

Materials Science and Engineering (BMEE209L)

by

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Content

□ **Module: 2 Crystallography and Defects** covers the following:

- **Crystallography – Fundamental Concepts**
 - **The Unit Cell**
 - **Bravais Lattices**
 - **Crystal Structures**
 - **Crystallographic Points, Directions, and Planes in the Unit Cell**
 - **Weiss Zone Law**
 - **Crystal Imperfections – Introduction**
 - **Classification of Defects Based on Dimensionality**
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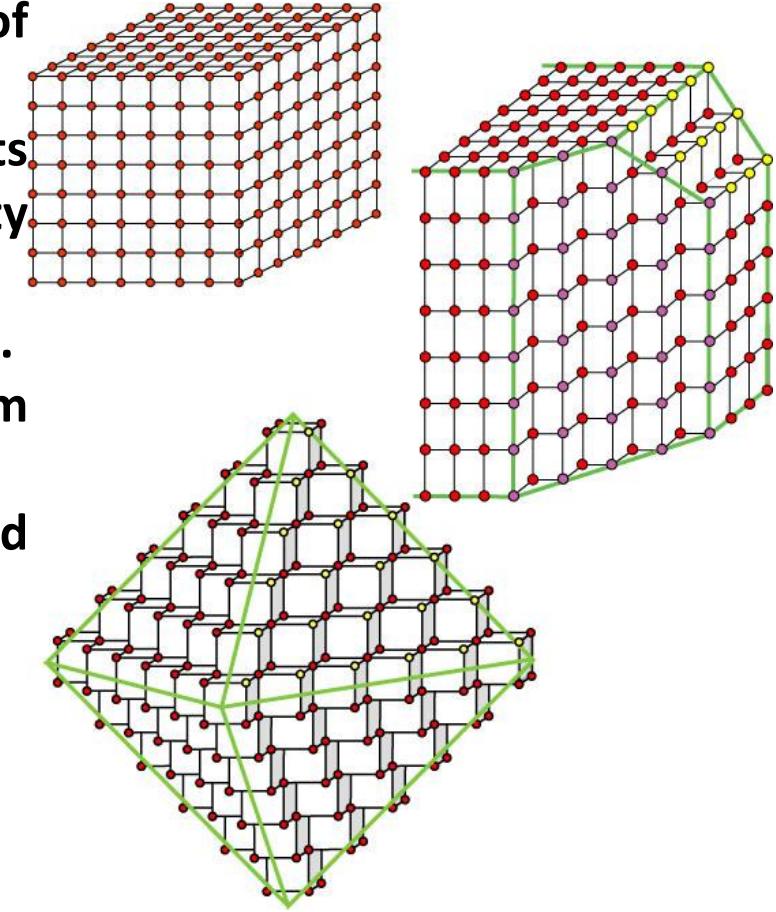
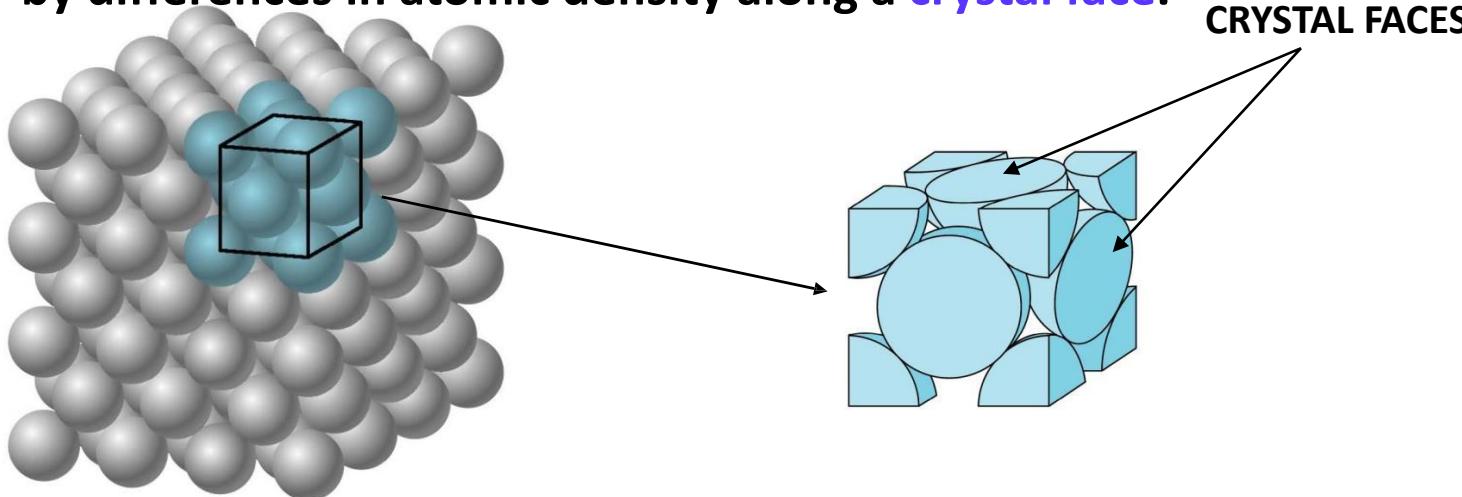


Crystallography – Fundamental Concepts

- Amorphous solids are homogeneous and isotropic (having a physical property which has the same value when measured in different directions) because there is no long range order or periodicity in their internal atomic arrangement.
- In contrast, the crystalline state is characterized by a regular arrangement of atoms over large distances.
- Crystals are therefore anisotropic – their properties vary with direction.
- For example, the interatomic spacing varies with orientation within the crystal, as does the elastic response to an applied stress.
- Note that crystals can be solid or liquid, and can have arbitrary shapes.
- Engineering materials are usually aggregates of many crystals of varying sizes and shapes; these polycrystalline materials have properties which depend on the nature of the individual crystals, but also on aggregate properties such as the size and shape distributions of the crystals, and the orientation relationships between the individual crystals.
- The crystallography of interfaces connecting adjacent crystals can determine the deformation behaviour of the polycrystalline aggregate; it can also influence the toughness through its effect on the degree of segregation of impurities to such interfaces.

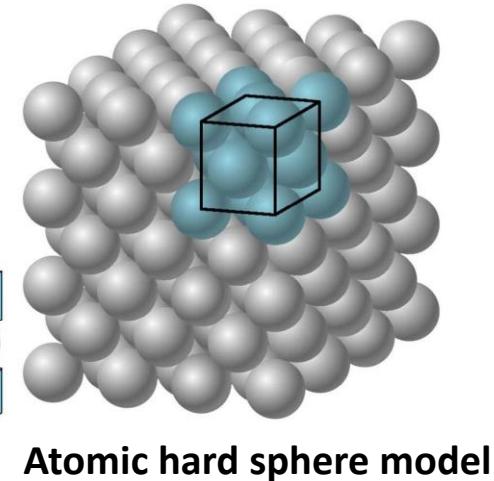
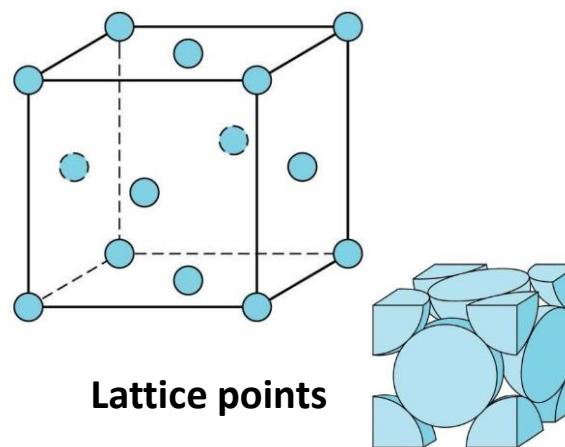
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- **Crystallography** is the experimental science of the arrangement of atoms in solids.
- A **crystal** consists of atoms arranged in a pattern that repeats periodically in three dimensions and whose surface regularity reflects its **internal symmetry**.
- A **crystal structure** is a regular arrangement of atoms or molecules.
- Growth of crystal is affected by the conditions and matrix from which they grow.
- That one face grows quicker than another is generally determined by differences in atomic density along a **crystal face**.

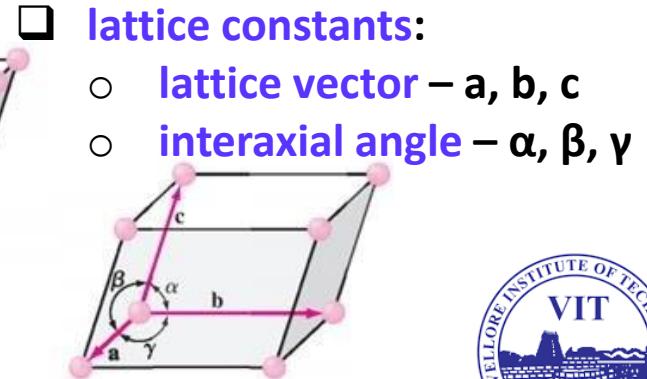
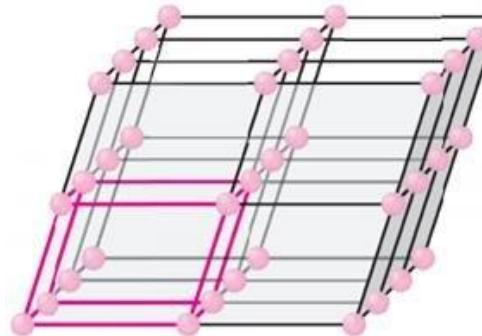


The Unit Cell

- Crystals have translational symmetry: it is possible in a crystal, to identify a regular set of points, known as the **lattice points**, each of which has an **identical environment**.
- The set of these lattice points constitutes a **three dimensional lattice**.
- A **unit cell** may be defined within this lattice as a space-filling parallelepiped with origin at a lattice point, and with its edges given by three non-coplanar basis vectors a , b , and c , each of which represents translations between two adjacent lattice points.
- The entire lattice can then be generated by stacking unit cells in three dimensions.
- Any vector representing a translation between lattice points is called a **lattice vector**.
- **Unit cell** is the smallest unit of volume that permits identical cells to be stacked together to fill all space.
- By repeating the pattern of the unit cell over and over in all directions, the entire **crystal lattice** can be constructed.



- **Space lattice** – a network composed of an infinite three-dimensional array of points and the repeating unit in a space lattice is known as **unit cell**.



- **lattice constants:**
 - **lattice vector** – a , b , c
 - **interaxial angle** – α , β , γ



Crystal Systems: Possible Unit Cell Shapes

- **Symmetry** is a the set of mathematical rules that describe the shape of an object.
- A **sphere** (perfect symmetry) has an Infinite planes of symmetry pass through its center, infinite rotational axes are present, and no matter how little or much you rotate it on any of its infinite number of axes, it appears the same.
- Goal is to quantitatively describe:
 - Shape and Size of the Unit Cell (point symmetry)
 - **Point Symmetry** is when every part has a matching part the same distance from the central point but in the opposite direction.
 - Location of the Lattice Points (translational symmetry)
 - **Translational symmetry** is when something has undergone a movement, a shift or a slide, in a specified direction through a specified distance without any rotation or reflection.

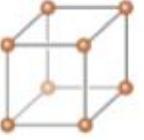
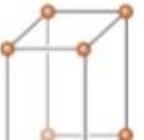
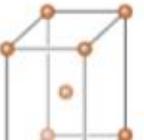
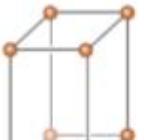
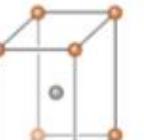
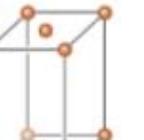
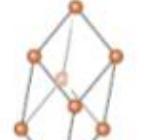
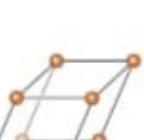
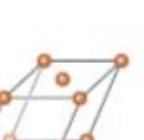
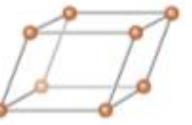
Bravais Lattices

- The number of ways in which points can be arranged regularly in three dimensions, such that the stacking of unit cells fills space, is not limitless; Bravais showed in year 1848 that all possible arrangements can be represented by just **fourteen lattices**.

- The **fourteen Bravais lattices** can be categorized into **seven crystal systems**, such as:
 - Cubic
 - Tetragonal
 - Orthorhombic
 - Trigonal
 - Hexagonal
 - Monoclinic
 - Triclinic

- Each crystal system can be characterized uniquely by a set of defining symmetry elements, which any crystal within that system must possess as a minimum requirement.

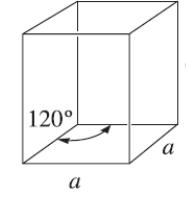
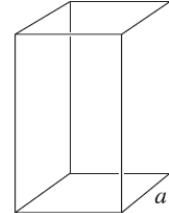
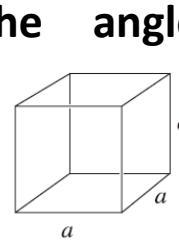
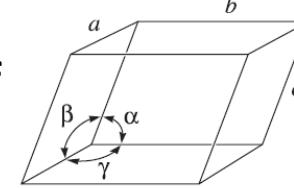
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Simple cubic	Face-centered cubic	Body-centered cubic
		
Simple tetragonal	Body-centered tetragonal	Hexagonal
		
Simple orthorhombic	Body-centered orthorhombic	Base-centered orthorhombic
		
Rhombohedral	Simple monoclinic	Base-centered monoclinic
		Triclinic

Structure	Axes	Angles between Axes	Volume of the Unit Cell
Cubic	$a = b = c$	All angles equal 90°	a^3
Tetragonal	$a = b \neq c$	All angles equal 90°	$a^2 c$
Orthorhombic	$a \neq b \neq c$	All angles equal 90°	abc
Hexagonal	$a = b \neq c$	Two angles equal 90° . One angle equals 120° .	$0.866a^2 c$
Rhombohedral or trigonal	$a = b = c$	All angles are equal and none equals 90°	$a^3 \sqrt{1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha}$
Monoclinic	$a \neq b \neq c$	Two angles equal 90° . One angle (β) is not equal to 90°	$abc \sin \beta$
Triclinic	$a \neq b \neq c$	All angles are different and none equals 90°	$abc \sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}$

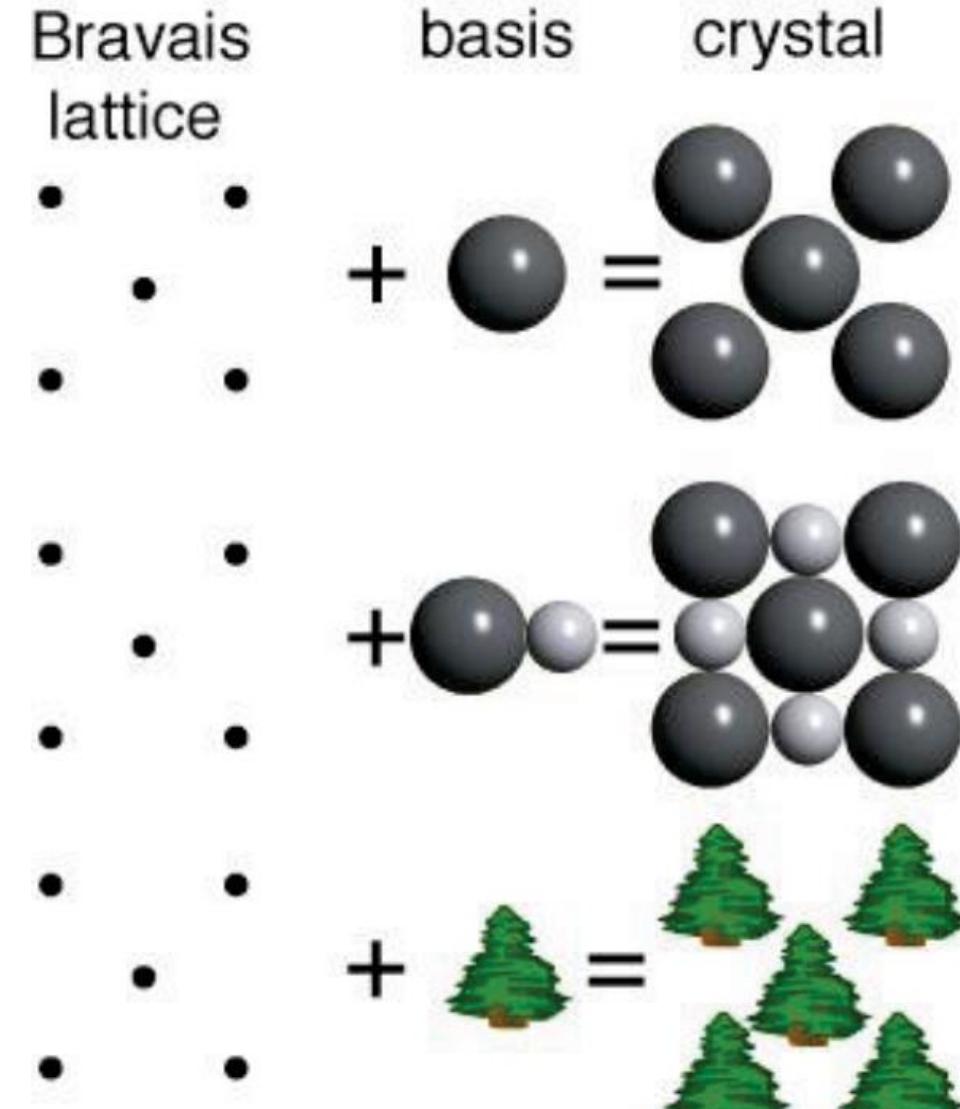
Illustration of 14 Bravais lattices categorized into 7 crystal systems

- The **lattice parameters**, which describe the size and shape of the unit cell, include the dimensions of the sides of the unit cell and the angles between the sides.



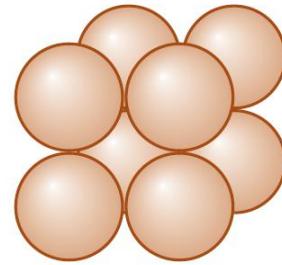
Basis or Motif

- Group of one or more atoms, located in a particular way with respect to each other and associated with each lattice point, is known as the **basis or motif**.
- In other words, these points all have exactly the same surroundings, and they are identical in position relative to the **repeating pattern or motif**.
- **Lattice:** The underlying periodicity of the crystal.
- **Basis:** Entity associated with each lattice points.
- We obtain a **crystal structure** by adding the lattice and basis (i.e., **crystal structure = lattice + basis**).

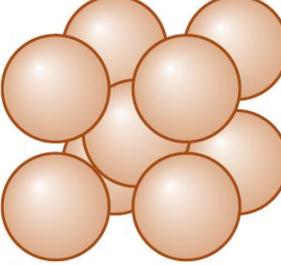


Crystal Structures

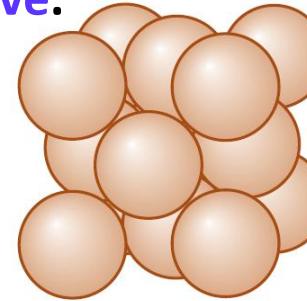
- The **unit cell** defined earlier has lattice points located at its corners.
- Since these are shared with seven other such cells, and since each cell has eight corners, there is only one lattice point per unit cell and such a unit cell is **primitive**.



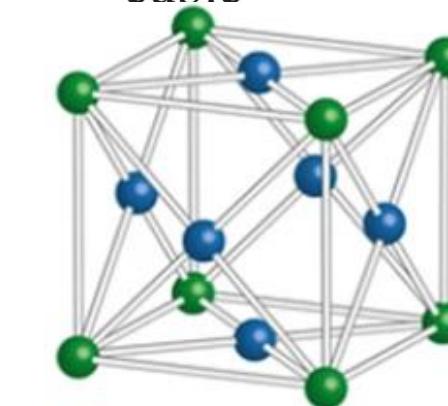
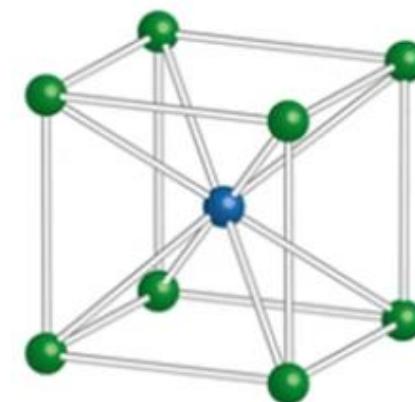
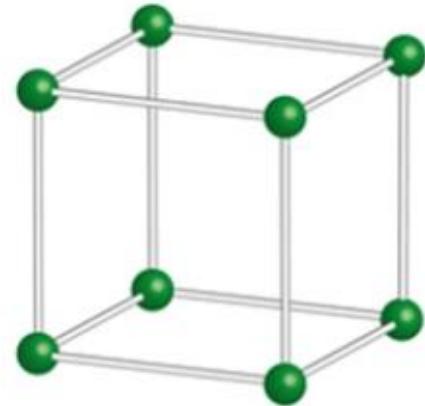
Simple cubic



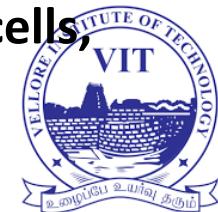
Body-centered
cubic



Face-centered
cubic



The models for simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) unit cells, assuming only one atom per lattice point

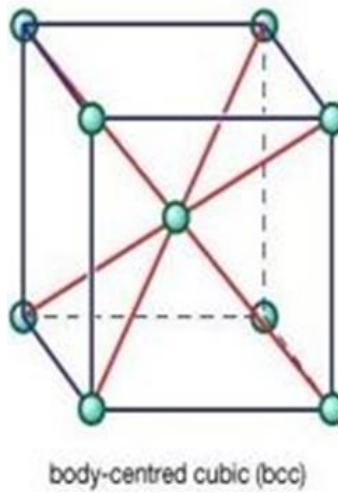


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□ Metallic crystal structures – 90% elemental metals crystallize into three crystal structures:

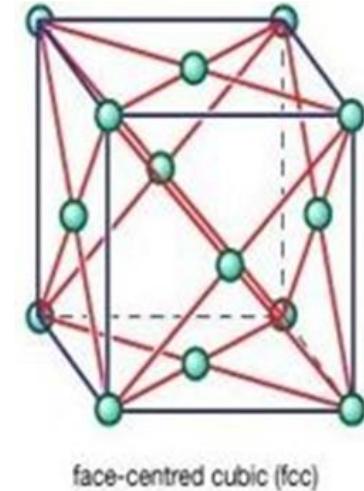
- body-centered cubic (BCC)

	a (nm)	R (nm)
Cr	0.289	0.125
Fe	0.287	0.124
Mo	0.315	0.136
K	0.533	0.231
Na	0.429	0.186
Ta	0.330	0.143
W	0.316	0.137
V	0.304	0.132



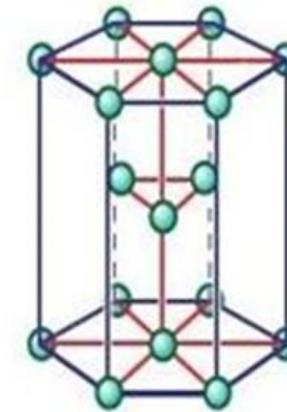
- face-centered cubic (FCC)

	a (nm)	R (nm)
Al	0.405	0.143
Cu	0.3615	0.128
Au	0.408	0.144
Pb	0.495	0.175
Ni	0.352	0.125
Pt	0.393	0.139
Ag	0.409	0.144



- hexagonal close-packed (HCP)

	a	c (nm)	R (nm)
Al	0.2973	0.5618	0.143
Zn	0.2665	0.4947	0.133
Mg	0.3209	0.5209	0.160
Co	0.2507	0.4069	0.125
Zr	0.3231	0.5148	0.160
Ti	0.2950	0.4683	0.147
Be	0.2286	0.3584	0.113



hexagonal close-packed (hcp)



Determination of Number of Atoms in Unit Cell

- We know that a crystal lattice comprises of several unit cells.
- In a unit cell, every constituent particle (atom, molecule, or ion) has a specific and fixed position called **lattice site**.
- We can calculate a number of atoms/molecules and ions in a unit cell easily by analyzing the nature and position of constituent particles in unit cells.
- **Number of atoms per unit cell:** The number of atoms per unit cell is the product of the number of atoms per lattice point and the number of lattice points per unit cell.
- In most metals, one atom is located at each lattice point.

Determine the number of lattice points per cell in the cubic crystal systems. If there is only one atom located at each lattice point, calculate the number of atoms per unit cell.

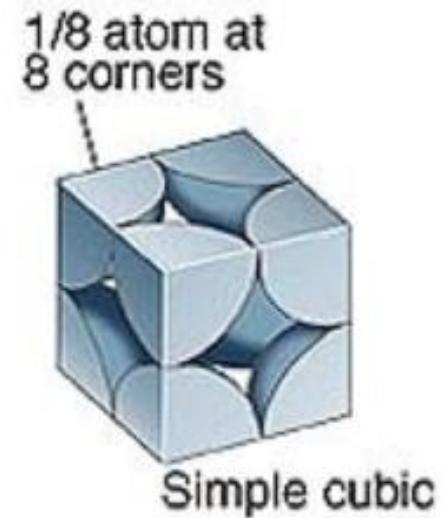
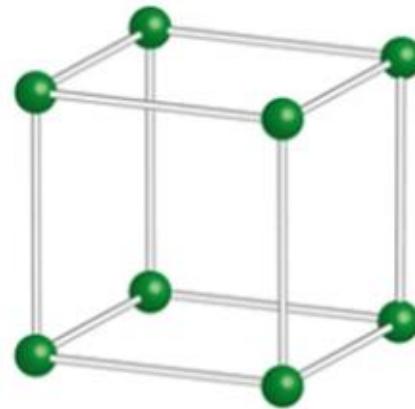


Simple Cubic Unit Cell (SC)

In the primitive cubic unit cell, the atoms are only located on the corners. That means 8 atoms are located on 8 corners of the lattice. Each atom located on the corner contributes $1/8^{\text{th}}$ of the original volume of the cell. So since there are total 8 atoms in a primitive cubic unit cell, the total number of atoms in the primitive cubic unit cell.

$$8 \times \frac{1}{8} = 1 \text{ atom}$$

So there is only 1 atom in a primitive cubic unit cell.



Body-Centred Cubic Unit Cell (BCC)

In a body-centred unit cell, 8 atoms are located on the 8 corners and 1 atom is present at the center of the structure. So total atoms in the body-centred unit cell will be:

Since 8 atoms are present at the corners, each will contribute $1/8^{\text{th}}$ of the original volume of the cell. Thus in the body-centred cubic unit cell:

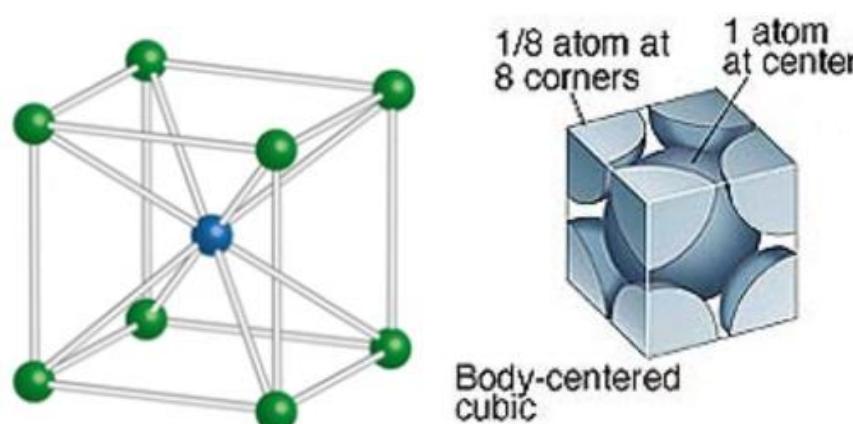
- There are 8 corners and 1 corner shares $1/8^{\text{th}}$ volume of the entire cell, so

$$8 \times \frac{1}{8} = 1 \text{ atom}$$

- Also, the atom at the centre is wholly present at the centre of the cell and can't be shared

$$1 \times 1 = 1 \text{ atom}$$

So there are total 2 atoms present in a body centred unit cell.



Face-Centred Cubic Unit Cell (FCC)

In face-centred cubic unit cell atoms are present on 8 corners and center of all the faces. Also, each atom located on the centre of the unit cell is shared by two adjacent unit cells. Therefore only half atom belongs to a single unit cell.

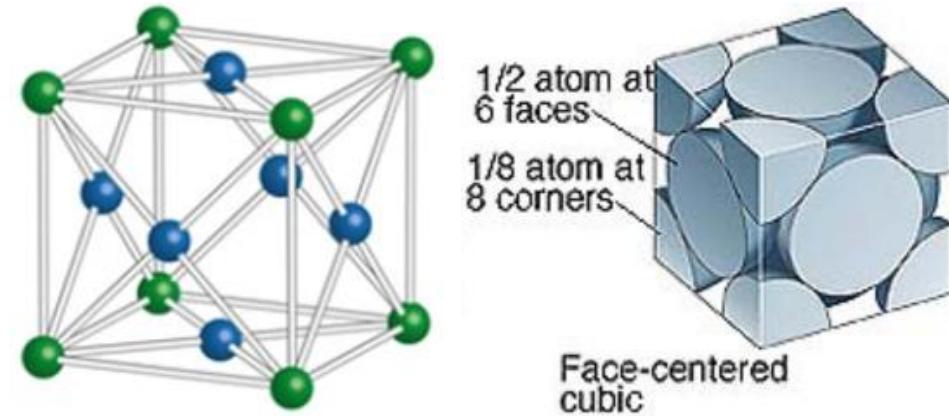
Thus in Face-centred cubic unit cell

- There are 8 atoms present on 8 corners, therefore, each corner will get $1/8$ part of atom

$$8 \times \frac{1}{8} = 1 \text{ atom}$$

- There are six faces and each face gets $1/2$ part of atom then

$$6 \times \frac{1}{2} = 3 \text{ atoms}$$

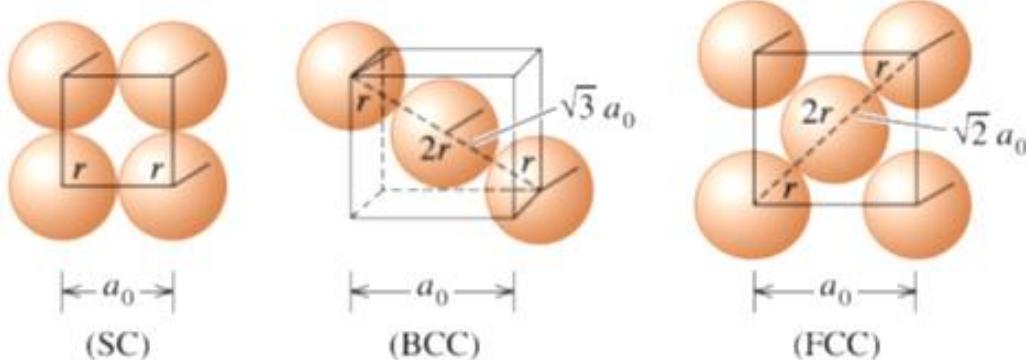


Total atoms present in a face-centred unit cell = $1 + 3 = 4$ atoms



Relationship Between the Atomic Radius and the Lattice Parameter

Determine the relationship between the atomic radius (r) and the lattice parameter (a_0) in SC, BCC, and FCC structures when one atom is located at each lattice point.



The relationships between the atomic radius (r) and the lattice parameter (a_0) in cubic systems

- If refer to the above figure, we find that atoms touch along the edge of the cube in an SC structure.
- The corner atoms are centered on the corners of the cube, so:

$$a_0 = 2r$$

In a BCC structure, atoms touch along the body diagonal, which is $\sqrt{3}a_0$ in length. There are two atomic radii from the center atom and one atomic radius from each of the corner atoms on the body diagonal, so:

$$a_0 = \frac{4r}{\sqrt{3}}$$

In an FCC structure, atoms touch along the face diagonal of the cube, which is $\sqrt{2}a_0$ in length. There are four atomic radii along this length—two radii from the face-centered atom and one radius from each corner, so:

$$a_0 = \frac{4r}{\sqrt{2}}$$



Coordination Number

- The coordination number is the number of atoms touching a particular atom, or the number of nearest neighbors for that particular atom.
- This is one indication of how tightly and efficiently atoms are packed together.

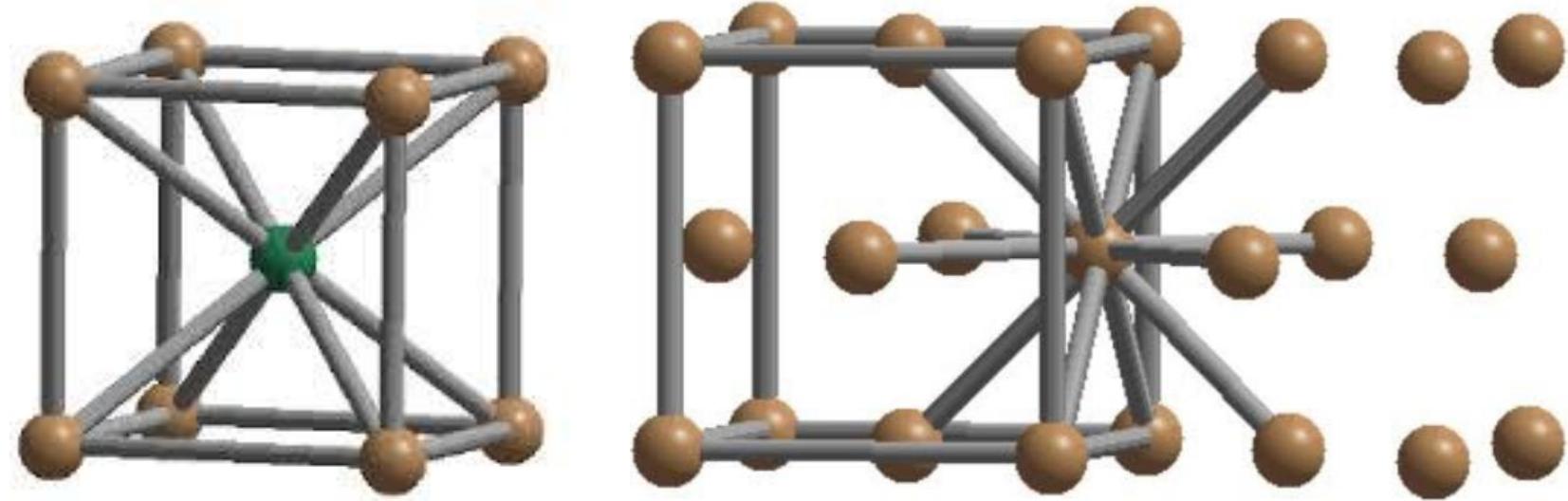
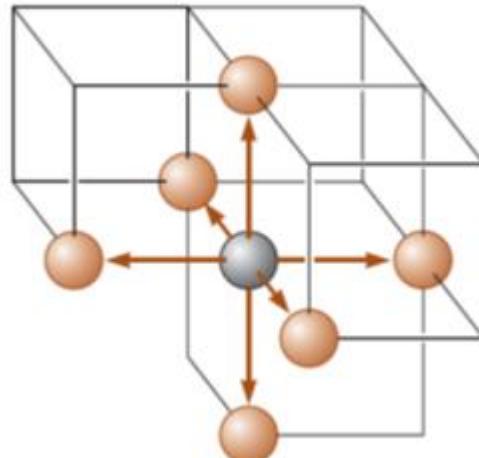


Illustration of coordination in (a) SC, (b) BCC, and (c) FCC unit cells. 6 atoms touch each atom in SC, 8 atoms touch each atom in the BCC, and 12 atoms touch each atom in the FCC unit cell.



Packing Factor

- The **packing factor** is the fraction of space occupied by atoms, assuming that atoms are hard spheres sized so that they touch their closest neighbor.
- The general expression for the **packing factor** is:

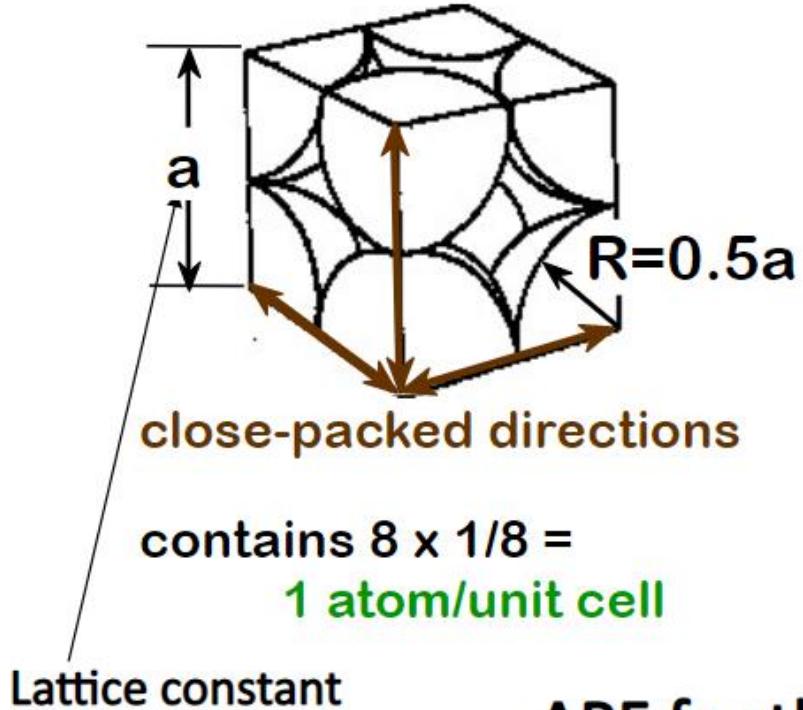
$$\text{Packing factor} = \frac{(\text{number of atoms/cell})(\text{volume of each atom})}{\text{volume of unit cell}}$$



Atomic Packing Factor: SC

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

*assume hard spheres



$$APF = \frac{\frac{\text{atoms}}{\text{unit cell}} \cdot \frac{4}{3} \pi (0.5a)^3}{a^3}$$

atoms
unit cell → 1

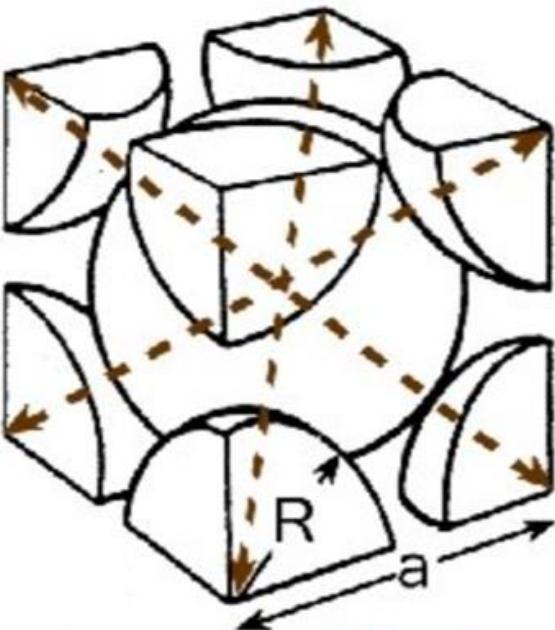
volume
atom → $\frac{4}{3} \pi (0.5a)^3$

volume
unit cell → a^3

APF for the simple cubic structure = 0.52



Atomic Packing Factor: BCC



Close-packed directions:
length = $4R$
 $= \sqrt{3} a$

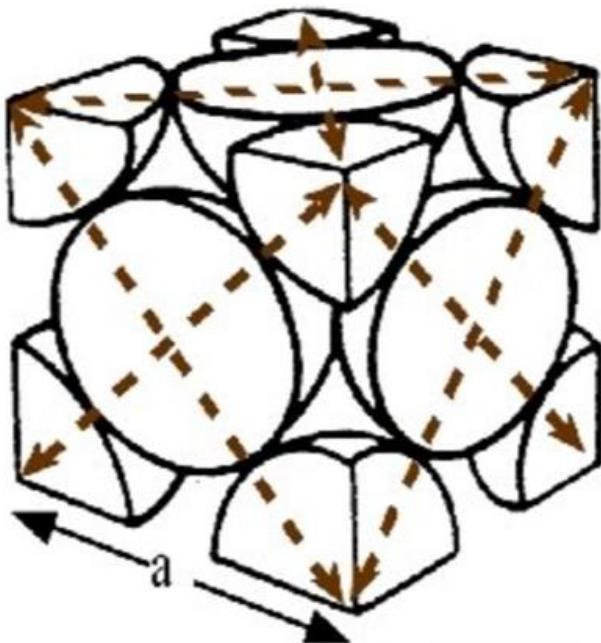
Unit cell contains:
 $1 + 8 \times 1/8$
 $= 2 \text{ atoms/unit cell}$

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

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



Atomic Packing Factor: FCC



Close-packed directions:

$$\text{length} = 4R \\ = \sqrt{2} a$$

Unit cell c contains:

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

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

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



Density Computations

- **Density:** The theoretical density of a material can be calculated using the properties of the crystal structure.
- The general formula is:

$$\text{Density } \rho = \frac{(\text{number of atoms/cell})(\text{atomic mass})}{(\text{volume of unit cell})(\text{Avogadro's number})}$$

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

where n = number of atoms/unit cell
 A = atomic weight
 V_C = Volume of unit cell = a^3 for cubic
 N_A = Avogadro's number
 = 6.022×10^{23} atoms/mol



Density Computations: BCC



- Ex: Cr (BCC)
 $A = 52.00 \text{ g/mol}$
 $R = 0.125 \text{ nm}$
 $n = 2 \text{ atoms/unit cell}$

$$a = 4R\sqrt{3} = 0.2887 \text{ nm}$$

$$\rho = \frac{\frac{\text{atoms}}{\text{unit cell}} \times 2 \times 52.00}{\frac{\text{volume}}{\text{unit cell}} \times a^3 \times 6.022 \times 10^{23}} \times \frac{\text{g}}{\text{mol}}$$

$\rho_{\text{theoretical}} = 7.18 \text{ g/cm}^3$
$\rho_{\text{actual}} = 7.19 \text{ g/cm}^3$



Theoretical Density Computation for Cu

- Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density, and compare the answer with its measured density.
- **Solution:** The crystal structure is FCC, n, the number of atoms per unit cell, is 4. Furthermore, the atomic weight A_{Cu} is given as 63.5 g/mol. The unit cell volume V_c for FCC is as $16R^3\sqrt{2}$, where R, the atomic radius, is 0.128 nm. Substitution for the various parameters into the previous equation, yields:

$$\begin{aligned}\rho_{\text{Cu}} &= \frac{nA_{\text{Cu}}}{V_c N_A} = \frac{nA_{\text{Cu}}}{(16R^3\sqrt{2})N_A} \\ &= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.022 \times 10^{23} \text{ atoms/mol})} \\ &= 8.89 \text{ g/cm}^3\end{aligned}$$

The literature value for the density of copper is 8.94 g/cm³, which is in very close agreement with the foregoing result.



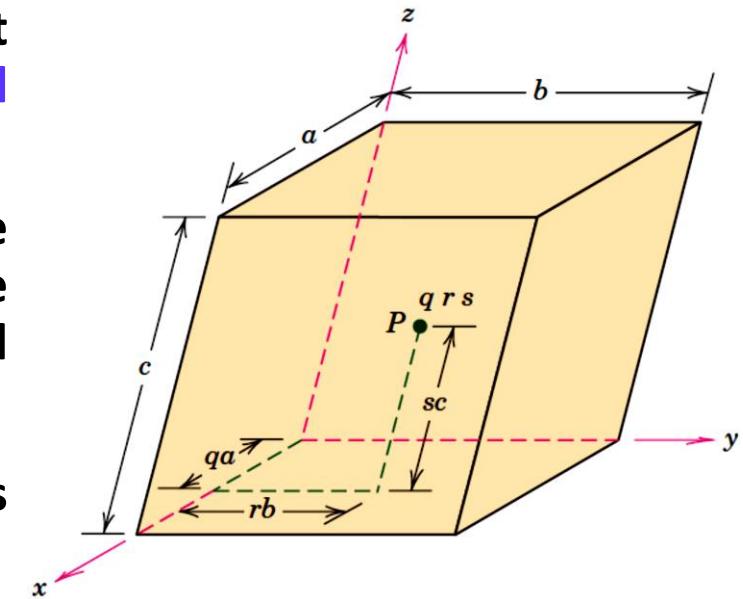
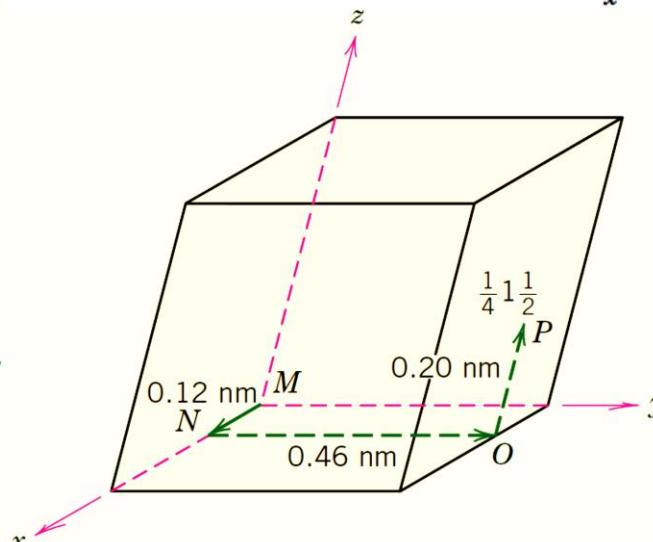
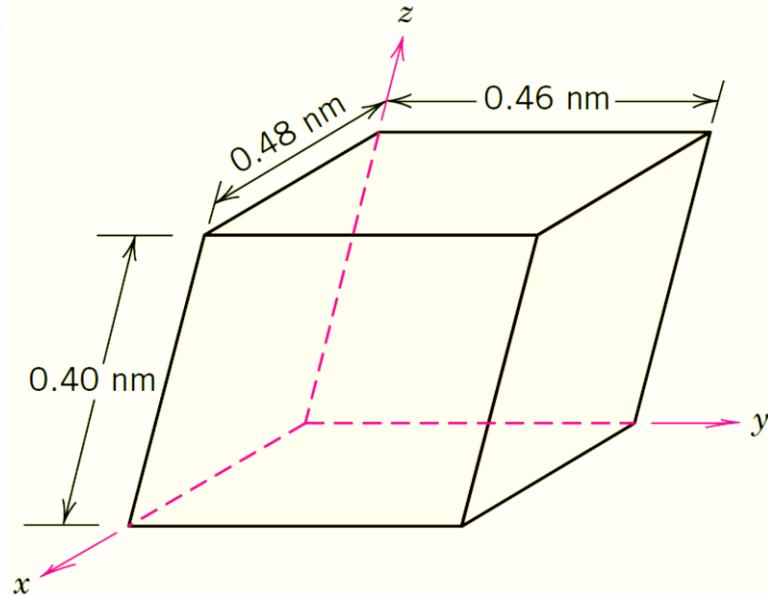
Allotropic or Polymorphic Transformations

- Materials with more than one crystal structure are called allotropic or polymorphic.
- The term allotropy is normally reserved for this behavior in pure elements, while the term polymorphism is used for compounds.
- For example, graphite (hexagonal) and diamond (FCC) are both allotropes of carbon that occur in the solid state.
- Graphite is soft, while diamond is extremely hard.
- Allotropes of phosphorus display different colors, such as red (Tetrahedral), yellow (BCC), and white (SC/Hexagonal).
- Classical examples of polymorphism are the pair of minerals calcite (Trigonal) and aragonite (Orthorhombic), both forms of calcium carbonate.

Structure	a_0 versus r	Atoms per Cell	Coordination Number	Packing Factor	Examples
Simple cubic (SC)	$a_0 = 2r$	1	6	0.52	Polonium (Po), α -Mn
Body-centered cubic	$a_0 = 4r/\sqrt{3}$	2	8	0.68	Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Zr, Cr
Face-centered cubic	$a_0 = 4r/\sqrt{2}$	4	12	0.74	Fe, Cu, Au, Pt, Ag, Pb, Ni
Hexagonal close-packed	$a_0 = 2r$ $c_0 \approx 1.633a_0$	2	12	0.74	Ti, Mg, Zn, Be, Co, Zr, Cd

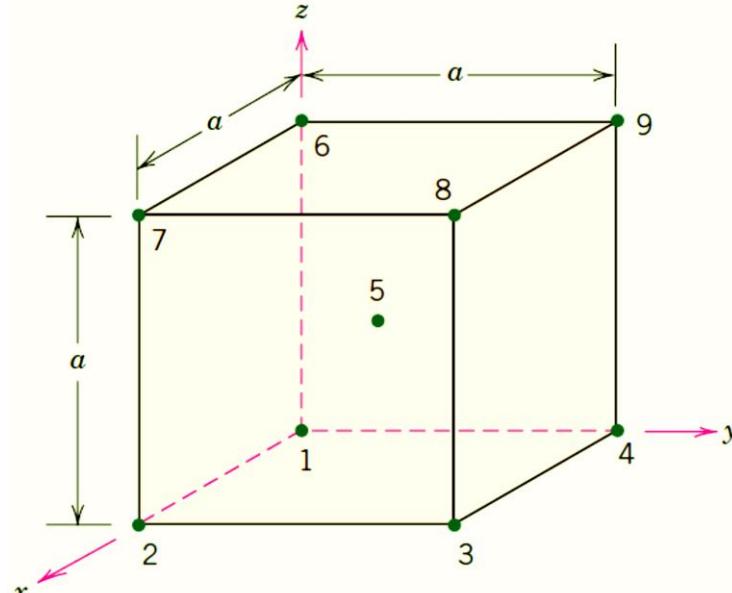
Crystallographic Points, Directions, and Planes in the Unit Cell

- **Point coordinates:** The position of any point located within a unit cell may be specified in terms of its coordinates as **fractional multiples of the unit cell edge lengths** (i.e., in terms of a , b , and c).
- 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.
- For the unit cell shown below, locate the point having coordinates $\frac{1}{4} \ 1 \frac{1}{2}$.



Contd...

- Specify point coordinates for all atom positions for a BCC unit cell.



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



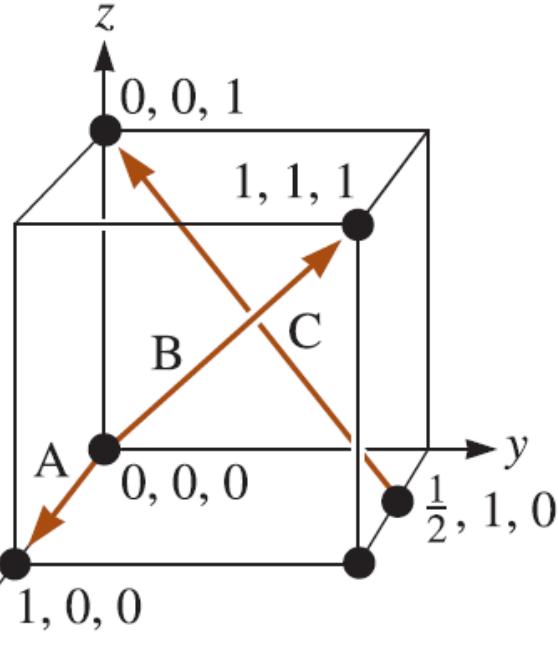
Crystallographic Directions

- A crystallographic direction is a unit vector used to represent various directions within the crystal system.
- The following steps are used to determine the three directional indices:
 - A vector of convenient length is positioned such that it passes through the origin of the coordinate system. Any vector may be translated throughout the crystal lattice without alteration, if parallelism is maintained.
 - The length of the vector projection on each of the three axes is determined; these are measured in terms of the unit cell dimensions **a**, **b**, and **c**.
 - Using a right-handed coordinate system, determine the coordinates of two points that lie on the direction.
 - Subtract the coordinates of the “tail” point from the coordinates of the “head” point to obtain the number of lattice parameters traveled in the direction of each axis of the coordinate system.
 - Clear fractions and/or reduce the results obtained from the subtraction to lowest integers.
 - These three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
 - The three indices, not separated by commas, are enclosed in square brackets, thus: **[uvw]**. The **u**, **v**, and **w** integers correspond to the reduced projections along the **x**, **y**, and **z** axes, respectively.
- Miller indices for directions are the shorthand notation used to describe these directions.



Contd...

- Determine the Miller indices of directions A, B, and C in figure below:



SOLUTION

Direction A

1. Two points are 1, 0, 0, and 0, 0, 0
2. $1, 0, 0 - 0, 0, 0 = 1, 0, 0$
3. No fractions to clear or integers to reduce
4. [100]

Direction B

1. Two points are 1, 1, 1 and 0, 0, 0
2. $1, 1, 1 - 0, 0, 0 = 1, 1, 1$
3. No fractions to clear or integers to reduce
4. [111]

Direction C

1. Two points are 0, 0, 1 and $\frac{1}{2}, 1, 0$
2. $0, 0, 1 - \frac{1}{2}, 1, 0 = -\frac{1}{2}, -1, 1$
3. $2(-\frac{1}{2}, -1, 1) = -1, -2, 2$
4. $[\bar{1}\bar{2}2]$

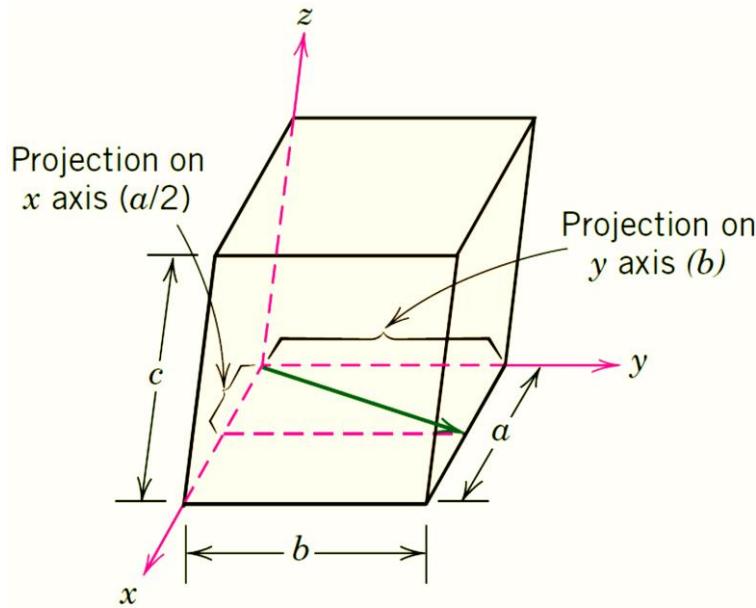
□ Representation of negative indices:

- For each of the three axes, there will exist both positive and negative coordinates.
- Thus negative indices are also possible, which are represented by a bar over the appropriate index.
- For example, the $[1\bar{1}1]$ direction would have a component in the y direction.



Contd...

- Determine the indices for the direction shown in the accompanying figure.



Solution:

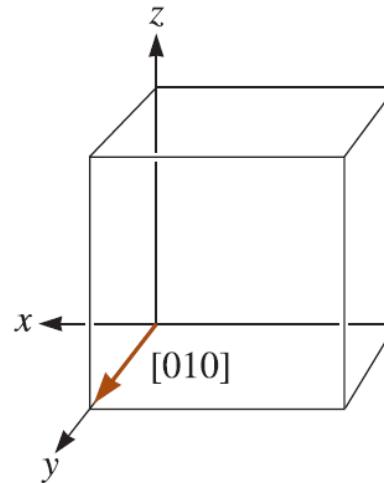
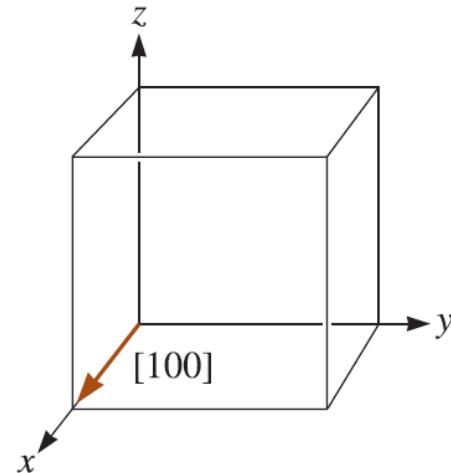
- The vector, as drawn, passes through the origin of the coordinate system, and therefore no translation is necessary.
- Projections of this vector on to the x, y, and z axes are, respective $\frac{1}{2}a$, $1b$, and $0c$, which become $\frac{1}{2}$, 1 , and 0 in terms of the unit cell parameters (i.e., when the a , b , and c are dropped).
- Reduction of these numbers to the lowest set of integers is accompanied by multiplication of each by the factor 2.
- This yields the integers 1, 2, and 0, which are then enclosed in brackets as [120].



Equivalency of Crystallographic Directions of a Form in Cubic Systems

□ Several points should be noted about the use of Miller indices for directions:

- Because directions are vectors, a direction and its negative are not identical; $[100]$ is not equal to $[\bar{1}00]$. They represent the same line, but opposite directions.
- A direction and its multiple are identical; $[100]$ is the same direction as $[200]$. We just forgot to reduce to lowest integers.
- Certain groups of directions are equivalent; they have their particular indices because of the way we construct the coordinates.
- For example, in a cubic system, a $[100]$ direction is a $[010]$ direction if we redefine the coordinate system as shown in figure below:



$$\langle 110 \rangle = \left\{ \begin{array}{ll} [110] & [\bar{1}\bar{1}0] \\ [101] & [\bar{1}0\bar{1}] \\ [011] & [0\bar{1}\bar{1}] \\ [1\bar{1}0] & [\bar{1}10] \\ [10\bar{1}] & [\bar{1}01] \\ [01\bar{1}] & [0\bar{1}1] \end{array} \right. \quad \text{Cubic edge directions}$$

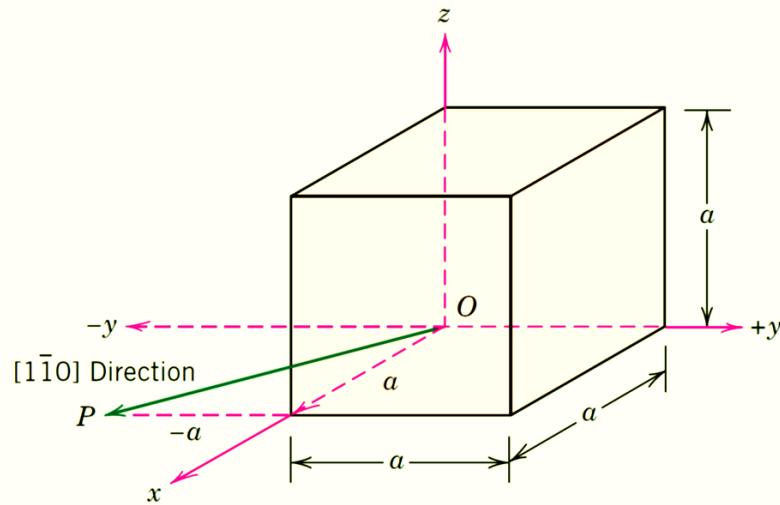


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- Draw a $[1\bar{1}0]$ direction within a cubic unit cell.

Solution

First construct an appropriate unit cell and coordinate axes system. In the accompanying figure the unit cell is cubic, and the origin of the coordinate system, point O , is located at one of the cube corners.



This problem is solved by reversing the procedure of the preceding example. For this $[1\bar{1}0]$ direction, the projections along the x , y , and z axes are a , $-a$, and $0a$, respectively. This direction is defined by a vector passing from the origin to point P , which is located by first moving along the x axis a units, and from this position, parallel to the y axis $-a$ units, as indicated in the figure. There is no z component to the vector, because the z projection is zero.



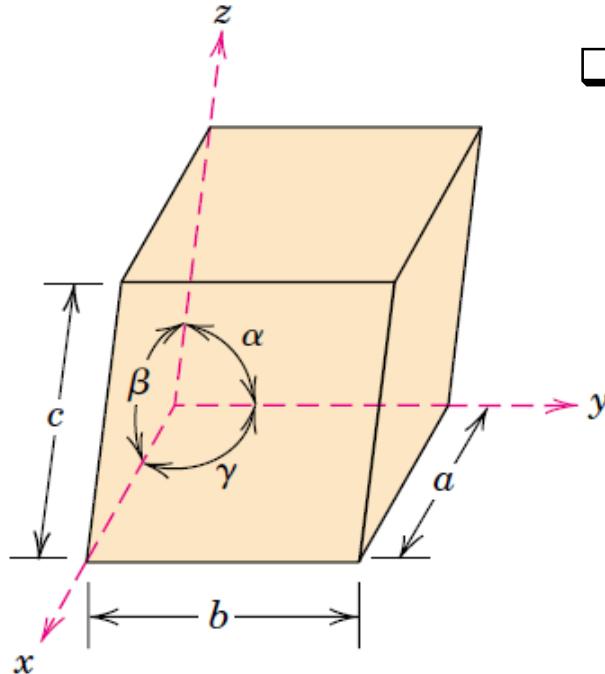
Significance of Crystallographic Directions

- Strength and failure of the materials is controlled by crystal structure and that means the planes which all structures have will move in the directions under stress.
- If and how they move determines strength and failure also called plastic deformation.
- The defects in these planes move in crystallographic directions and weaken the material.
- It can be used to predict the properties and behavior of the material.



Crystallographic Planes

- The orientations of planes for a crystal structure are represented in a similar manner.

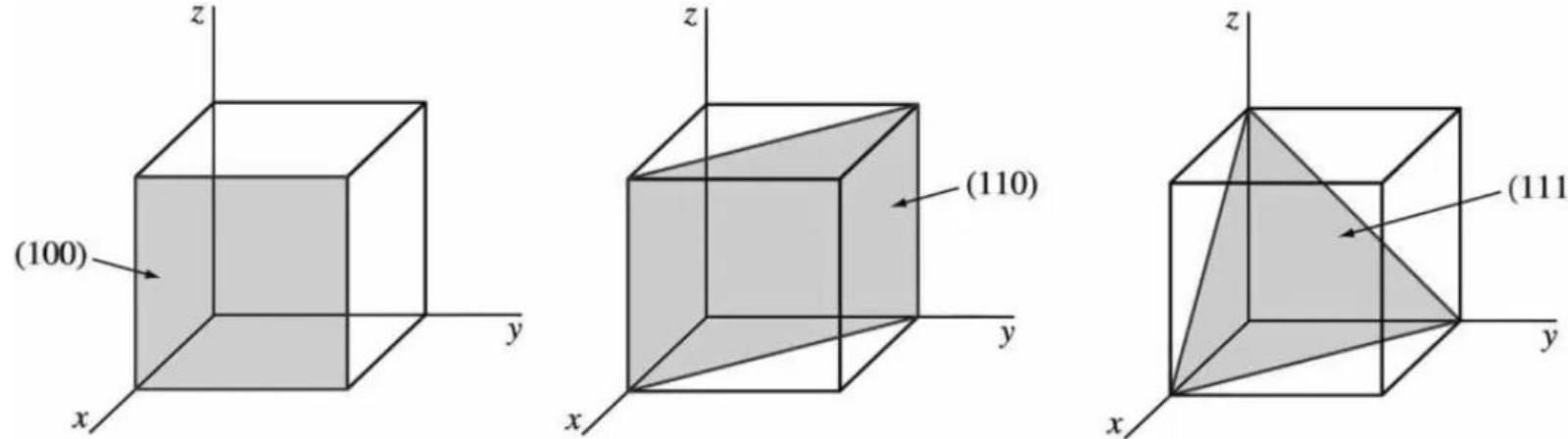


- The procedure used to determine the h , k , and l index numbers is as follows:
 - Choose a plane that does not pass through the origin at $(0, 0, 0)$.
 - Determine the intercepts of the plane (points on the x , y , and z axis where the plane cuts their axes) in terms of the crystallographic x , y , and z axes for a unit cube. These intercepts may be fractions.
 - Form the reciprocals of these intercepts.
 - Clear fractions and determine the smallest set of whole numbers that are in the same ratio as the intercepts.
 - These whole numbers are the Miller indices of the crystallographic plane and are enclosed in parentheses without the use of commas.
 - The notation (hkl) is used to indicate Miller indices in a general sense, where h , k , and l are the Miller indices of a cubic crystal plane for the x , y , and z axes, respectively.
 - Planes and their negatives are identical (not the case for directions) and therefore, $(010) = (0\bar{1}0)$.



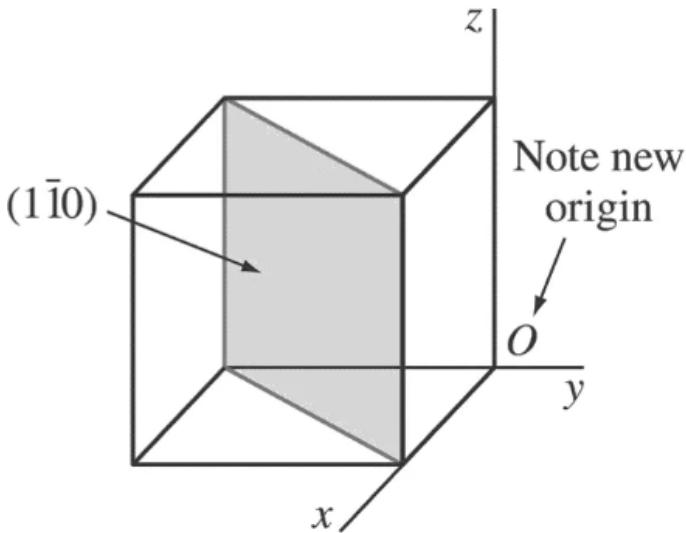
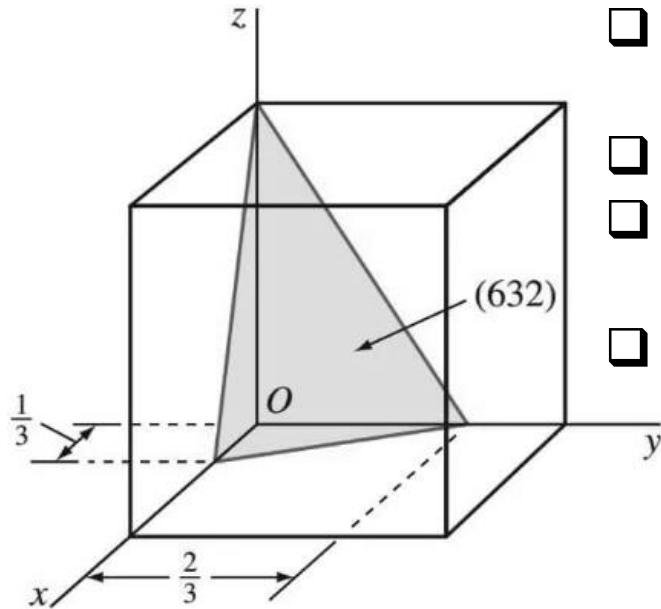
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- The following figure shows three of the most important crystallographic planes of cubic crystal structures.



- Let us first consider the shaded crystal plane in first figure, which has the intercepts $1, \infty, \infty$ for the x, y, and z axes, respectively.
- Take the reciprocals of these intercepts to obtain the Miller indices, which are therefore $1, 0, 0$.
- Since these numbers do not involve fractions, the Miller indices for this plane are (100) , which is read as the one-zero-zero plane.
- Let us consider the second plane shown in figure. The intercepts of this plane are $1, 1, \infty$.
- Since the reciprocals of these numbers are $1, 1, 0$, which do not involve fractions, the Miller indices of this plane are (110) .
- The third plane in the figure has the intercepts $1, 1, 1$, which give the Miller indices (111) for this plane.

Contd...



- Let us Consider now the cubic crystal plane is shown in figure that has the intercepts $1/3$, $2/3$, 1.
- The reciprocals of these intercepts are 3, $3/2$, 1.
- Since fractional intercepts are not allowed, these fractional intercepts must be multiplied by 2 to clear the $3/2$ fractions.
- The reciprocal intercepts become 6, 3, 2, and the Miller indices are (632).
 - If the crystal plane passes through the origin so that one or more intercepts are zero, the plane must be moved to an equivalent position in the same unit cell, and the plane must remain parallel to the original plane.
- This is possible because all equi-spaced parallel planes are indicated by the same Miller indices.
- If sets of equivalent lattice planes are related by the symmetry of the crystal system, they are called planes of a family or form, and the indices of one plane of the family are enclosed in braces as {hkl} to represent the indices of a family of symmetrical planes.
- The Miller indices of the cubic surface planes (100), (010), and (001) are designated as a family or form by the notation {100}.



Calculation of the Angle Between Two Planes

- For cubic crystals, the angle, θ between two planes, $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is given by:

$$\cos \theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)}}$$

Example:

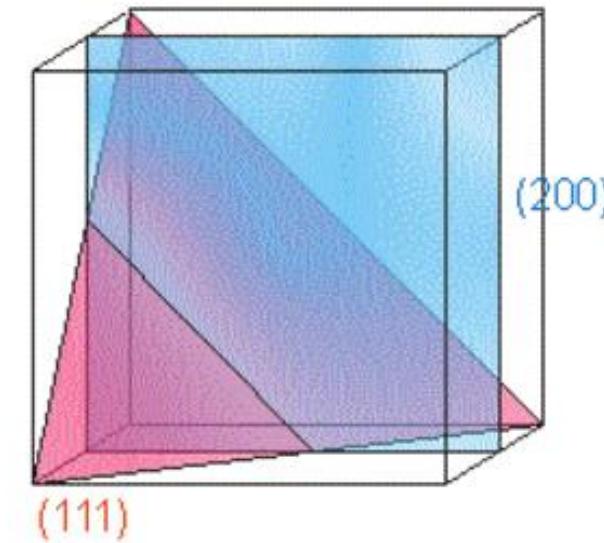
Calculate the angle between the (111) and (200) planes.

From the above,

$$\cos \phi = \frac{(1 \times 2) + (1 \times 0) + (1 \times 0)}{\sqrt{1+1+1}\sqrt{4+0+0}}$$

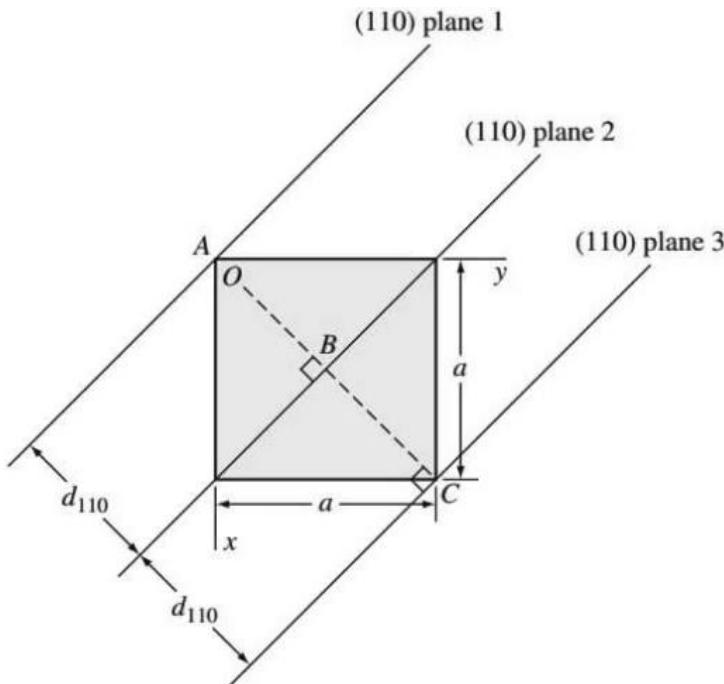
$$\cos \phi = \frac{1}{\sqrt{3}}$$

which produces the result, $\phi = 54.75^\circ$.



Inter-planar Spacing

- An important relationship for the cubic system, is that the direction indices of a direction perpendicular to a crystal plane are the same as the Miller indices of that plane.
- For example, the [100] direction is perpendicular to the (100) crystal plane.
- In cubic crystal structures, the inter-planar spacing between two closest parallel planes with the same Miller indices is designated d_{hkl} , where h , k , and l are the Miller indices of the planes.
- This spacing represents the distance from a selected origin containing one plane and another parallel plane with the same indices that are closest to it.



- For example, the distance between (110) planes 1 and 2, d_{110} , in the figure is AB.
 - Also, the distance between (110) planes 2 and 3 is d_{110} and is the length BC in the figure.
 - From simple geometry, it can be shown that for cubic crystal structure,
- $$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

where

d_{hkl} = interplanar spacing between parallel closest planes with Miller indices h , k , and l

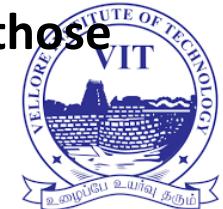
a = lattice constant (edge of unit cube)

h , k , l = Miller indices of cubic planes being considered



Weiss Zone Law

- The Weiss zone law states that, if the direction $[uvw]$ lies in the plane (hkl) , then: $hu + kv + lw = 0$.
- In a cubic system this is exactly analogous to taking the scalar product of the direction and the plane normal, so that if they are perpendicular, the angle between them, θ , is 90° , then $\cos\theta = 0$, and the direction lies in the plane.
- Indeed, in a cubic system, the scalar product can be used to determine the angle between a direction and a plane.
- However, the Weiss zone law is more general, and can be shown to work for all crystal systems, to determine if a direction lies in a plane.
- From the Weiss zone law the following rule can be derived.
- The direction, $[uvw]$, of the intersection of $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is given by:
 - $u = k_1l_2 - k_2l_1$
 - $v = l_1h_2 - l_2h_1$
 - $w = h_1k_2 - h_2k_1$
- As it is derived from the Weiss zone law, this relation applies to all crystal systems, including those that are not orthogonal.



Linear and Planar Density

- Linear density (LD) is defined as the number of atoms per unit length whose centres lie on the direction vector for a specific crystallographic direction; that is,

$$LD = \frac{\text{number of atoms centered on direction vector}}{\text{length of direction vector}}$$

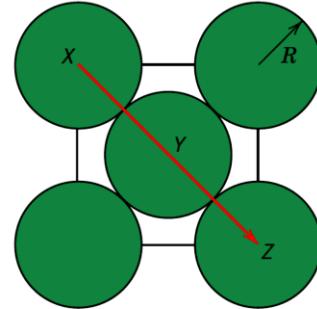
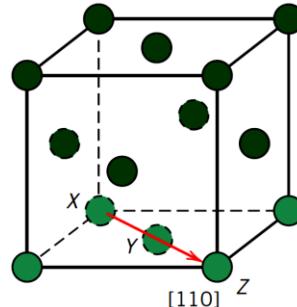
The units of LD are reciprocal length
(e.g., nm⁻¹, m⁻¹)

- Planar density (PD) is taken as the number of atoms per unit area that are centered on a particular crystallographic plane,

$$PD = \frac{\text{number of atoms centered on a plane}}{\text{area of plane}}$$

The units of PD are reciprocal area
(e.g., nm⁻², m⁻²)

- Example: determine the linear density of the [110] direction for the FCC crystal structure.



$$LD_{110} = \frac{2 \text{ atoms}}{4R} = \frac{1}{2R}$$

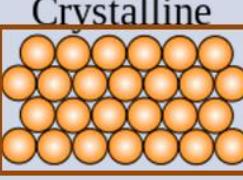
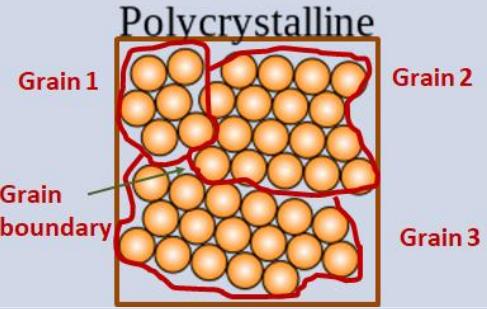
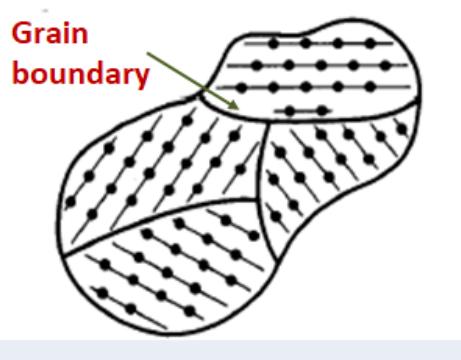
(110) atomic plane for FCC crystal structure

$$PD_{110} = \frac{2 \text{ atoms}}{8R^2\sqrt{2}} = \frac{1}{4R^2\sqrt{2}}$$

- Example:
- Although six atoms have centers that lie on this plane, only one-quarter of each of atoms A, C, D, and F, and one-half of atoms B and E, for a total equivalence of just 2 atoms, are on that plane. The area of this rectangular section is,

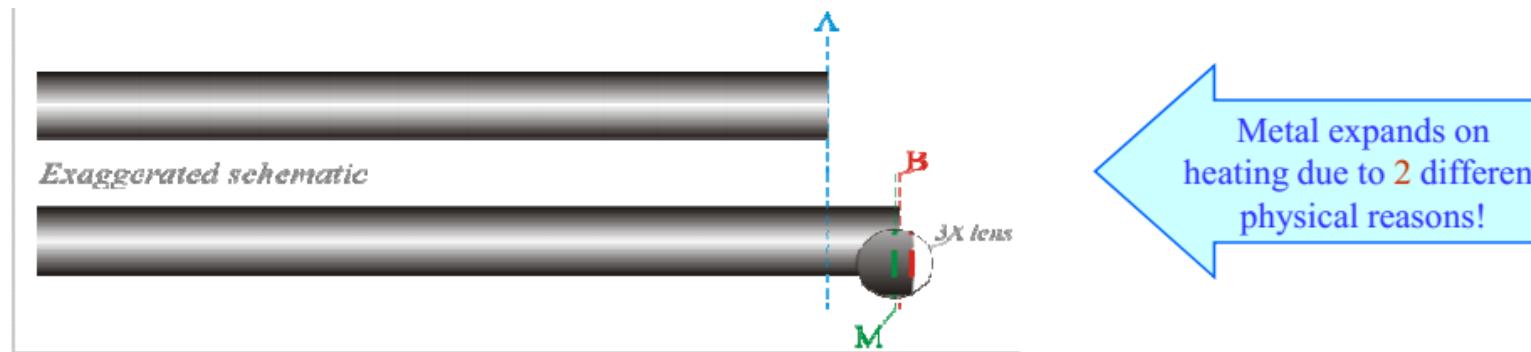
$$(4R)(2R\sqrt{2}) = 8R^2\sqrt{2}$$

Single Crystals vs. Polycrystalline Materials

Single crystals	Polycrystalline		
An ideal single crystal has an atomic structure that repeats periodically across its whole volume.	A polycrystalline solid or polycrystal is comprised of many individual grains or crystallites. Each grain can be thought of as a single crystal, within which the atomic structure has long-range order.	Popularly used in electronic microcircuits, which employ single crystals of silicon and other semiconductors	
They are ordinarily difficult to produce, because the environment must be carefully controlled	Generally, most of the crystalline materials exist in polycrystalline form when they solidify in normal conditions.	On the quantum scale that microprocessors operate on, the presence of grain boundaries would have a significant impact on the functionality of field effect transistors by altering local electrical properties. Therefore, microprocessor fabricators have invested heavily in facilities to produce large single crystals of silicon.	Used in all generic engineering applications
 <p>Crystalline</p>	 <p>Polycrystalline</p> <p>Grain 1</p> <p>Grain boundary</p> <p>Grain 2</p> <p>Grain 3</p>		 <p>Grain boundary</p>
No grain boundaries. Hence, no defects related to the grain boundaries were present.	Grain boundaries were present (Grain boundaries are interfaces where crystals of different orientations meet.)		
Properties vary with direction (called anisotropic): The physical properties of single crystals of some substances depend on the crystallographic direction in which measurements are taken. For example, the elastic modulus, the electrical conductivity, and the index of refraction may have different values in the [100] and [111] directions. This directionality of properties is termed anisotropy .	Properties may not vary with direction if the grains are randomly oriented (called isotropic): For many polycrystalline materials, the crystallographic orientations of the individual grains are totally random. Under these circumstances, even though each grain may be anisotropic, a specimen composed of the grain aggregate behaves isotropically .		

Stability and Equilibrium

- The fields of Thermodynamics and Kinetics are vast oceans and this chapter will introduce the bare essentials required to understand the remaining chapters.
- Let us start by performing the following (thought) experiment:-
 - Heat a rod of Al from room temperature to 500 °C → As expected the rod will expand (**A → B** in figure below).
- The expansion occurs because of **two reasons**:
- Vibration of atoms (leading to an increase in average spacing between atoms → the usual reason) (**A → M** in figure below).
- Increase in the concentration of vacancies* (a vacancy is created when a Al atom goes to the surface and for every **4** vacancies created the volume equal to **1** unit cell is added). (**M → B** in figure below).
- The 2nd reason is a smaller effect in terms of its contribution to the overall increase in length of the specimen.

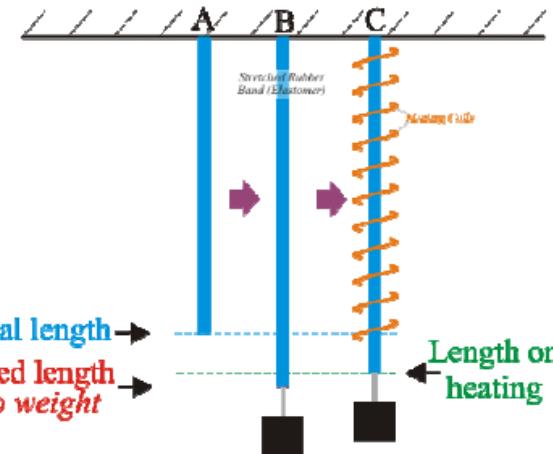


*It costs energy for the system to put vacancies (broken bonds, distortion to the lattice)
→ then why does the system tolerate vacancies?

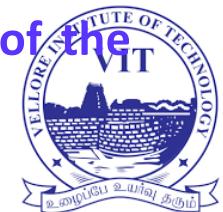


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- Now let us perform another (thought) experiment to put in perspective the previous experiment:
 - Heat a **elastomer** (cut rubber band) which has been stretched by a small weight by about 20°C (room temperature + 20°C) → **the stretched rubber band will contract**.
- **The 2nd reason for the expansion of the Al rod is closely related to the contraction of the stretched rubber band** → occurs because of thermodynamic reasons (quantities like Gibbs Free Energy (G) and Entropy (S)).
- In the case of the heating of the **Al rod**- “how ^{Natural length}_{Extended length Due to weight} the vacancies form” is an issue of **kinetics** (chapter on diffusion).
- Let us next consider the **melting of a pure metal at its melting point (MP)** (at constant T and P) → by supplying heat to the sample of metal (so that the metal sample is only partly molten). At the MP the liquid metal is in equilibrium with the solid metal.
- The **liquid has higher potential energy as well as higher kinetic energy than the solid**.
- Then **why does the liquid co-exist with the solid?**
- The answer to this question lies in the fact that **internal energy is not the measure of stability of the system** (under the circumstances).



A 'stretched' elastomer contracts on heating!



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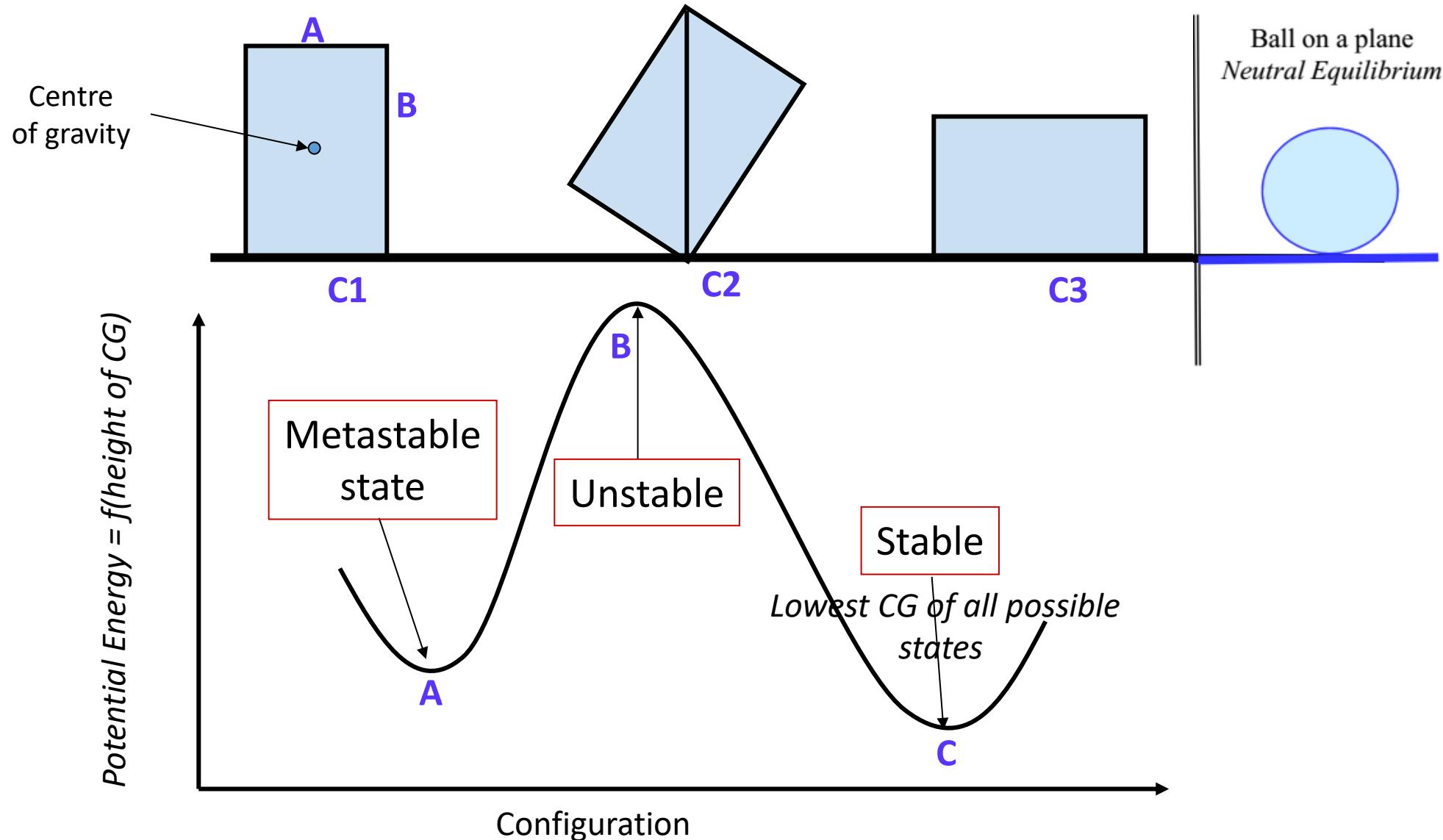
- Equilibrium refers to a state → wherein there is a balance of ‘forces’* (as we shall see equilibrium points have zero slope in a energy-parameter plot)
- Stability relates to perturbations (usually small perturbations** about an equilibrium state) (as we shall see stable relates to the curvature at the equilibrium points).
- Let us start with a simple mechanical system → a rectangular block (figure in next slide) (under an uniform gravitational potential).
- The potential energy (PE) of the system depends on the height of the center of gravity (CG).
- The system has higher PE when it rests on face-A, than when it rests on face-B.
- The PE of the system increases when one tilts it from C1 → C2 configuration.
- In configurations such as C1, C2, and C3 the system will be in equilibrium (i.e., will not change its configuration if there are no perturbations).
- In configuration C2 the system has the highest energy (point B) and any small perturbations to the system will take it downhill in energy → unstable state.
- Configuration C3 has the lowest energy (point C) and the system will return to this state if there are small perturbations → stable state.
- Metastable state is a state of apparent equilibrium although capable of changing to a more stable state.

*Force has been used here in a generalized sense (as an agent which can cause changes)

** Perturbation is usually a small ‘force/displacement’ imposed in a short span of time.



Mechanical Equilibrium of a Rectangular Block



Contd...

- Configuration C1 also lies in an ‘energy well’ (like point C) and small perturbations will tend to bring back the system to state C1. However this state is not the global energy minimum and hence is called a **metastable state**.
- Additionally, one can visualize a state of **neutral equilibrium**, like a ball on a plane (wherein the system is in a constant energy state with respect to configurations).
- **Points to be noted:**
 - A system can exist in many states (as seen even for a simple mechanical system: block on a plane).
 - These states could be **stable**, **metastable** or **unstable**.
 - Using the relevant (thermodynamic) **potential** the stability of the system can be characterized (in the case of the block it is the potential energy, measured by the height of the CG for the case of the block on the plane).
 - System will ‘evolve’ towards the stable state provided ‘**sufficient activation**’ is provided (in the current example the system will go from C1 to C3 by ‘sufficient jolting/shaking’ of the plane).
- **Four kinds of equilibrium (with respect to energy)**
 - Global minimum → Stable state
 - Local minimum → Metastable state
 - Maximum → Unstable state
 - Constant energy → Neutral state/Equilibrium



Crystal Imperfections – Introduction

- You have been introduced to the lattice structures and types of bonding in crystalline solids earlier.
- You know that the behavior of electrons determine the way the atoms interact – the type of bonding (metallic, ionic, covalent and vanderwaals), that holds atoms in a solid together.
 - ✓ But is the knowledge of bonding and crystal structure is sufficient to predict the macroscopic properties of materials?
- So far in our study of crystalline solids, we have assumed a correspondence between the abstract three-dimensional lattice and the actual structure of solids. This implies that crystals are perfect.
- Perfect crystal: A crystal, in which all the atoms are at rest on their correct lattice position in the crystal.
- Such perfect crystals could only exist at absolute zero, and thermal vibrations can be treated as a form of defect in crystal structures.
- For $T > 0K$, defects always exist in the structure.

REAL CRYSTALS ARE NEVER PERFECT, THERE ARE ALWAYS DEFECTS



Contd...

- **For example:** If a bulk metal (i.e., steel) were a single perfect crystal, it would have a strength far exceeding the strongest steel ever produced from metallurgical research. May be this is one of the limitation, in the strength of a metal comes from the number and type of defect, rather than from the nature of the ideal crystal lattice.
- **Many other important properties of materials are due to the imperfections caused by crystal defects (may be...).**

- In this topic we will discuss different types of imperfections or defects in the ideal arrangement of atoms in a crystal.
- **For example:** If you buy a diamond ring, it is mostly the number and type of defects in the diamond crystal that define the amount of money you pay for a given crystal size.
- **Another example:** Forging a metal tool introduces defects and increases strength and elasticity of the tool. Note, that in the case the required properties are achieved without changes in composition of the material, but just by manipulating the crystal defects.

“Crystals are like people, it is the defects in them which tend to make them interesting”

- Colin Humphreys



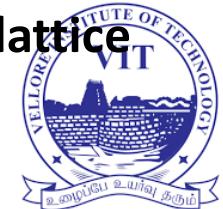
Thermodynamic Cause of Crystal Imperfections

- Crystal defects are thermodynamically-controlled phenomena.
 - ✓ To understand how defects come about, consider the effect of probability on entropy in the following two examples.
- A typical single crystal of a large gemstone contains about 1 mole of atoms. Now compare the effect of adding a single additional defect to:-

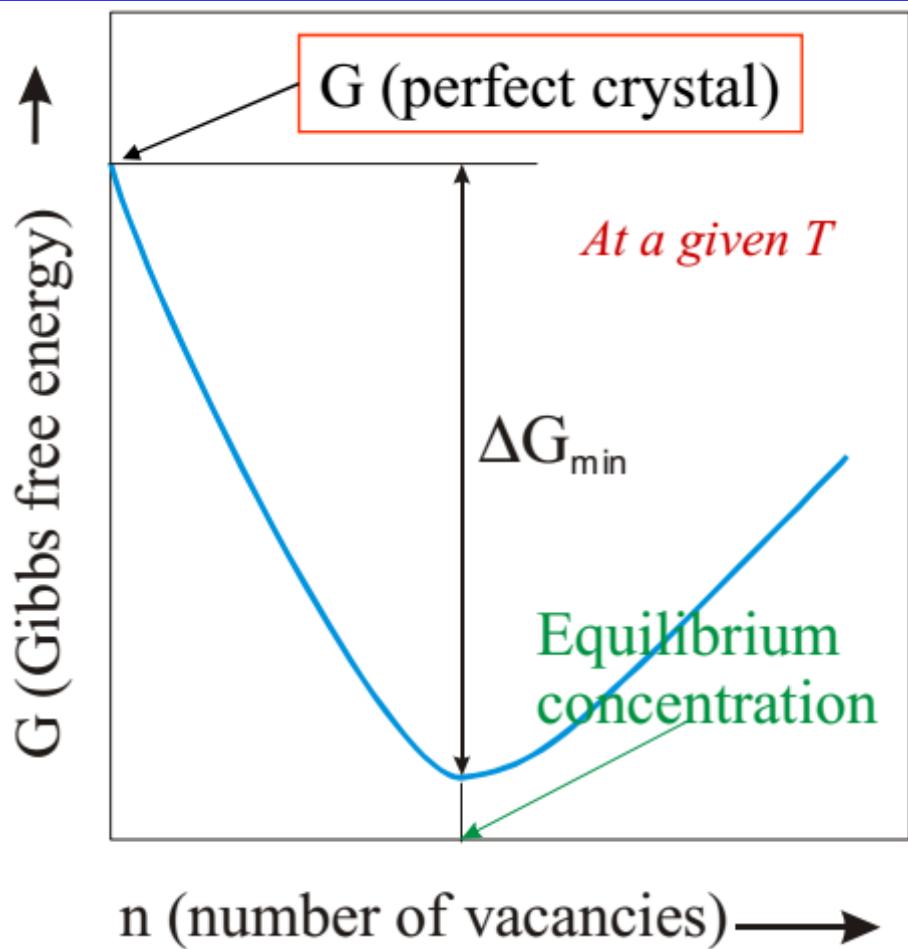
- An ideal crystal → 1 defect {
 - Probability for defect location is 10^{23}
 - There is large increase in the system's entropy}
- A lattice which already has 10% defects → 10% + 1 defect {
 - Probability for defect location is 10
 - There is only a small increase in total entropy}
- This kind of entropy is called **configurational entropy**. It is given by the equation:-

$$S = K \ln(\omega) \quad K = \text{Boltzmann constant}$$
$$\omega = \text{Probability}$$

- So far the effect of entropy; however, the creation of any kind of defect costs energy, since the total lattice energy will be reduced. The competing effects of the energy required to disturb the lattice and the initial large gain in entropy causes a minimum in the free energy.



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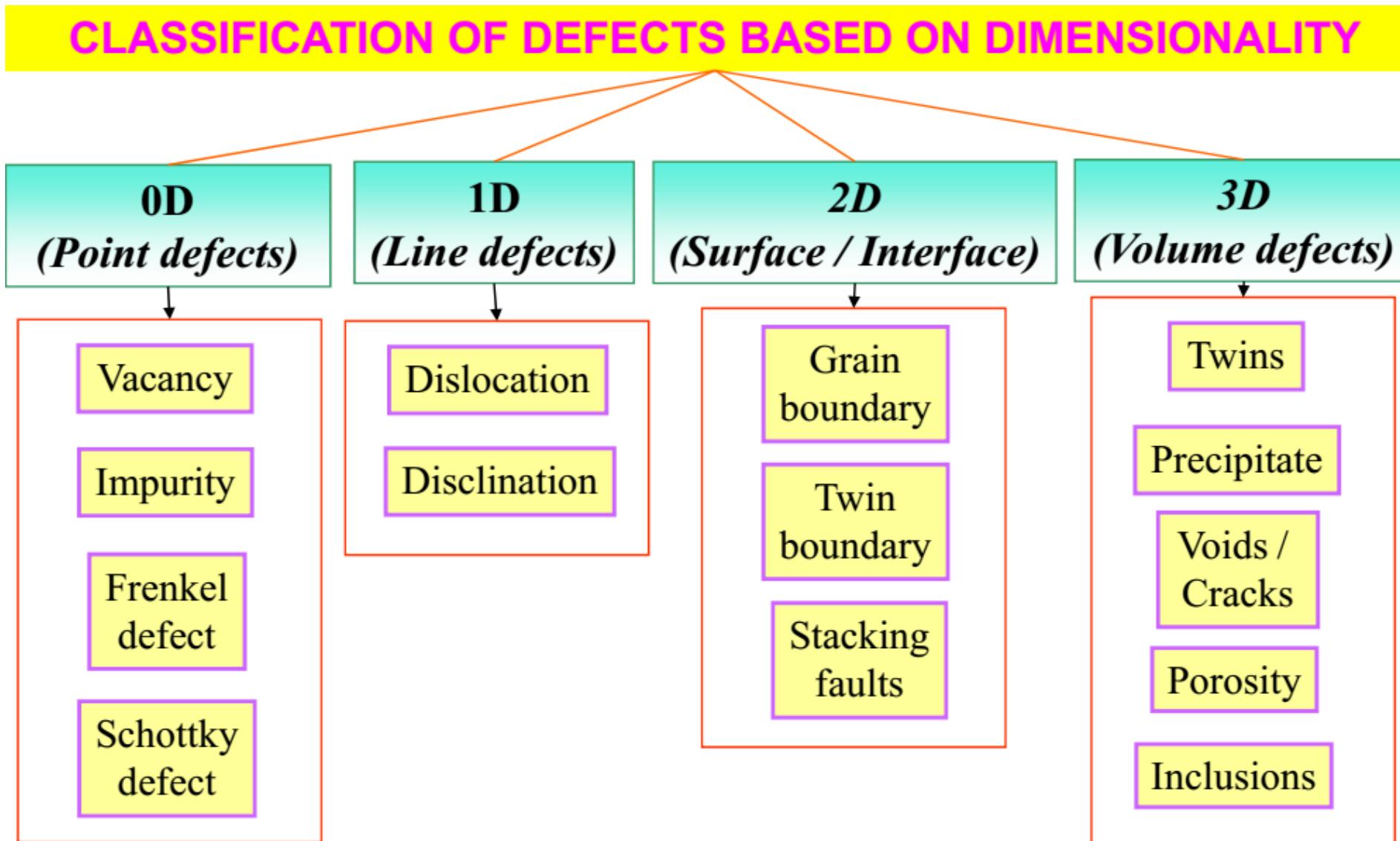
T (°C)	n/N
500	1×10^{-10}
1000	1×10^{-5}
1500	5×10^{-4}
2000	3×10^{-3}

$\Delta H_f = 1 \text{ eV/vacancy}$
 $= 0.16 \times 10^{-18} \text{ J/vacancy}$

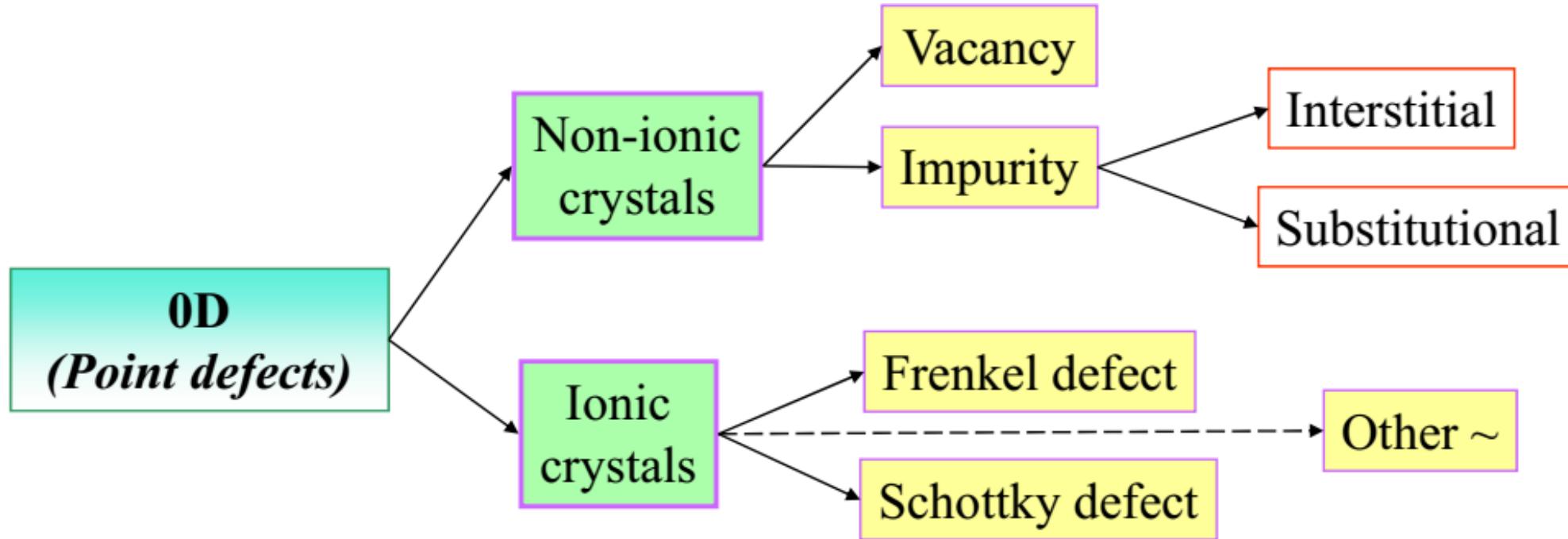
- ❑ Certain equilibrium number of vacancies are preferred at $T > 0 \text{ K}$.
- ❑ n = Number of vacancies.
- ❑ N = For a system of N particles.



Classification of Defects Based on Dimensionality



Point Defects



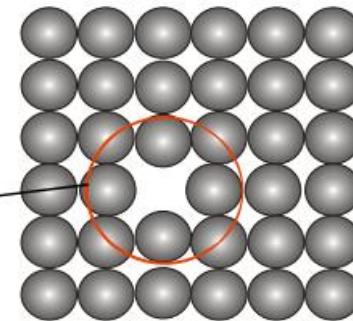
- Imperfect point-like regions in the crystal about the size of 1–2 atomic diameters.



Point Defects: Non-Ionic Crystals

Vacancy

- Missing atom from an atomic site
- Atoms around the vacancy displaced
- Tensile stress field produced in the vicinity



Impurity

Interstitial

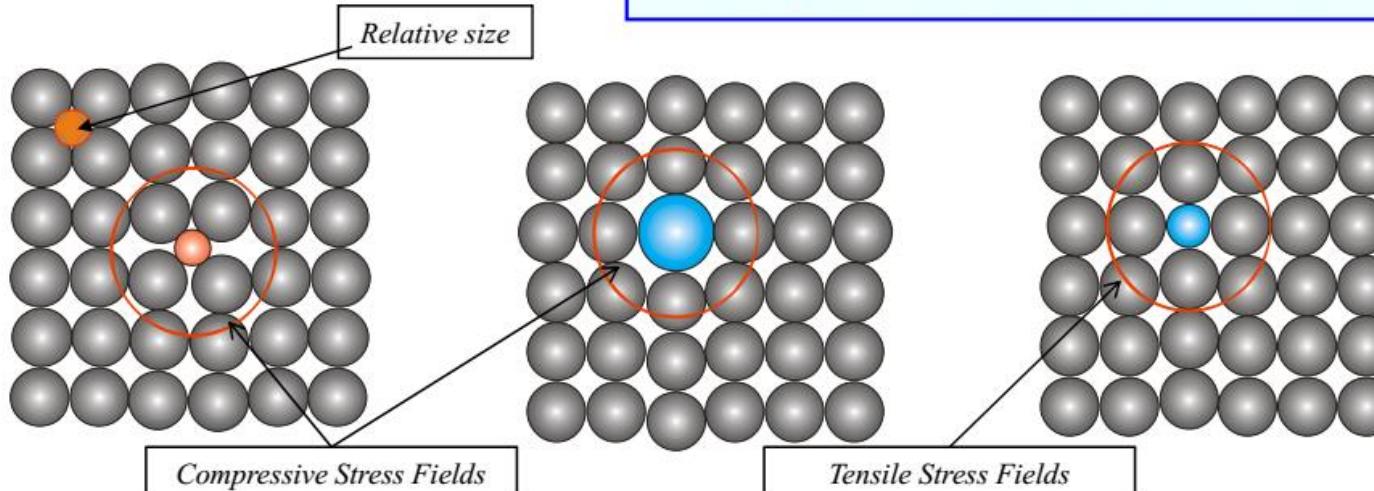
Substitutional

Substitutional Impurity

- Foreign atom replacing the parent atom in the crystal
- E.g. **Cu** sitting in the lattice site of FCC-**Ni**

Interstitial Impurity

- Foreign atom sitting in the void of a crystal
- E.g. **C** sitting in the octahedral void in HT FCC-**Fe**

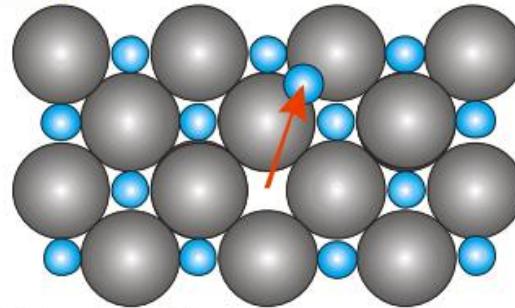


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- Overall electrical neutrality has to be maintained

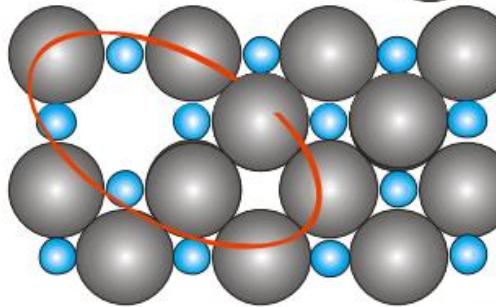
Frenkel defect

- Cation (being smaller get displaced to interstitial voids)
- E.g. AgI, CaF₂



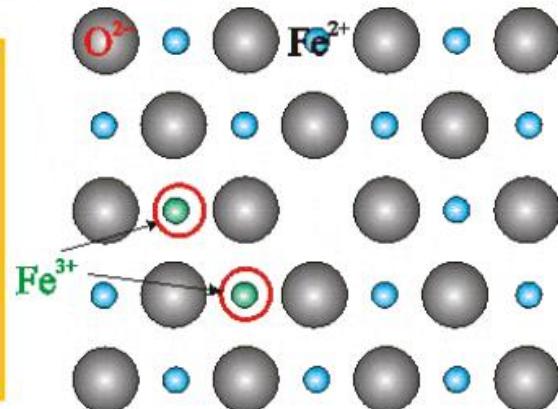
Schottky defect

- Pair of anion and cation vacancies
- E.g. Alkali halides



Other defects due to charge balance

- FeO heated in oxygen atmosphere → Fe_xO ($x < 1$)
- Vacant cation sites are present
- Charge is compensated by conversion of ferrous to ferric ion:
$$\text{Fe}^{2+} \rightarrow \text{Fe}^{3+} + \text{e}^-$$
- For every vacancy (of Fe cation) two ferrous ions are converted to ferric ions → provides the 2 electrons required by excess oxygen



How Many Vacancies are Present?

- The higher is the temperature, more often atoms are jumping from one equilibrium position to another and larger number of vacancies can be found in a crystal.
- Actually, the number of vacancies, N_v , increases exponentially with the absolute temperature, T and can be estimated using the equation:

$$N_v = N_s \exp\left(\frac{-E_v}{K_B T}\right)$$

N_s = Number of regular lattice sites

K_B = Boltzman constant

E_v = Energy needed to form a vacant lattice site in a perfect crystal

- Using this simple equation we can estimate vacancy per 10^n lattice atoms.



Example – 1

- Calculate the equilibrium number of vacancies per cubic meter for copper at 1000 °C. The energy for vacancy formation is 0.9ev/atom. The atomic weight and density (at 1000 °C) for copper are 63.5 g/mol and 8.4 g/cm³ respectively.
- **Solution:** This problem may be solved by using following equations:
- It is first necessary to determine the value of N_s , the number of atomic sites per cubic meter for copper, from its atomic weight A_{Cu} , its density ρ , and Avogadro's number N_A .

$$\begin{aligned}N_s &= \frac{N_A \rho}{A_{Cu}} \\&= \frac{(6.023 \times 10^{23} \text{ atoms/mol})(8.4 \text{ g/cm}^3)(10^6 \text{ cm}^3/\text{m}^3)}{63.5 \text{ g/mol}} \\&= 8.0 \times 10^{28} \text{ atoms/m}^3\end{aligned}$$

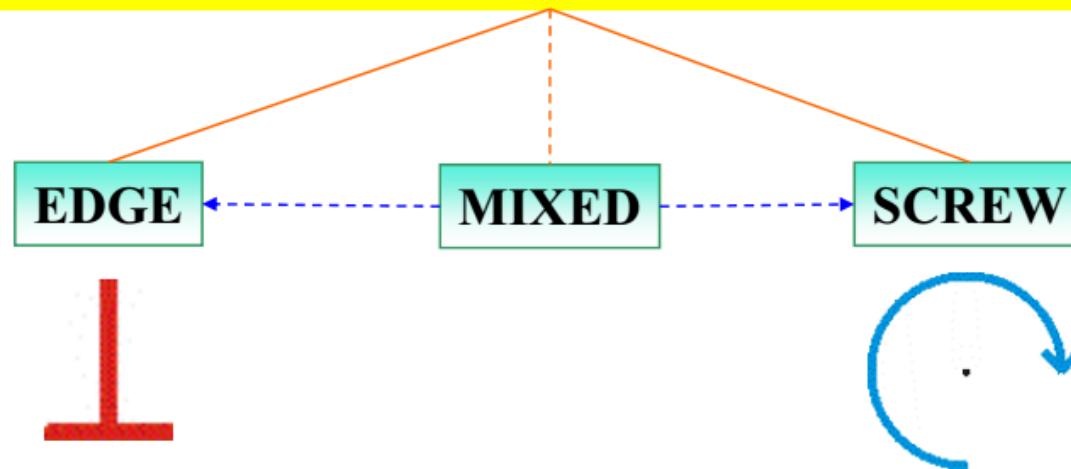
Thus the number of vacancies at 1000°C is equal to

$$\begin{aligned}N_v &= N_s \exp\left(\frac{-E_V}{K_B T}\right) \\&= (8.0 \times 10^{28} \text{ atoms/m}^3) \exp\left[\frac{-0.9 \text{ e.v}}{(8.62 \times 10^{-5} \text{ eV/K})(1273 \text{ K})}\right] \\&= 2.2 \times 10^{25} \text{ vacancies/m}^3\end{aligned}$$

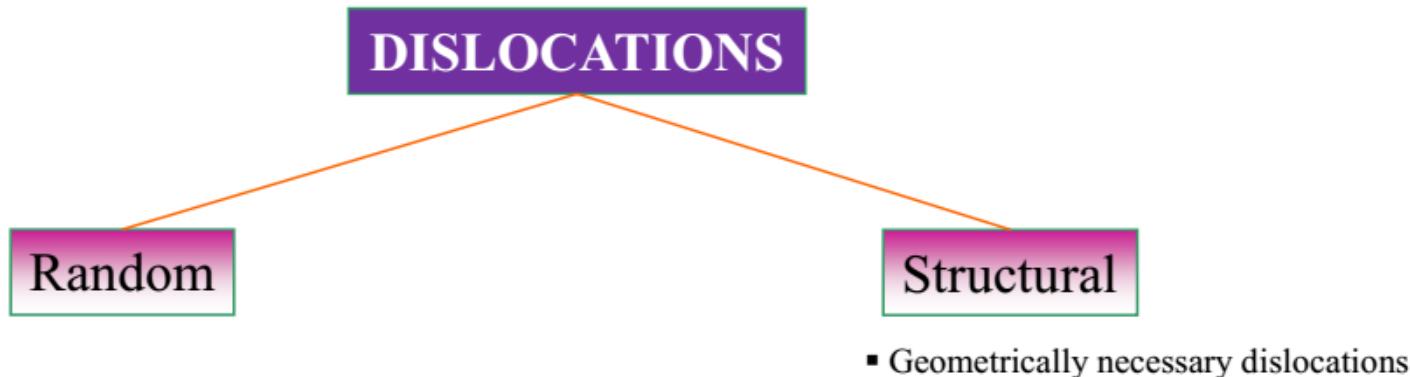


1D Defects: Dislocations

1D Defects : DISLOCATIONS



- Usually dislocations have a mixed character and edge and screw dislocations are the ideal extremes.



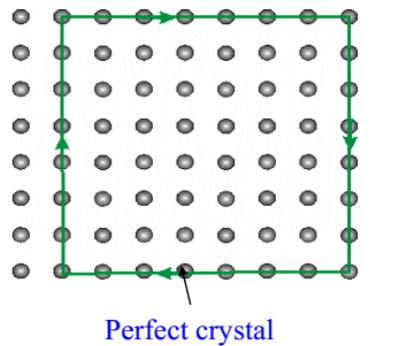
Contd...

- Dislocation is a boundary between the slipped and the un-slipped parts of the crystal lying over a slip plane.
- The intersection of the extra half-plane of atoms with the slip plane defines the dislocation line (for an edge dislocation).
- Direction and magnitude of slip is characterized by the Burgers vector of the dislocation (A dislocation is born with a Burgers vector and expresses it even in its death).
- The Burgers vector is determined by the Burgers circuit.
- Right hand screw (finish to start) convention is used for determining the direction of the Burgers vector.
- As the periodic force field of a crystal requires that atoms must move from one equilibrium position to another \Rightarrow b must connect one lattice position to another (for a full dislocation).
- Dislocations tend to have as small a Burgers vector as possible.
- The edge dislocation has compressive stress field above and tensile stress field below the slip plane.
- Dislocations are non-equilibrium defects and would leave the crystal if given an opportunity.

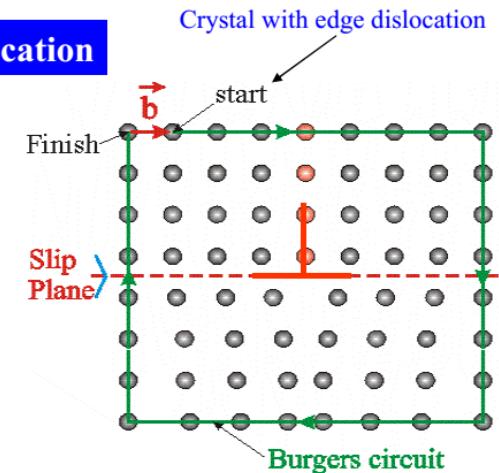
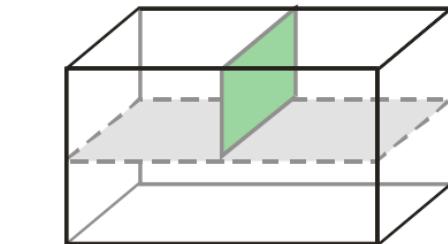
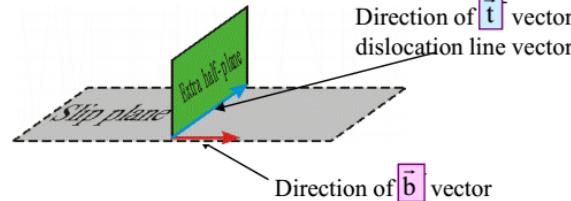


Burgers Vector

- An edge dislocation is a defect where an extra half-plane of atoms is introduced mid way through the crystal, distorting nearby planes of atoms.
- When enough force is applied from one side of the crystal structure, this extra plane passes through planes of atoms breaking and joining bonds with them until it reaches the grain boundary.
- The most useful definition of a dislocation is given in terms of the **Burgers circuit**. A burgers circuit is any atom-to-atom path taken in a crystal containing dislocations which forms a closed loop.



RHFS:
Right Hand Finish to Start convention



- Determination of Burgers vector in a dislocated crystal using **right hand finish to start rule (RHFS)**.
- In a perfect crystal, make a circuit (e.g. 7 atomic steps to right, 7 down, 7 left & 7 up). The circuit is right handed.
- Do the same in the dislocated crystal. The 'missing link' (using some convention like RHFS) is the Burgers vector.
- The edge dislocation is not the 'extra half-plane', neither the 'missing half-plane'. It is the line between the 'extra' and the 'missing' half-planes.
- The regions far away from the dislocation line are perfect → all the 'deformation' is concentrated around the dislocation line.

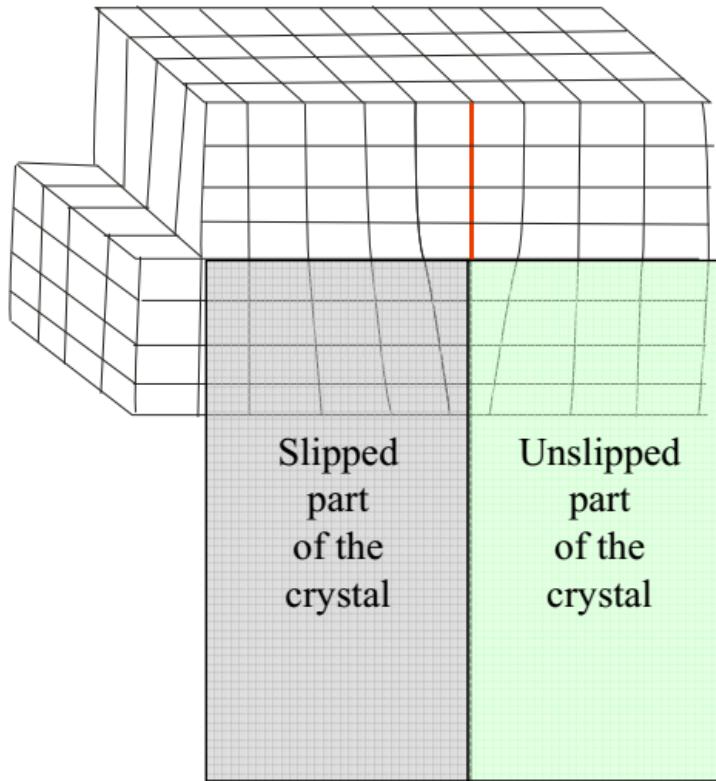
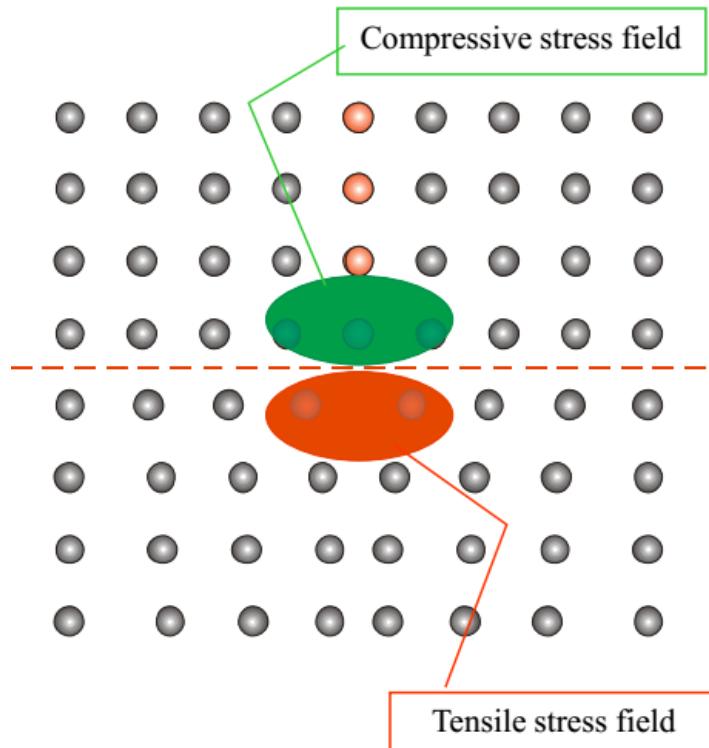


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A dislocation has associated with it two vectors:

\vec{t} → A unit tangent vector along the dislocation line

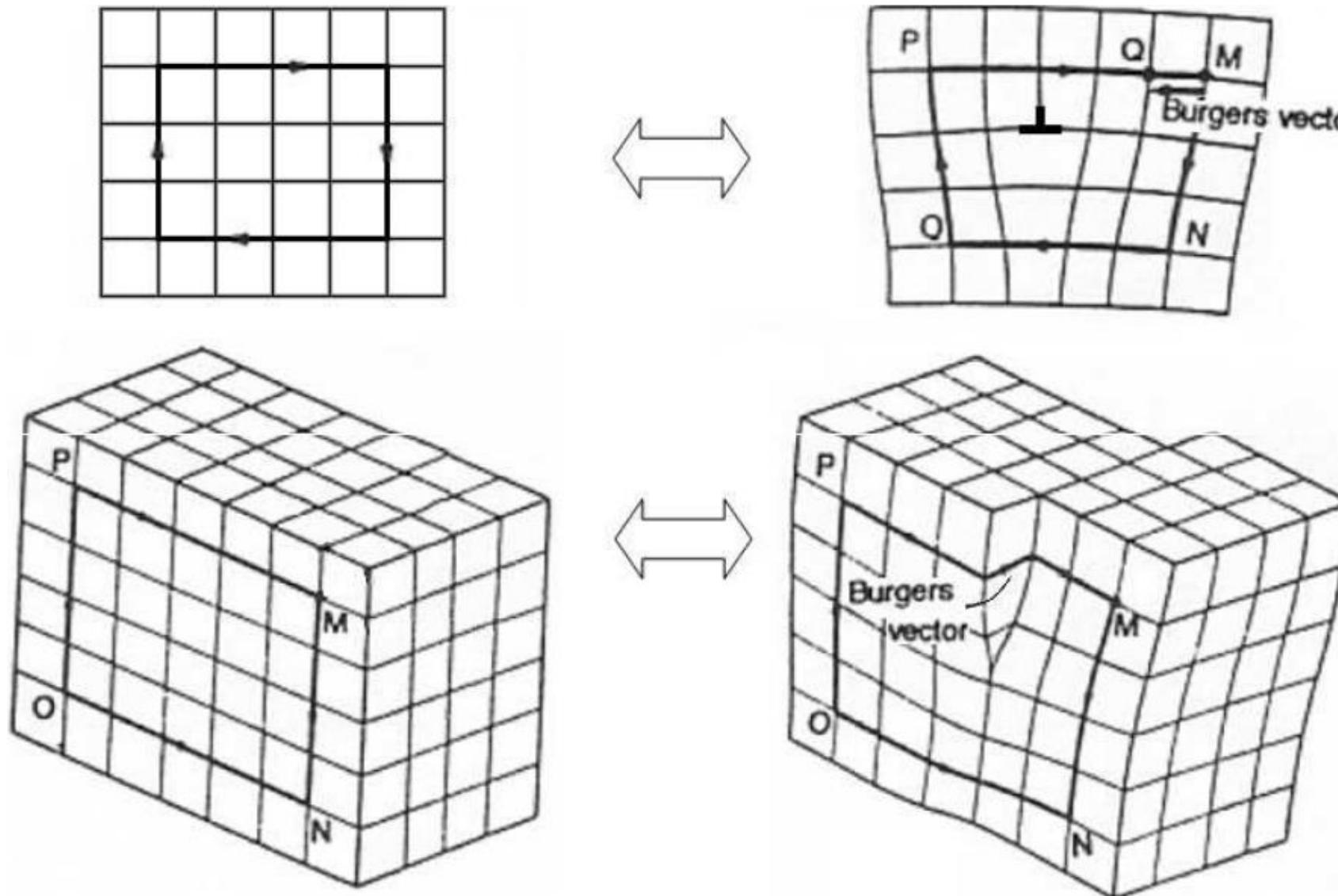
\vec{b} → The Burgers vector



Dislocation is a boundary between the slipped and the unslipped parts of the crystal lying over a slip plane



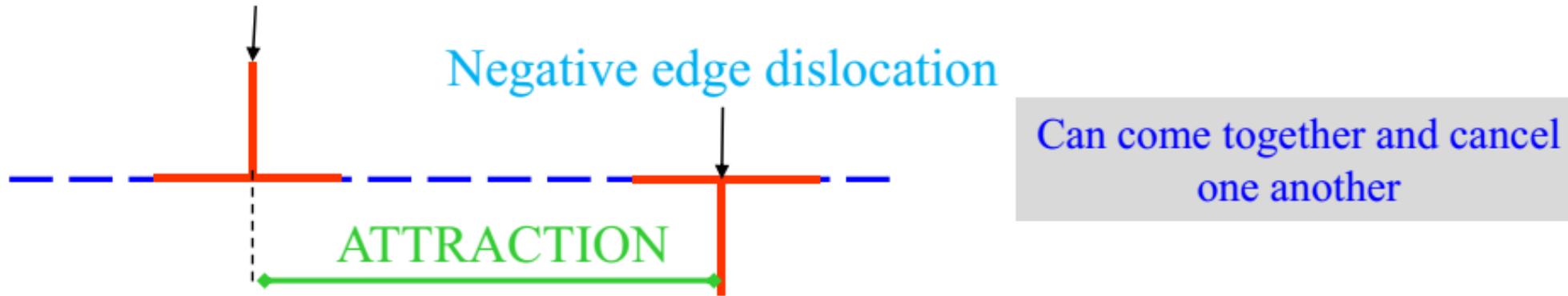
Burgers Vector in Edge and Screw Dislocations



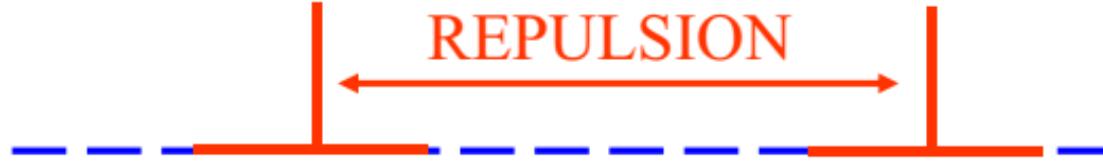
+ve and -ve Edge Dislocations

- Elastic interactions between edge dislocations on the same slip plane can be either attractive or repulsive.
- Consider two dislocations present on the same slip plane with the extra half-plane on two different sides of the slip plane. One of them is positive and the other is negative.

Positive edge dislocation

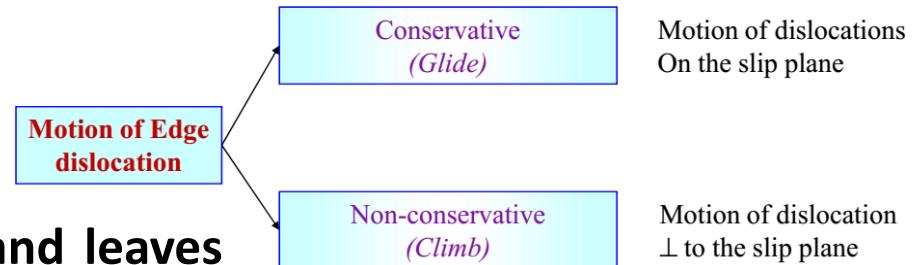


Can come together and cancel one another

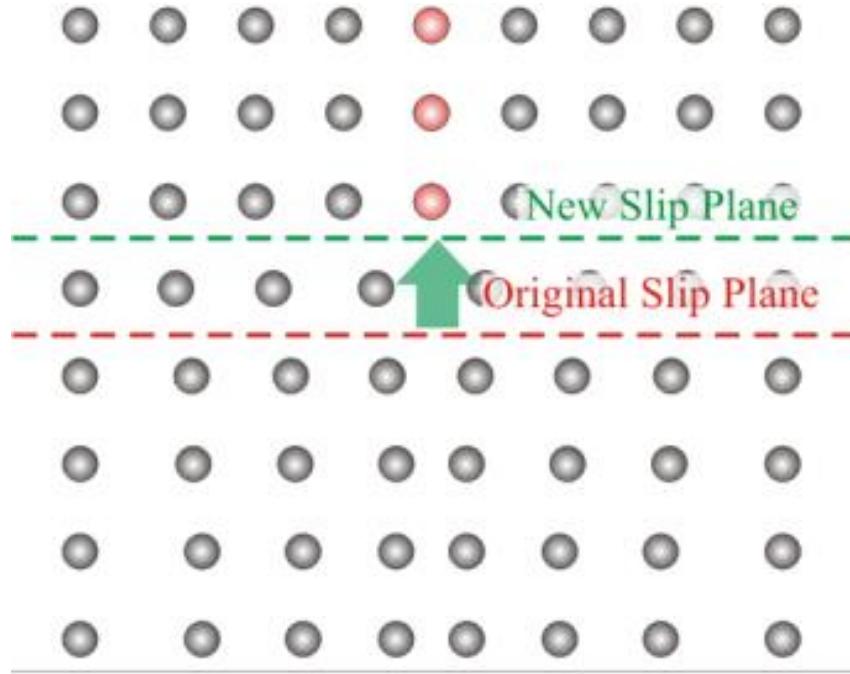


Motions of Dislocations

- Dislocations can move under an externally applied stress. Two possible motions of a dislocation:
Glide and **Climb**.
- Local shear stresses on the slip plane can drive the motions of dislocations. The minimum stress required to move a dislocation is called the **Peierls-Nabarro (PN) stress**.
- Dislocations may also move under the influence of other internal stress fields produced by other dislocations, precipitates, or those by phase transformations etc.
- Dislocations are attracted by free-surfaces and interfaces with softer materials and may move because of the attractive **Image Force**.
- In any case, the Peierls stress must be exceeded for the dislocation to move. The value of the Peierls stress is different for the edge and the screw dislocations.
- Plastic deformation is due to that the dislocation moves and leaves the crystal. When the dislocation leaves the crystal, a surface step with a height 'b' is created and the stress and energy stored in the crystal due to the dislocation is relieved.
- For edge dislocation: as $b \perp t \rightarrow$ they define a plane \rightarrow **the slip plane**.
- Climb involves addition or subtraction of a row of atoms below the half plane.
 - +ve climb = climb up \rightarrow removal of a plane of atoms
 - -ve climb = climb down \rightarrow addition of a plane of atoms

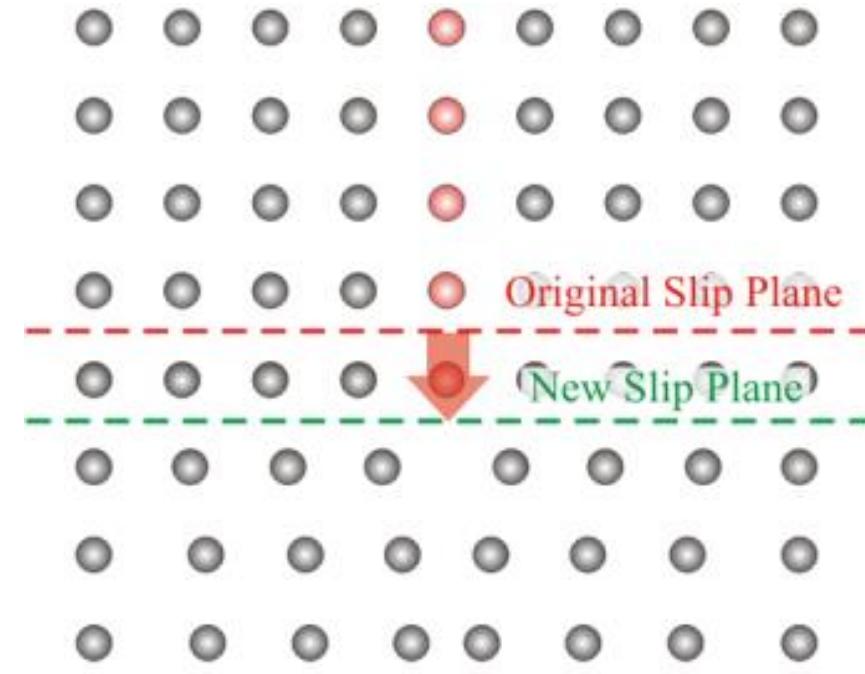


Edge Climb



Positive climb

Removal of a row of atoms



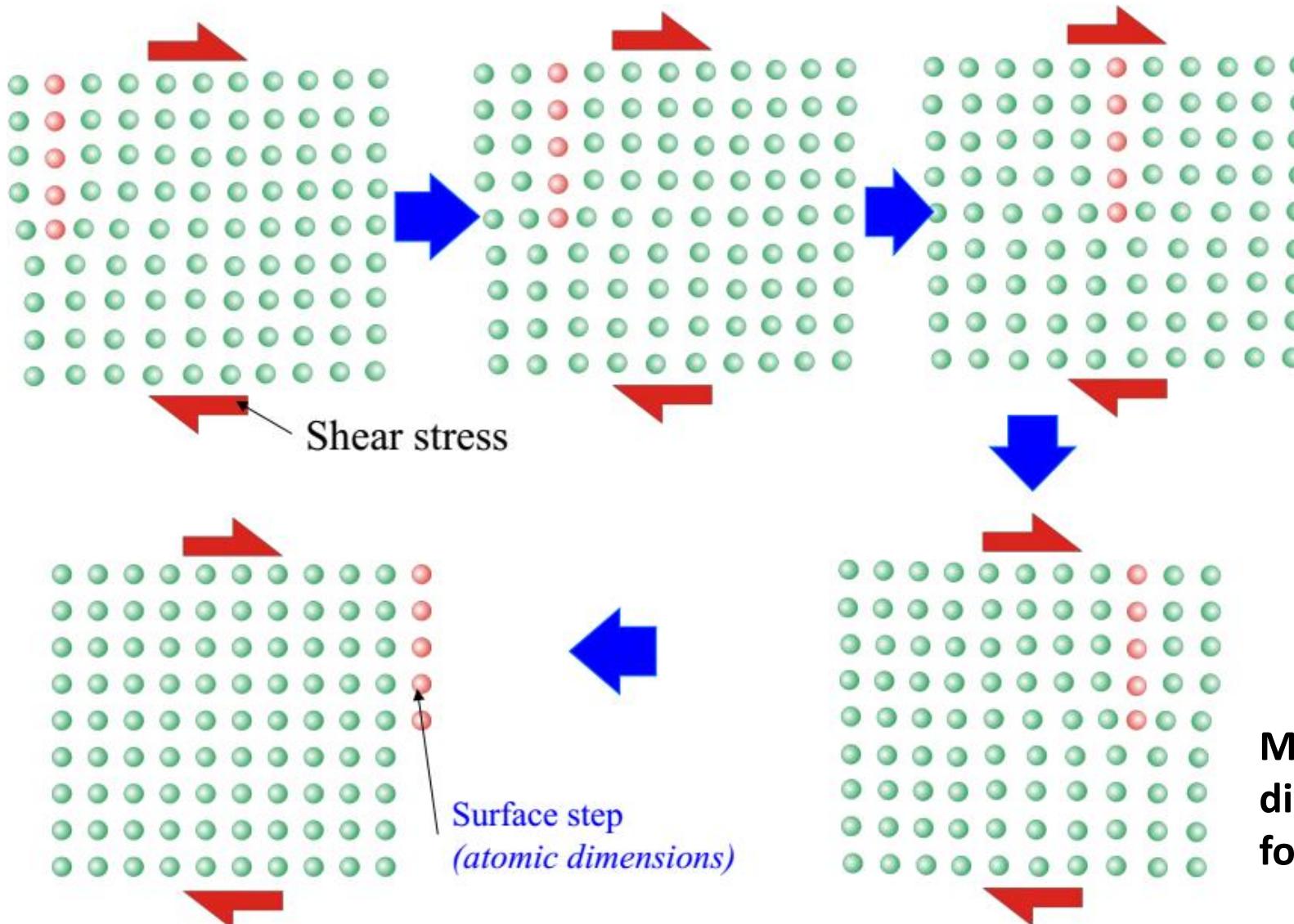
Negative climb

Addition of a row of atoms

- Removal of a row of atoms lead to a decrease in vacancy concentration in the crystal and negative climb leads to an increase in vacancy concentration in the crystal.



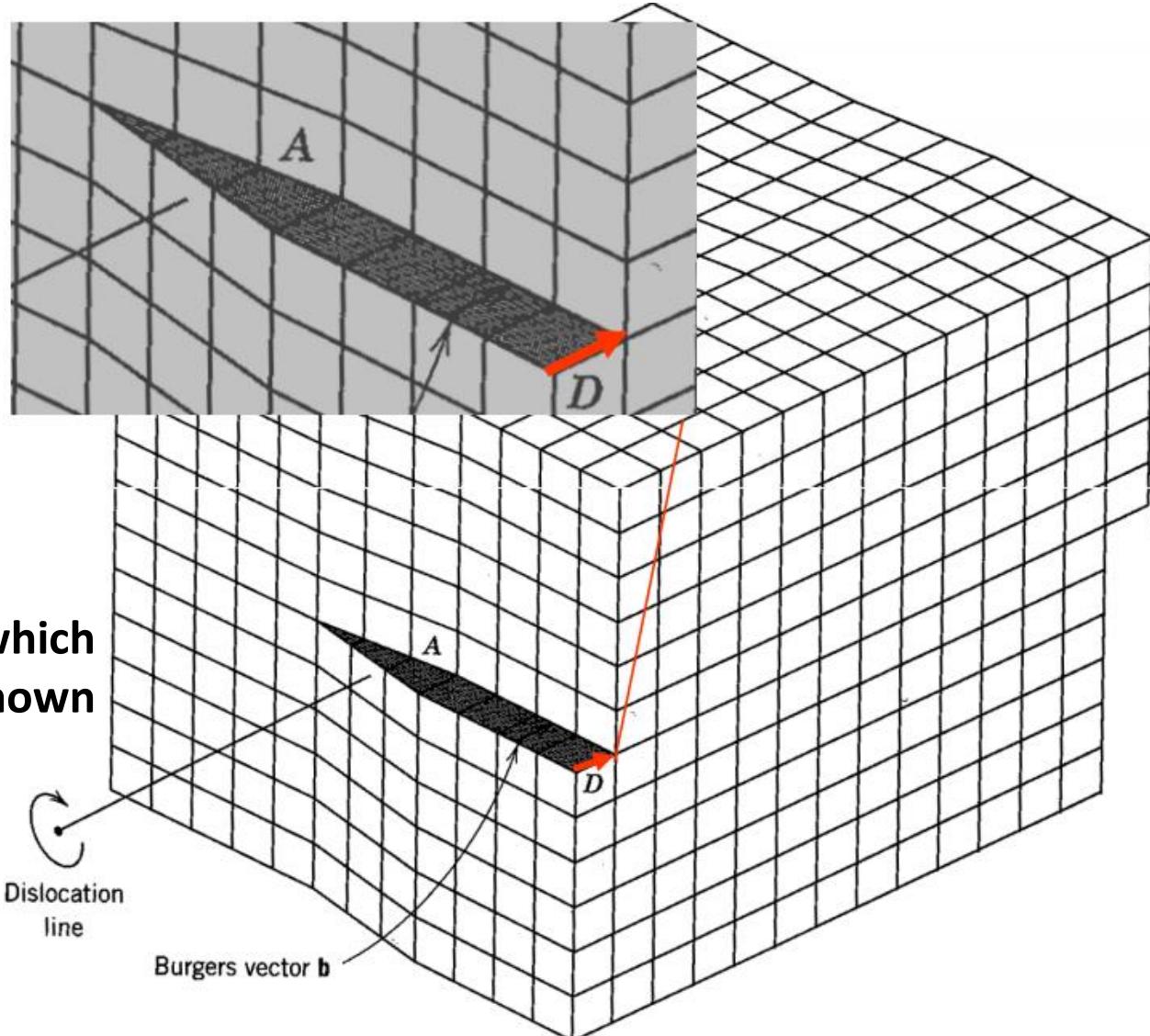
Edge Dislocation Glide



Motion of an edge dislocation leading to the formation of a step b.



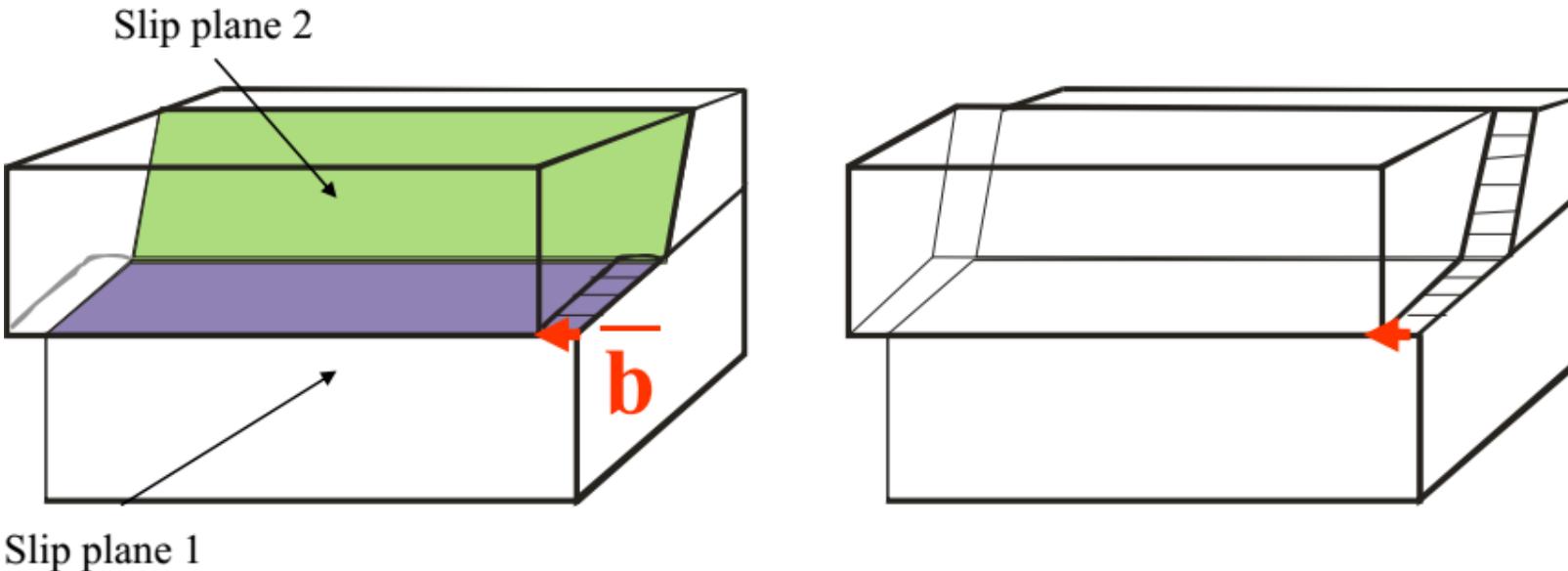
Screw Dislocation



The line along which shearing occurs is known as a **screw dislocation**.



Screw Dislocation Cross-Slip



The dislocation is shown cross-slipping from the blue plane to the green plane

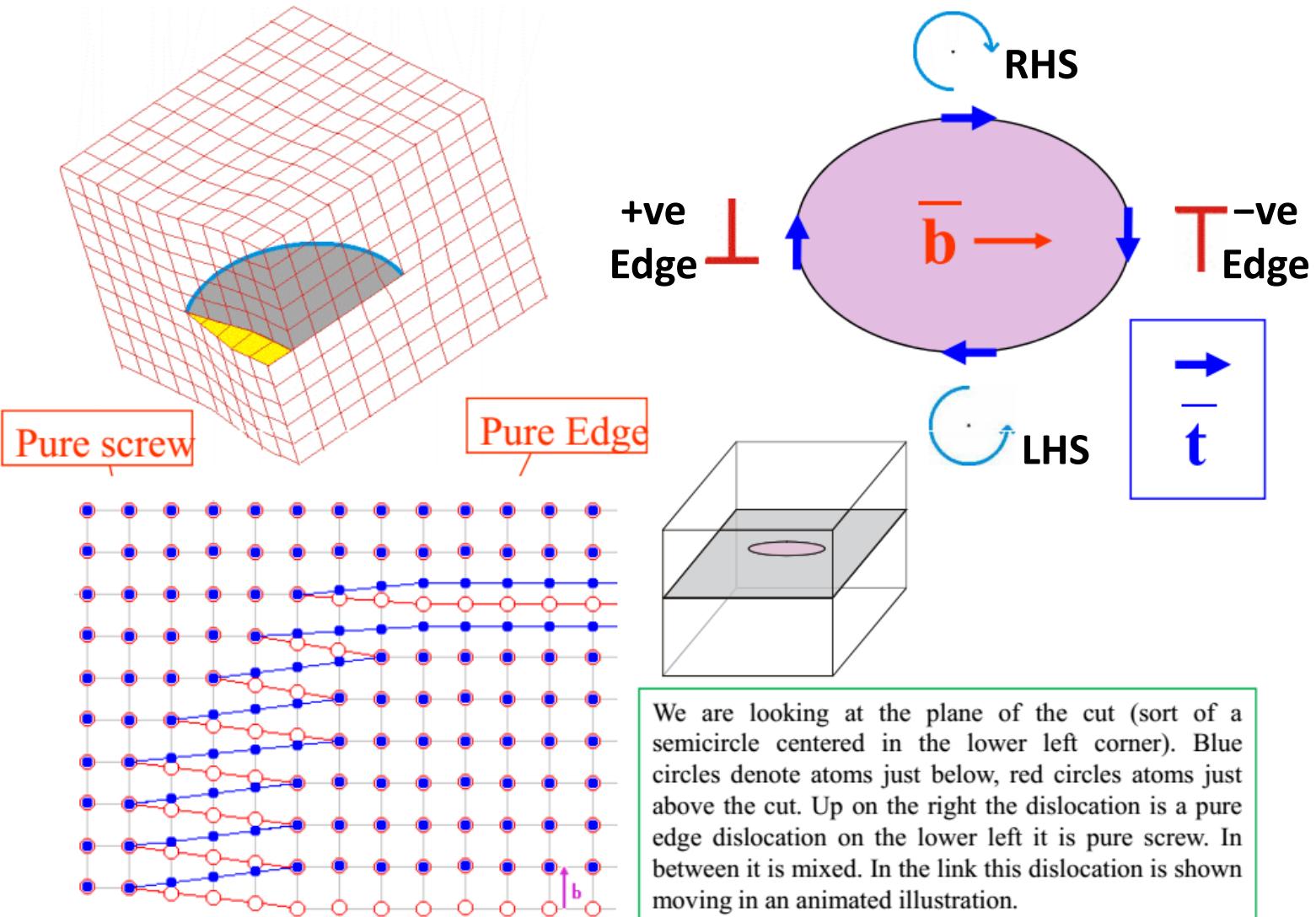
- The dislocation line ends on:
 - ✓ The free surface of the crystal
 - ✓ Internal surface or interface
 - ✓ Closes on itself to form a loop
 - ✓ Ends in a node
- A node is the intersection point of more than two dislocations.
- The vectoral sum of the Burgers vectors of dislocations meeting at a node = 0.

Geometric Properties of Dislocations

Dislocation Property	Type of dislocation	
	Edge	Screw
Relation between dislocation line (t) and \mathbf{b}	\perp	\parallel
Slip direction	\parallel to \mathbf{b}	\parallel to \mathbf{b}
Direction of dislocation line movement relative to \mathbf{b}	\parallel	\perp
Process by which dislocation may leave slip plane	Glide/Climb	Cross-slip



Mixed Dislocations



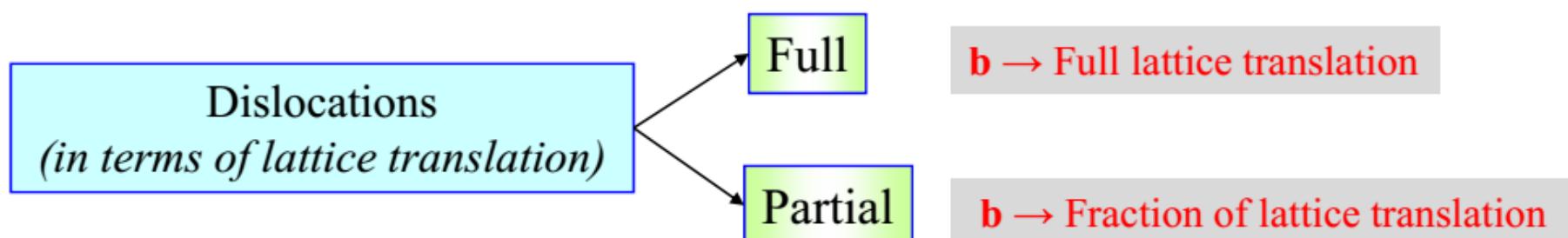
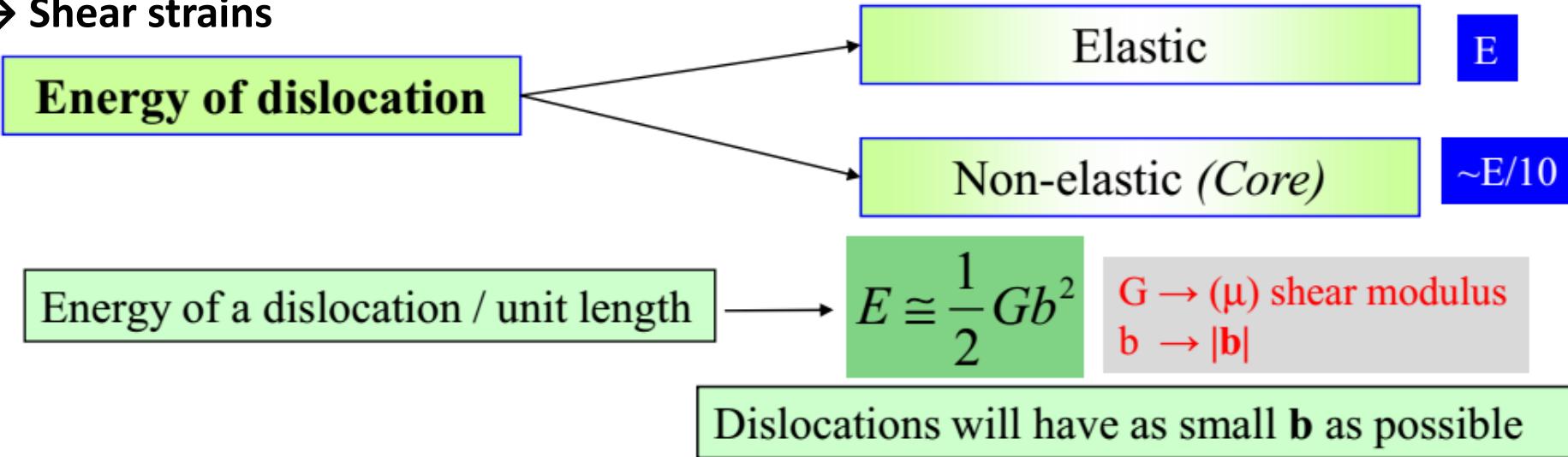
Energy of Dislocations

□ Dislocations have distortion energy associated with them

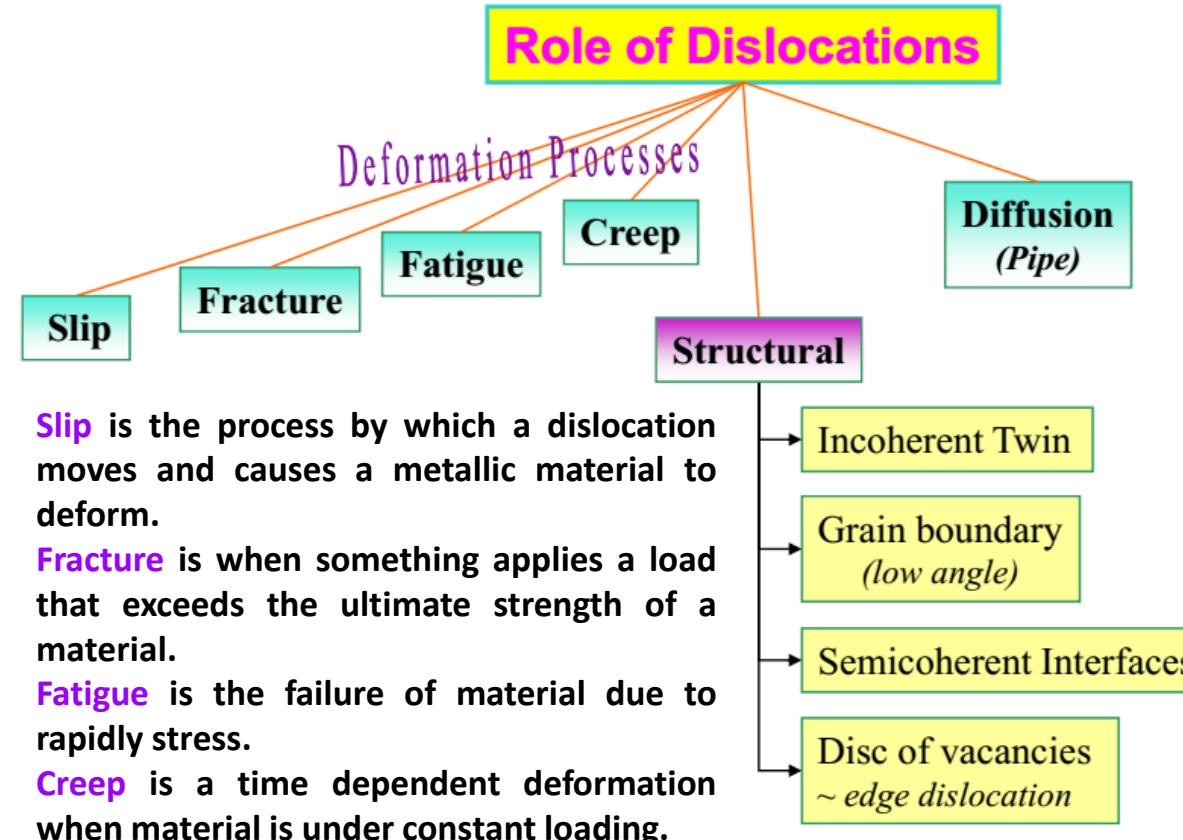
□ E per unit length

□ Edge → Compressive and tensile stress fields

□ Screw → Shear strains



Role of Dislocations



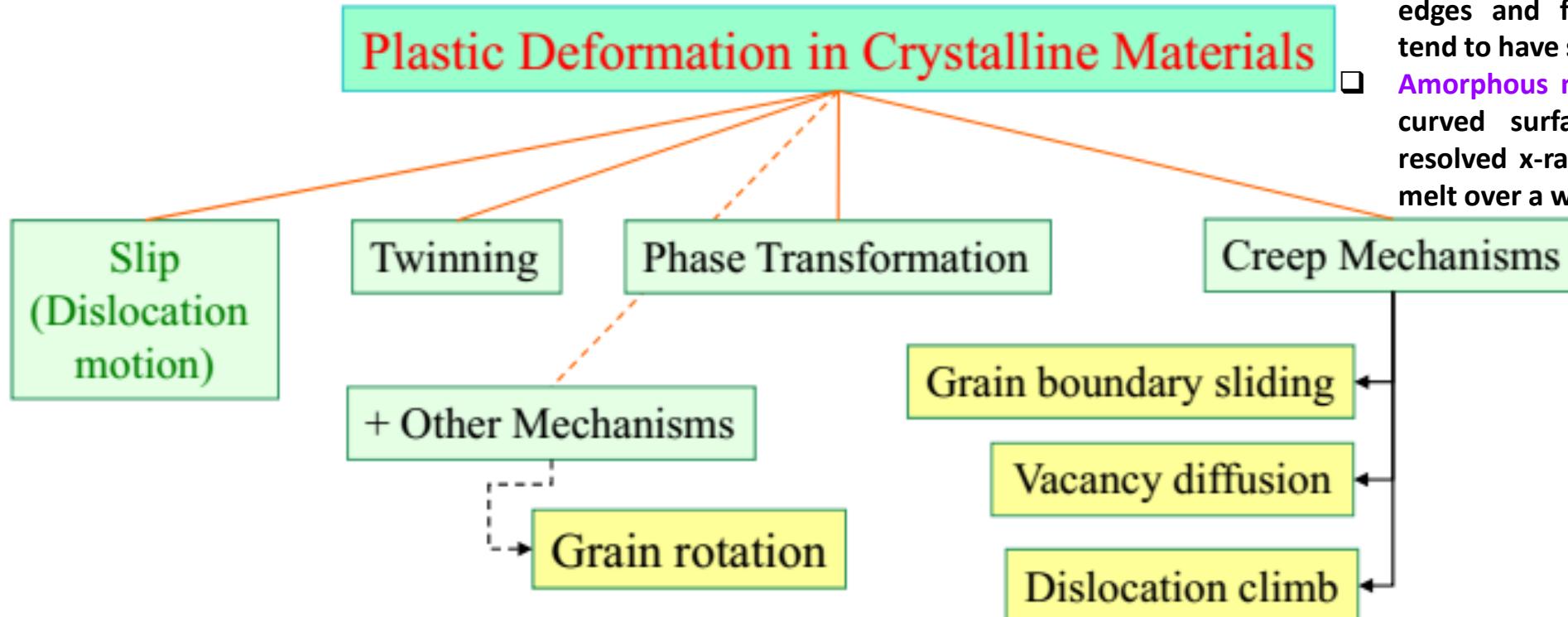
Formation of dislocations (in the bulk of the crystal)

- Due to accidents in crystal growth from the melt.
- Mechanical deformation of the crystal.



Mechanisms/Modes of Plastic Deformation

- Plastic deformation in crystalline solid is accomplished by means of various processes mentioned below, among which slip is the most important mechanism.
- Plastic deformation of crystalline materials takes place by mechanisms which are very different from that for amorphous materials (glasses).
- Plastic deformation in amorphous materials occur by other mechanisms including flow (~viscous fluid) and shear banding.

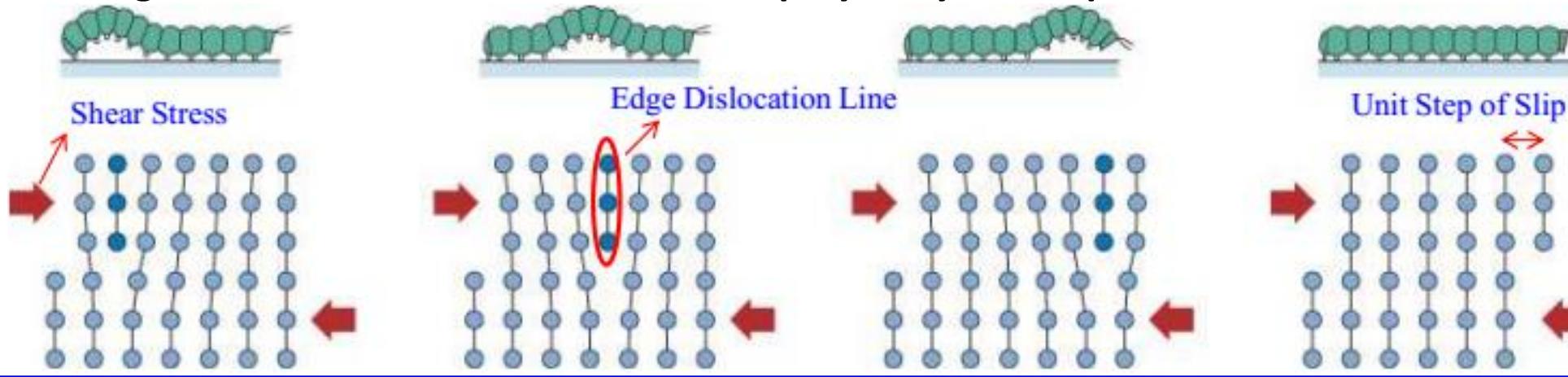


- Crystalline materials have well-defined edges and faces, diffract x-rays, and tend to have sharp melting points.
- Amorphous materials have irregular or curved surfaces, do not give well-resolved x-ray diffraction patterns, and melt over a wide range of temperatures.

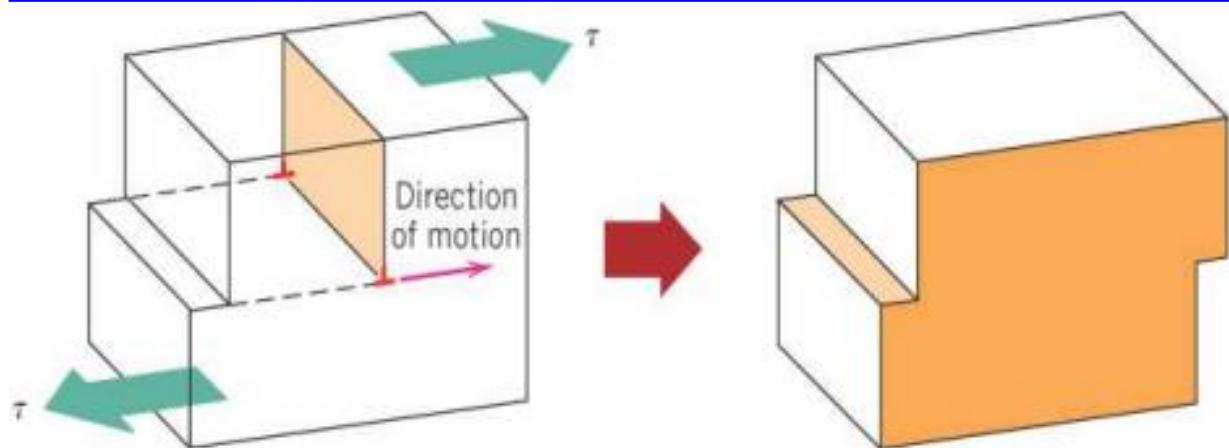
Dislocation Motion (SLIP)

Basic concepts:

- SLIP is the most important mechanism of plastic deformation.
- At low temperatures (especially in BCC metals) twinning may also become important.
- At the fundamental level plastic deformation (in crystalline materials) by slip involves the motion of dislocations on the slip plane (creating a step of Burgers vector).
- Burgers vector represents the magnitude and direction of the lattice distortion resulting from a dislocation in a crystal lattice.
- Slip is caused by shear stresses (at the level of the slip plane).
- Hence, a purely hydrostatic state of stress cannot cause slip.
- A slip system consists of a slip direction lying on a slip plane.
- Slip is analogous to the mode of locomotion employed by a caterpillar.



Direction of Dislocation Motion



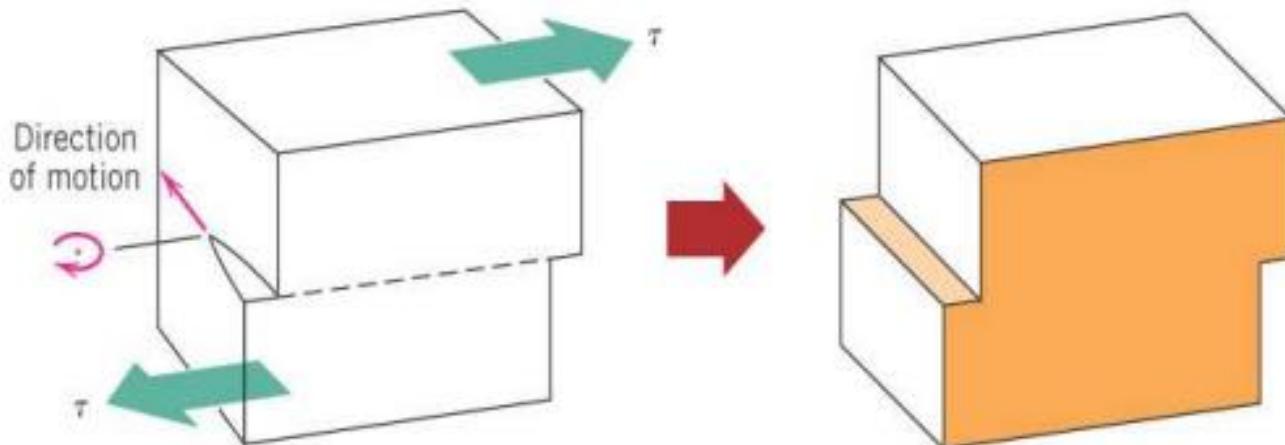
Edge dislocation line moves parallel to applied stress

□ Edge Dislocation:

- An edge dislocation is a defect where an extra half-plane of atoms is introduced midway through the crystal, distorting nearby planes of atoms.
- An edge dislocation therefore moves in the **direction of the Burgers vector**.

□ Screw Dislocation:

- A screw dislocation is a topological defect of a crystal lattice. If one moves around the dislocation, the lattice plane shifts by one layer (or more layers), like a spiral staircase.
- A screw dislocation moves in a **direction perpendicular to the Burgers vector**.

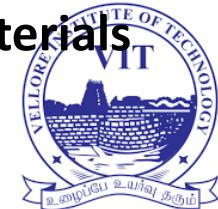


Screw dislocation line moves perpendicular to applied stress



Slip Systems

- Dislocations move more easily on specific planes and in specific directions.
- Ordinarily, there is a preferred plane (**slip plane**), and specific directions (**slip direction**) along which dislocations move.
- The combination of slip plane and slip direction is called the **slip system**.
- The slip system depends on the **crystal structure** of the metal.
- The **slip plane** is the plane that has the **most dense atomic packing** (the **greatest planar density**).
- The **slip direction** is most closely packed with atoms (**highest linear density**).
- In Cubic closed packing (CCP), HCP materials the slip system consists of a close packed direction on a close packed plane.
- Just the existence of a slip system does not guarantee slip → slip is competing against other processes like twinning and fracture.
- If the **stress to cause slip is very high** (i.e., **Critical Resolved Shear Stress (CRSS) is very high**), then fracture may occur before slip (like in brittle ceramics).
- For slip to occur in polycrystalline materials, **5 independent slip systems** are required.
- Hence, materials which are ductile in single crystalline form, may not be ductile in polycrystalline form.
- At **higher temperatures** more slip systems may become active and hence polycrystalline materials which are brittle at low temperature, may become ductile at high temperature.



Example of Slip Systems

Crystal	Slip plane(s)	Slip direction	Number of slip systems
FCC	{111}	$\frac{1}{2}\langle 110 \rangle$	12
HCP	(0001)	$\langle 11\bar{2}0 \rangle$	3
BCC	{110}, {112}, {123}	$\frac{1}{2}[111]$	48
NaCl (<i>Ionic</i>)	{110} {111} not a slip plane	$\frac{1}{2}\langle 110 \rangle$	6
C (<i>Diamond cubic</i>)	{111}	$\frac{1}{2}\langle 110 \rangle$	12
TiO ₂ (<i>Rutile</i>)	{101}	$\langle 10\bar{1} \rangle$	
CaF ₂ , UO ₂ , ThO ₂ <i>Fluorite</i>	{001}	$\langle 1\bar{1}0 \rangle$	
CsCl	{110}	$\langle 001 \rangle$	
NaCl, LiF, MgO <i>Rock Salt</i>	{110}	$\langle 110 \rangle$	6
C, Ge, Si <i>Diamond cubic</i>	{111}	$\langle 110 \rangle$	12
MgAl ₂ O ₄ <i>Spinel</i>	{111}	$\langle 1\bar{1}0 \rangle$	
Al ₂ O ₃ <i>Hexagonal</i>	(0001)	$\langle 11\bar{2}0 \rangle$	

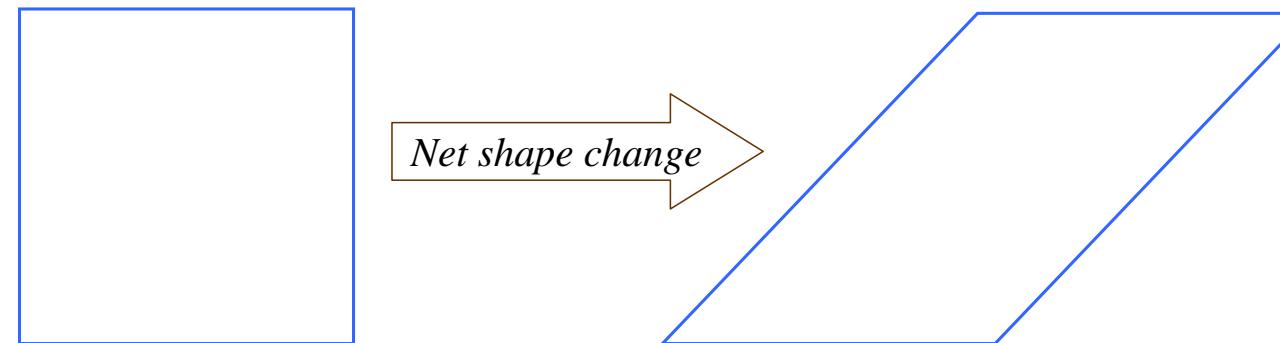


Microscopic Slip to Macroscopic Deformation

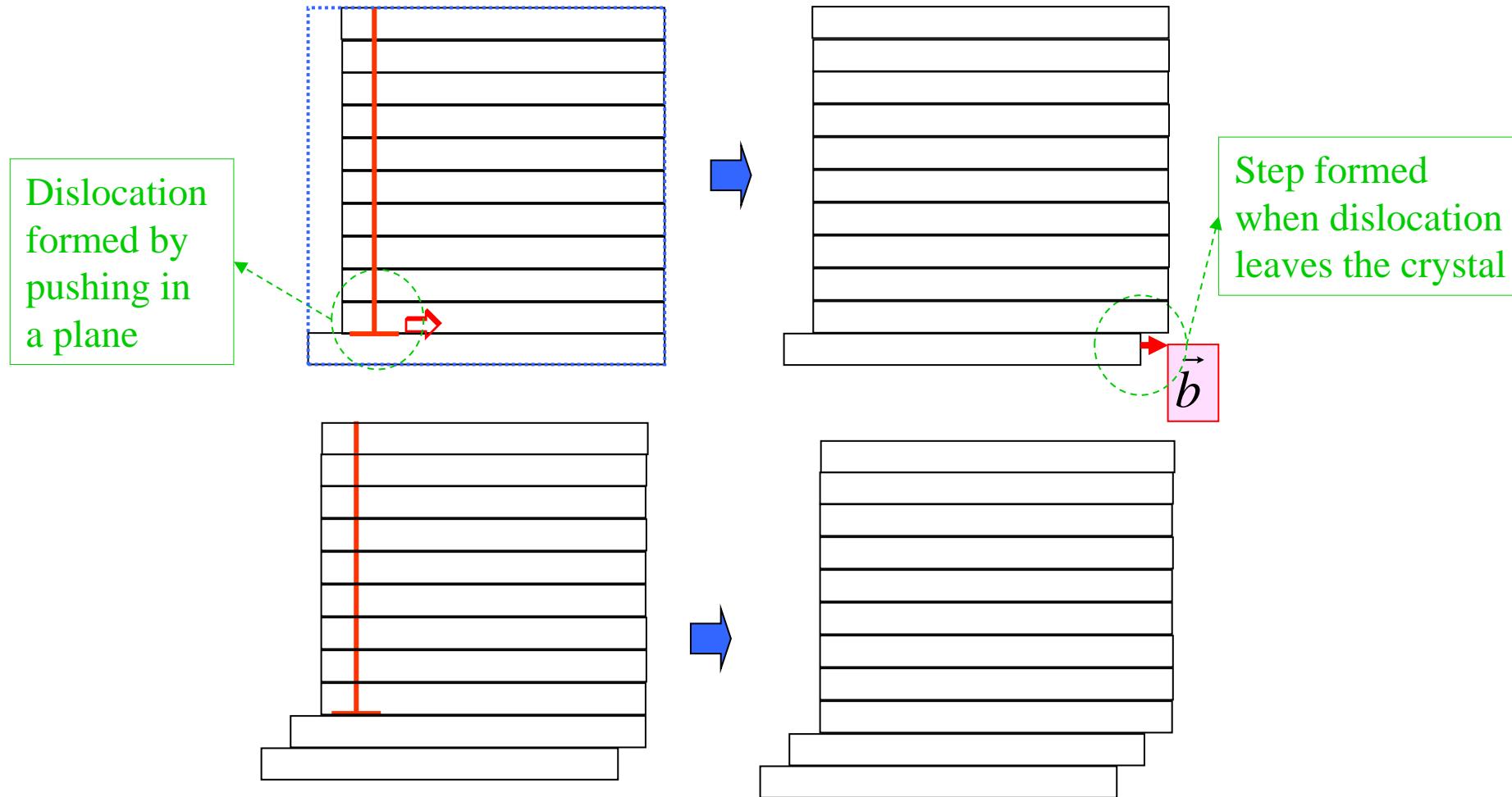
How does the motion of dislocations lead to a macroscopic shape change?

(From microscopic slip to macroscopic deformation \Rightarrow a first feel!)

- When one bends a rod of Al to a new shape, it involves processes occurring at various length scales and understanding these is a difficult task.
- However, at the fundamental level slip is at the heart of the whole process.
- To understand how slip can lead to shape change? We consider a square crystal deformed to a rhombus (as below).



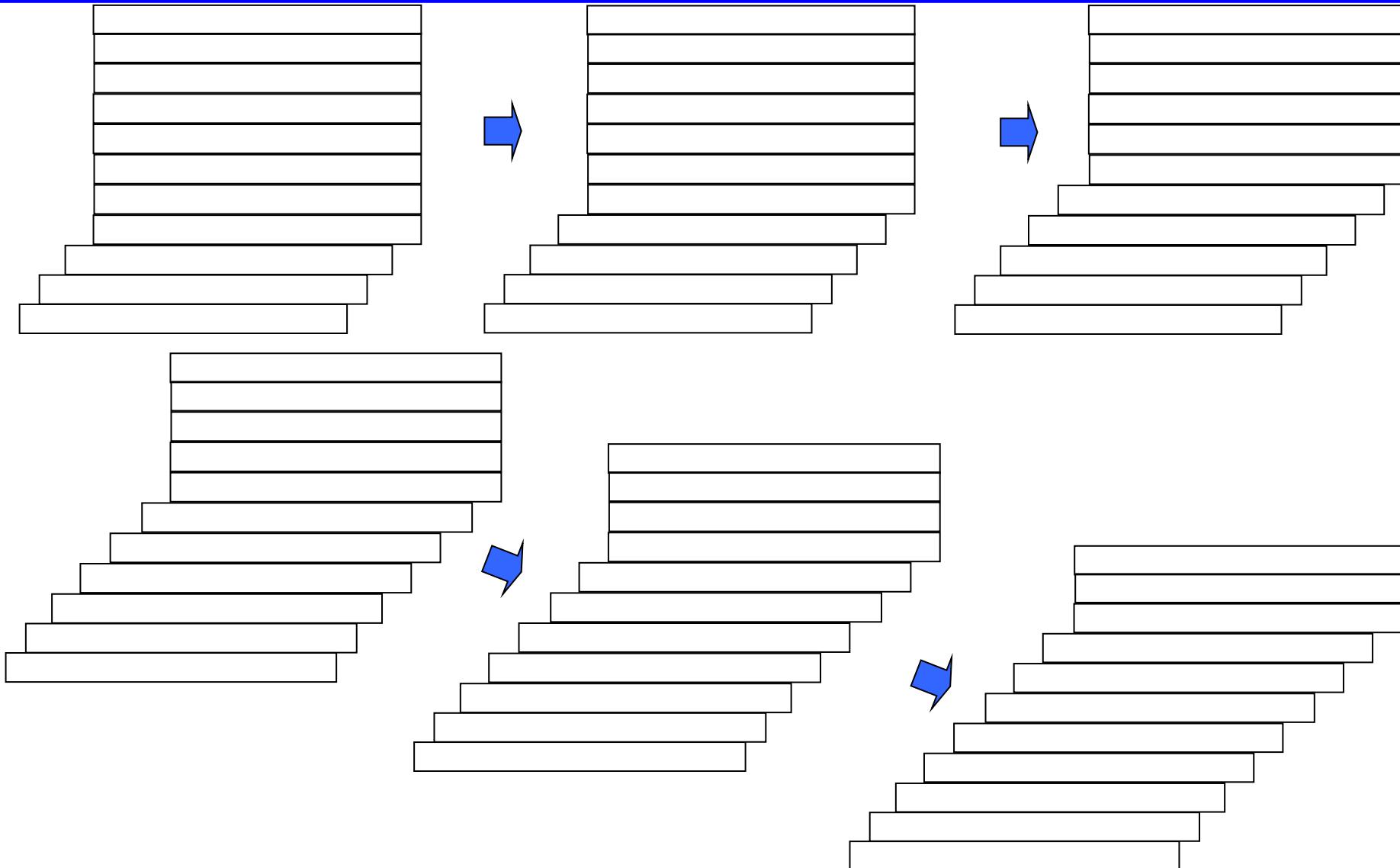
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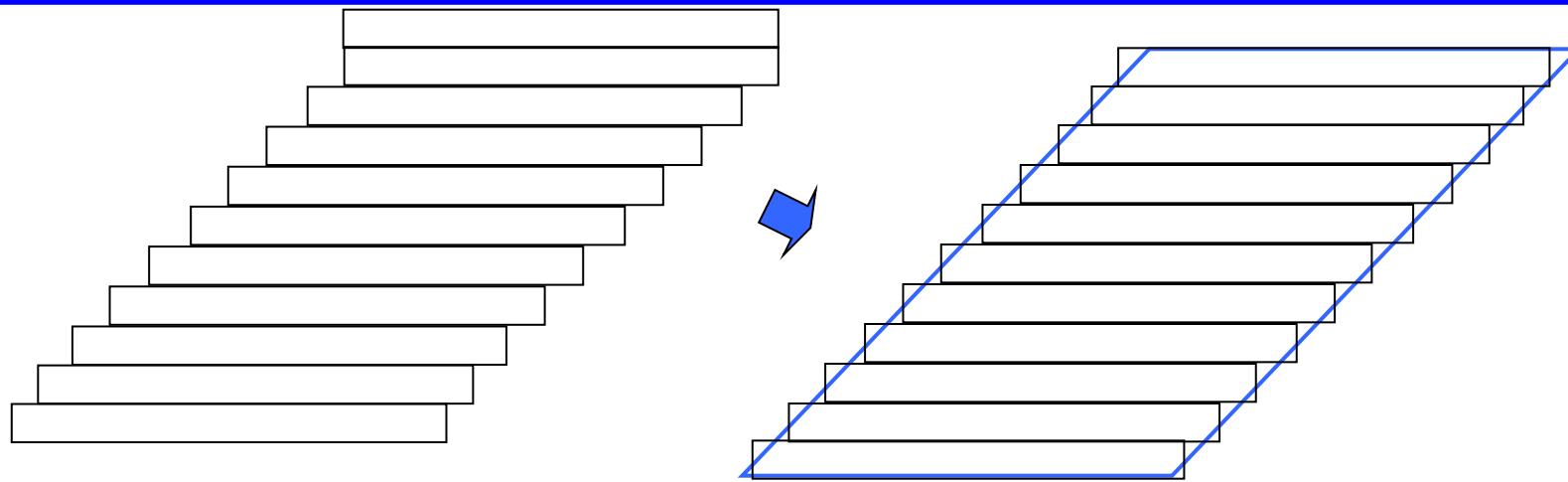
Now visualize dislocations being punched in on successive planes → moving and finally leaving the crystal



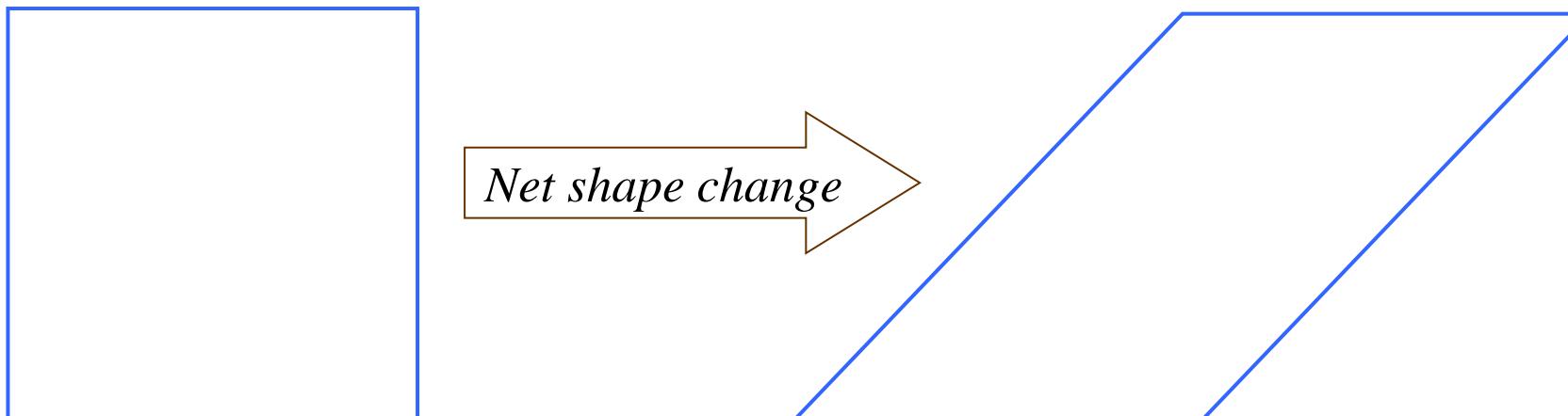
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This sequence of events finally leads to deformed shape which can be approximated to a rhombus.



Stress to Move a Dislocation: Peierls–Nabarro (PN) Stress

- We have seen that there is a **critical stress** required to **move a dislocation**.
- At the fundamental level the motion of a dislocation involves the **rearrangement of bonds** → **requires application of shear stress on the slip plane**.
- When **sufficient stress** is applied the dislocation moves from one metastable energy minimum to another.
- The original model is due to **Peierls & Nabarro** (formula as below) and the **sufficient stress** which needs to be applied is called **Peierls-Nabarro stress (PN stress)** or simply **Peierls stress**.
- Width of the dislocation is considered as a basis for the ease of motion of a dislocation in the model which is a function of the bonding in the material.

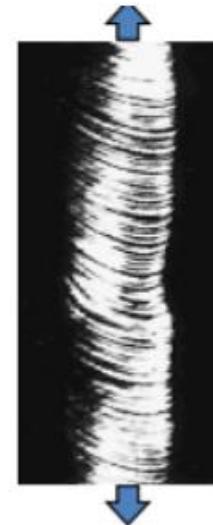
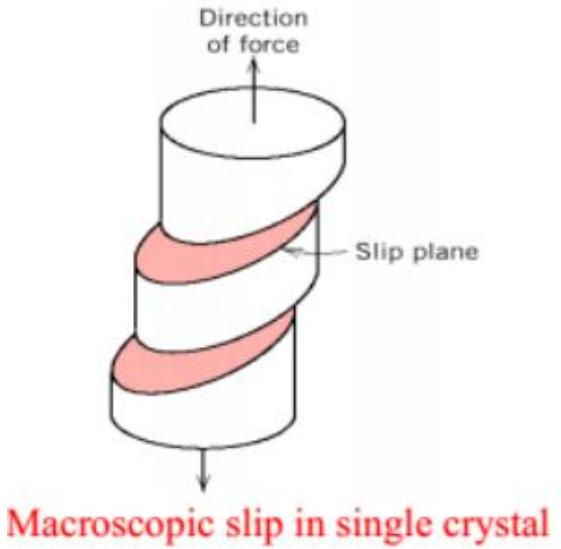
$$\tau_{PN} = G e^{-\left(\frac{2\pi w}{b}\right)}$$

- G → shear modulus of the crystal (ratio of shear stress to shear strain)
- w → width of the dislocation
- b → $|\mathbf{b}|$ slip distance or Burgers vector



Slip in Single Crystal

- If a **single crystal** of a metal is **stressed in tension beyond its elastic limit**, it elongates slightly and a step appears on the surface due to the relative displacement of one part of the crystal with respect to the others and the elongation stops.
- **Further increase in the load** causes movement of another parallel plane, resulting in another step.
- Similarly number of small steps are formed on the surface of the single crystal that are parallel to one another and loop around the circumference of the specimen.
- Each step (shear band) results from the movement of a large number of dislocations and their propagation in the slip system.

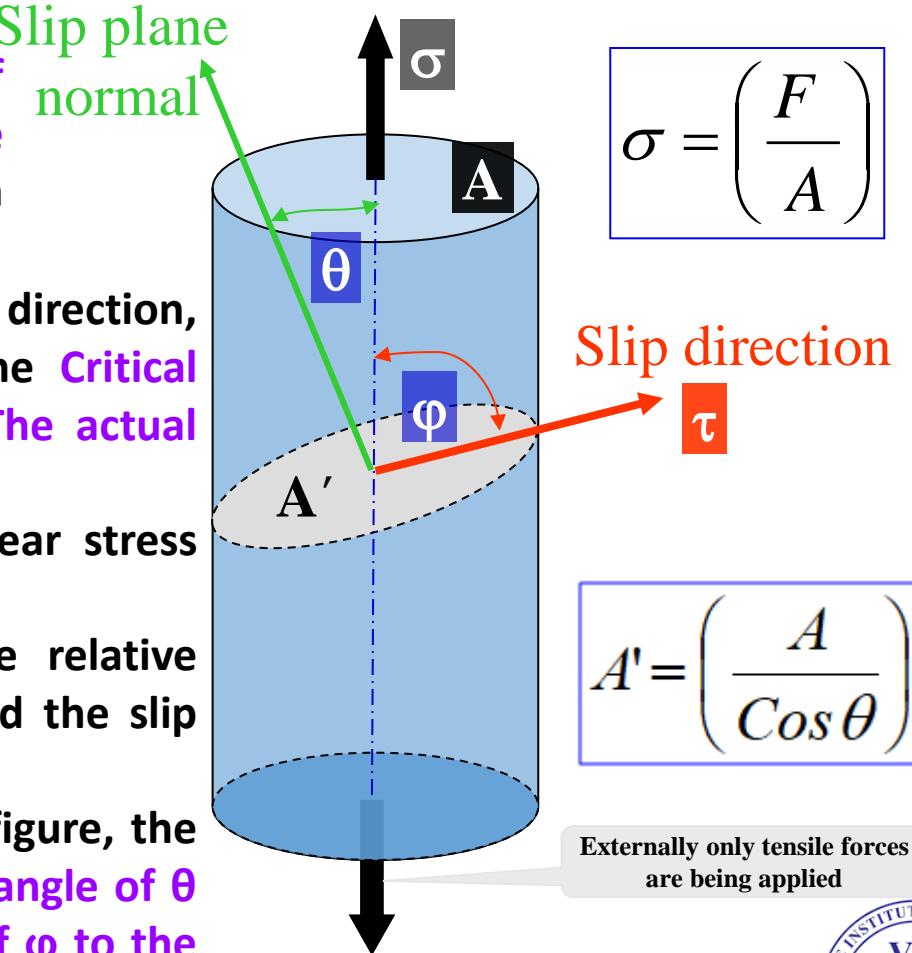


Slip in a zinc single crystal



Critical Resolved Shear Stress (CRSS)

- Resolved shear stress (RSS) is component of the applied stress that causes shear on a given plane in a given direction and critical resolved shear stress (CRSS) is the minimum shear needed to cause dislocation motion for a certain material in a certain state condition.
- Extent of slip in a single crystal depends on the magnitude of shearing stress produced by external loads, geometry of the crystal structure and the orientation of the active slip planes with respect to the shearing stress.
- Slip begins when the shearing stress on slip plane in the slip direction, Resolved Shear Stress (RSS) reaches a critical value called the Critical Resolved Shear Stress (CRSS) and plastic deformation starts (The actual Schmid's law).
- Even if we apply an tensile force on the specimen → the shear stress resolved onto the slip plane is responsible for slip.
- The stress at which slip starts in a crystal depends on the relative orientation of the stress axis with respect to the slip plane and the slip direction.
- When a tensile stress σ is applied to a crystal, as illustrated in figure, the shear stress τ resolved on a slip plane whose normal makes an angle of θ with the stress axis, along a slip direction inclined at an angle of φ to the stress axis.



Contd...

$$\text{Stress} = \left(\frac{\text{Force}}{\text{Area}} \right)_{1D}$$
$$\tau = \left(\frac{F \cos\varphi}{A / \cos\theta} \right)$$

$$\tau_{RSS} = \sigma \cos\theta \cos\varphi$$

Schmid factor

Schmid's law

Slip is initiated when

$$\tau_{RSS} \geq \tau_{CRSS}$$

τ_{CRSS} is a material parameter, which is determined from experiments

Yield strength of a single crystal

$$\sigma_y = \frac{\tau_{CRSS}}{\cos\theta \cos\varphi}$$

- Maximum shear stress is in a plane inclined at ($\theta = 45^\circ$).
- The vertical (90°) and horizontal plane (0°) feel no shear stresses.



Example – 2

□ Consider a single crystal of BCC-Fe oriented such that a tensile stress is applied along a [010] direction.

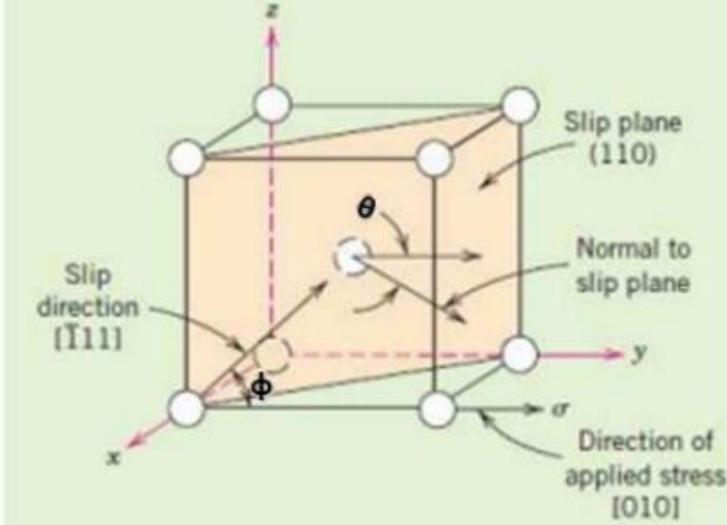
- Compute the resolved shear stress along a (110) plane and in a $\bar{[111]}$ direction when a tensile stress of 52 MPa is applied.
- If slip occurs on a (110) plane and in a direction $\bar{[111]}$, and the critical resolved shear stress is 30 MPa, calculate the magnitude of the applied tensile stress necessary to initiate yielding.

□ Solution: (a) Determine the value of the angle between the normal to the (110) slip plane (i.e., the $\bar{[111]}$ direction) and the [010] direction using $[u_1v_1w_1] = [110]$, $[u_2v_2w_2] = [010]$ and the following equation:

$$\theta = \cos^{-1} \left(\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)(u_2^2 + v_2^2 + w_2^2)}} \right)$$

$$\theta = \cos^{-1} \left(\frac{(1)(0) + (1)(1) + (0)(0)}{\sqrt{[(1)^2 + (1)^2 + (0)^2][(0)^2 + (1)^2 + (0)^2]}} \right)$$

$$= \cos^{-1} \left(\frac{1}{\sqrt{2}} \right) = 45^\circ$$



Contd...

- Similarly determine the value of φ , the angle between $\bar{[111]}$ and $[010]$ directions as follows:

$$\varphi = \cos^{-1} \left(\frac{(-1)(0) + (1)(1) + (1)(0)}{\sqrt{[(-1)^2 + (1)^2 + (1)^2][(0)^2 + (1)^2 + (0)^2]}} \right) = \cos^{-1} \left(\frac{1}{\sqrt{3}} \right) = 54.7^\circ$$

- Then calculate the value of τ_{RSS} using the following expression:

$$\begin{aligned}\tau_{RSS} &= \sigma \cos \theta \cos \varphi \\ &= (52 \text{ MPa}) (\cos 45) (\cos 54.7) \\ &= 21.3 \text{ MPa}\end{aligned}$$

- (b) Yield Strength, $\sigma_y =$

$$\sigma_y = \frac{30 \text{ MPa}}{(\cos 45)(\cos 54.7)} = 73.4 \text{ MPa}$$



Example – 3

- Determine the tensile stress that is applied along the $[1\bar{1}0]$ axis of a Ag crystal to cause slip on the $(\bar{1}\bar{1}\bar{1})$ $[0\bar{1}\bar{1}]$ system. The critical resolved shear stress is 6 MPa.
- Solution: Determine the angle θ between the tensile axis $[1\bar{1}0]$ and normal to $(\bar{1}\bar{1}\bar{1})$ using the following equation:

$$\cos \theta = \left(\frac{u_1 u_2 + v_1 v_2 + w_1 w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)(u_2^2 + v_2^2 + w_2^2)}} \right)$$

$$\cos \theta = \left(\frac{(1)(1) + (-1)(-1) + (0)(-1)}{\sqrt{[(1)^2 + (-1)^2 + (0)^2][(1)^2 + (-1)^2 + (-1)^2]}} \right) = \frac{2}{\sqrt{2}\sqrt{3}} = \frac{2}{\sqrt{6}}$$

- Determine the angle ϕ between tensile axis $[1\bar{1}0]$ and slip direction $[0\bar{1}\bar{1}]$ using the following equation:

$$\cos \phi = \left(\frac{(1)(0) + (-1)(-1) + (0)(-1)}{\sqrt{[(1)^2 + (-1)^2 + (0)^2][(0)^2 + (-1)^2 + (-1)^2]}} \right) = \frac{1}{\sqrt{2}\sqrt{2}} = \frac{1}{2}$$

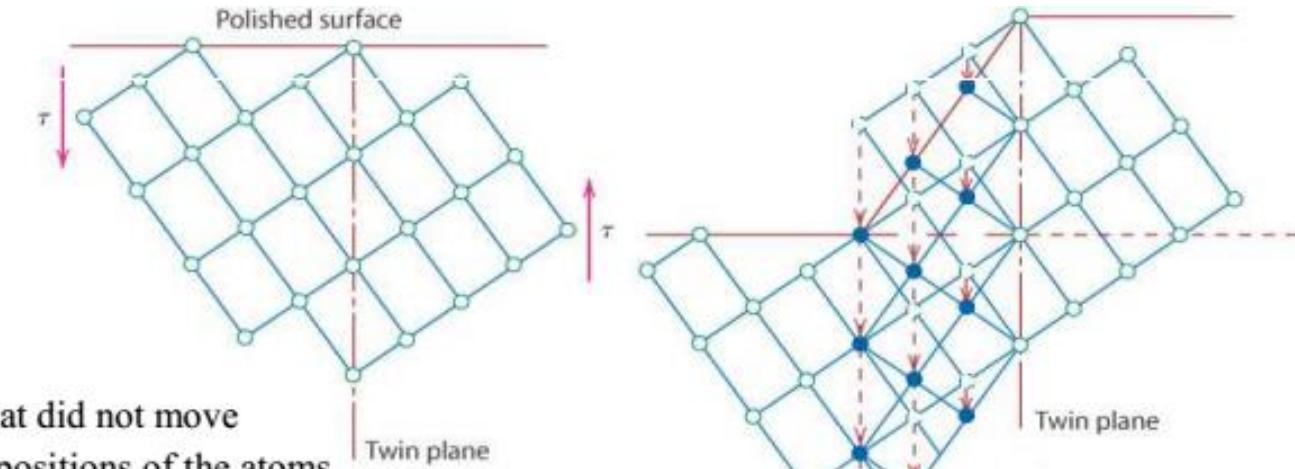
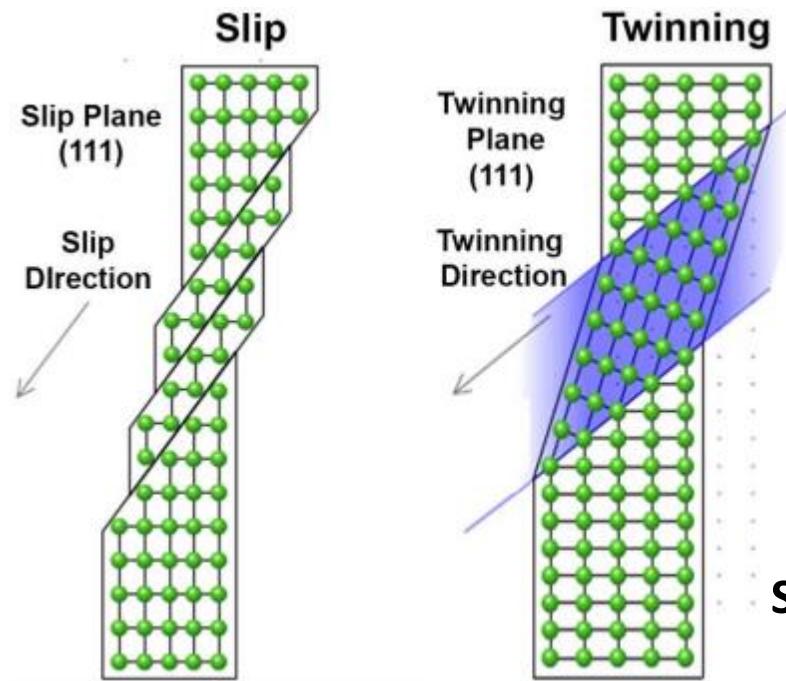
- Then calculate the tensile stress using the expression:

$$\sigma = \frac{P}{A} = \frac{\tau_{RSS}}{\cos \theta \cos \phi} = \frac{6 \text{ MPa}}{\frac{2}{\sqrt{6}} \times \frac{1}{2}} = 6\sqrt{6} = 14.7 \text{ MPa}$$



Deformation by Twin

- In addition to **slip** (dislocation movement), plastic deformation can also occur by **twinning**.
- **Twinning** is a shear force that can produce **atomic displacements**.
- **Twinning** results when a portion of the crystal takes up an orientation that is related to the orientation of the rest of the un-twinned lattice in a definite, symmetrical way.
- Twinned portion of the crystal is a mirror image of the parent crystal and the plane of symmetry between the two portions is called **twinning plane**.
- Twinning may favorably reorient slip systems to promote dislocation movement.



Schematic diagram showing how twinning results from an applied shear stress



Contd...

❑ Twins are generally of two types:

- Mechanical Twins

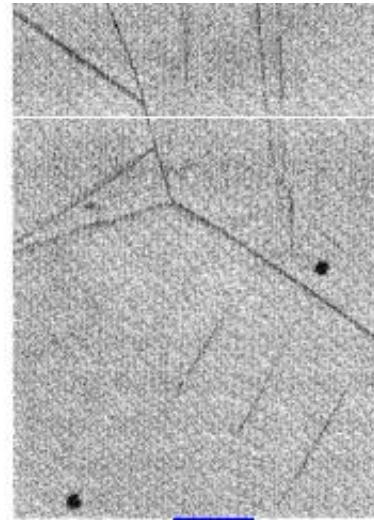
- Mechanical twins are generally seen in BCC or HCP metals and produced under conditions of rapid rate of loading and decreased temperature.

- Annealing twins

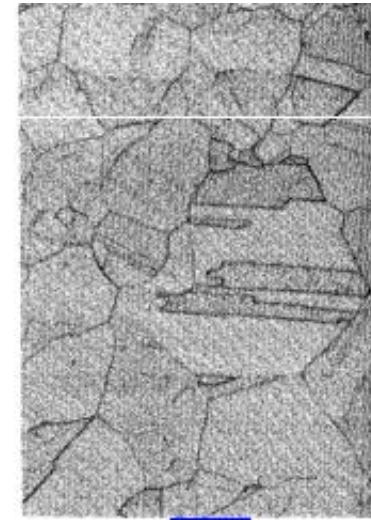
- Annealing twins are produced as the result of annealing. These twins are generally seen in FCC metals.
 - Annealing twins are usually broader and with straighter sides than mechanical twins.



(a)



(b)



(c)

(a) Mechanical Twins (Neumann bands in Fe),
(b) Mechanical Twins in Zn produced by polishing,
(c) Annealing Twins in Au-Ag alloy



Contd...

- Twinning generally occurs when the slip systems are restricted or when something increases the critical resolved shear stress so that the twinning stress is lower than the stress for slip.
- So, twinning generally occurs at low temperatures or high strain rates in BCC or FCC metals or in HCP metals.
- Twinning occurs on specific twinning planes and twinning directions.

Twin Planes and Twin Directions

Crystal Structure	Typical Examples	Twin Plane	Twin Direction
BCC	α -Fe, Ta	(112)	[111]
HCP	Zn, Cd, Mg, Ti	(10̄12)	[̄1011]
FCC	Ag, Au, Cu	(111)	[112]



Difference Between Slip and Twin

Slip

The crystallographic orientation above and below the slip plane is the same both before and after the deformation.

Slip occurs in distinct atomic spacing multiples.

Slip leaves a series of steps (lines).

Normally slip results in relatively large deformations.

Mostly seen in FCC and BCC structure, as they have more slip systems.

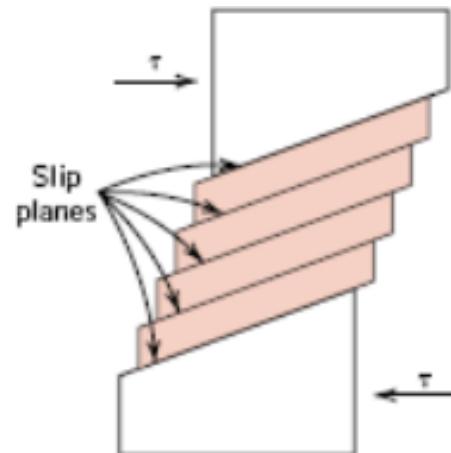
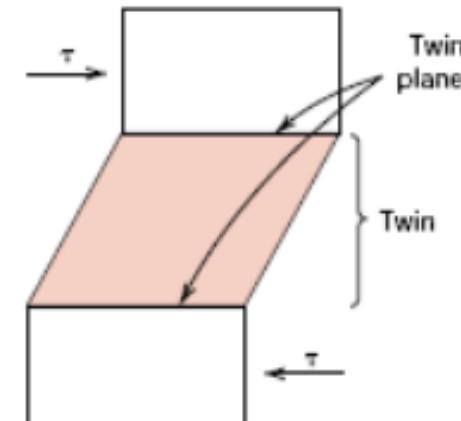
Twin

Orientation difference is seen across the twin plane.

The atomic displacement for twinning is less than the interatomic separation.

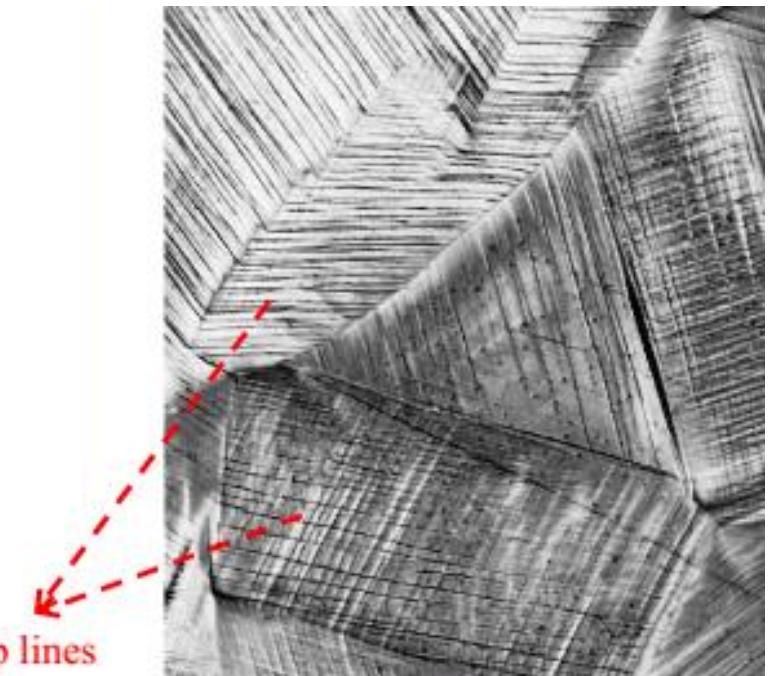
Twinning leaves small but well defined regions of the crystal deformed.

Only small deformations result for twinning.



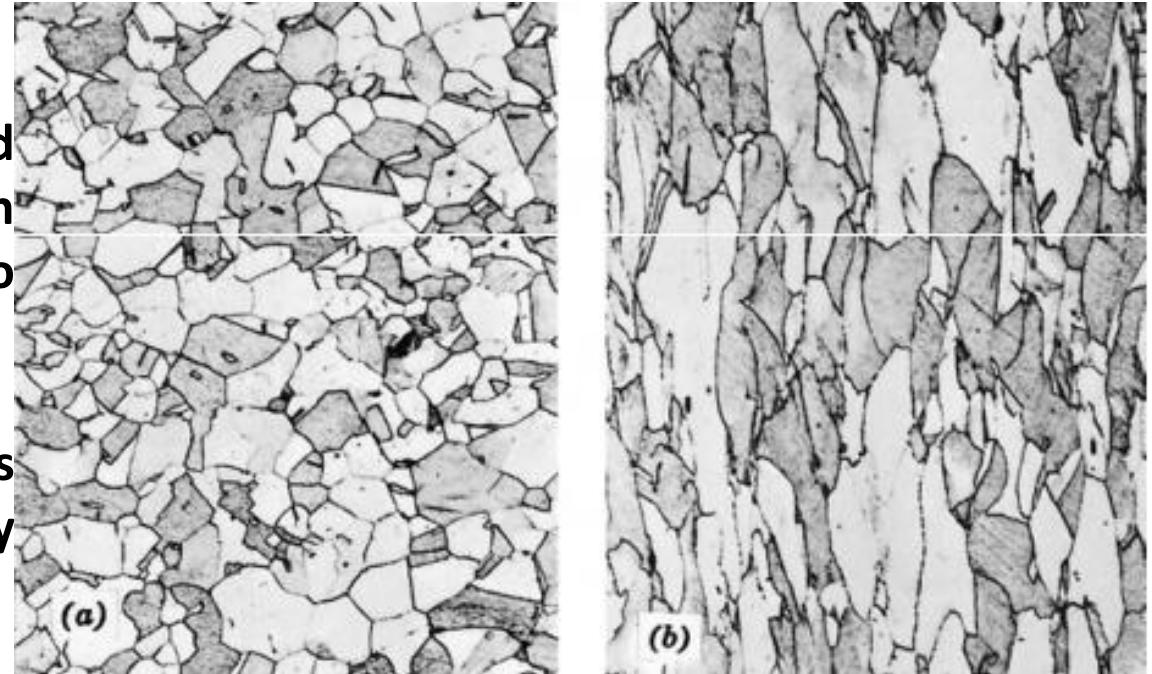
Deformation of Polycrystalline Materials

- Plastic deformation in polycrystalline materials is very complex than those in the single crystals due to the presence of grain boundaries, different orientation of neighboring crystals, presence of several phases etc.
- Due to random crystallographic orientations, the slip planes and slip direction varies from one grain to another.
- As a result the resolved shear stress τ_{RSS} will vary from one crystal to another and the dislocations will move along the slip systems with favorable orientation (i.e. the highest resolved shear stress).
- When a polished polycrystalline specimen of Cu is plastically deformed, two slip systems operate for most of the grains (evidenced by two sets of parallel yet intersecting sets of lines).
- Slip lines are visible, and the variation in grain orientation is indicated by the difference in alignment of the slip lines for several grains.



Contd...

- During deformation, **mechanical integrity** and **coherency** are maintained along the grain boundaries; i.e. the grain boundaries usually do not come apart or open up.
- As a consequence, each individual grain is constrained, to some degree in the shape it may assume by its neighboring grains.



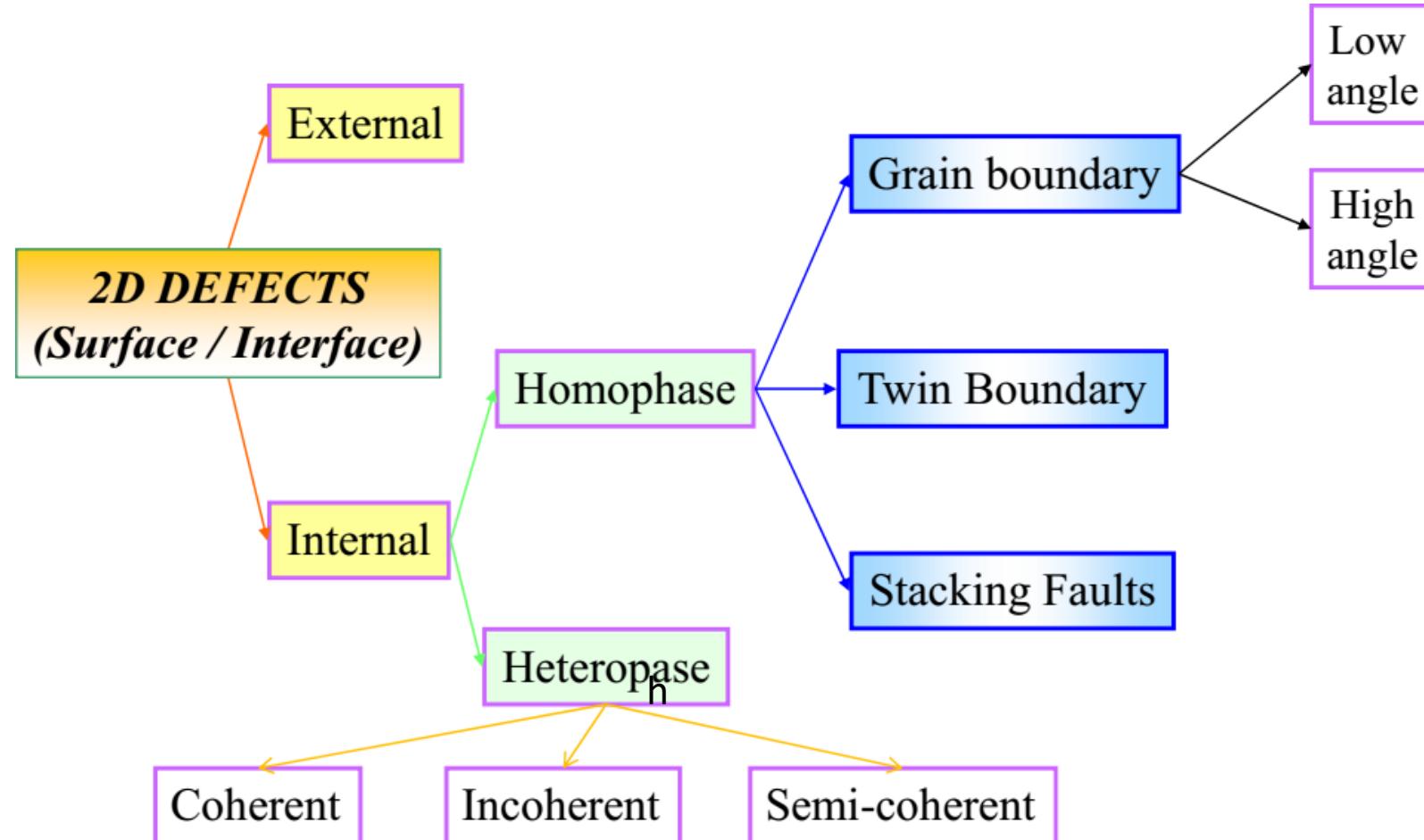
Alteration of the grain structure of a polycrystalline metal as a result of plastic deformation

- (a) Before deformation the grains are equi-axed.
- (b) After deformation elongated grains are produced



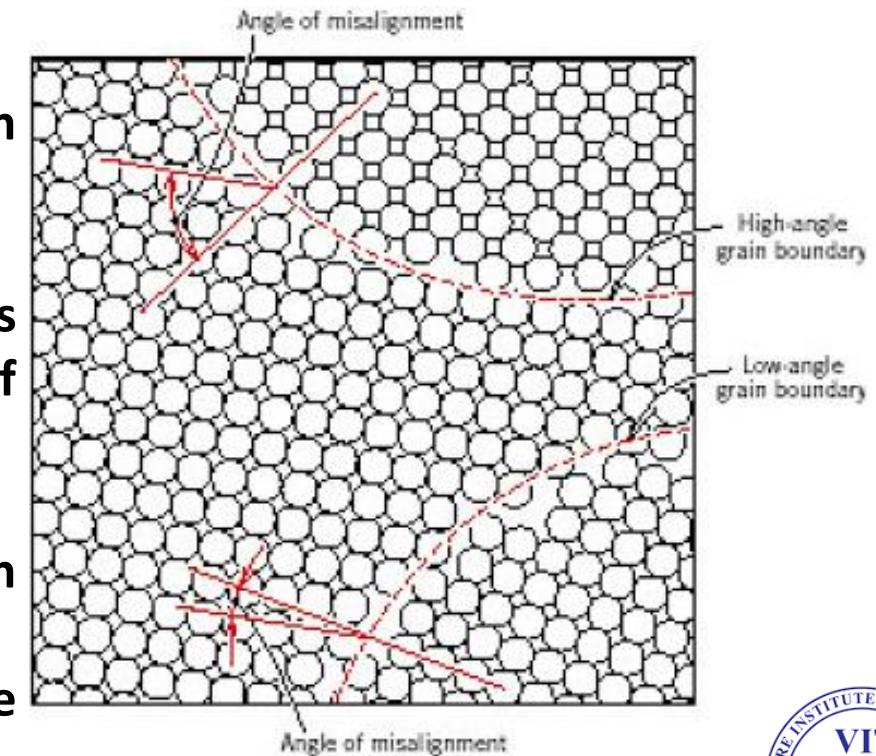
2D Defects: Surface Defects

- 2D in a mathematical sense.
- The region of distortion is ~ few atomic diameters in thickness.



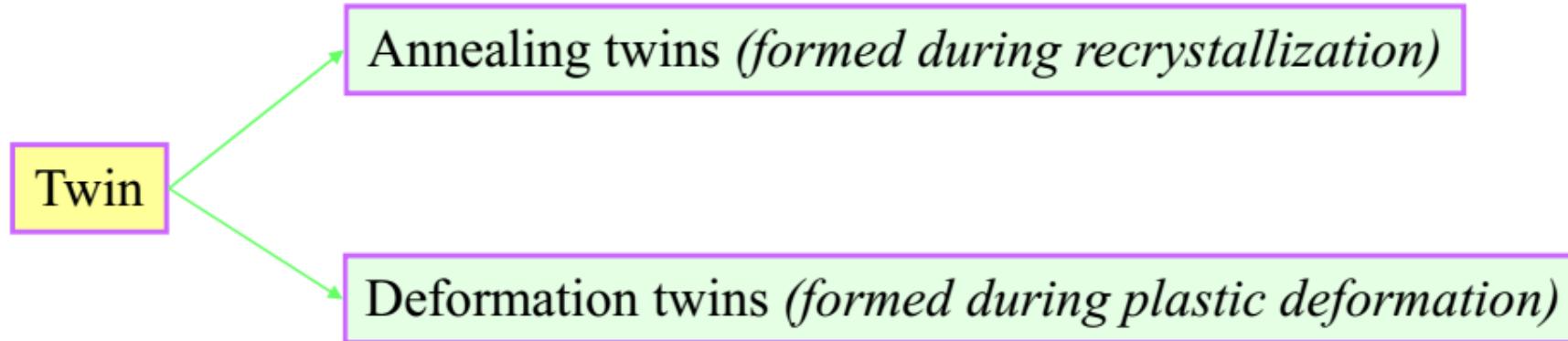
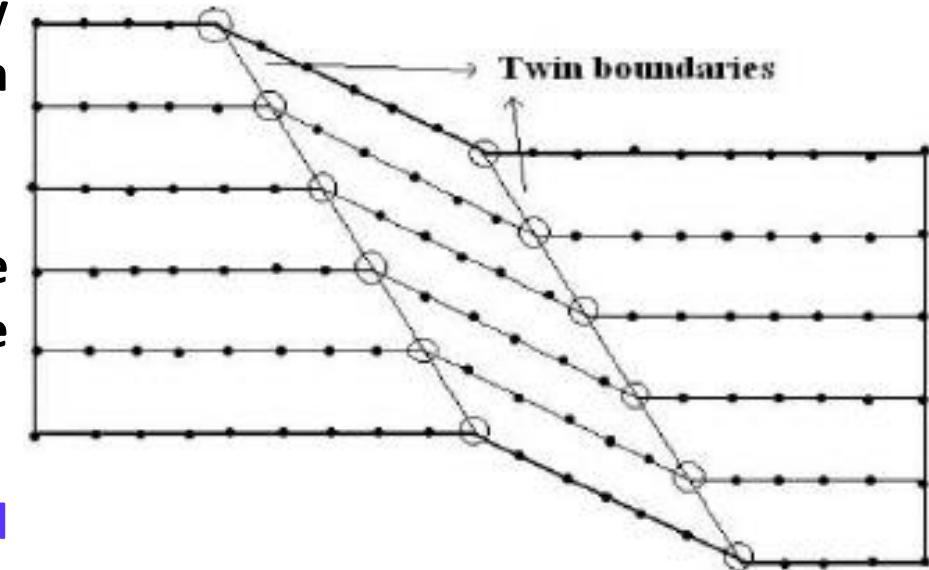
Homo-Phase (Grain Boundary)

- Single-phase polycrystalline material consist many crystals or grains that have different crystallographic orientation. There exist atomic mismatch within the regions where grains meet. These regions are **grain boundaries**.
- The grain boundary region may be distorted with atoms belonging to neither crystal.
- The thickness may be of the order of few atomic diameters.
- The crystal orientation changes abruptly at the grain boundary.
- In an low angle boundary the orientation difference is $< 15^{\circ}$.
- In the low angle boundary the distortion is not so drastic as the high-angle boundary → can be described as an array of dislocations.
- Large grains grow at the expense of smaller ones.
- Grain boundary energy is responsible for grain growth on heating $\sim (> 0.5 T_m)$.
- The average number of nearest neighbors for an atom in the grain boundary of a close packed crystal is 11.



Homo-Phase (Twin Boundary)

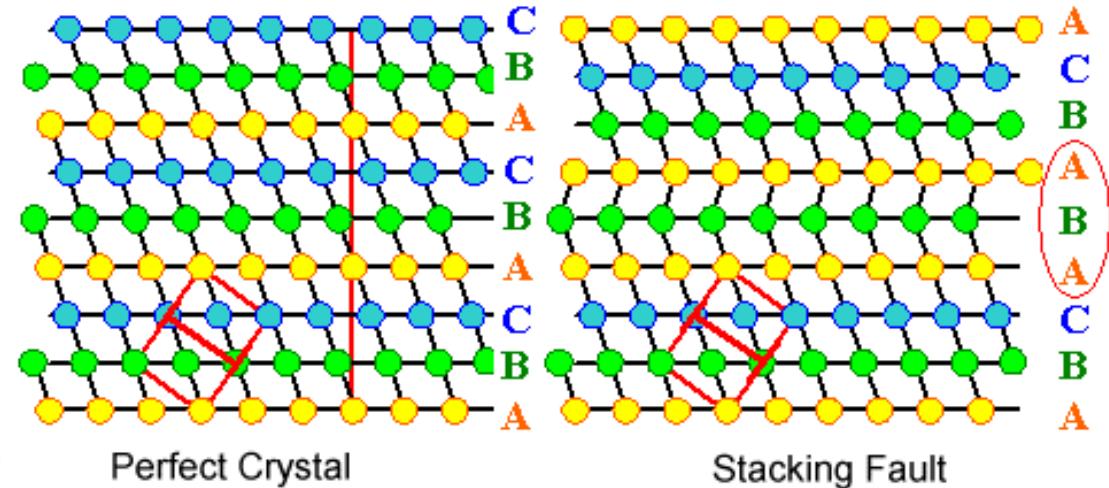
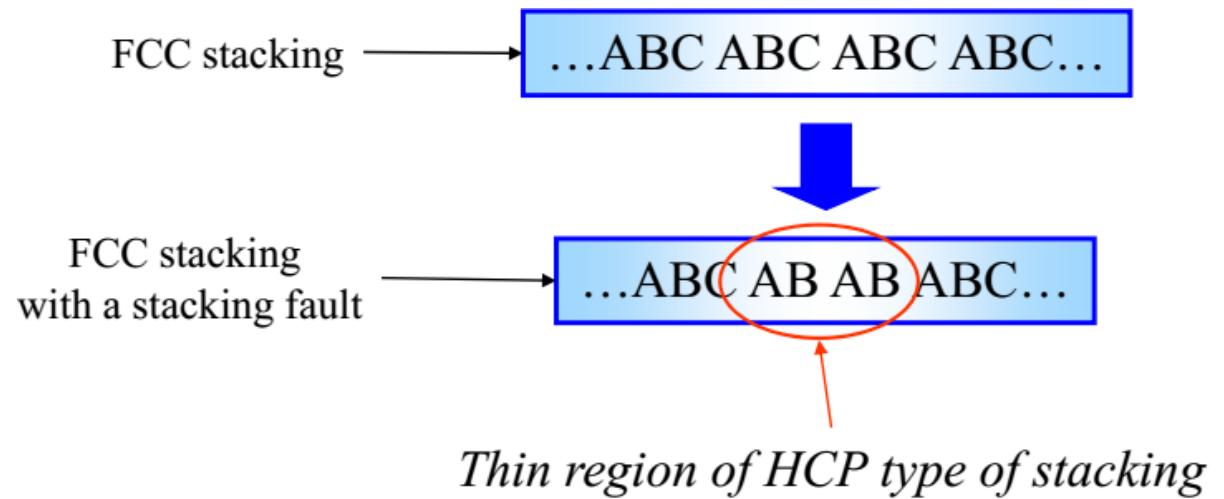
- The atomic arrangement on one side of the twin boundary is related to the other side by a symmetry operation (usually a mirror).
- Twin boundaries usually occur in pairs such that the orientation difference introduced by one is restored by the other.
- The region between the regions is called the twinned region.



Homo-Phase (Stacking Fault)

- Error in the sequence of stacking atomic planes → Stacking fault

- Defined by a shift vector



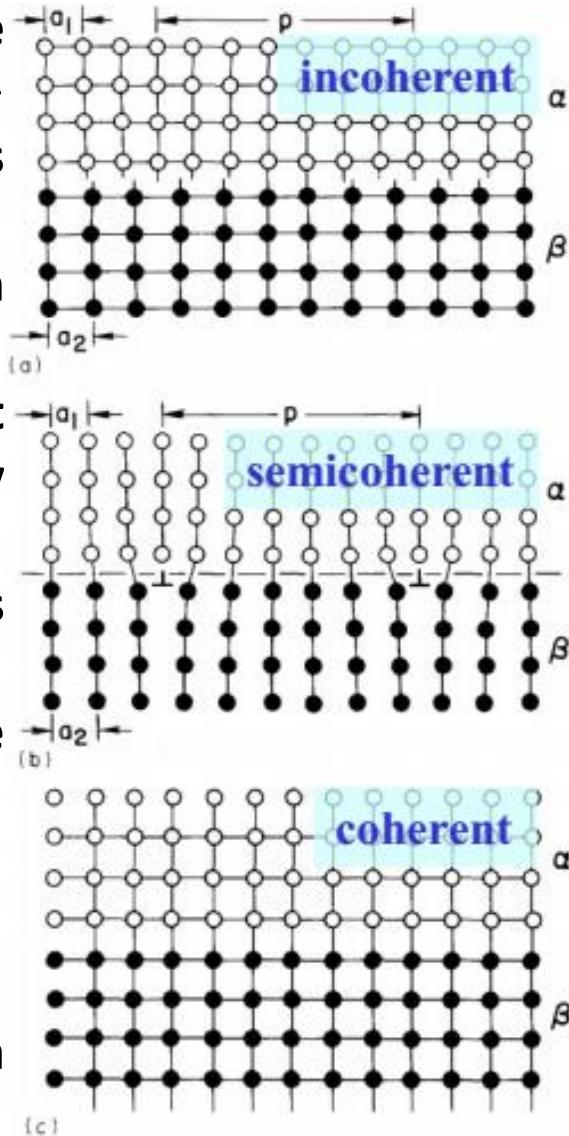
- In above the number of nearest neighbors remains the same but next-nearest neighbors are different than that in FCC.
- Stacking fault energy $\sim 0.01 - 0.05 \text{ J/m}^2$.
- Stacking fault in HCP can lead to thin region of FCC kind of stacking.

Hetero-Phase

- Interphase boundary separates two different phases which may have different composition, crystal structure and/or lattice parameter → limited (if any) options for perfect matching of planes and directions in the two crystals.
- Depending on atomic structure, 3 types of interphase boundaries can be distinguished: **coherent**, **semi-coherent**, and **incoherent**.
- **Coherent (commensurate) interface:** two crystals match perfectly at the interface plane (small lattice mismatch can be accommodated by elastic strain in the adjacent crystals).
- **Semi-coherent (dis-commensurate) interface:** lattice mismatch is accommodated by periodic array of misfit dislocations.
- **Incoherent (in-commensurate) interface:** disordered atomic structure of the interface.
- lattice misfit at the interface:

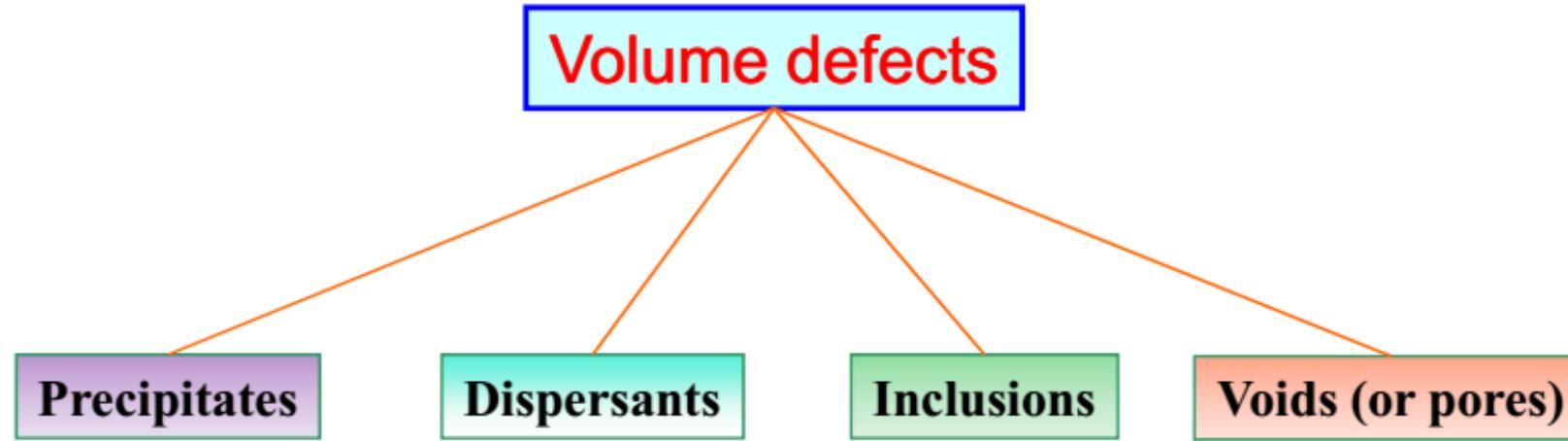
$$\delta = \frac{a_2 - a_1}{a_1}$$

- even in the case of perfect atomic matching, there is always a chemical contribution to the interface energy.

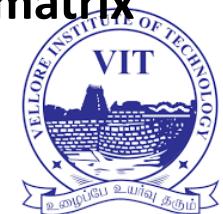


3D Defects: Volume Defects

- Volume defects in crystals are three dimensional aggregates of atoms or vacancies.



- Precipitates:** Precipitates are small particles that are introduced into the matrix by solid state reactions. While precipitates are used for several purposes, their most common purpose is to increase the strength of structural alloys by acting as obstacles to the motion of dislocations.
- Their efficiency in doing this depends on their size, their internal properties, and their distribution through the lattice. However, their role in the microstructure is to modify the behavior of the matrix rather than to act as separate phases in their own right.



Contd...

- **Dispersants:** Dispersants are larger particles that behave as a second phase as well as influencing the behavior of the primary phase. They may be large precipitates, grains, or poly-granular particles distributed through the microstructure. When a microstructure contains dispersants such properties as mechanical strength and electrical conductivity are some average of the properties of the dispersant phase and the parent.

- **Inclusions:** Inclusions are foreign particles or large precipitate particles. They are usually undesirable constituents in the microstructure. For example, inclusions have a deleterious effect on the useful strength of structural alloys since they are preferential sites for failure. They are also often harmful in microelectronic devices since they disturb the geometry of the device by interfering in manufacturing, or alter its electrical properties by introducing undesirable properties of their own.

- **Voids (or pores):** Voids (or pores) are caused by gases that are trapped during solidification or by vacancy condensation in the solid state. They are almost always undesirable defects. Their principal effect is to decrease mechanical strength and promote fracture at small loads.

