

UNIT - 1

Crystallography Defects in Materials and Deformations

UNIT - 1

- Types of Materials –
- Properties of Materials –
↓
- Microstructure – internal arrangement of atoms and/or molecules

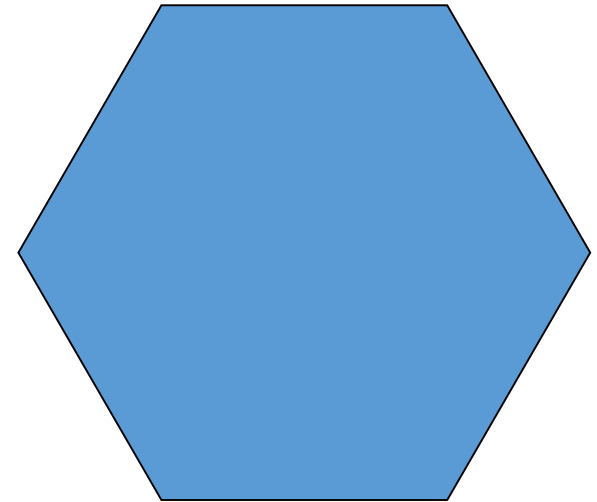
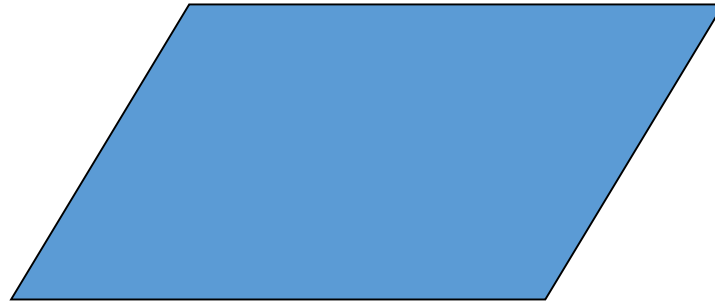
- Matter – Solids
 - Crystalline -
 - Amorphous -

- Repetition = Symmetry

Types of repetition: Rotation and Translation

Rotation - What is rotational symmetry?

Imagine that this object will be rotated (maybe)



The object is obviously symmetric...it has symmetry

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What about translation?

Same as rotation

Ex: one dimensional array of points

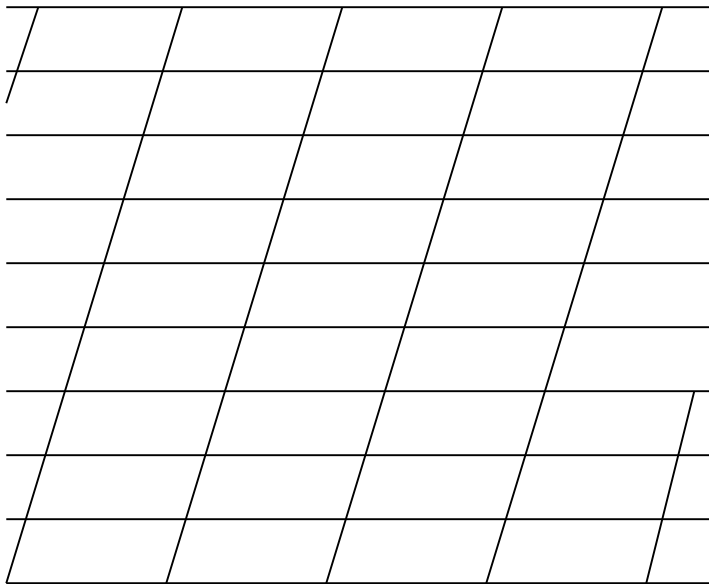


Translations are restricted to only certain values to get symmetry (periodicity)

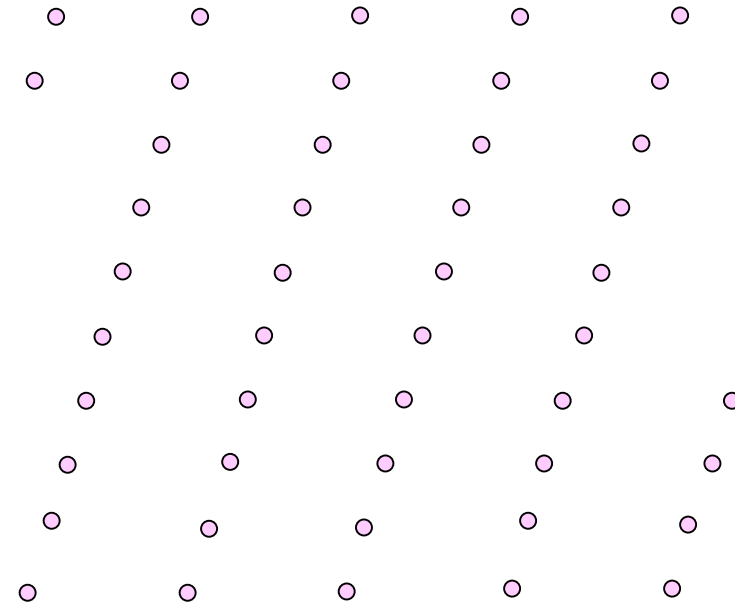
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2D translations

Lots of common examples

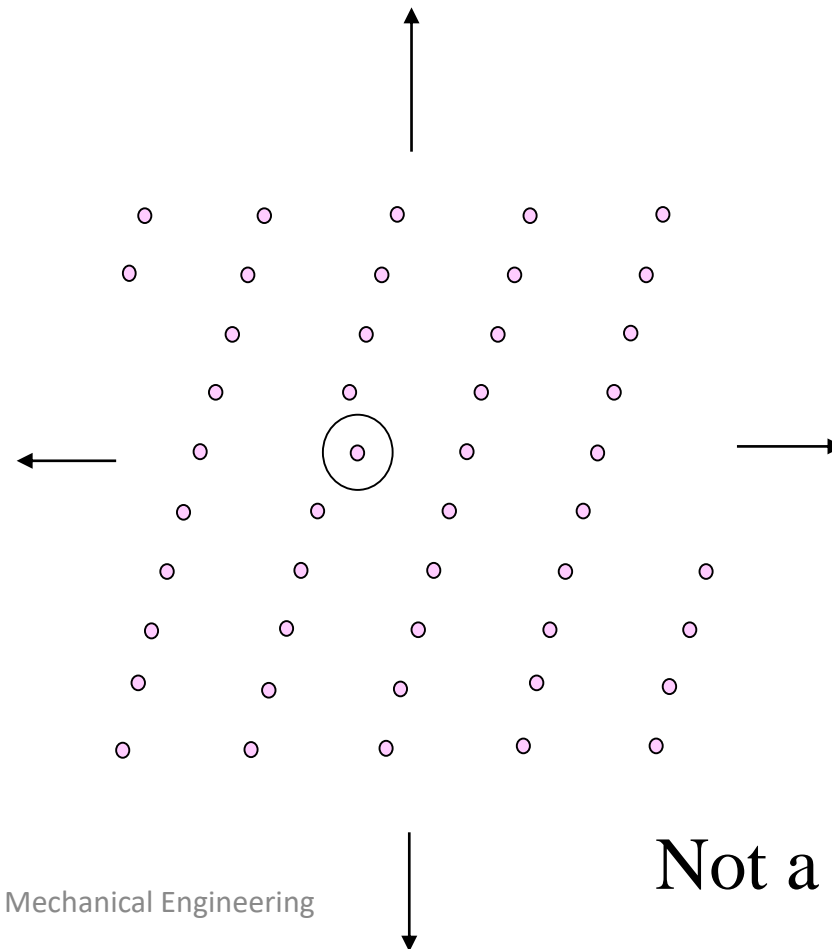
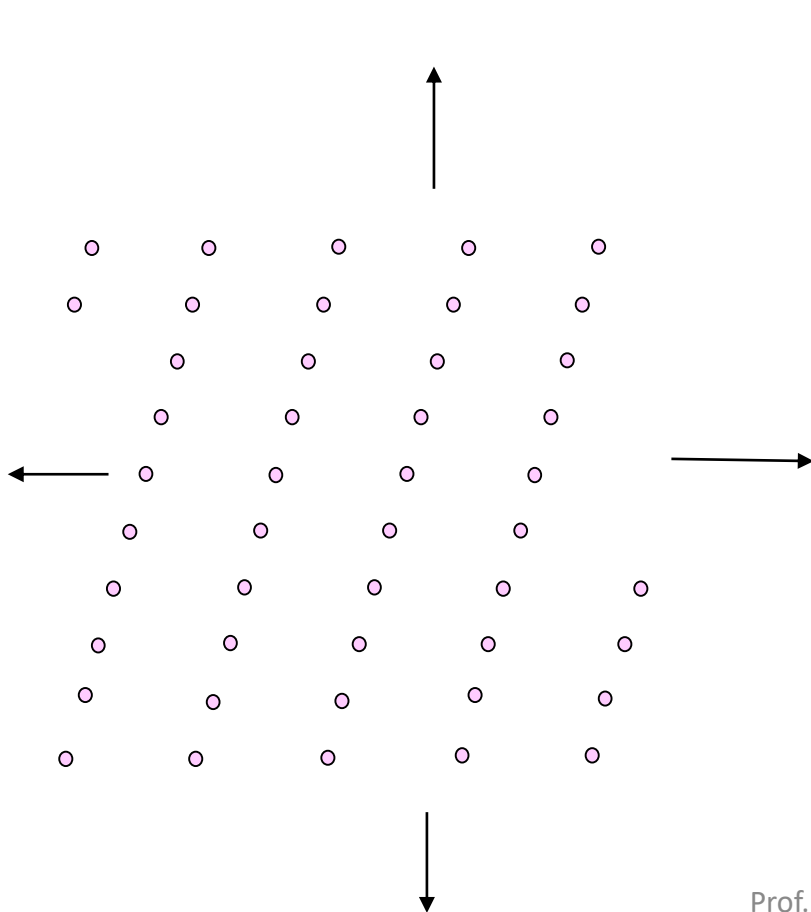


Each block is represented by a point



This array of points is a LATTICE

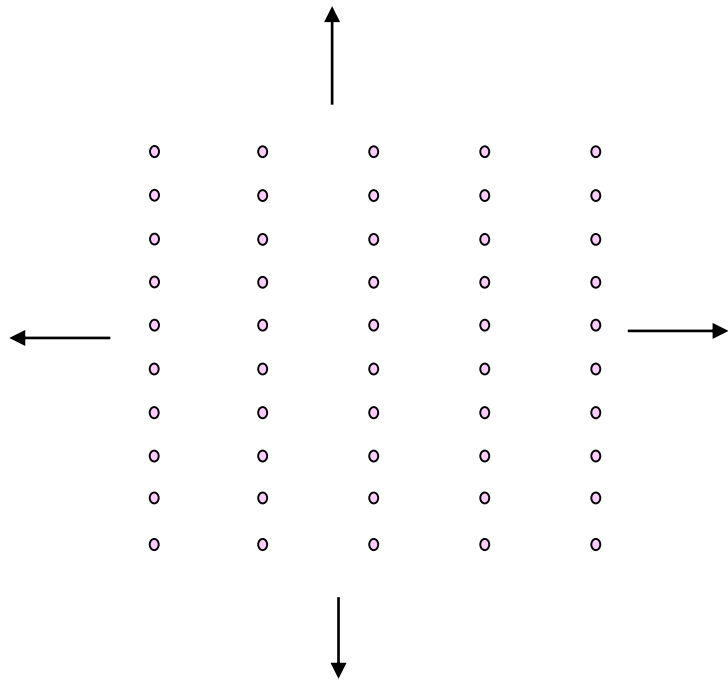
Lattice - infinite, perfectly periodic array of points in a space



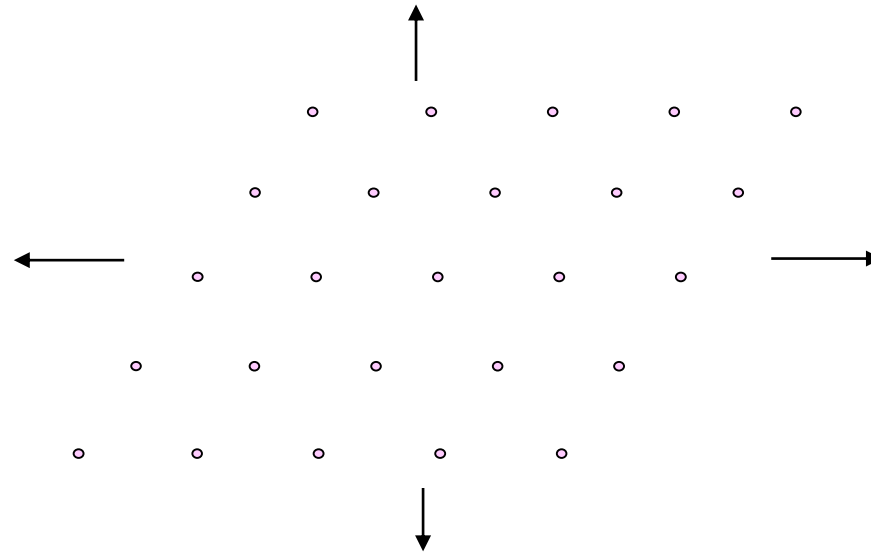
Not a lattice

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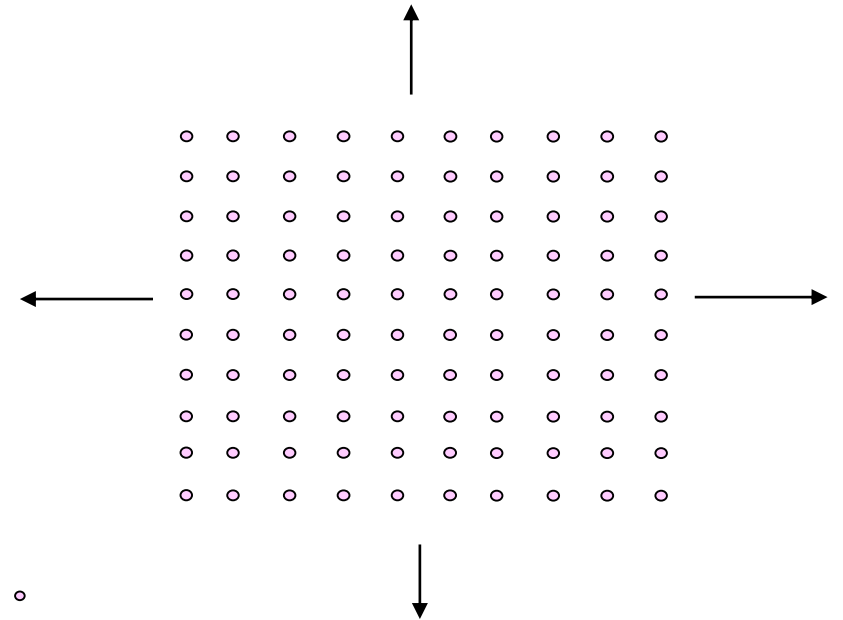
Another type of lattice - with a different symmetry



rectangular



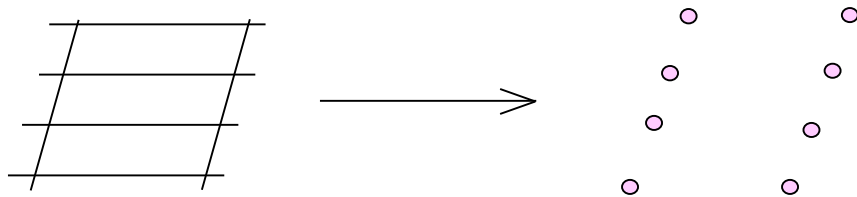
hexagonal



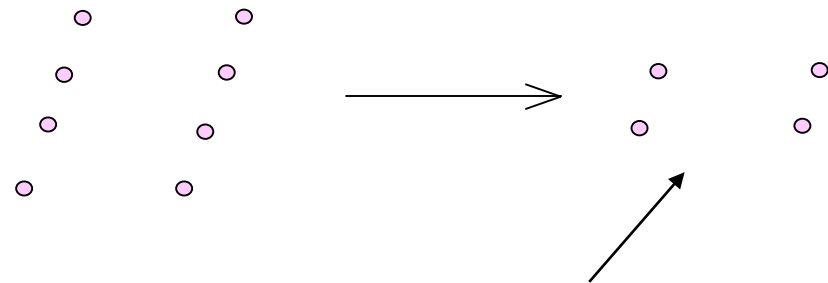
square

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We abstracted points from the shape:



Now we abstract further:



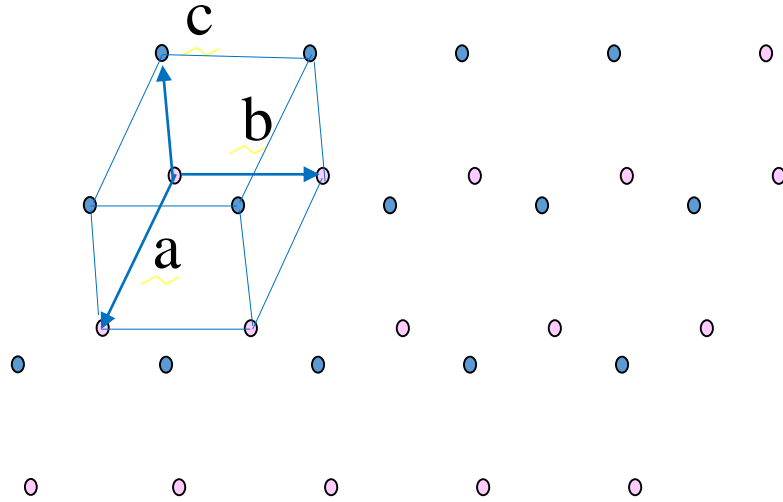
Unit cell: smallest repetitive volume which contains the complete *lattice pattern* of a crystal.

This is a UNIT CELL

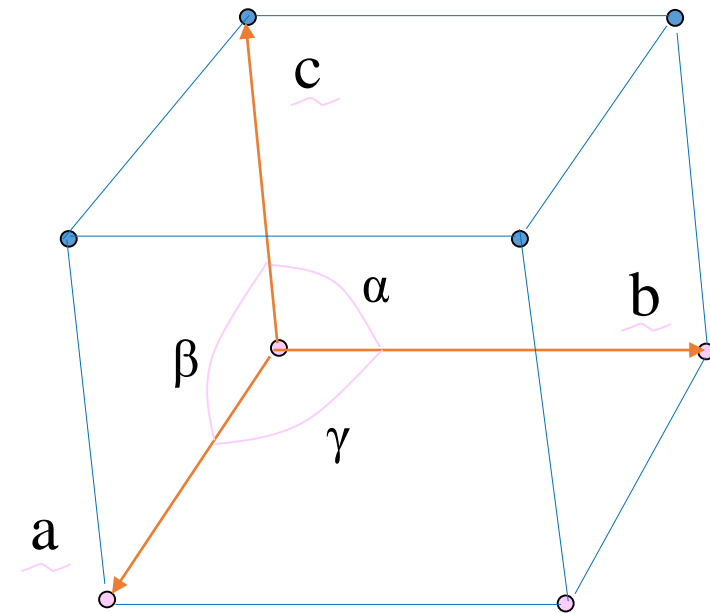
Represented by two lengths and an angle

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In 3-D:



Lattice parameters:



a , b , and c are the basis vectors for the lattice

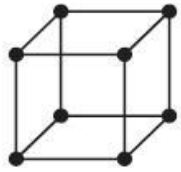
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The many thousands of lattices classified into **crystal systems**

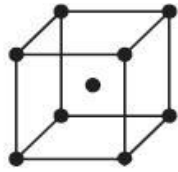
System	Interaxial Angles	Axial lengths
Cubic	$a = b = c = 90^\circ$	$a = b = c$
Tetragonal	$a = b \neq c = 90^\circ$	$a = b \neq c$
Orthorhombic	$a \neq b \neq c = 90^\circ$	$a \neq b \neq c$
Monoclinic	$a \neq b \neq c, \alpha = \beta = 90^\circ \neq \gamma$	$a \neq b \neq c$
Hexagonal	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	$a = b \neq c$
Rhombohedral	$a = b = c \neq 90^\circ$	$a = b = c$
Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$	$a \neq b \neq c$

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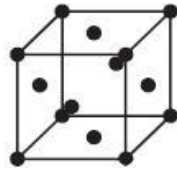
The 14 Crystal (Bravais) Lattices



Simple cubic



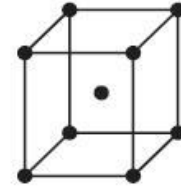
Body-centered
cubic



Face-centered
cubic



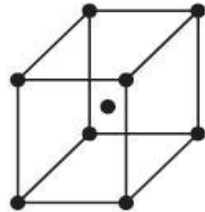
Simple
tetragonal



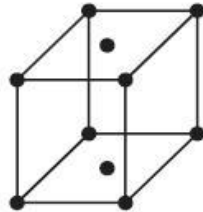
Body-centered
tetragonal



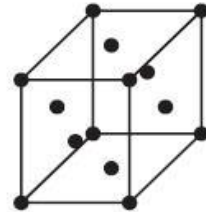
Simple
orthorhombic



Body-centered
orthorhombic



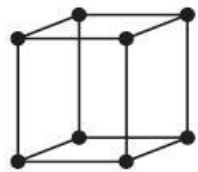
Base-centered
orthorhombic



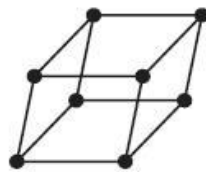
Face-centered
orthorhombic



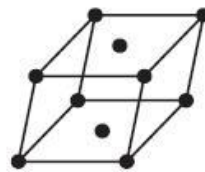
Rhombohedral



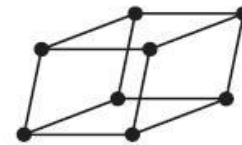
Hexagonal



Simple
monoclinic



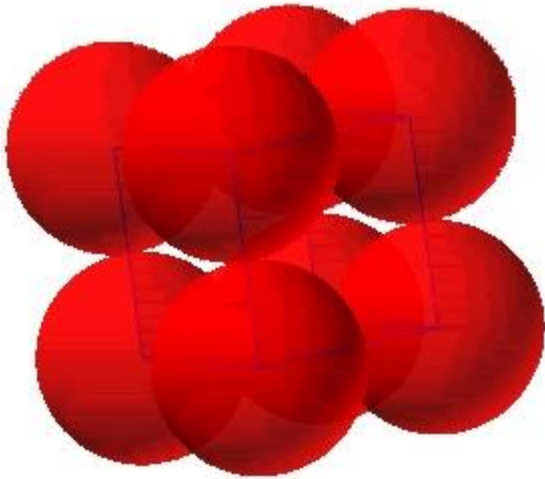
Base-centered
monoclinic



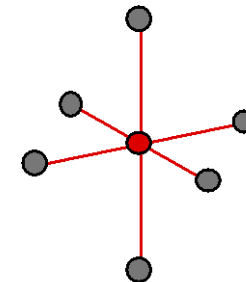
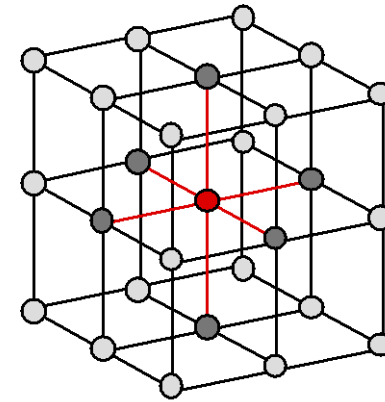
Triclinic

Simple Cubic Structure (SC)

- Rare due to low packing density (only Po – Polonium -- has this structure)
- **Close-packed directions** are *cube edges*.



- **Coordination No.** = 6
(# nearest neighbors) for each atom as seen

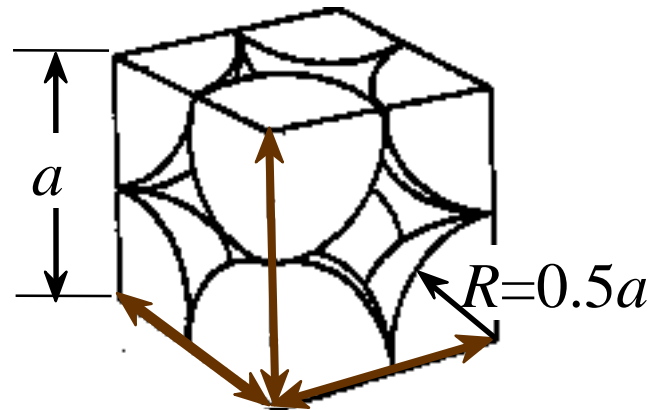


(Courtesy P.M. Anderson)

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Atomic Packing Factor (APF)

- APF for a simple cubic structure = 0.52



close-packed directions
contains $(8 \times 1/8) =$
1 atom/unit cell

Adapted from Fig. 3.23,
Callister 7e.

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

*assume hard spheres

$$\text{APF} = \frac{\overbrace{1}^{\text{atoms}} \overbrace{\frac{4}{3} \pi (0.5a)^3}^{\text{volume atom}}}{\underbrace{a^3}_{\text{volume unit cell}}}$$

Here: $a = R_{\text{at}} * 2$

Where R_{at} is the 'handbook' atomic radius

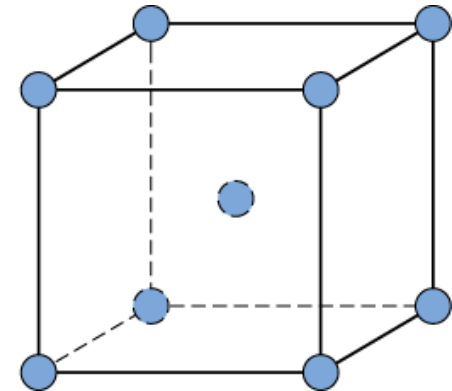
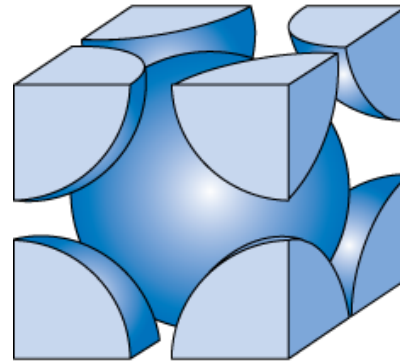
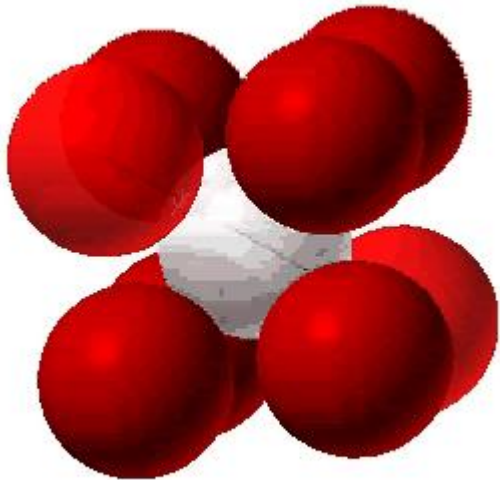
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Body Centered Cubic Structure (BCC)

- Atoms touch each other along *cube diagonals within a unit cell*.

--Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr, W, Fe (α), Tantalum, Molybdenum

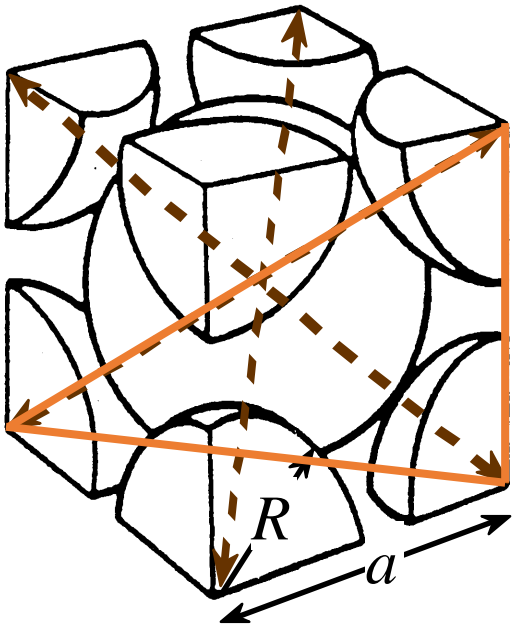


Adapted from Fig. 3.2,
Callister 7e.

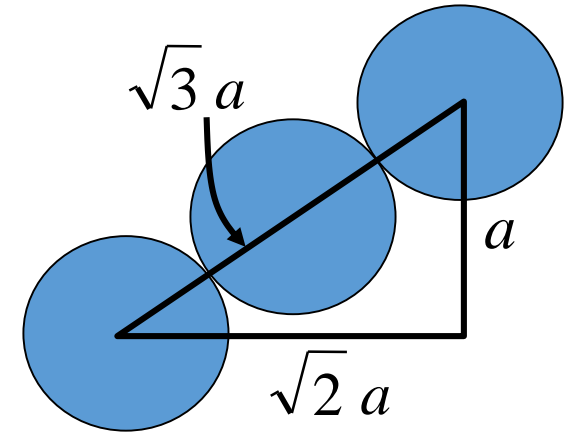
- Coordination # = 8

2 atoms/unit cell: (1 center) + (8 corners x 1/8)

Atomic Packing Factor: BCC



Adapted from
Fig. 3.2(a), Callister 7e.



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

$$\text{APF} = \frac{\text{atoms unit cell} \times \frac{4}{3} \pi \left(\frac{\sqrt{3}a}{4}\right)^3}{a^3}$$

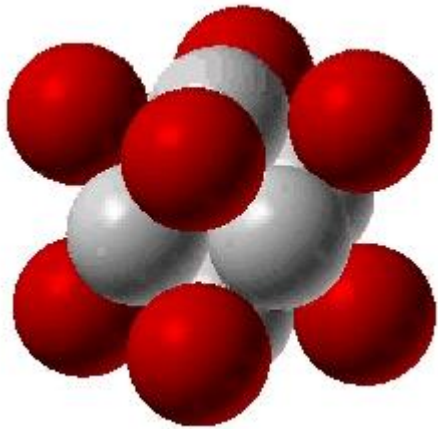
atoms unit cell → 2 $\frac{4}{3} \pi \left(\frac{\sqrt{3}a}{4}\right)^3$ ← volume atom
volume unit cell ← a^3

- APF for a body-centered cubic structure = 0.68

UNIT - 1

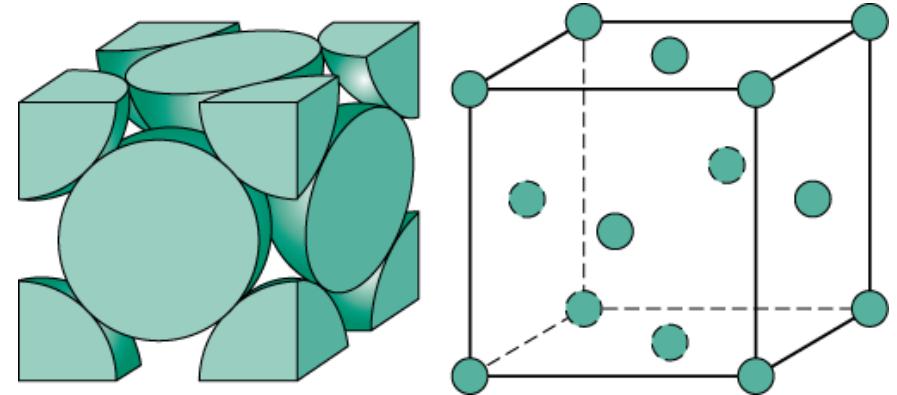
Face Centered Cubic Structure (FCC)

- Atoms touch each other along *face diagonals*.
- Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.



- Coordination # = 12

ex: Al, Cu, Au, Pb, Ni, Pt, Ag



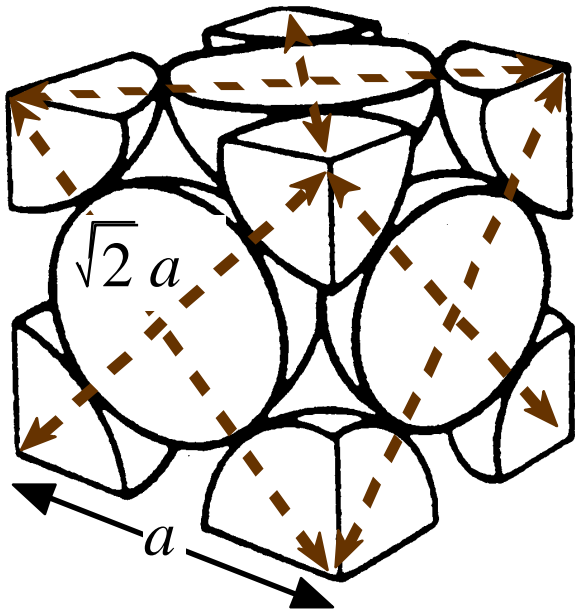
Adapted from Fig. 3.1, *Callister 7e*.

4 atoms/unit cell: $(6 \text{ face} \times \frac{1}{2}) + (8 \text{ corners} \times \frac{1}{8})$

UNIT - 1

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74



Adapted from Fig. 3.1(a),
Callister 7e.

The maximum achievable APF!

Close-packed directions:

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

$$(a = 2\sqrt{2}R)$$

Unit cell contains:

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

$$\text{APF} = \frac{\frac{\text{atoms}}{\text{unit cell}} \times \frac{4}{3} \pi \left(\frac{\sqrt{2}a}{4}\right)^3}{a^3}$$

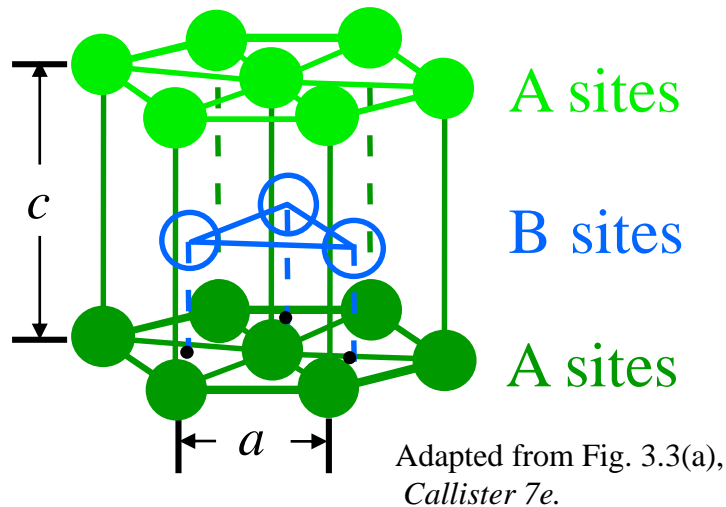
The diagram shows the APF formula with color-coded components and arrows indicating their origin:

- atoms/unit cell** (green text) points to the **4** in the numerator.
- volume/atom** (brown text) points to the $\frac{4}{3} \pi \left(\frac{\sqrt{2}a}{4}\right)^3$ term in the numerator.
- volume/unit cell** (blue text) points to the a^3 in the denominator.

UNIT - 1

Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection



- Coordination # = 12

6 atoms/unit cell

- APF = 0.74

Prof. Roopa T.S. Dept. of Mechanical Engineering

ex: Cd, Mg, Ti, Zn

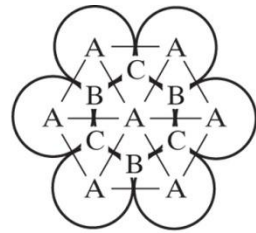
- 2D Projection



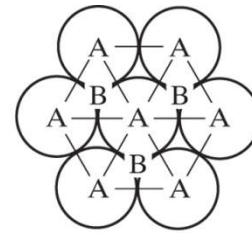
- $c/a = 1.633$ (*ideal*)

UNIT - 1

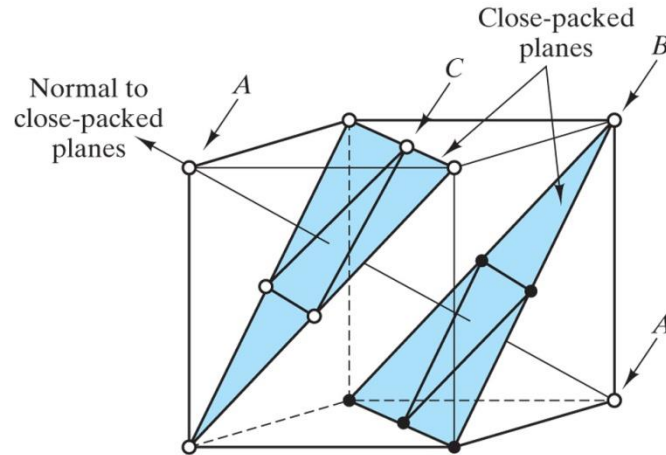
We find that both FCC & HCP are highest density packing schemes ($APF = .74$) – this illustration shows their differences as the closest packed planes are “built-up”



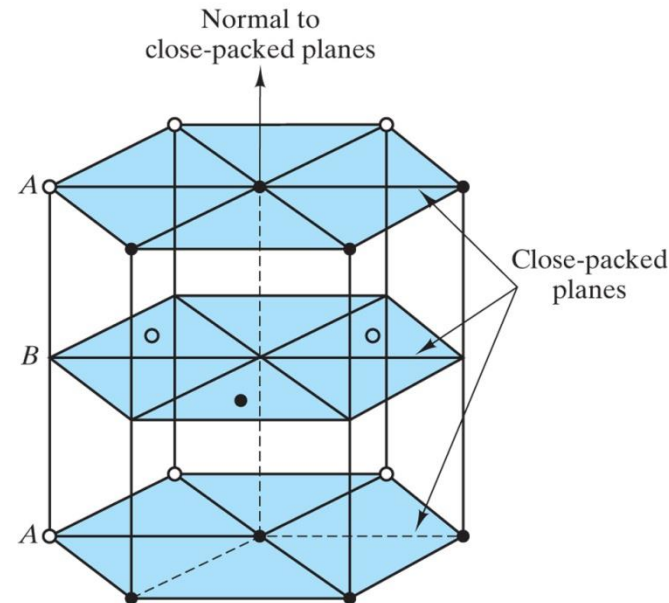
(a) Stacking of close-packed planes



(b) Stacking of close-packed planes



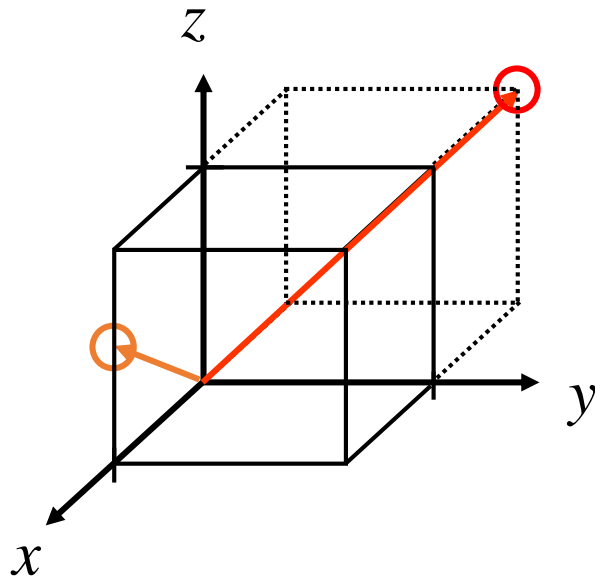
(c) Face-centered cubic



(d) Hexagonal close packed

UNIT – 1 Crystallographic Directions and Planes

Crystallographic Directions



ex: $1, 0, \frac{1}{2} \Rightarrow 2, 0, 1 \Rightarrow [201]$

$-1, 1, 1 \Rightarrow [\bar{1}11]$

where 'overbar' represents a negative index

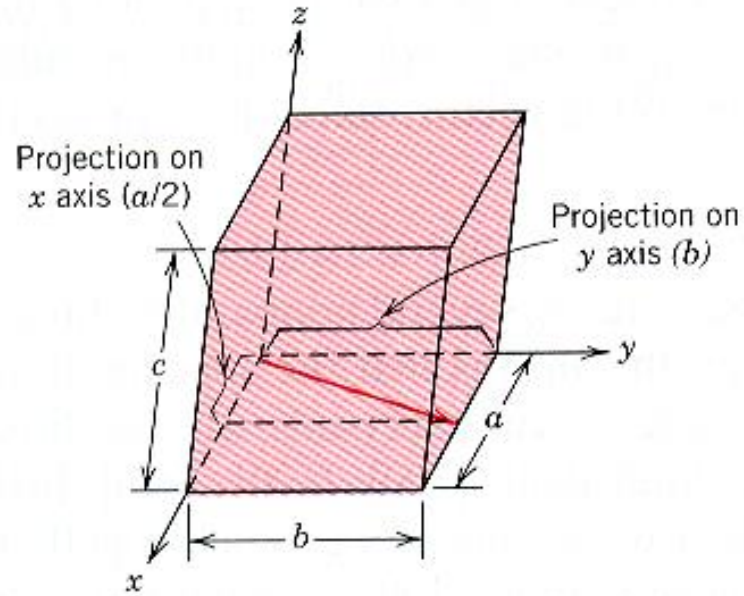
families of directions $\langle uvw \rangle$

Algorithm

1. Vector is repositioned (if necessary) to *pass through the Unit Cell origin*.
2. Read off line projections (to principal axes of U.C.) in terms of unit cell dimensions a , b , and c
3. Adjust to smallest **integer values**
4. Enclose in square brackets, *no commas*

$[uvw]$

UNIT - 1



What is this *Direction* ?????

Projections:

Projections in terms of a,b and c:

Reduction:

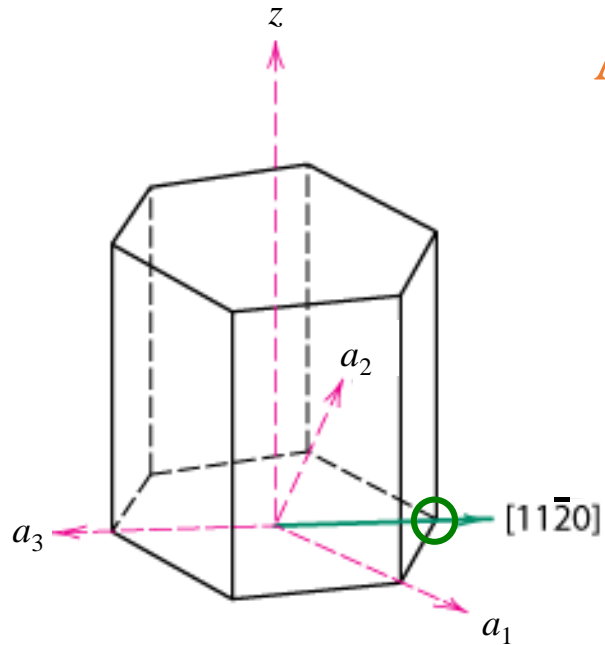
Enclosure [brackets]

<u>x</u>	<u>y</u>	<u>z</u>
a/2	b	0c
1/2	1	0
1	2	0

[120]

UNIT - 1

HCP Crystallographic Directions



Adapted from Fig. 3.8(a), Callister 7e.

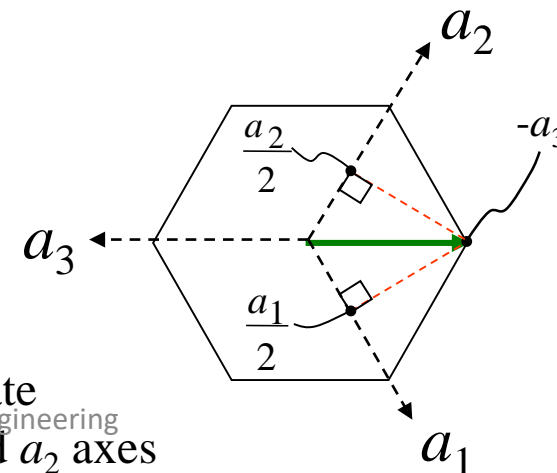
ex: $\frac{1}{2}, \frac{1}{2}, -1, 0 \Rightarrow [11\bar{2}0]$

dashed red lines indicate
projections onto a_1 and a_2 axes

Algorithm

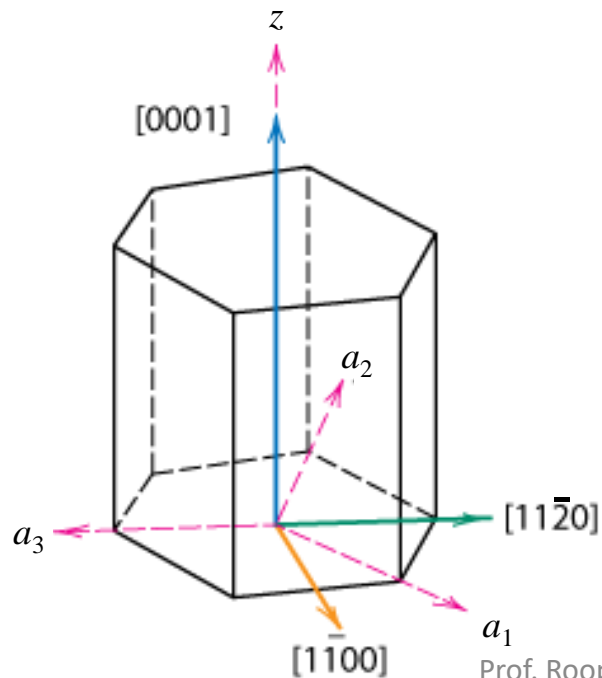
1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a_1 , a_2 , a_3 , or c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

$[uvw]$



HCP Crystallographic Directions

- Hexagonal Crystals
 - 4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., $u'v'w'$) in the '3 space' Bravais lattice as follows.



$$[u'v'w'] \text{ ® } [uvw]$$

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

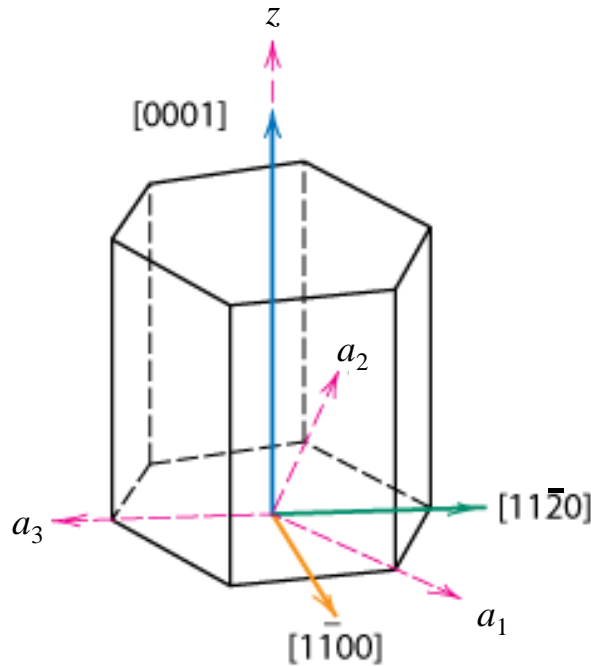
Fig. 3.8(a), Callister 7e.

UNIT - 1

Computing HCP Miller- Bravais Directional Indices (an alternative way):

We confine ourselves to the bravais parallelopiped in the hexagon: a_1 - a_2 - Z and determine: (u',v',w')

Here: $[1\ 1\ 0]$ - so now apply the models to create M-B Indices



$$u = \frac{1}{3} (2u' - v') = \frac{1}{3} (2 * 1 - 1) = \frac{1}{3} \rightarrow 1$$

$$v = \frac{1}{3} (2v' - u') = \frac{1}{3} (2 * 1 - 1) = \frac{1}{3} \rightarrow 1$$

$$t = -(u + v) = -\left(\frac{1}{3} + \frac{1}{3}\right) = -\frac{2}{3} \rightarrow -2$$

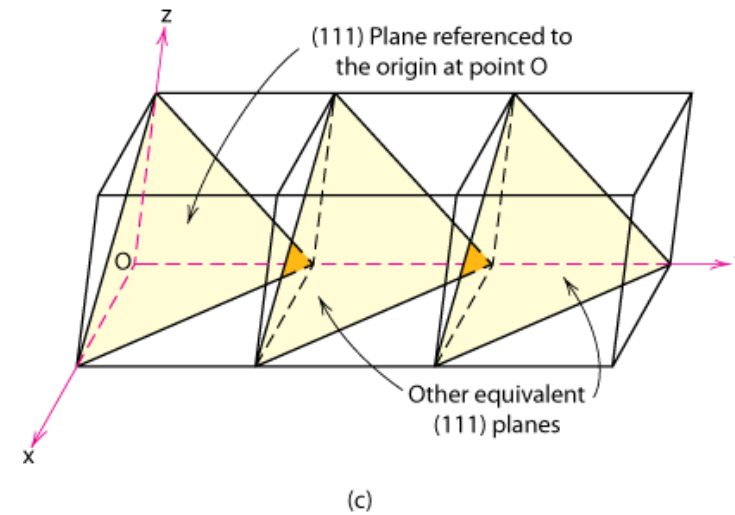
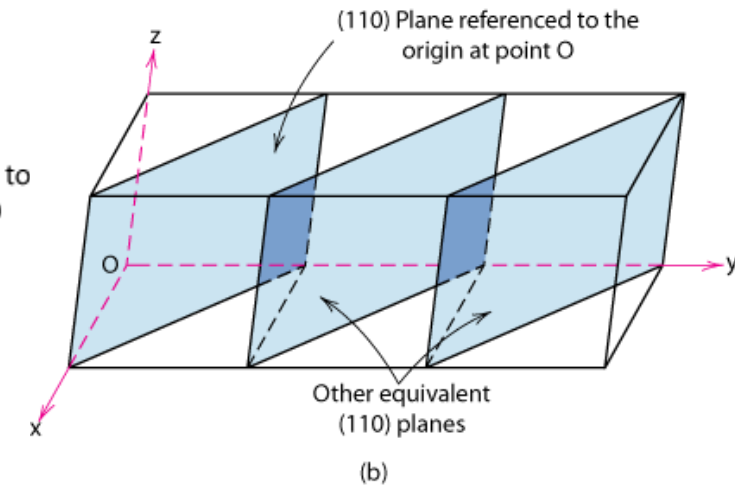
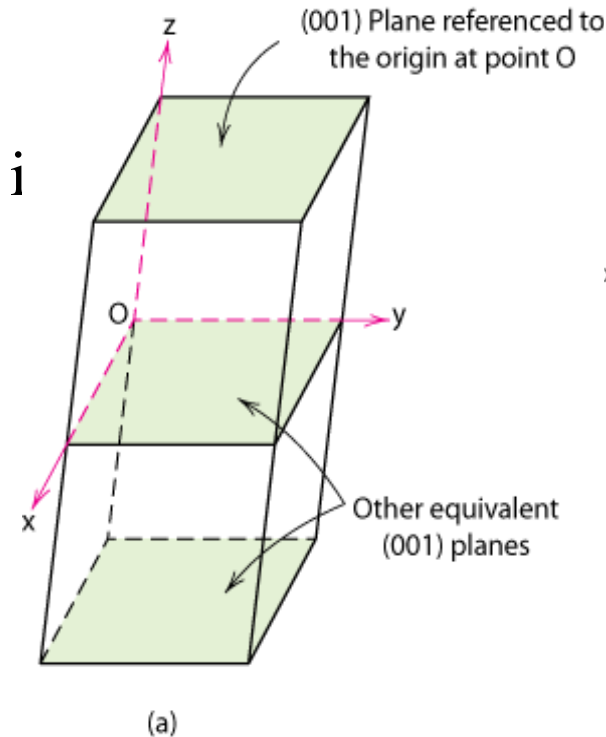
$$w = w' = 0$$

M-B Indices: $[11\bar{2}0]$

UNIT - 1

Defining Crystallographic Planes

- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.
- Algorithm (in cubic lattices this is direct)
 1. Read off intercepts of plane with axes in terms of a , b , c
 2. Take reciprocals of intercepts
 3. Reduce to smallest integer values
 4. Enclose in parentheses,
No commas i.e., (hkl) → families $\{hkl\}$

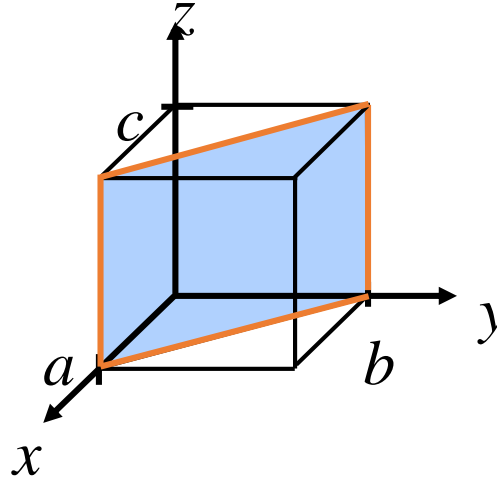


UNIT - 1

Crystallographic Planes

example

	a	b	c
1. Intercepts	1	1	∞
2. Reciprocals	$1/1$	$1/1$	$1/\infty$
	1	1	0
3. Reduction	1	1	0
4. Miller Indices	(110)		

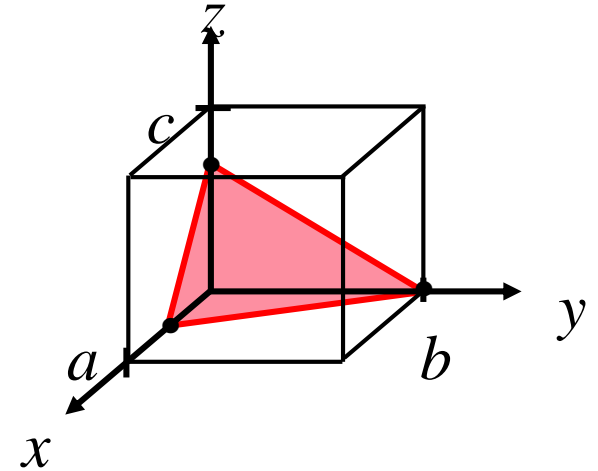
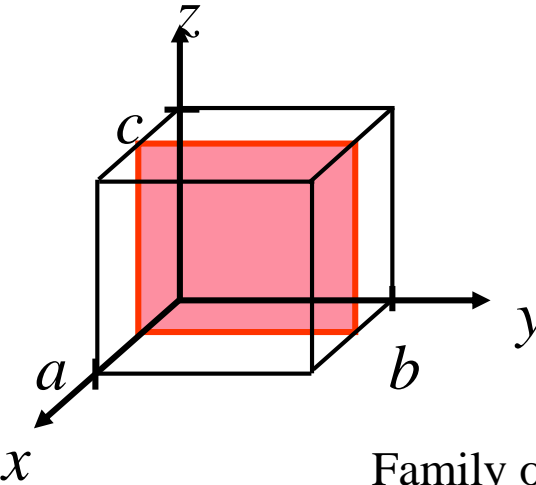


example

	a	b	c
1. Intercepts	$1/2$	1	$3/4$
2. Reciprocals	$1/(1/2)$	$1/1$	$1/(3/4)$
	2	1	$4/3$
3. Reduction	6	3	4
4. Miller Indices	(634)		

example

	a	b	c
1. Intercepts	$1/2$	∞	∞
2. Reciprocals	$1/(1/2)$	$1/\infty$	$1/\infty$
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(100)		

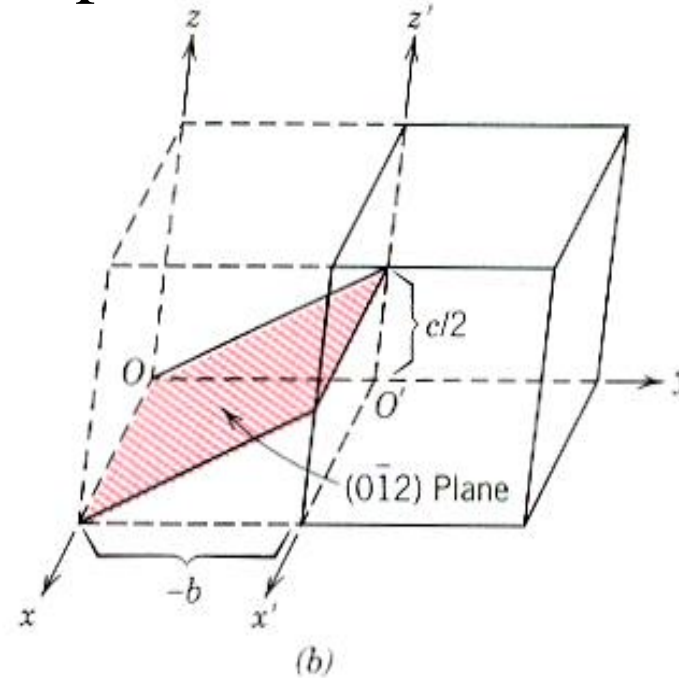
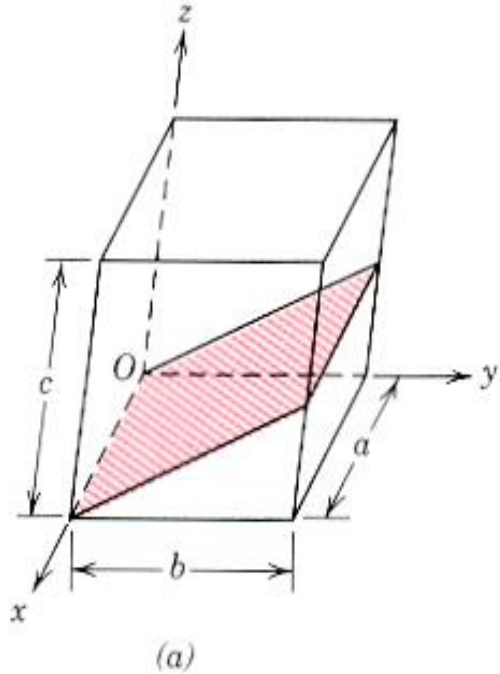


Family of Planes $\{hkl\}$

Ex: $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

UNIT - 1

Determine the Miller indices for the plane shown in the sketch



Intercepts

Intercept in terms of lattice parameters

Reciprocals

Reductions

Enclosure

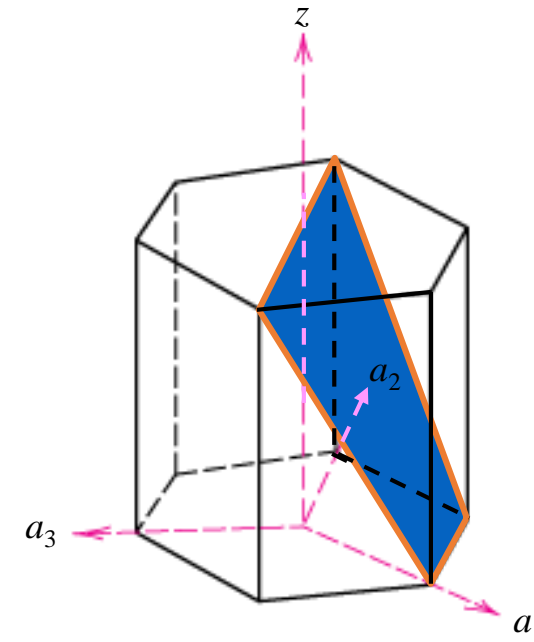
x	y	z
$\propto a$	$-b$	$c/2$
\propto	-1	$1/2$
0	-1	2
	N/A	

(012)

Crystallographic Planes (HCP)

- In hexagonal unit cells the same idea is used

<u>example</u>	a_1	a_2	a_3	c
1. Intercepts	1	∞	-1	1
2. Reciprocals	1	$1/\infty$	-1	1
	1	0	-1	1
3. Reduction	1	0	-1	1
4. Miller-Bravais Indices	(1011)			



There is no such thing as a perfect crystal.

- What are these imperfections?
- Why are they important?

Many of the important properties of materials are due to the presence of imperfections.

The study of imperfections has a two fold purpose, namely,

- A better understanding of crystals and how they affect the properties of metals.
- Exploration of possibilities of minimizing or eliminating these defects.

The term “*defect*” or “*imperfection*” is generally used to describe any deviation from the perfect periodic array of atoms in the crystal.

UNIT – 1 Types of Imperfections

- Vacancy atoms
- Interstitial atoms
- Substitutional atoms

Point defects

- Dislocations

Line defects

- Grain Boundaries

Area/surface/Plane defects

- Voids

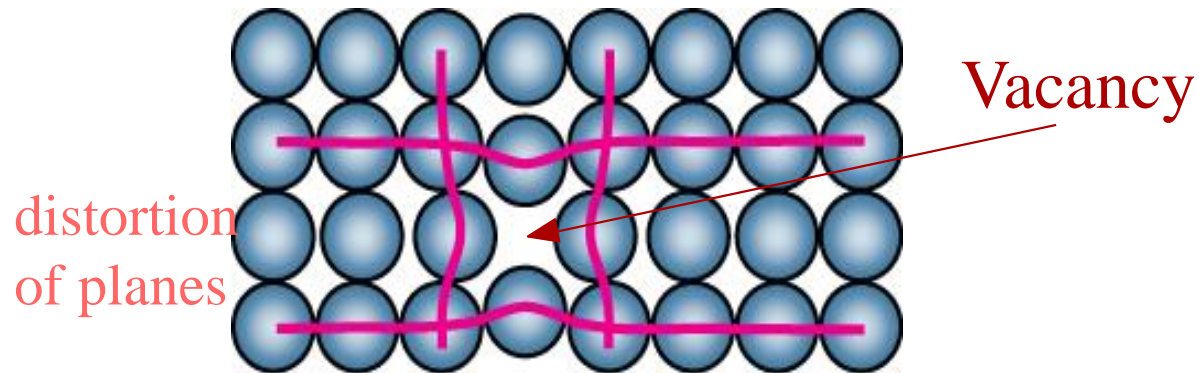
Volume defects

UNIT - 1

Point Defects in Metals

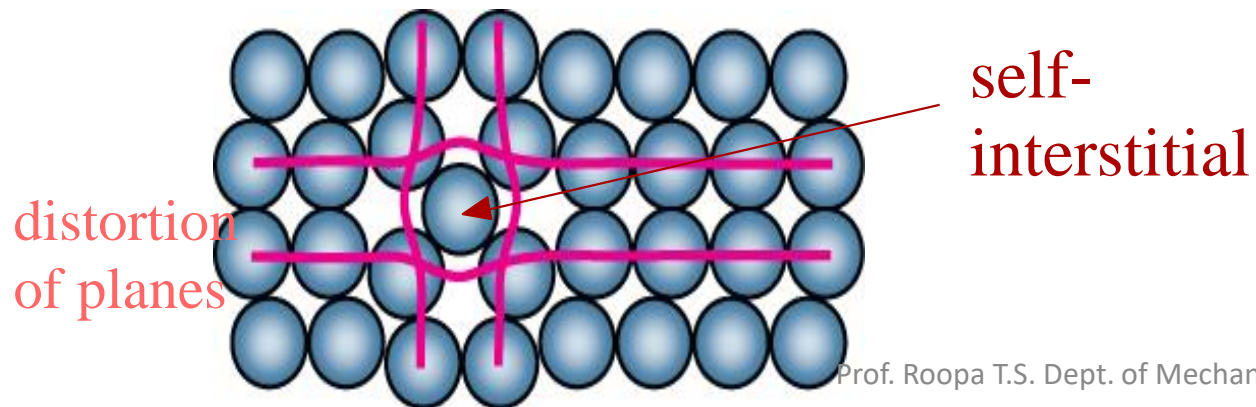
- **Vacancies:**

-vacant atomic sites in a structure.



- **Self-Interstitials:**

-"extra" atoms positioned between atomic sites.



They are imperfect point- like regions, one or two atomic diameters in size and hence referred to as ‘zero dimensional imperfections’.

There are different kinds of point imperfections.

VACANCIES

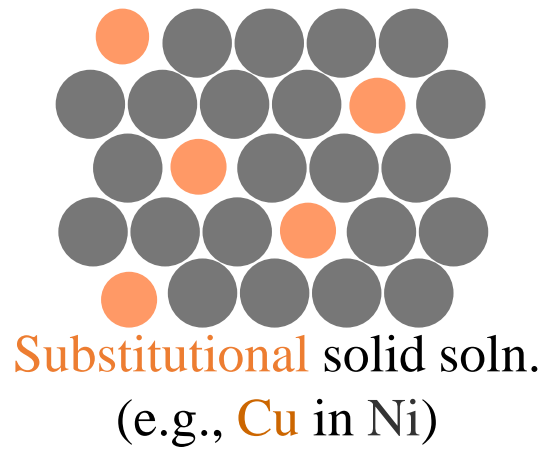
If an atom is missing from its normal site in the matrix, the defect is called a *vacancy defect*.

It may be a single vacancy, divacancy or a trivacancy.

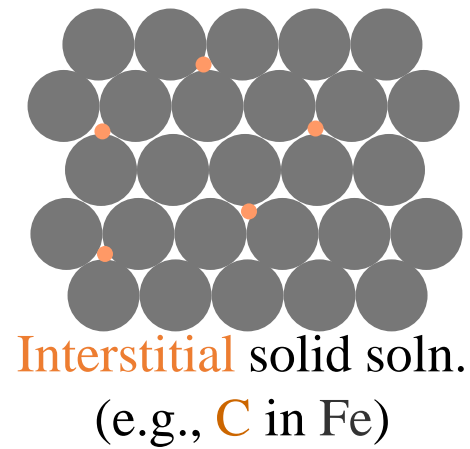
Imperfections in Metals

Two outcomes if impurity (B) added to host (A):

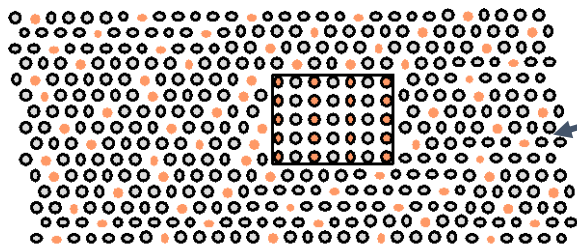
- **Solid solution** of **B** in A (i.e., random dist. of point defects)



OR



- Solid solution of **B** in A plus particles of a new phase (usually for a larger amount of B)

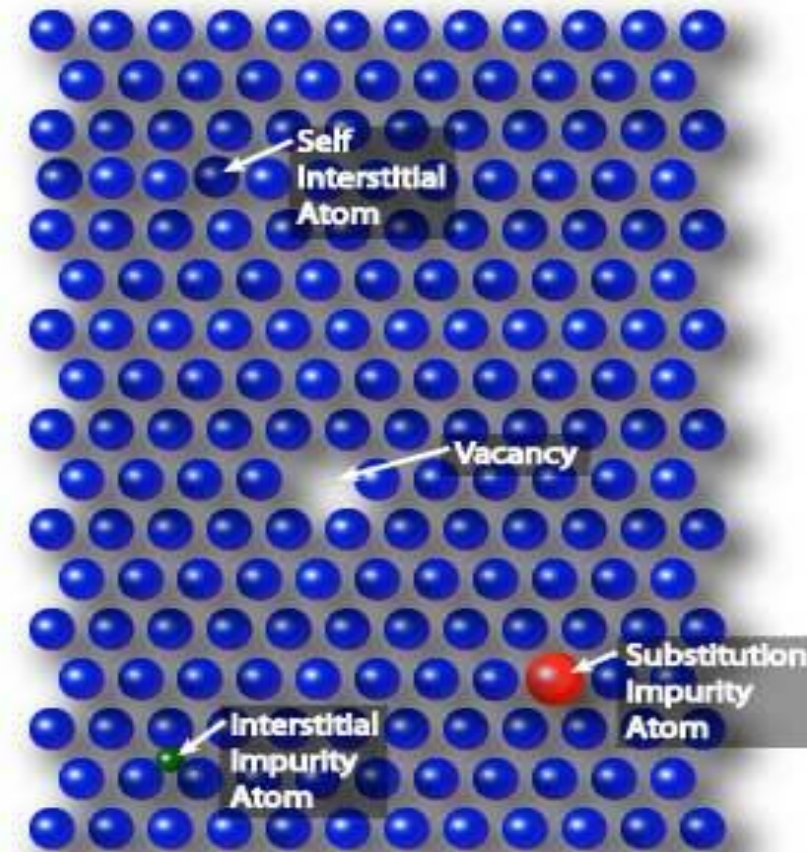


Second phase particle

-- different **composition**

-- often different structure.

Prof. Roopa T.S. Dept. of Mechanical Engineering



UNIT - 1

• Line Defects (**Dislocations**)

- Are one-dimensional defects around which atoms are misaligned
- slip between crystal planes result when dislocations move,
- produce permanent (plastic) deformation.

Edge dislocation: extra half-plane of atoms inserted in a crystal structure. **b** perpendicular (\perp) to dislocation line

- Edge dislocations are represented by ' \perp ' or 'T' depending on whether the incomplete plane starts from the top or from the bottom of the crystal.
- These two configurations are referred to as positive and negative edge dislocations respectively.

Screw dislocation:

spiral planar ramp resulting from shear deformation

b parallel (\parallel) to dislocation line

Burger's vector, b: measure of lattice distortion

Schematic of Zinc (HCP):

- before deformation • after tensile elongation

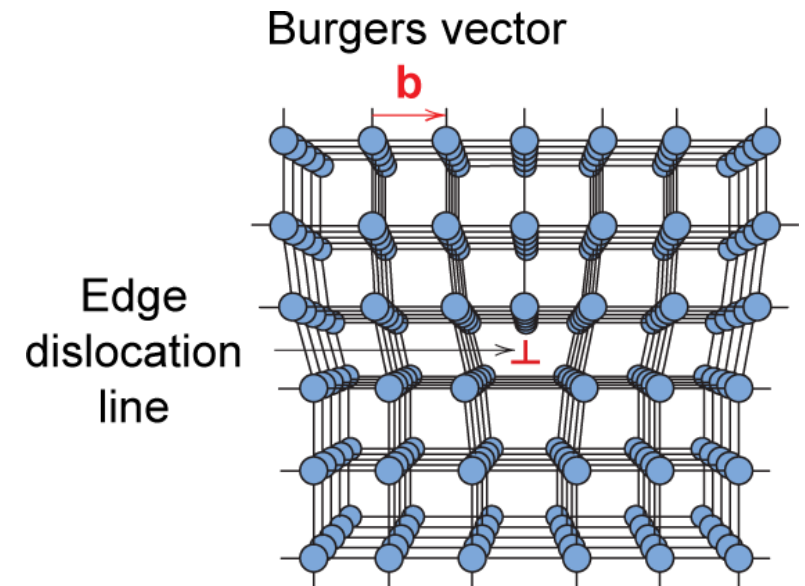
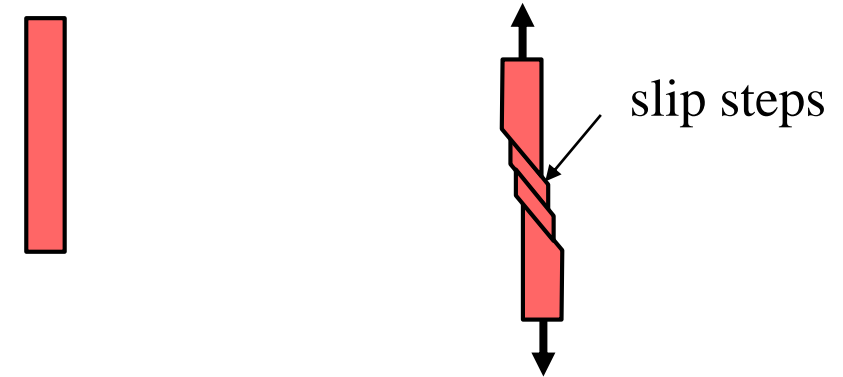
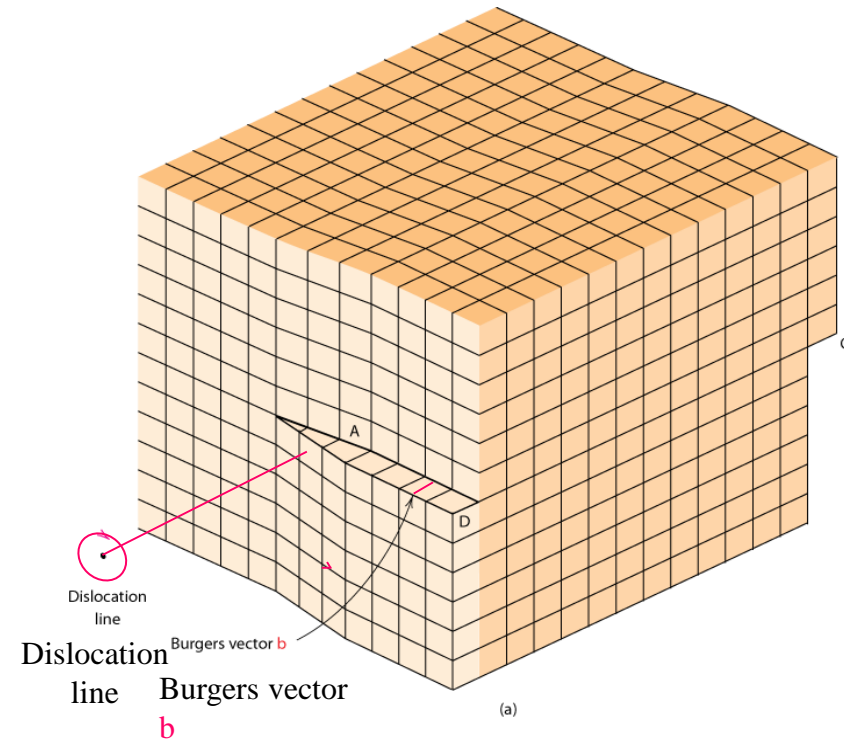


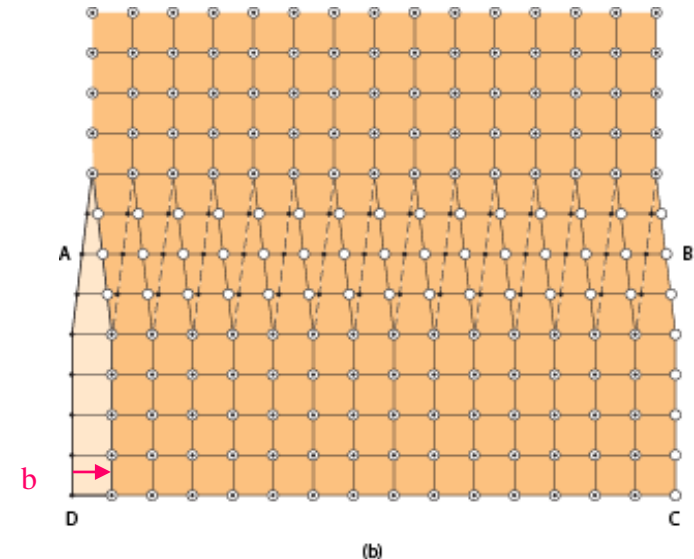
Fig. 4.3, Callister & Rethwisch 8e.

• UNIT - 1

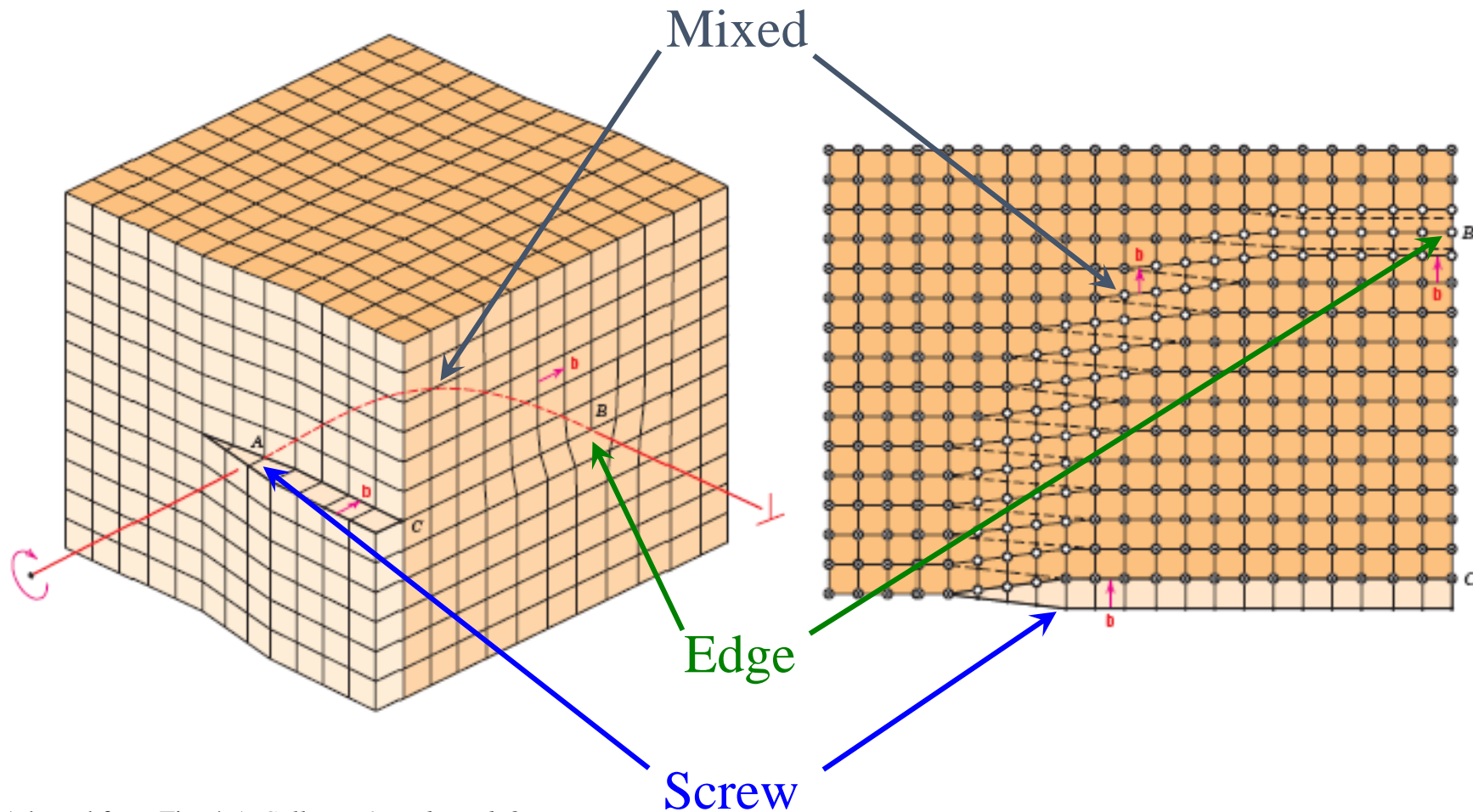
Screw Dislocation



- In this dislocation, the atoms are displaced in two separate planes perpendicular to each other.
- It forms a spiral ramp around the dislocation.
- The Burgers Vector is parallel to the screw dislocation line.
- Speed of movement of a screw dislocation is lesser compared to edge dislocation. Normally, the real dislocations in the crystals are the mixtures of edge and screw dislocation.



Edge, Screw, and Mixed Dislocations



Adapted from Fig. 4.5, *Callister & Rethwisch 8e*.

UNIT - 1

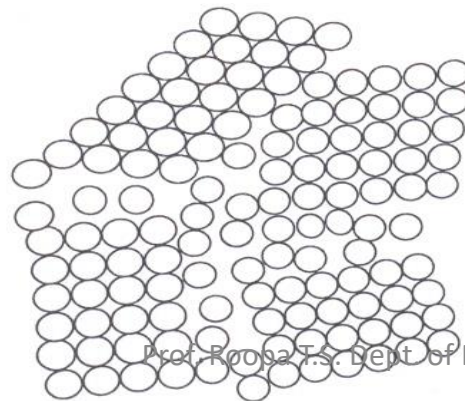
SURFACE IMPERFECTIONS

- **Internal surface imperfections** : are the imperfections which occurred inside a crystal.
- It is caused by the defects such as, grain boundaries, tilt boundaries, twin boundaries and stacking faults.
- **External surface imperfections** : They are the imperfections represented by a boundary. At the boundary the atomic bonds are terminated.
- The atoms on the surface cannot be compared with the atoms within the crystal. The reason is that the surface atoms have neighbours on one side only. Whereas the atoms inside the crystal have neighbours on either sides. This is shown in figure 4.38. Since these surface atoms are not surrounded by others, they possess higher energy than that of internal atoms.
- For most metals, the energy of the surface atoms is of the order of 1J/m^2 .

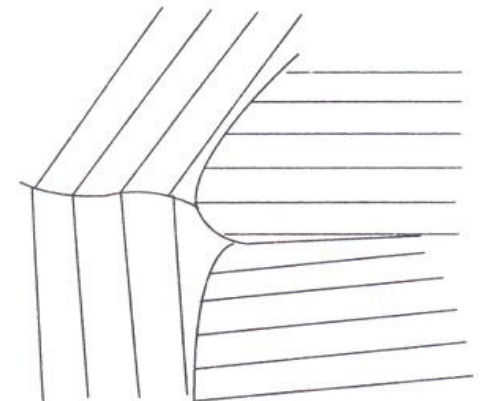
UNIT - 1

Grain Boundaries

- They are the imperfections which separate crystals or grains of different orientation in a poly crystalline solid during nucleation or crystallization.
- It is a two dimensional imperfection. During crystallization, new crystals form in different parts and they are randomly oriented with respect to one another.
- They grow and impinge on each other.
- The atoms held in between are attracted by crystals on either side and depending on the forces, the atoms occupy equilibrium positions.



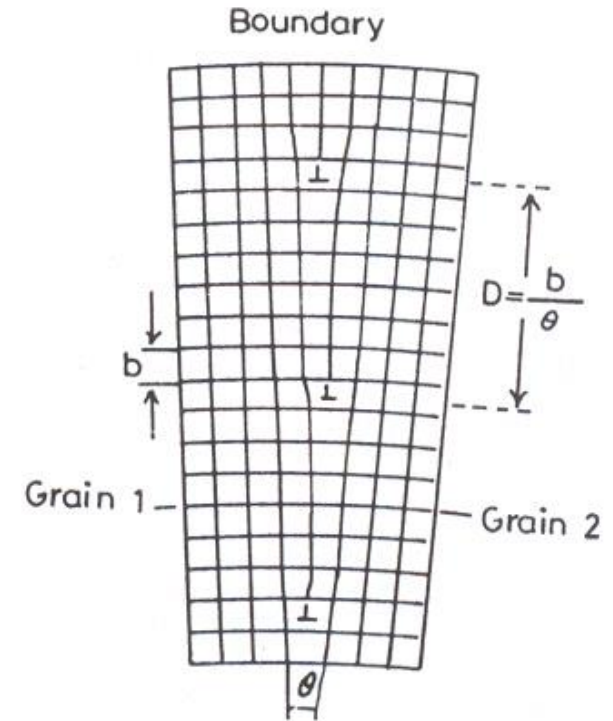
- These positions at the boundary region between two crystals are distorted. As a result, a region of transition exists in which the atomic packing is imperfect.
- The thickness of this region is 2 to 10 or more atomic diameters.
- The boundary region is called a **crystal boundary** or a **grain boundary**.
- The boundary between two crystals which have different crystalline arrangements or different compositions, is called as interphase boundary or commonly an interface.



UNIT - 1

Tilt Boundaries

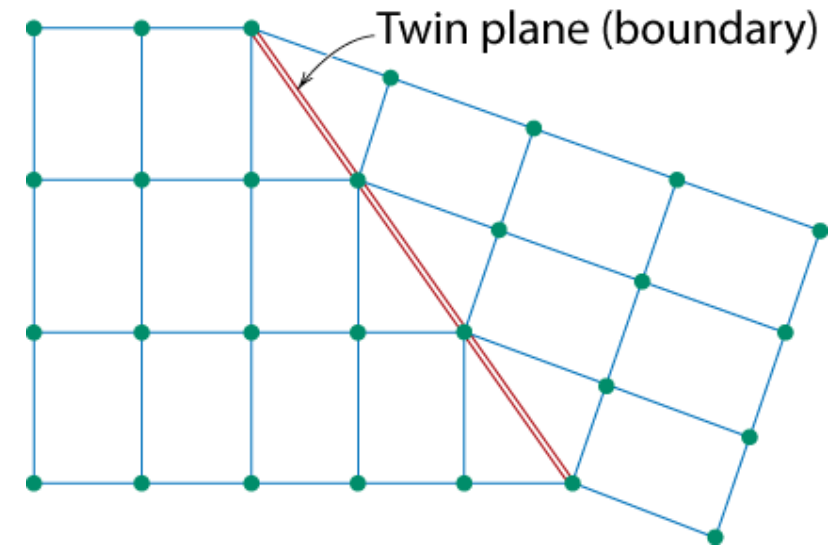
- This is called low-angle boundary as the orientation difference between two neighboring crystals is less than 10° .
- The disruption in the boundary is not so severe as in the high-angle boundary. In general low-angle boundaries can be described by suitable arrays of dislocation.
- Actually a low-angle ***tilt boundary*** is composed of edge dislocation lying one above the other
- The angle or tilt will be
- where b = Burgers vector and
- D = the average vertical distance between dislocations.



UNIT - 1

Twin Boundaries

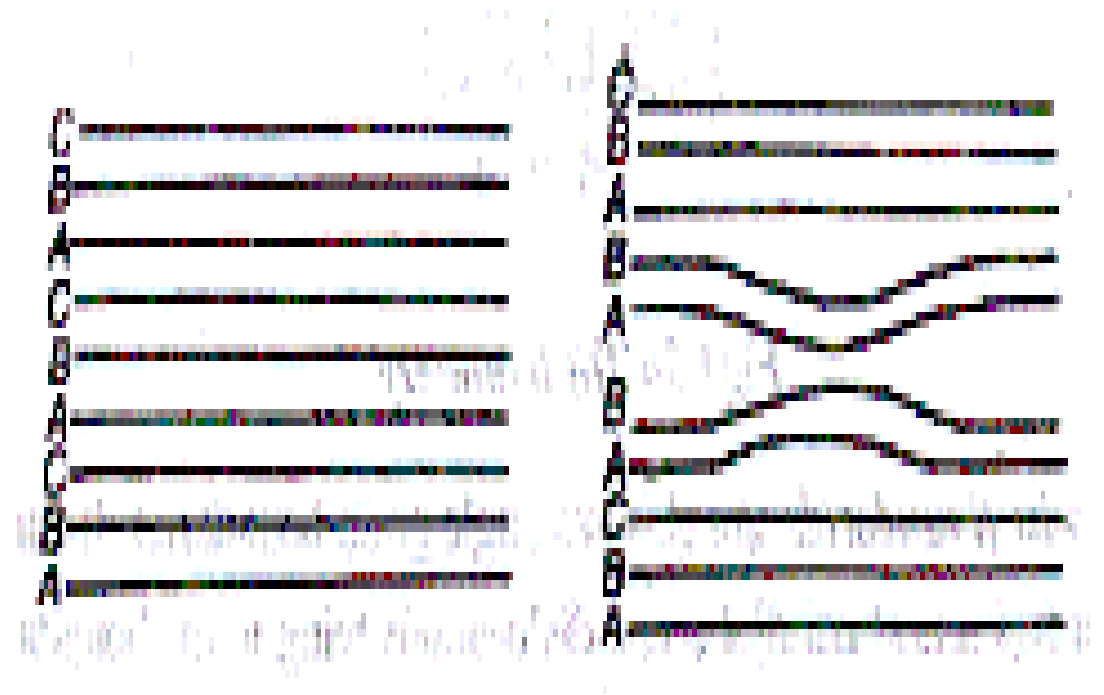
- If the atomic arrangement on one side of a boundary is a mirror reflection of the arrangement on the other side, then it is called as *twin boundary*.
- As they occur in pair, they are called twin boundaries. At one boundary, orientation of atomic arrangement changes.
- At another boundary, it is restored back. The region between the pair of boundaries is called the twinned region.
- These boundaries are easily identified under an optical microscope.



UNIT - 1

Stacking Faults

- Whenever the stacking of atomic planes is not in a proper sequence throughout the crystal, the fault caused is known as *stacking fault*.
- For example, the stacking sequence in an ideal FCC crystal may be described as A-B-C-A-B-C- A-B-C- But the stacking fault may change the sequence to A-B-C-A-B-A-B-A-B-C. The region in which the stacking fault occurs (A-B-A-B) forms a thin region and it becomes HCP.
- This thin region is a surface imperfection and is called a stacking fault.



UNIT - 1

Volume imperfections

- Volume defects such as cracks may arise in crystals when there is only small electrostatic dissimilarity between the stacking sequences of close packed planes in metals. Presence of a large vacancy or void space, when cluster of atoms are missed is also considered as a volume imperfection.
- Foreign particle inclusions and non crystalline regions which have the dimensions of the order of 0.20 nm are also called as volume imperfections.
- 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.

UNIT – 1 Grain Size- ASTM Grain size number

The grain size is often determined when the properties of a polycrystalline material are under consideration.

- Affects the **mechanical properties** of the material
- The smaller the grain size, more are the grain boundaries.
- More grain boundaries means higher resistance to **slip** (plastic deformation occurs due to slip).
- More grains means more **uniform** the mechanical properties are.

In this regard, there exist a number of techniques by which size is specified in terms of average grain volume, diameter, or area.

Comparison Method – Metal Specimen is prepared etched, photomicrographed at 100X and compared with a series of graded standard grain size ASTM charts

Intercept method - Straight lines all the same length are drawn through several photomicrographs that show the grain structure. The grains intersected by each line segment are counted; the line length is then divided by an average of the number of grains intersected, taken over all the line segments. The average grain diameter is found by dividing this result by the linear magnification of the photomicrographs.

$$G = -6.644 (\log l) - 3.288$$

Where l mean lineal intercept length, $l = 1/P^L = 1/N^L$

UNIT – 1 Grain Size- ASTM Grain size number

[number of grain-boundary intersections, P , or the number of grains intercepted, N , is counted. Dividing P or N by the true line length, L , gives P^L or N^L , which are identical (N or P can differ slightly due to tangent hits) for a single-phase grain structure.]

Planimetric method - A circle of known size (generally 5000 mm² area) is drawn on a photomicrograph. The number of grains completely within the circle, n^1 , and the number of grains intersecting the circle, n^2 , are counted.

The number of grains per square millimeter at $1\times$, N^A , is determined:

$$N^A = f(n^1 + n^2/2)$$

where f is the magnification squared divided by the circle area.

The ASTM grain size, G , can be found by using the tables in ASTM E 112 or by the following equation:

$$G = 3.322(\log N^A) - 2.95$$

UNIT – 1 Grain Size- ASTM Grain size number

ASTM has prepared several standard comparison charts, all having different average grain sizes. To each is assigned a number ranging from 1 to 10, which is termed the *grain size number*.

A specimen must be properly prepared to reveal the grain structure, which is photographed at a magnification of $100\times$. Grain size is expressed as the grain size number of the chart that most nearly matches the grains in the micrograph. Thus, a relatively simple and convenient visual determination of grain size number is possible.

Let n represent the grain size number, and N the average number of grains per square inch at a magnification of $100\times$. These two parameters are related to each other through the expression:

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

- (a) Determine the ASTM grain size number of a metal specimen if 45 grains per square inch are measured at a magnification of $100\times$.
- (b) For this same specimen, how many grains per square inch will there be at a magnification of $85\times$?

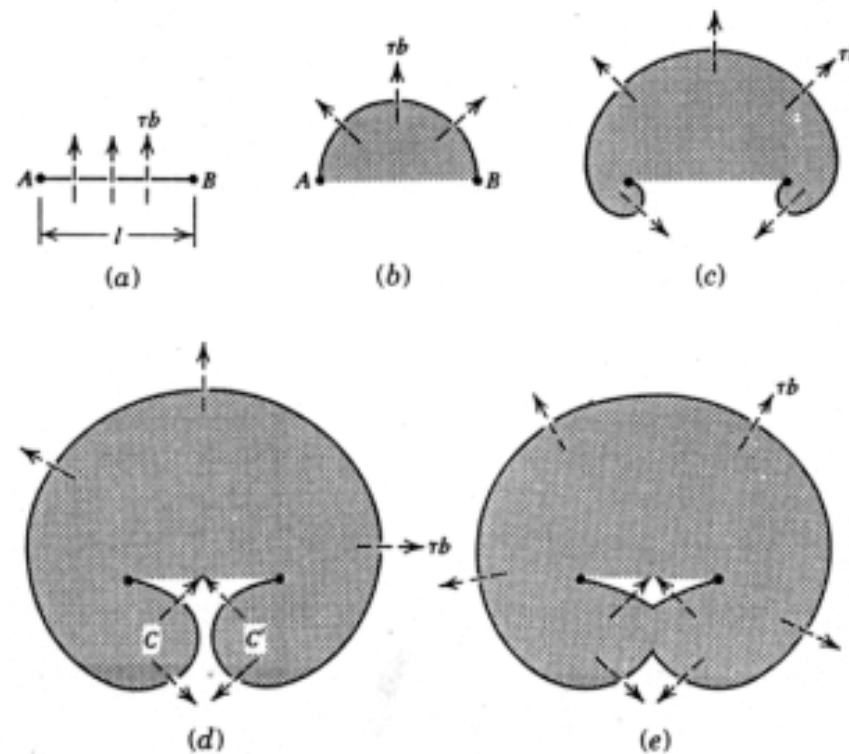
UNIT – 1

- Let $M = 200$
- $A = 2 \times 3 = 6 \text{ inch}^2$
- $n_m = 200 \text{ grain} / 6 \text{ inch}^2 = 33.3 \text{ grain} / \text{inch}^2$
- $n_{100} = n_m * [M / 100]^2$
- $= 33.3 * [200 / 100]^2$
- $n_{100} = 133.2 \text{ grain} / \text{inch}^2$
- $N = [\ln (n) / \ln (2)] + 1$
- $= [\ln (133.2) / \ln (2)] + 1$
- $= 8.06 \text{ grain} / \text{inch}^2$

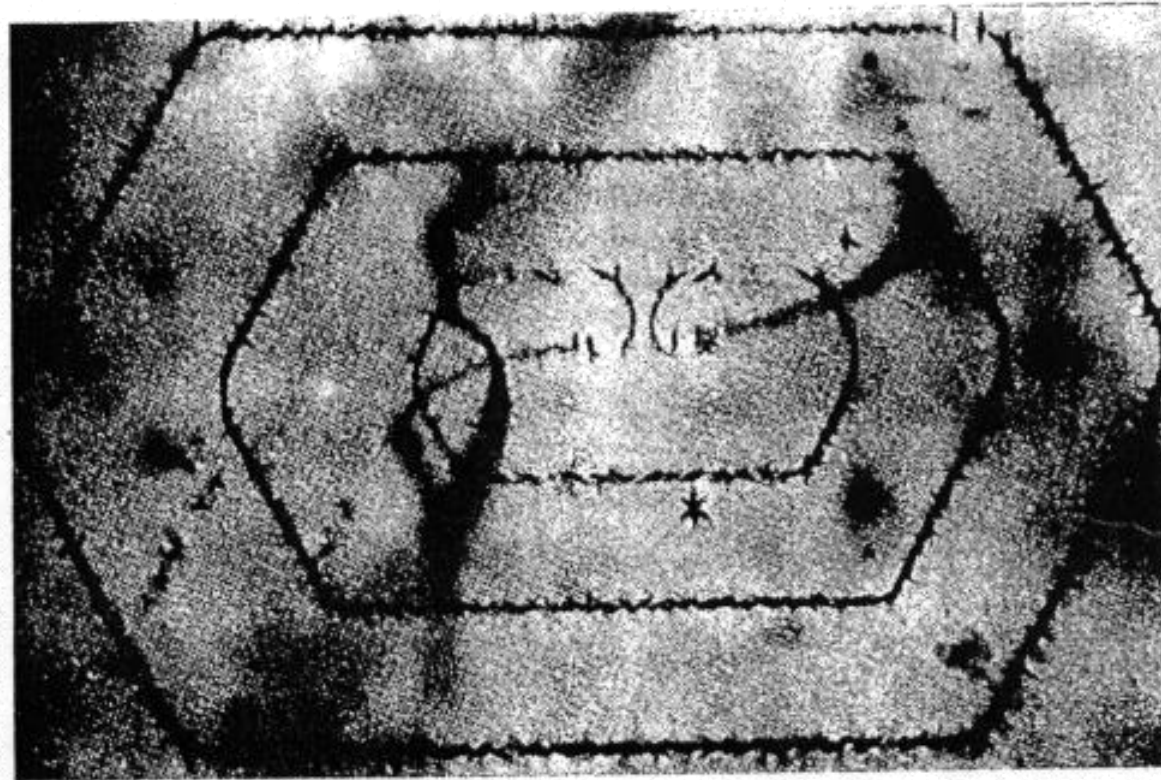
UNIT – 1

Dislocation multiplication

- Some dislocations form during the process of crystallization.
- More dislocations are created during plastic deformation.
- Frank-Read Sources: a dislocation breeding mechanism.



Frank-Read sources in Si



Dash, Dislocation and Mechanical Properties of Crystals, Wiley (1957).

Prof. Koopa, IS, Dep. of Mechanical Engineering

Thank You