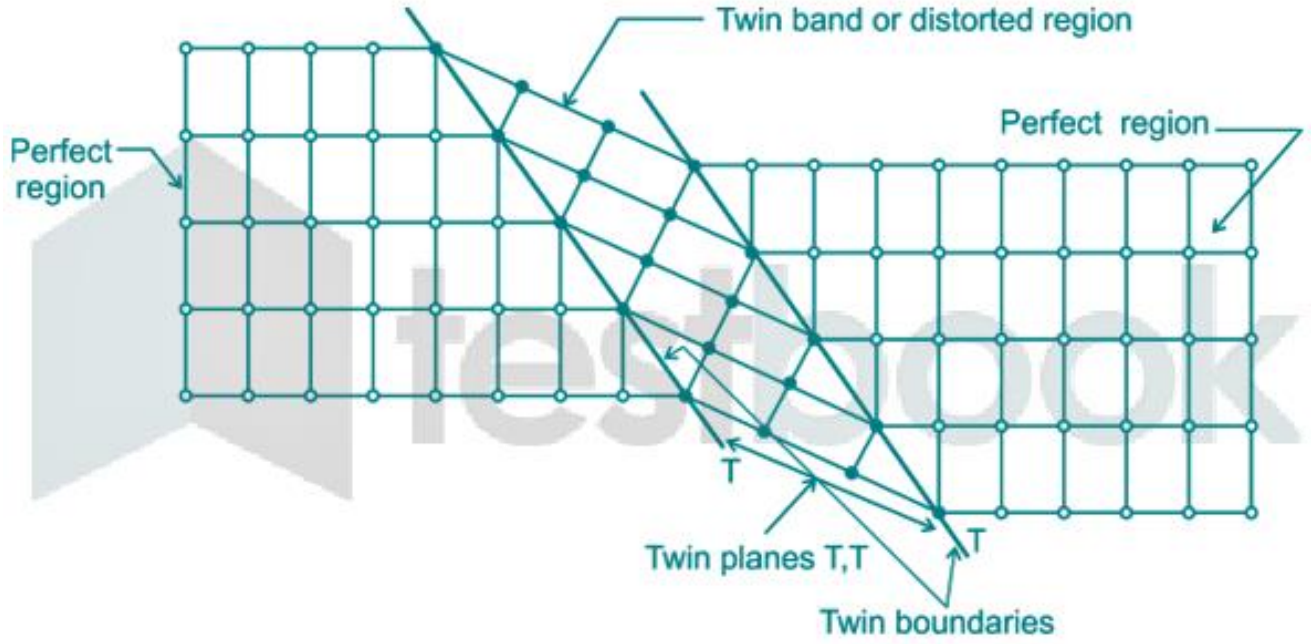
Two dimensional surface defect, which separate two orientations that are mirror image of one another are twin boundaries. The volume of the material which has an orientation that is a mirror image of the matrix orientation, called twin. (fairly thick, i.e. 10^3-10^5 atomic layer).

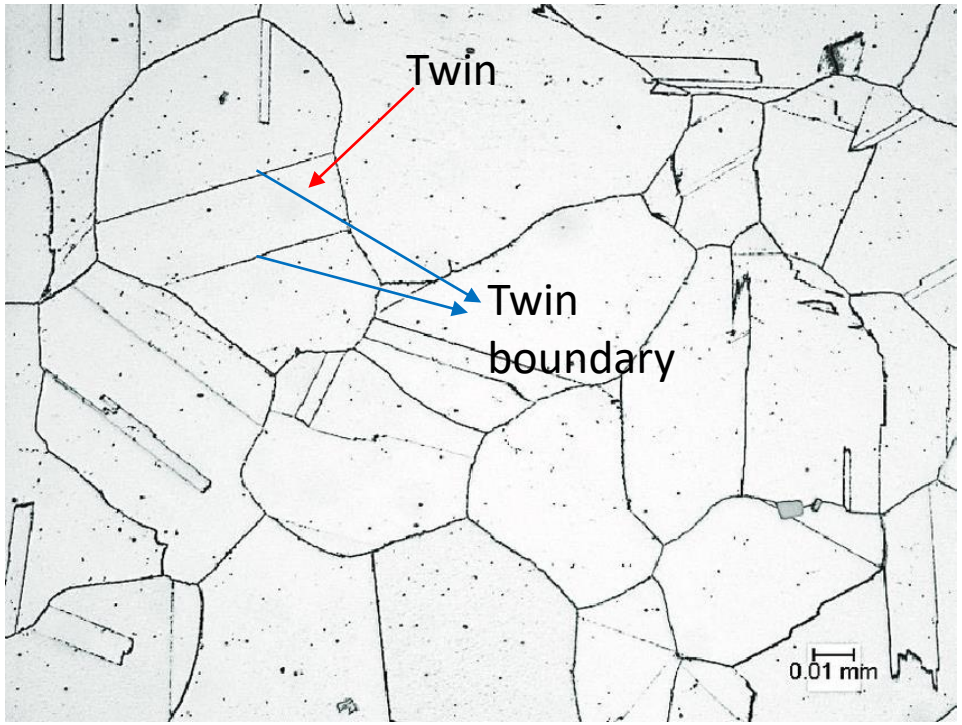
The mechanism that produces twin orientation requires that a given atom moves only a fraction of a lattice spacing.

Twins are formed as a result of :--

a) Plastic deformation, called deformation twin. Commonly observed in HCP and BCC metals when deformed at high strain rate and/or low temperatures.

b) By the process of growth during annealing, and are then called annealing twin, commonly observed in FCC metals.





Volume defects/ three dimensional defects

Four type :
1) Precipitate
2) Void
3) Pores
4) Blow holes

Precipitates : which break the continuity of regular crystalline structure of the matrix. Depending upon the nature of interface of the matrix, it divided into three.

Coherent precipitate: these precipitate form by the replacement of solvent atoms by an equal number of Solute atoms in localized region. The interfaces of precipitates are coherent with the matrix. Due to small difference In lattice parameter, interplaner spacing coherency strain (long range elastic strain filed) will generate.
(Due to bending of atomic plane at interface)
Surface energy is small at the interface, but elastic strain energy is high.
Misfit strain parameter $\delta < 5\%$.

Semi-coherent precipitate: in which, the interface between the precipitate and matrix consists of regular Network of dislocations. Size difference between precipitate and matrix is larger than the coherent precipitate.
Elastic strain smaller, dislocation get introduced. Elastic strain energy than coherent PPTs.

Incoherent precipitate : if misfit dislocation increasing more and more, every dislocation have energy associated.
Interfacial energy/ surface energy high but no coherency and no elastic strain.
Size difference between precipitate and matrix is very high, Misfit strain parameter $\delta > 15\%$.

Voids : Voids can be generated as agglomeration of vacancy. Voids formed when materials are subjected to irradiation with high energy particles. It offers nucleation sites for gas bubbles, octahedral in shape.

Pores: It is common in ceramic materials and powder metallurgy manufacturing processes like compacting, setting, sintering. Pores lead to decrease, strength, thermal conductivity, magnetic properties etc.

Blow holes : A hole in metal caused by a bubble of gas captured during solidification. Decrease electrical and thermal conductivity as well as strength.