MODULE 1

Crystallography:- Crystal, space lattice, unit cell- BCC, FCC, HCP structures - short and long range order - effects of crystalline and amorphous structure on mechanical properties. Coordination number and radius ratio; theoretical density; simple problems - Polymorphism and allotropy.

Miller Indices: - crystal plane and direction (brief review) - Attributes of miller indices for slip system, brittleness of BCC, HCP and ductility of FCC - Modes of plastic deformation: - Slip and twinning.

Schmid's law, equation, critical resolved shear stress, correlation of slip system with plastic deformation in metals and applications.

Crystallography

A **crystal** or **crystalline solid** is a solid material whose constituents, such as atoms, molecules or ions, are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions.

A lattice is a regular repeated three-dimensional arrangement of atoms, ions, or molecules in a metal or other crystalline solid.
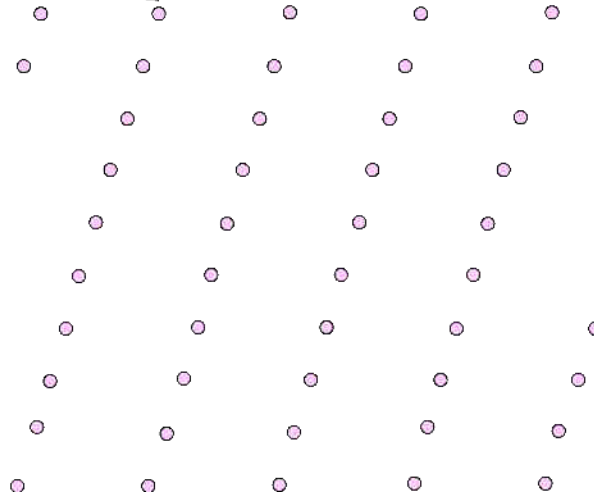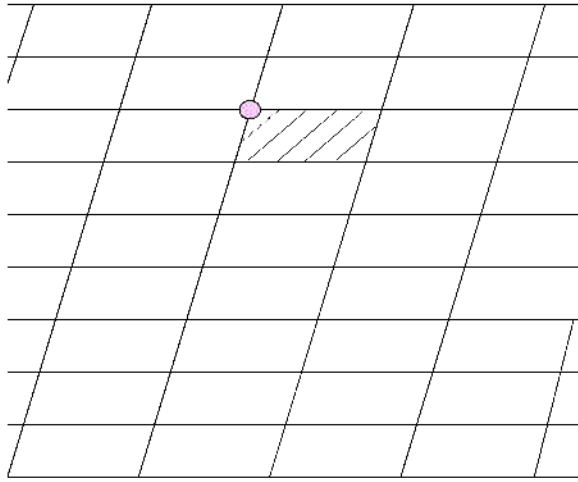
Repetition = Symmetry

Types of repetition can be

Rotation or Translation

Lattice

Each block is represented by a point

If the atoms are considered as points in space, then the array of infinite, perfectly periodic array of points in a space is a **LATTICE**

Unit cell

- The **smallest group of atoms** or **the smallest unit of lattice** which has the overall symmetry of a crystal, and from which the entire lattice can be built up by repetition in three dimensions.

- In other words a three-dimensional crystal can be described by specifying the size, shape, and contents of the simplest repeating unit and the way these repeating units stack to form the crystal.

In a lattice there can be a number of unit cells. These unit cells fall into seven categories, which differ in the three unit-cell edge lengths (a, b, and c) and three internal angles
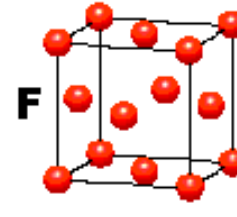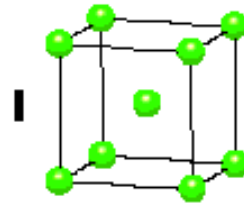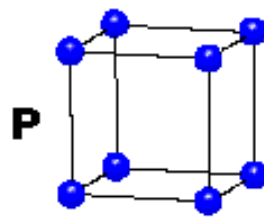
All unit cells may be described via these vectors and angles.
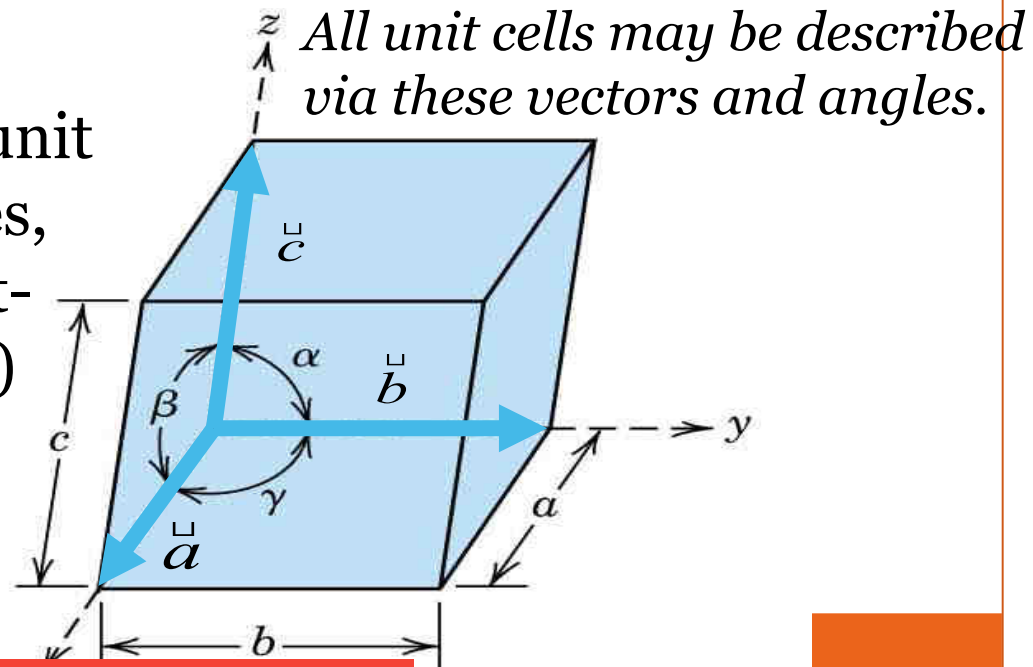
Unit cell (Bravais Lattices)

CUBIC
$a = b = c$
$\alpha = \beta = \gamma = 90°$

P **I** **F**

TETRAGONAL
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

P **I**
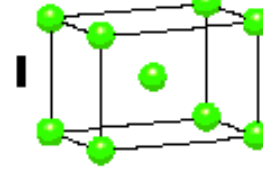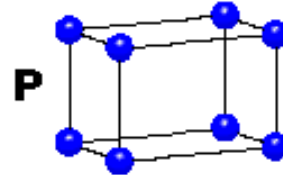
ORTHORHOMBIC
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$

P **I** **F** **C**
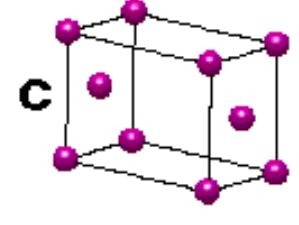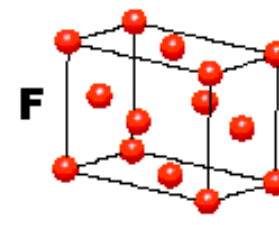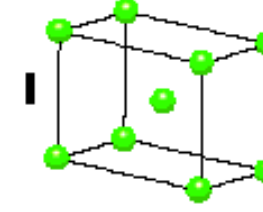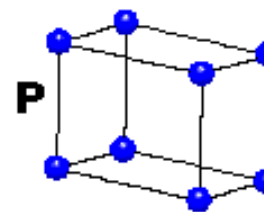
HEXAGONAL
$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$

P

TRIGONAL
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$

P
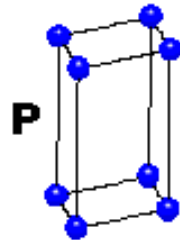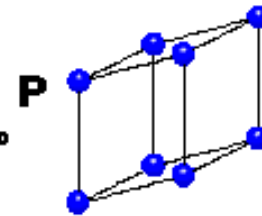
MONOCLINIC
$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$

P **C**

TRICLINIC
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

P
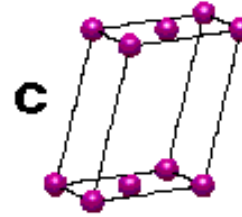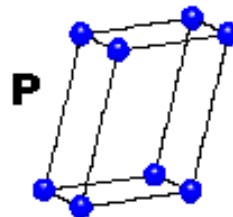
4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ **14 Bravais Lattices**

Coordination Number

- In general, **Coordination number** is the number of atoms or ions immediately surrounding a central atom in a crystal structure.

- The crystal structure can be either a metallic or ionic complex crystal

Atomic Packing Factor

- **Atomic packing factor** (APF), **packing efficiency** or **packing fraction** is the fraction of volume in a crystal structure that is occupied by constituent atoms.
- It is dimensionless and always less than unity.
- In atomic systems, by convention, the APF is determined by assuming that atoms are rigid spheres.
- The radius of the spheres is taken to be the maximal value such that the atoms do not overlap.

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

Simple Cubic Unit Cell

A simple cubic unit cell has one sphere/atom at each corner of the cube.
Rare due to poor packing (only Polonium has this structure)
Close-packed directions are cube edges.
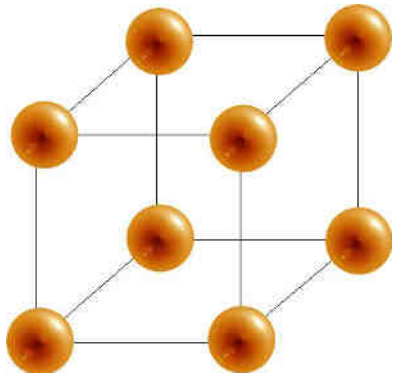
$\frac{1}{8}$ atom at each corner
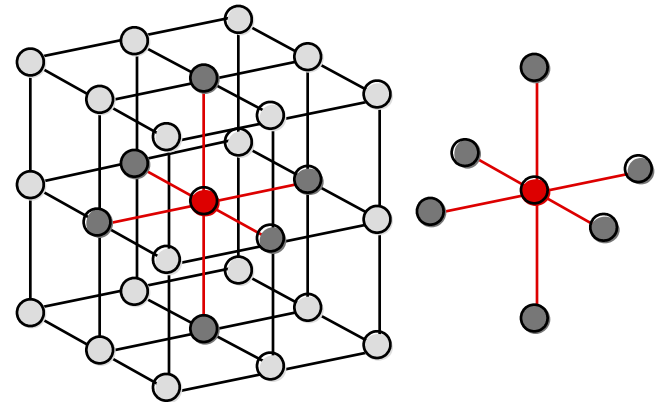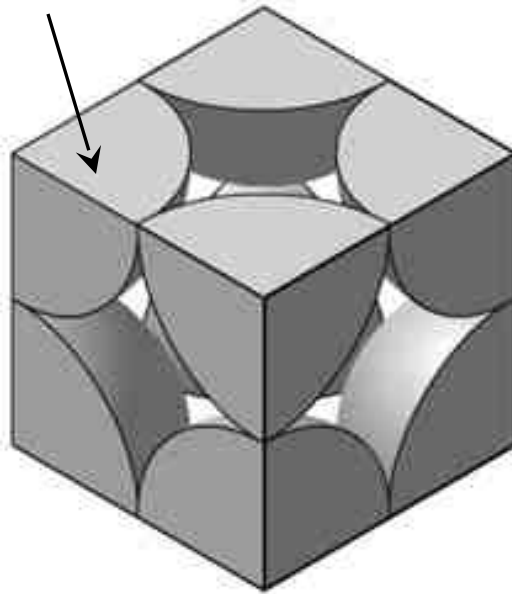
Coordination # = 6
(# nearest neighbors)

Atomic packing factor

APF for a simple cubic structure = 0.52

a

R=0.5a
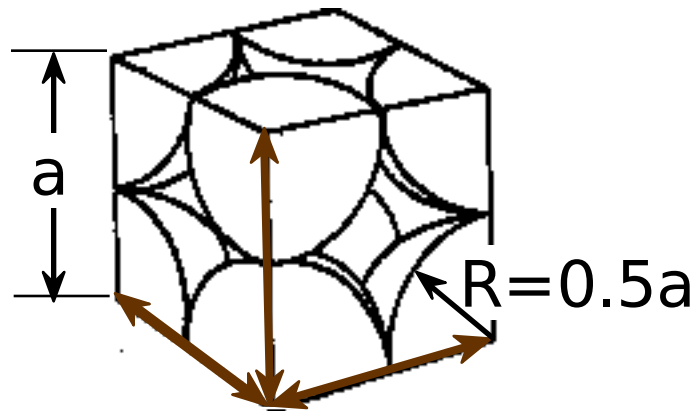
close-packed directions

contains 8 x 1/8 =
1 atom/unit cell

$$APF = \frac{1 \quad \frac{4}{3}\pi(0.5a)^3}{a^3}$$

atoms / unit cell

volume / atom

volume / unit cell

Face Centered Cubic Structure (FCC)

In this type of cubic cells, the lattice points are at the center of each face, as well as at each corner,
Close packed directions are face diagonals.

$\frac{1}{2}$ atom

at face center

Coordination number = 12

-Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

$\frac{1}{8}$ atom at each corner
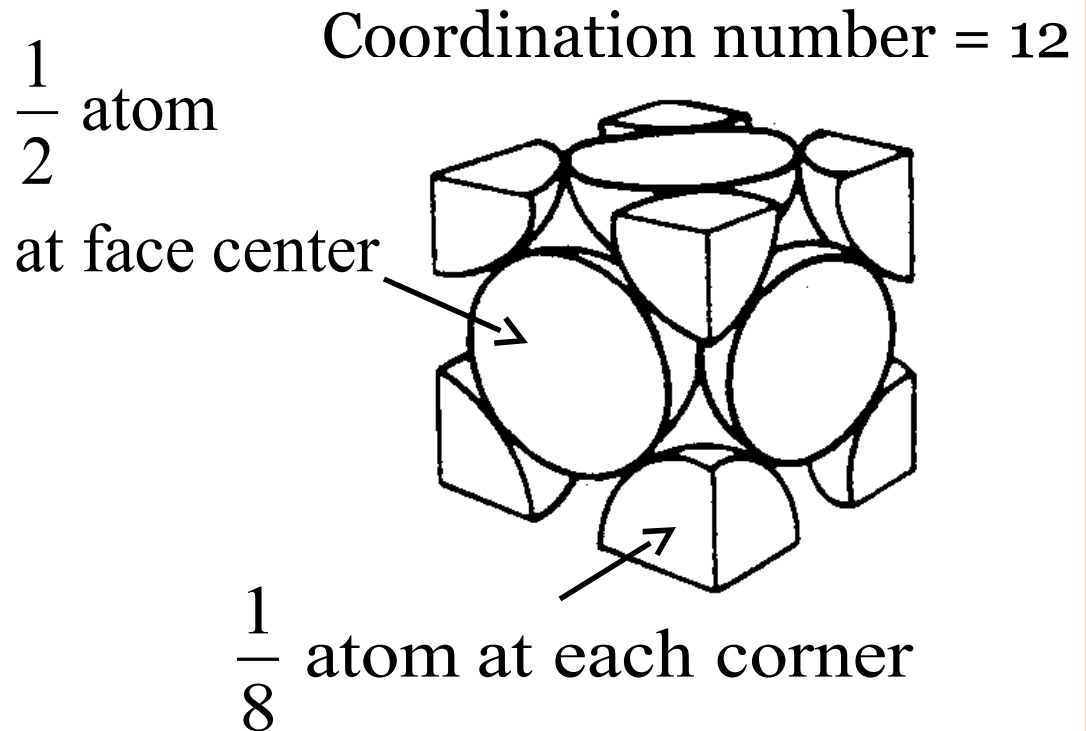
Atomic Packing Factor (APF): FCC

APF for a body-centered cubic structure = 0.74
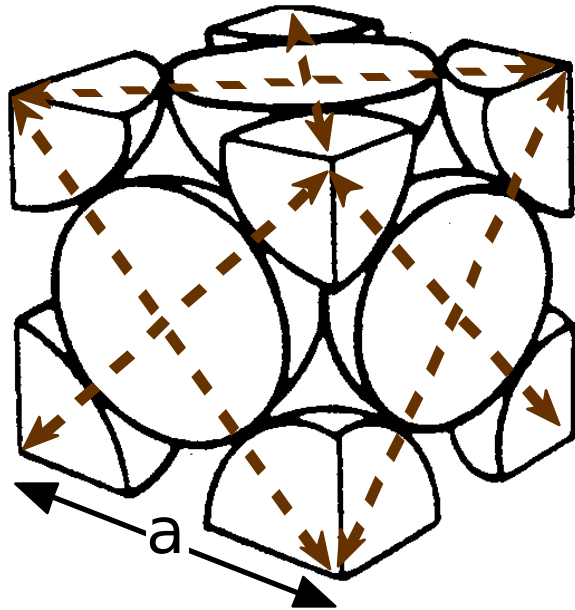
Close-packed directions:
length = 4R
= $\sqrt{2}$ a

Unit cell contains:
6 x 1/2 + 8 x 1/8
=4 atoms/unit cell

$$\text{APF} = \frac{\overset{\displaystyle\frac{\text{atoms}}{\text{unit cell}}}{4}\ \frac{4}{3}\,\pi\,(\sqrt{2}a/4)^3 \ \overset{\displaystyle\frac{\text{volume}}{\text{atom}}}{}}{\underset{\displaystyle\frac{\text{volume}}{\text{unit cell}}}{a^3}}$$

Body Centered Cubic Structure (BCC)

In this unit cells, the lattice points/atoms are at the center of the unit cell, as well as at each corner

Close packed directions are cube diagonals.

Coordination number = 8

1 atom
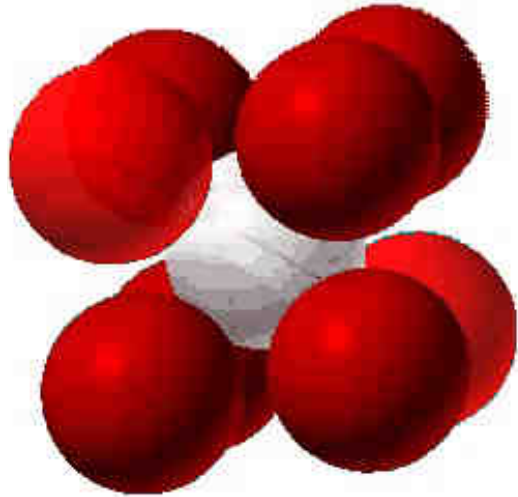
at body center

Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.
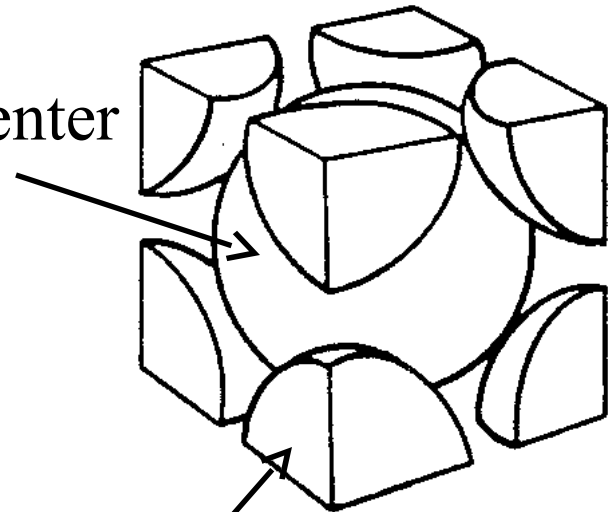
$\dfrac{1}{8}$ atom at each corner

Atomic Packing Factor (APF): BCC

APF for a body-centered cubic structure = 0.68
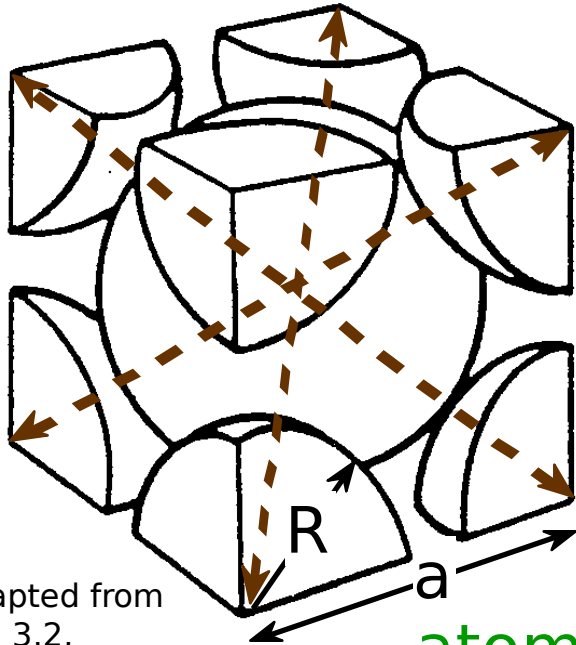
Adapted from Fig. 3.2, *Callister 6e.*

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

Unit cell contains:
1 + 8 x 1/8
= 2 atoms/unit cell

$$APF = \dfrac{2 \cdot \dfrac{4}{3}\pi\,(\sqrt{3}a/4)^3}{a^3}$$

atoms / unit cell

volume / atom

volume / unit cell

Three-Dimensional Cubic Lattices

Simple cubic

a a a

1/8 x 8 =1 particle

coordination number =6

Simple cubic

Body-centered cubic

a b a b

(1/8 x 8) + 1 = 2 particles

coordination number =8

Body-centered cubic

Face-centered cubic
cubic closest pack

a b c a b c

(1/8 x 8)+(1/2x 6) = 4 particles

coordination number =
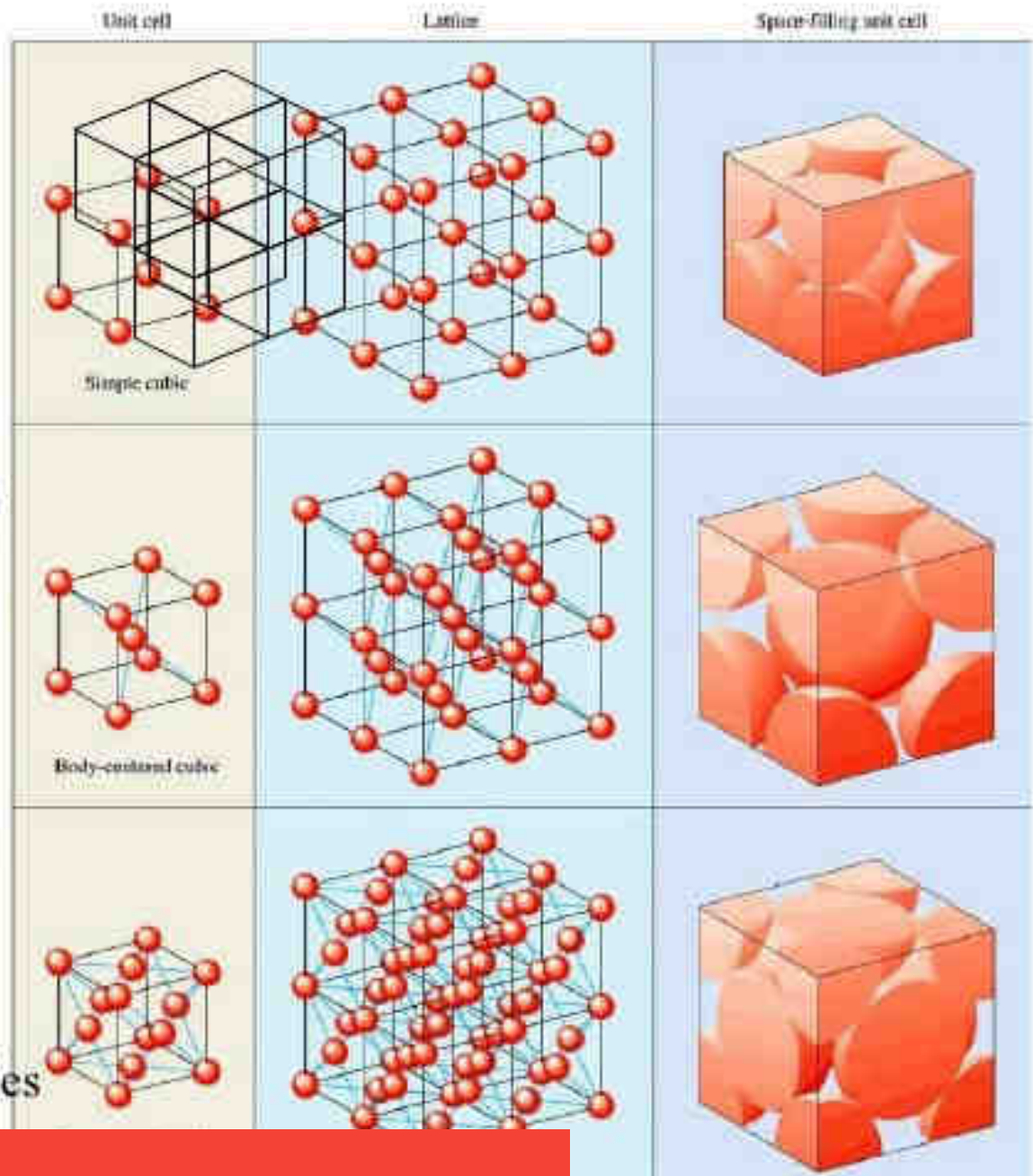
Close Packing

- **Close-packing of atoms** means the dense arrangement of atoms in an infinite, regular arrangement or lattice.

- The most efficient way to fill space with spheres

- It is proved that the highest packing density – that is, the greatest fraction of space occupied by spheres in a crystal structure– that can be achieved by a close packing is 0.74.

Close packed structures

- If the arrangement of spheres in the first layer is considered to be of A type, then the arrangement of spheres in the subsequent layers is also of A type. This three-dimensional arrangement is referred to as AAA type packing.

This arrangement has resulted in the formation of a simple cubic lattice
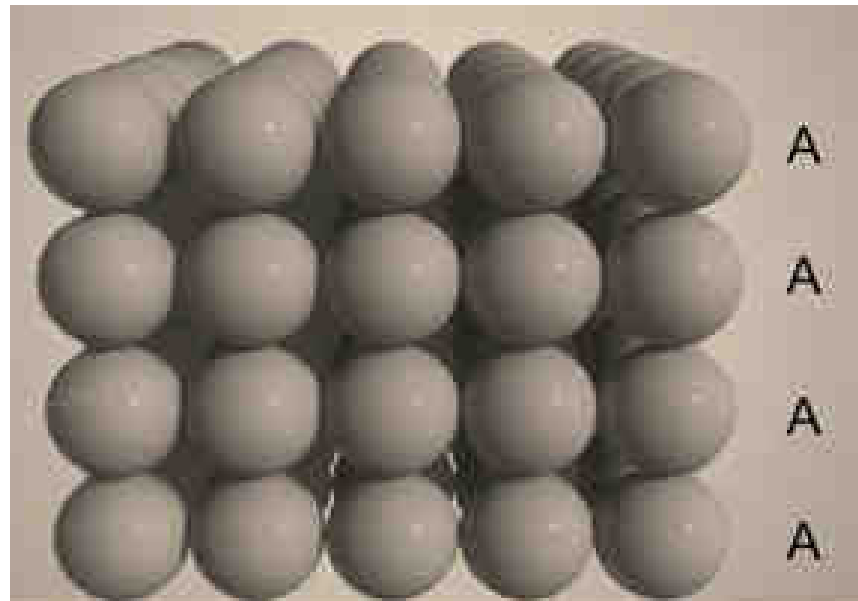
Close Packing

- As the spheres of the two layers are aligned differently, let the arrangement of spheres in the first layer be referred to as "A' type and in the second layer as 'B' type.

- The void formed when a sphere in the second layer is placed over a void in the first layer is **tetrahedral** or of "T' type. It is known as a tetrahedral void.

- Another type of void is formed when a void in the second layer lies on a void in the first layer. Such a void is called an octahedral void or an 'O' type void.

- In HCP structure a second layer of spheres is placed in the indentations left by the first layer.
- Space is trapped between the layers that is not filled by the spheres is called **voids**
- The **voids** in close packing can be called as **holes** or **interstitial sites.**

OCTAHEDRAL HOLES
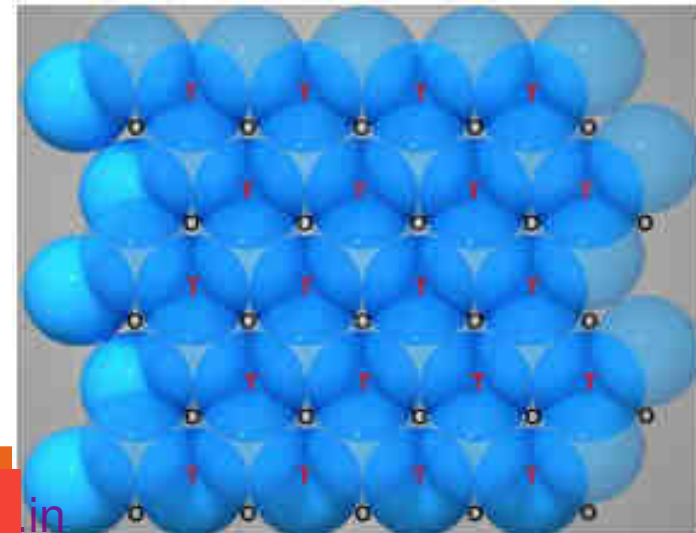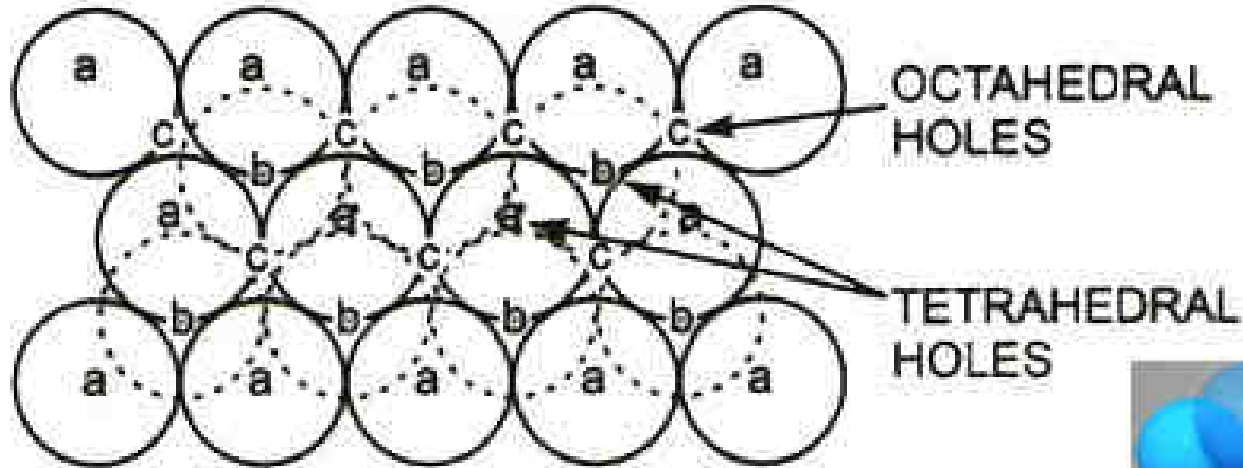
TETRAHEDRAL HOLES

Close Packing of Atoms

- The third layer can be stacked in two different ways. If the third layer is placed over the second layer in such a way that the tetrahedral voids of the second layer get covered, then a close packing is obtained. This type of an arrangement is called ABAB type packing or **hexagonal close packing.**

Close packing of atoms

- If continue to add the layers, then the arrangement of the spheres/atoms in the third layer called C layer are not aligned with those of either the first or the second layer. This type of packing is referred to as ABCABC type of packing.

- It is also called **cubic close packing** (CCP) or face-centered close packing (FCC).

- In hexagonal close packing and cubic close packing, a sphere has the coordination number 12. In hexagonal close packing and cubic close packing 74% of the space in the crystal is filled up.

- In a close packed structure, whether ccp or hcp if there are N spheres in the packing per unit cell, then The number of octahedral voids= N. The number of the tetrahedral voids =2N.

HCP and CCP
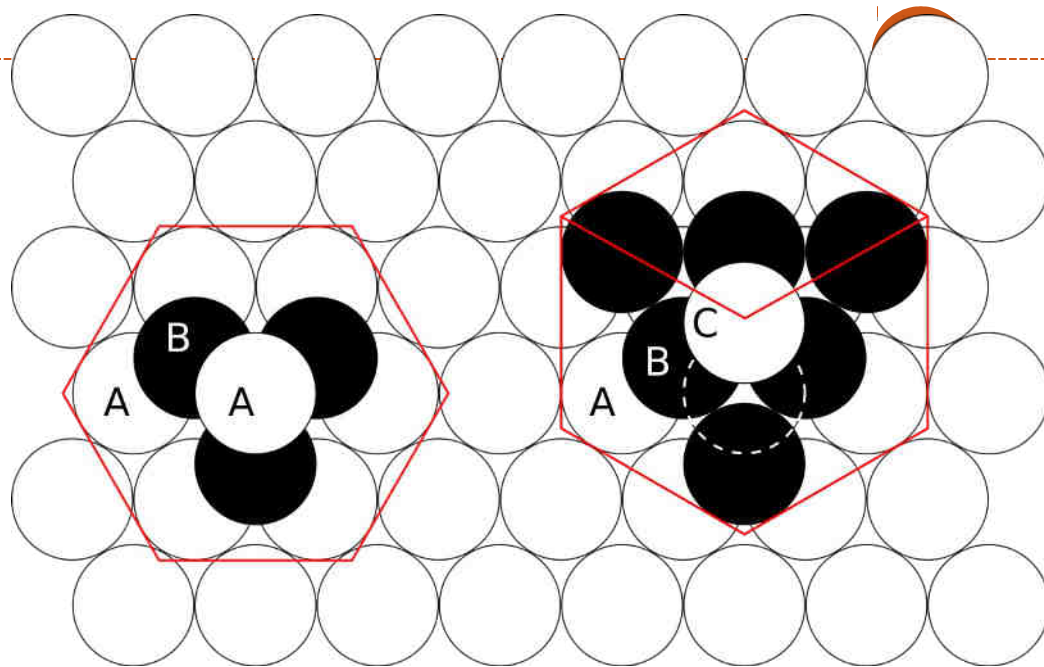
HCP

CCP/FCC
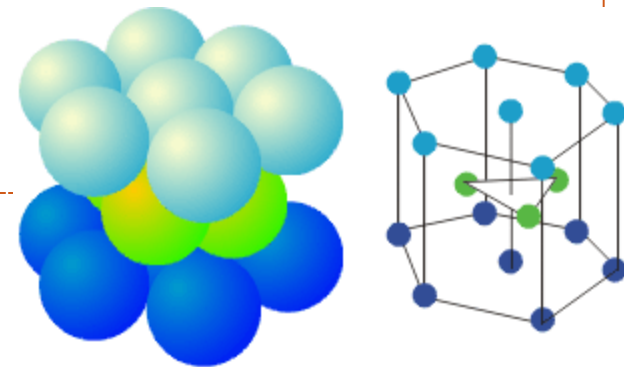
HCP
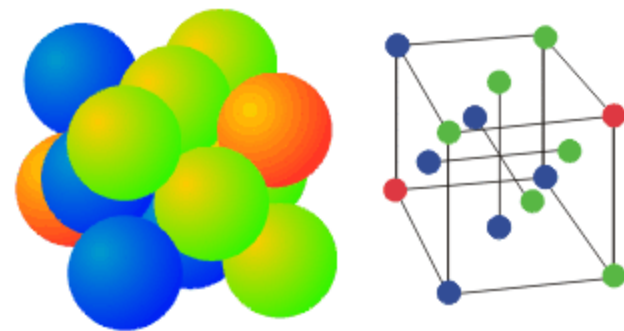
CCP/FCC
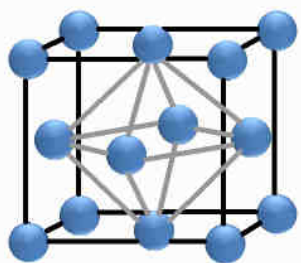
FCC
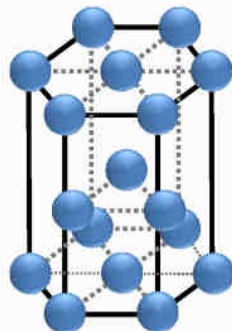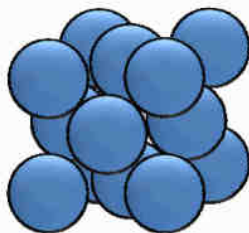
HCP
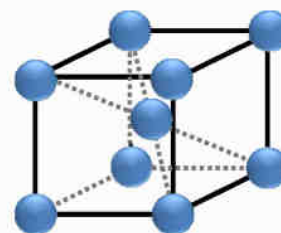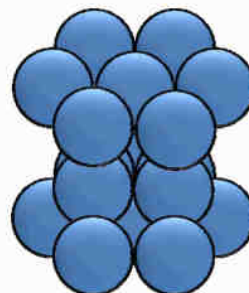
BCC
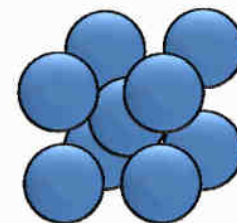
Hexagonal Close-packed Structure (HCP)

- ABAB... Stacking Sequence

3D Projection

A sites

B sites

A sites

2D Projection

Top layer

Middle layer

Bottom layer
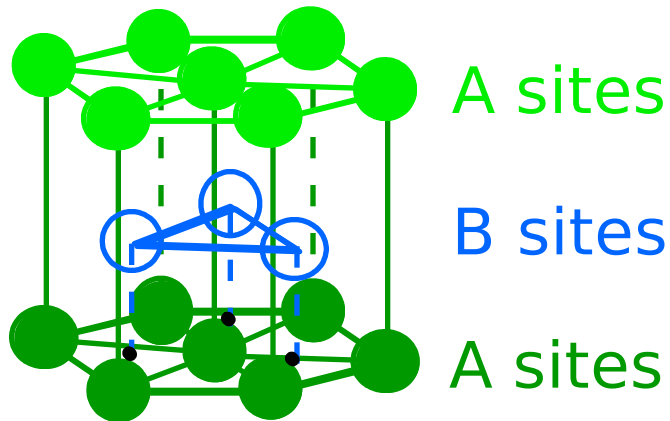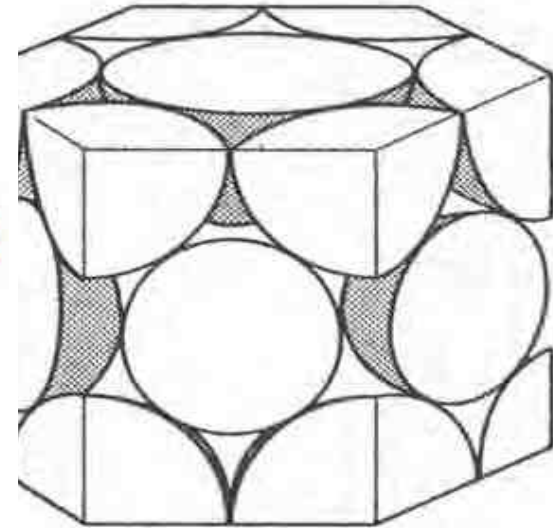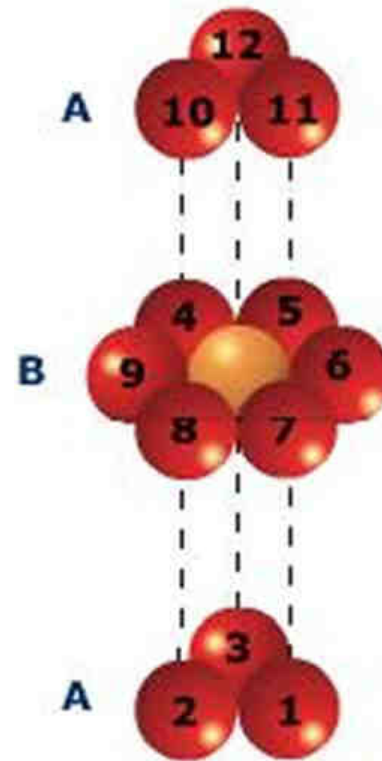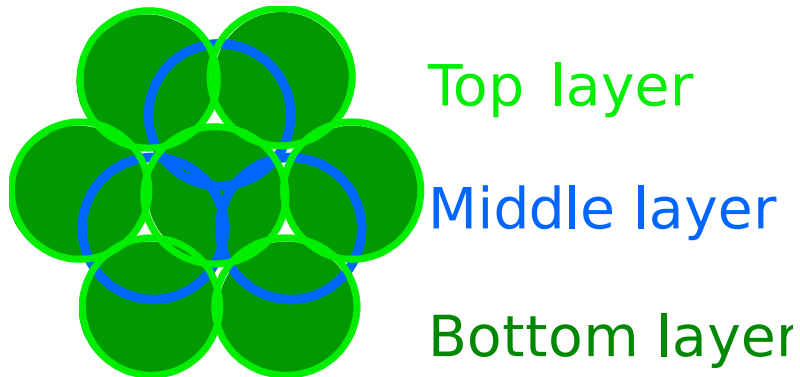
Coordination number = 12

APF for HCP

C=1.633a

Number of atoms in HCP unit cell=(12×1/6)+(2×1/2)+3=6atoms

Vol.of HCP unit cell= area of the hexagonal face X height of the hexagonal

Area of the hexagonal face=area of each triangle×6

a=2r
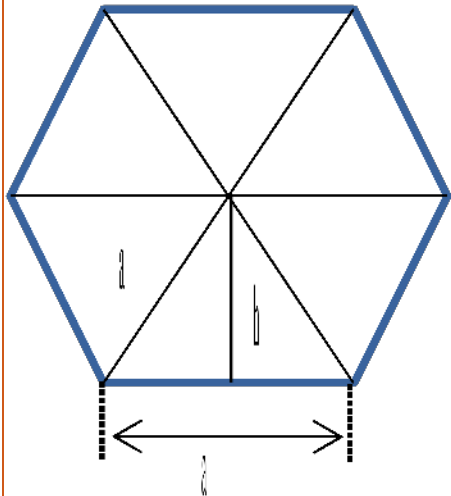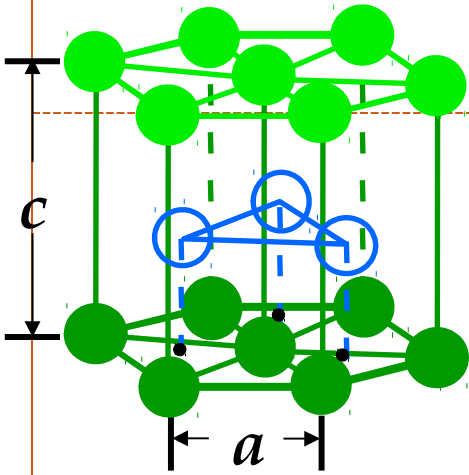
APF =0.74

To show that the ideal c/a ratio for HCP is 1.633. A sketch of one third of an HCP unit cell is shown below.
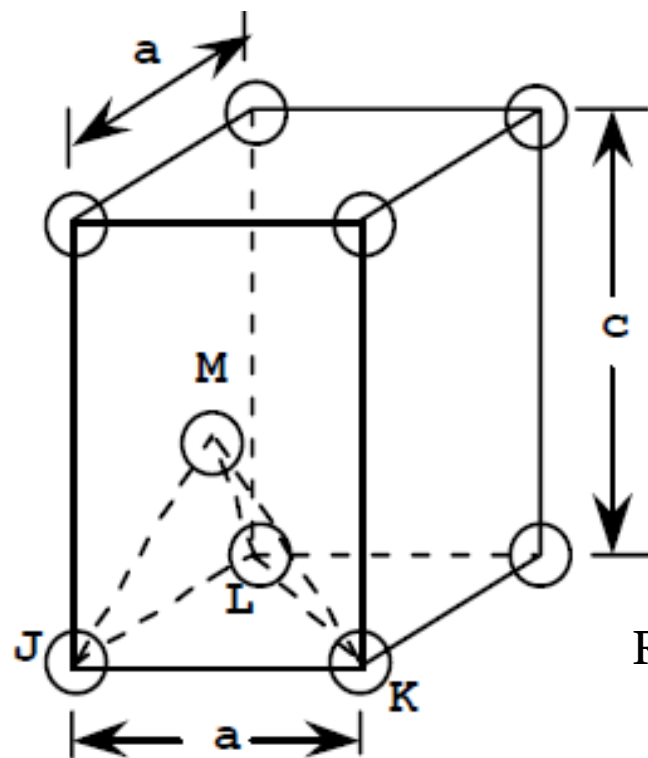
from triangle **JHM**,

$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2, \text{ or}$$

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$
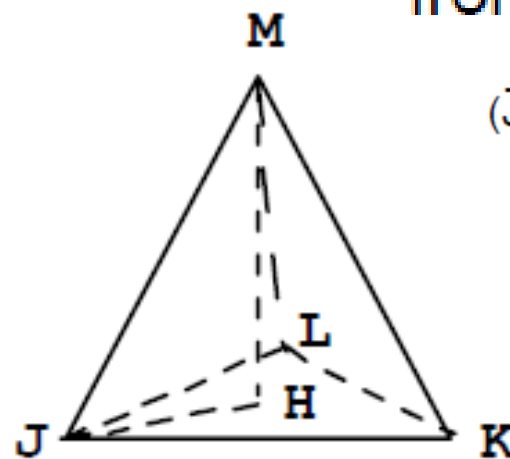
Refer Δ^{le} JHK

$\overline{MH} = c/2.$

$\overline{JM} = \overline{JK} = 2R = a$
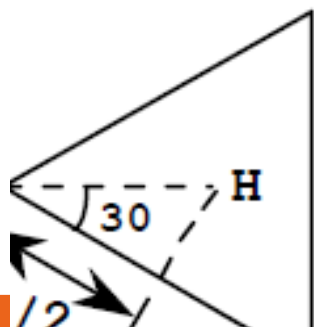
Solving for c/a
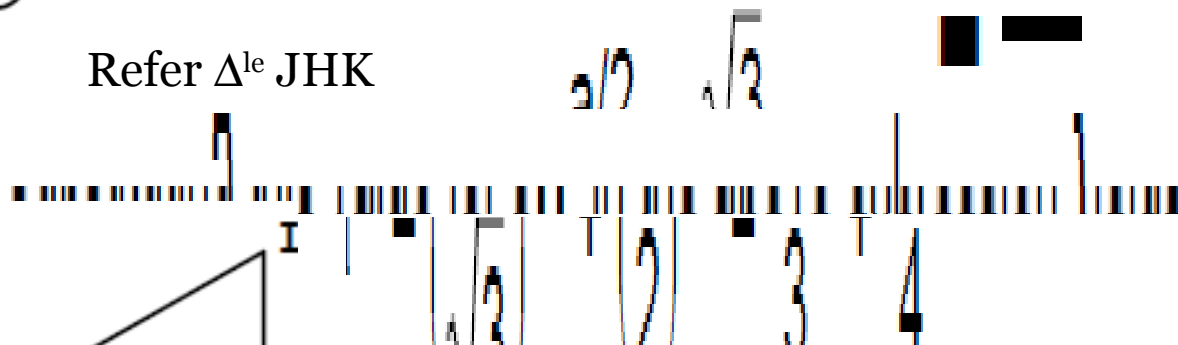
Short-Range Order versus Long-Range Order

- Short-range order - The regular and predictable arrangement of the atoms/ions over a short distance - usually one or two atom spacings.

- Long-range order (LRO) - A regular repetitive arrangement of atoms/ions in a solid which extends over a very large distance.

(a)

(b)

Ar

H — O — H

O

Si
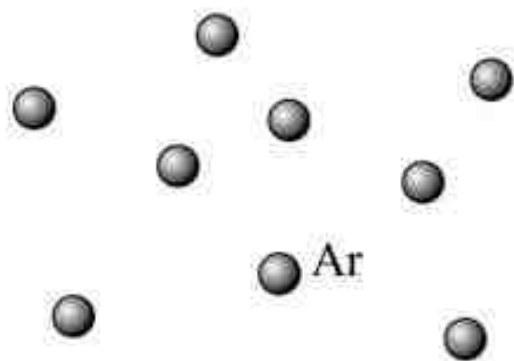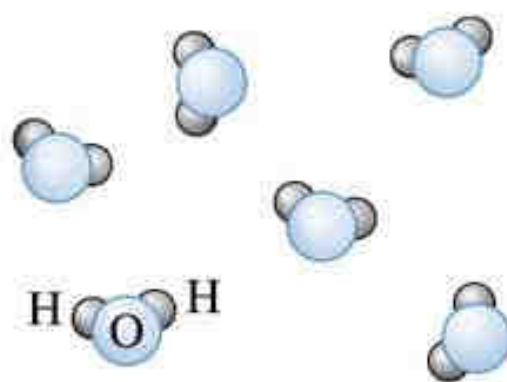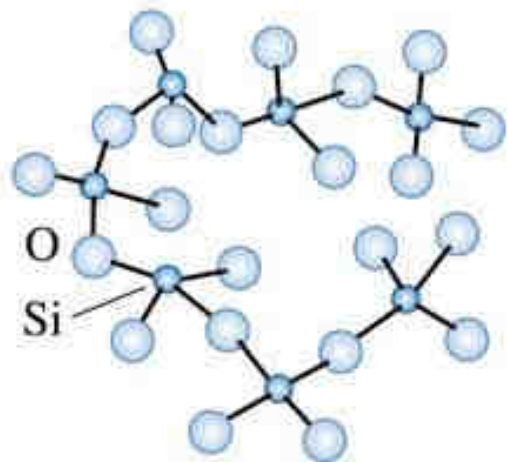
(c)
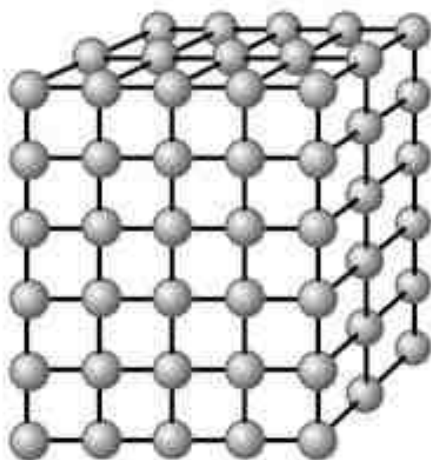
(d)

Levels of atomic arrangements in materials:

(a) Inert monoatomic gases have no regular ordering of atoms:

(b,c) Some materials, including water vapor, nitrogen gas, amorphous silicon and silicate glass have short-range order.

(d) Metals, alloys, many ceramics and some polymers have regular ordering of atoms/ions that extends through the material.

Classification of materials based on the type of atomic order.

Crystalline and Amorphous solids
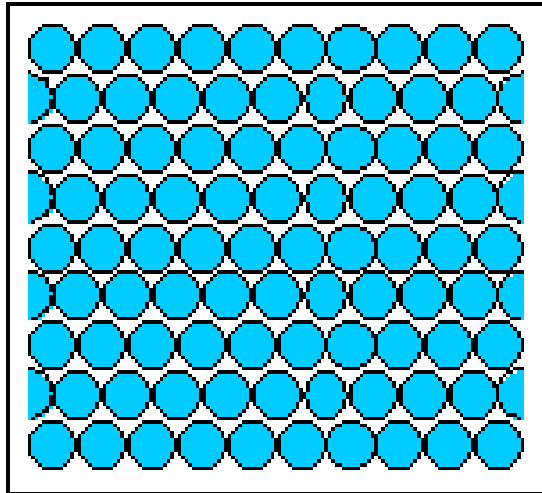
Single crystal	Polycrystal	Amorphous solid
Periodic across the whole volume.	Periodic across each grain.	Not periodic.
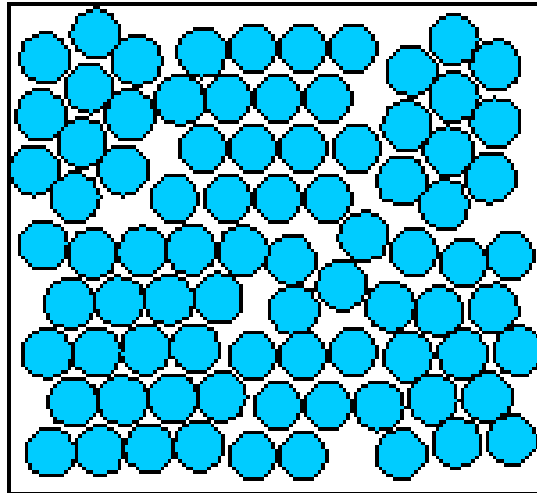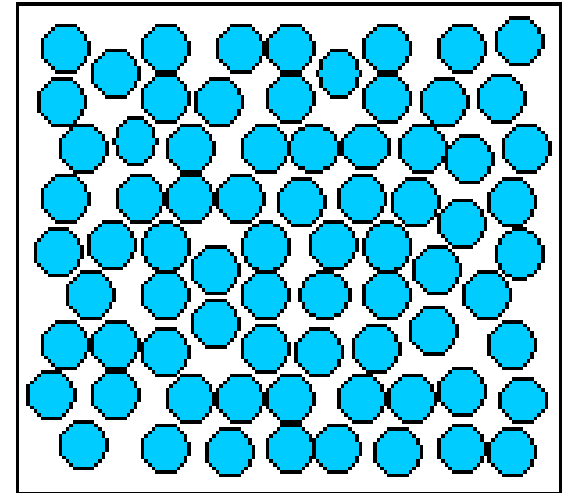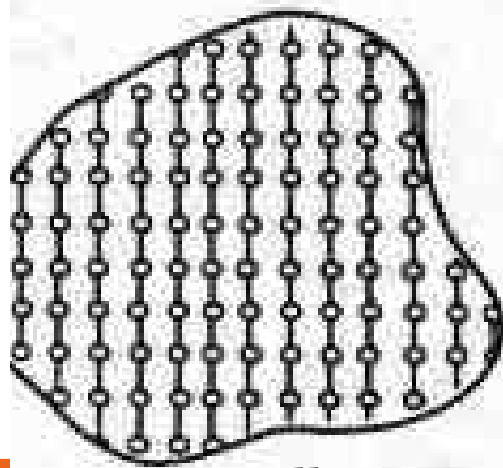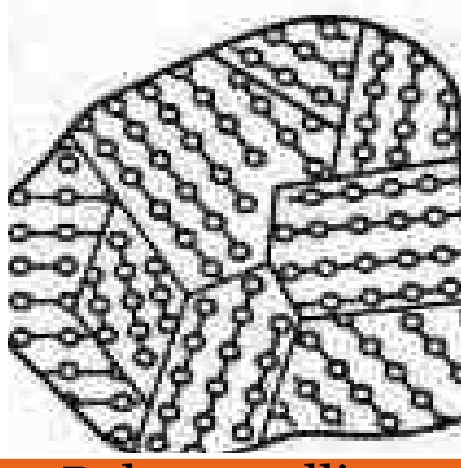
Crystalline	Polycrystalline	Amorphous
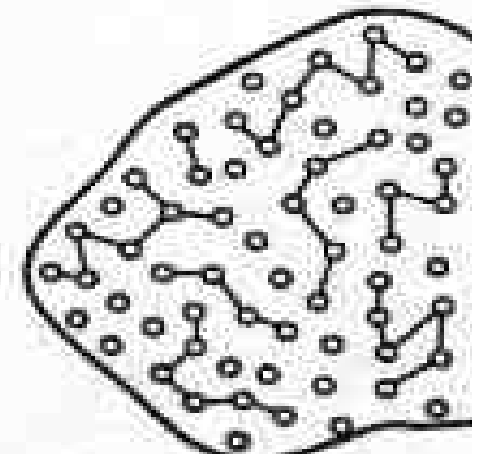
Single *vs* Polycrystals

Single Crystals

- ✓ Properties vary with direction: anisotropic.
- ✓ Example: the modulus of elasticity (E) in BCC iron:

E (diagonal) = 273 GPa

E (edge) = 125 GPa
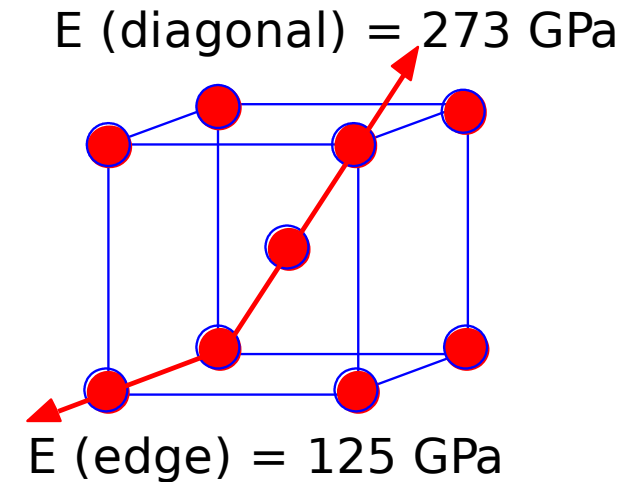
Polycrystals

- ✓ Properties may/may not vary with direction.
- ✓ If grains are randomly oriented:

  isotropic

  ($E_{polyiron}$ = 210 GPa)
- ✓ If grains are textured, anisotropic

200 μm
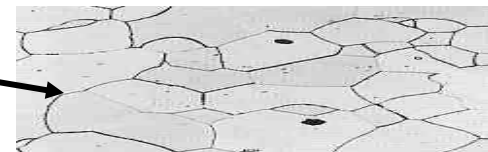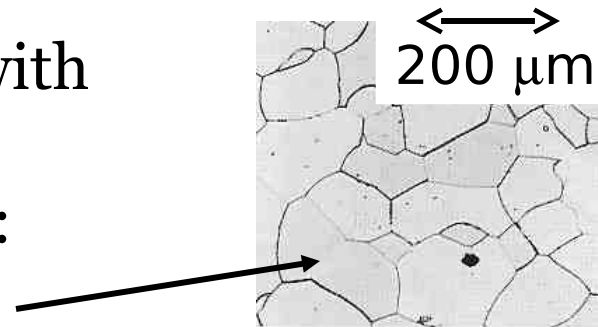
MATERIALS AND PACKING

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
  -many ceramics
  -some polymers
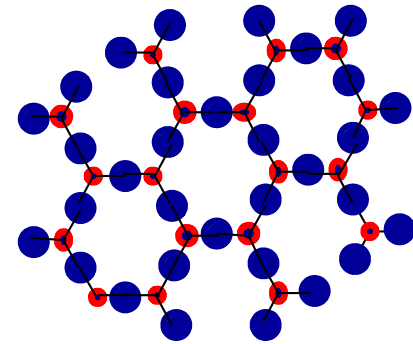
crystalline SiO_2 (Quartz)

Si • Oxygen

Noncrystalline materials...

- atoms have no periodic packing
- occurs for: -complex structures
  -rapid cooling
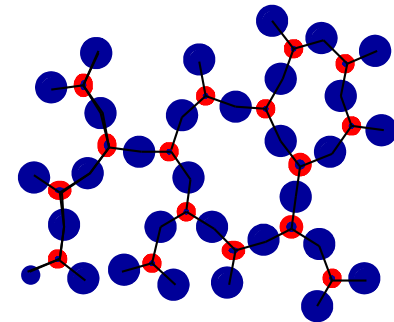
"Amorphous" = Noncrystalline

Amorphous SiO_2 (Glass)

Properties of crystalline solids

- Crystalline solids have a particular three dimensional geometrical structure.
- The arrangement order of the ions/atoms in crystalline solids is of long order.
- The strength of all the bonds between different ions, molecules and atoms is equal.
- Melting point of crystalline solids is extremely sharp. Mainly the reason is that the heating breaks the bonds at the same time.
- The physical properties like thermal conductivity, electrical conductivity, refractive index and mechanical strength of crystalline solids are different along different directions.
- These solids are the most stable solids as compared to other solids.

Properties of Amorphous solids

- The strength of different bonds is different in amorphous solids.
- There is no regularity in the external structure of amorphous solids.
- Amorphous solids don't have sharp melting point, due to the variable strength of bonds present between the molecules, ions or atoms. So, bonds having low strength on heating break at once. But the strong bonds take some time to break. This is the reason that the amorphous solids don't have sharp melting points.
- Amorphous solids are isotropic in nature. Isotropic means that in all the directions their physical properties will remain same.

Mechanical properties

○ The crystal structure is responsible for mechanical properties because of the shape/type of crystal and the boundaries between crystals.

○ Between the atoms within a material, there is an attractive force between atoms, whatever the type of bonding between atoms (metallic, covalent or ionic).

○ There is a repulsive force also due to resistance of overlapping of electron shells. The overall force is attractive at larger distances, repulsive at smaller distances, and at some point is zero (point of minimum potential energy).

○ Elastic deformations represent small disturbances in spacing from equilibrium, stretching the bonds but not breaking them, meaning when the applied force is removed the system goes back to equilibrium.

Potential Energy of Two Isolated Atoms
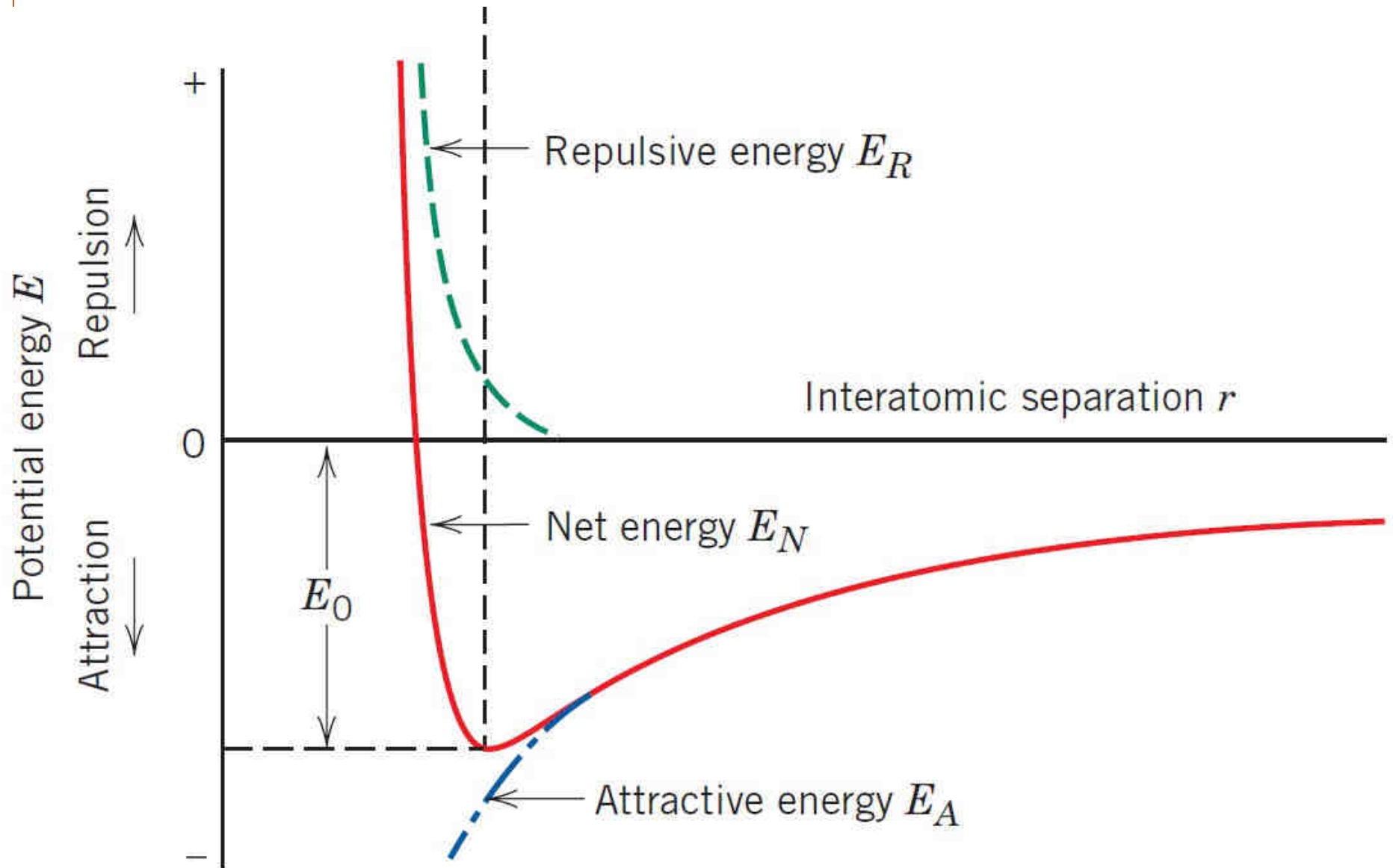
Mechanical properties

- Plastic (permanent) deformations occur when the bonds are broken, resulting in the atoms being rearranged and new bonds are formed. These can happen along all sorts of planes of failure.
- Crystal structure affects how the plastic deformation to occur.
- The orientation of the atoms relative to one another determines the planes on which they fail when loaded, how much energy the bonds can handle before breaking, the manner in which the bonds are likely to reform after a plane slips, etc.
- In crystalline materials new bonds with the neighboring atom can easily form as compared with the amorphous materials, because of the periodic arrangement of atoms in cryalline materials.
- As a result crystalline materials are stronger than amorphous materials

Theoretical Density

#atoms/unit cell

Atomic weight (g/mol)

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

Volume/unit cell
(cm^3/unit cell)

Avogadro's number
(6.023 x 10^{23} atoms/mol)

Example: Copper

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius R = 0.128 nm (1 nm = 10^{-7} cm)

$V_C = a^3$; For FCC, $a = 4R\sqrt{2}$ $V_C = 4.75 \times 10^{-23}$ cm^3

Result: theoretical ρ_{Cu} = 8.89 g/cm^3

Compare to actual: ρ_{Cu} = 8.94 g/cm^3

Theoretical Density

- Mass per atom: $m_A = \dfrac{\text{atomic weight from periodic table (g/mol)}}{6.02 \times 10^{23} \text{ (atoms/mol)}}$

- Volume per atom: $V_A = \dfrac{4}{3}\pi R_A^3$

- Number of atoms per unit cell (N)

   2 for bcc, 4 for fcc, 6 for hcp

Volume occupied by atoms in a unit cell $= NV_A$

- Volume of unit cell (V_C)

   - Depends on crystal structure

$$\text{Packing Factor} = \frac{NV_A}{V_C}$$

- Mass density: $\rho = \dfrac{Nm_A}{V_C}$

Problem on Density

1. Calculate the radius of a palladium atom, given that Pd has an FCC crystal structure, a density of 12.0 g/cm³, and an atomic weight of 106.4 g/mol.

2. Calculate the radius of a tantalum atom, given that Ta has a BCC crystal structure, a density of 16.6 g/cm³, and an atomic weight of 180.9 g/mol.

3. Titanium has an HCP crystal structure and a density of 4.51 g/cm³.

   a) What is the volume of its unit cell in cubic meters?

   b) If the ratio is 1.58, compute the values of *c and a.*

4. Niobium has an atomic radius of 0.1430 nm and a density of 8.57 g/cm³. Determine whether it has an FCC or BCC crystal structure.

Polymorphism

Existence of substance/material/compound into more than one crystalline forms is known as "POLYMORPHISM".
In other words: Under different conditions of temperature and pressure, a substance can form more than one type of crystals. This phenomenon is called Polymorphism and different crystalline forms are known as 'POLYMORPHICS'
 Example:
1) Mercuric iodide (HgI_2) forms two types of crystals.

    a. Orthorhombic
    b. Trigonal

2) $SiO2$
    a. Quartz
    b. Glass

- Silicon atom
- Oxygen atom

Quartz

Glass
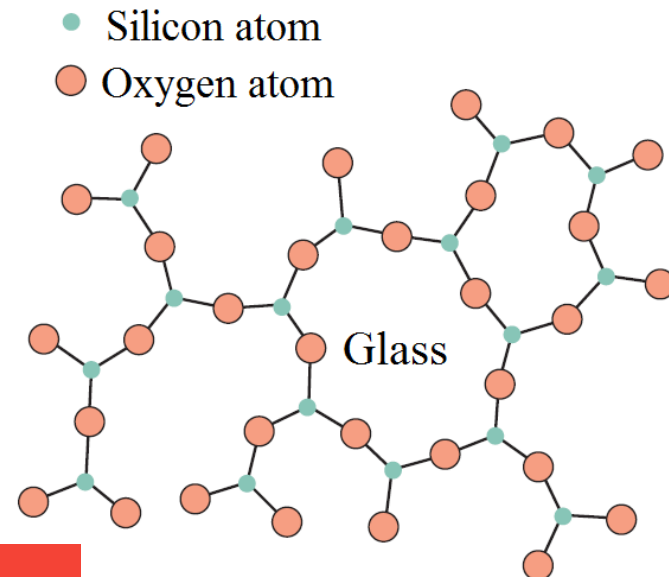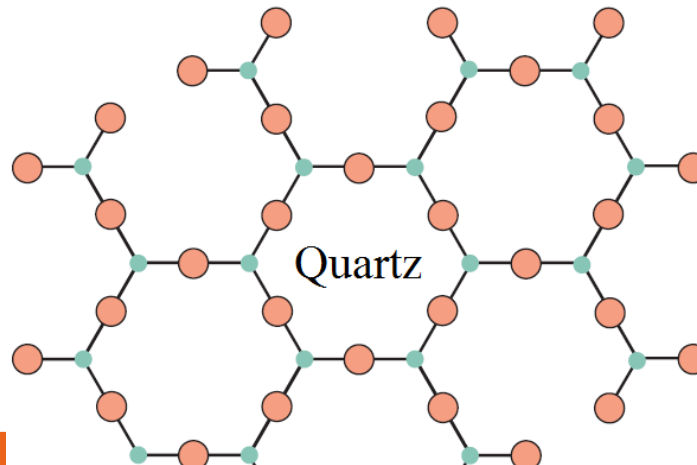
Allotropy

- Allotropes are different forms of the same element.
- Different bonding arrangements between atoms result in different structures with different chemical and physical properties.
- Under different conditions of temperature and pressure an element can exist in more than one physical forms. This phenomenon is known as Allotropy and different forms are known as "Allotropes"
Example:
   Coal, lamp black, coke, Diamond, graphite etc. are all allotropic forms of carbon.
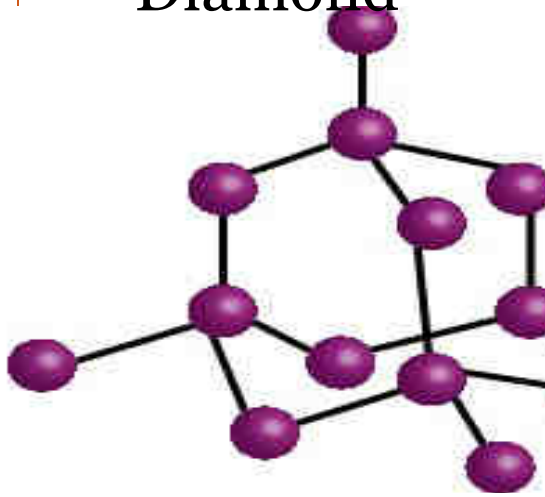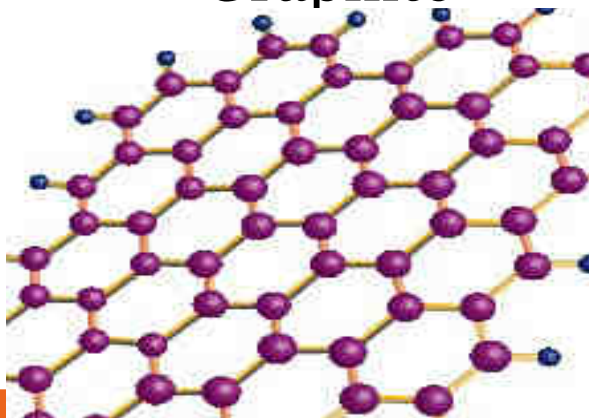
Diamond   Graphite   Fullerene
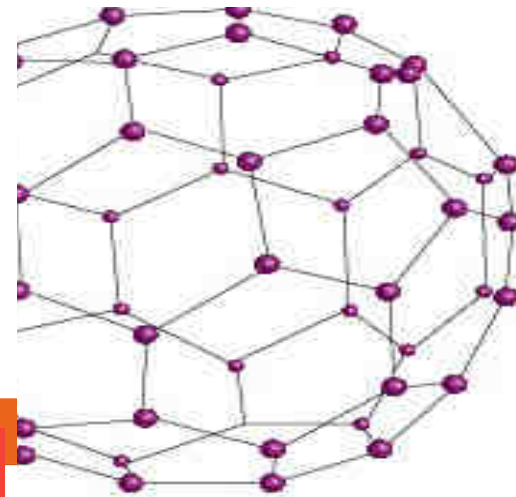
Radius ratio

- Many ionic crystals (cation and anion) are generated by close packing of larger anions.

- Cations then can be viewed as smaller ions that fit into the interstitial sites of the close-packed anions.

- The radius ratios described as **the ratios of the radius of the cation to that of the anion**.

- The packing in ionic crystals is not as tight as that in FCC or HCP metals.

- Interstitial atoms or ions whose radii are slightly larger than the radius of the interstitial site may enter that site, pushing the surrounding atoms slightly apart.

- Atoms with radii smaller than the radius of the hole are not allowed to fit into the interstitial site because the ion would "rattle" around in the site.

- If the interstitial atom becomes too large, it prefers to enter a site having a larger

Radius Ratio Rule

- In ideal ionic crystals, coordination numbers are determined largely by electrostatic considerations.
- Cations surround themselves with as many anions as possible and vice-versa. This can be related to the relative sizes of the ions, which is determined by radius ratio rule
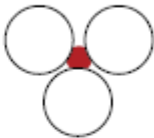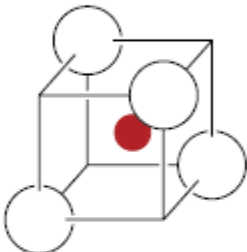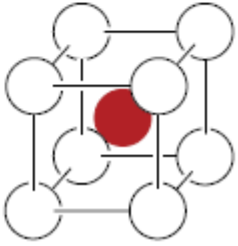
- **Radius ratio rule states:**
- As the size (ionic radius r) of a cation increases, more anions of a particular size can pack around it. Thus, knowing the size of the ions, one can predict which type of crystal packing will be observed.
- We can account for the relative size of both ions by using the RATIO of the ionic radii:

$$\rho = \frac{r^+}{r^-}$$

- The stability of the ionic crystal depend on the minimum allowable value of the ionic radius ratio, which is also called as limiting radius ratio

TABLE 3-6 ■ *The coordination number and the radius ratio*

Coordination Number	Location of Interstitial	Radius Ratio	Representation
2	Linear	0–0.155	
3	Center of triangle	0.155–0.225	
4	Center of tetrahedron	0.225–0.414	
6	Center of octahedron	0.414–0.732	
8	Center of cube	0.732–1.000	

Computation of Minimum Cation-to-Anion Radius Ratio for a Coordination Number of 3
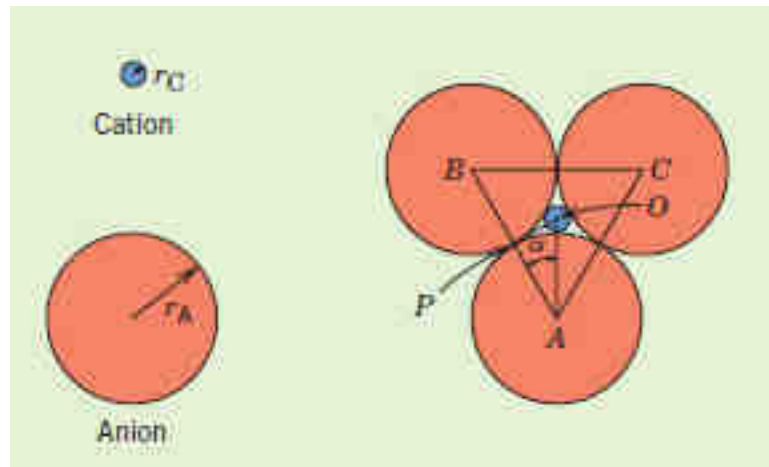
$$\overline{AP} = r_A$$

$$\frac{\overline{AP}}{\overline{AO}} = \cos\alpha$$

The magnitude of α is $30°$, since line AO bisects the $60°$ angle BAC. Thus,

$$\frac{\overline{AP}}{\overline{AO}} = \frac{r_A}{r_A + r_C} = \cos 30° = \frac{\sqrt{3}}{2}$$

Solving for the cation–anion radius ratio,

$$\frac{r_C}{r_A} = \frac{1 - \sqrt{3}/2}{\sqrt{3}/2} = 0.155$$

Points, Directions, and Planes in the Unit Cell

Coordinates of Points

- We can locate certain points, such as atom positions, in the lattice or unit cell by constructing the right-handed coordinate system.

- Distance is measured in terms of the number of lattice parameters we must move in each of the *x, y, and z coordinates to get from the origin to the point in* question. The coordinates are written as the three distances, with commas separating the numbers.
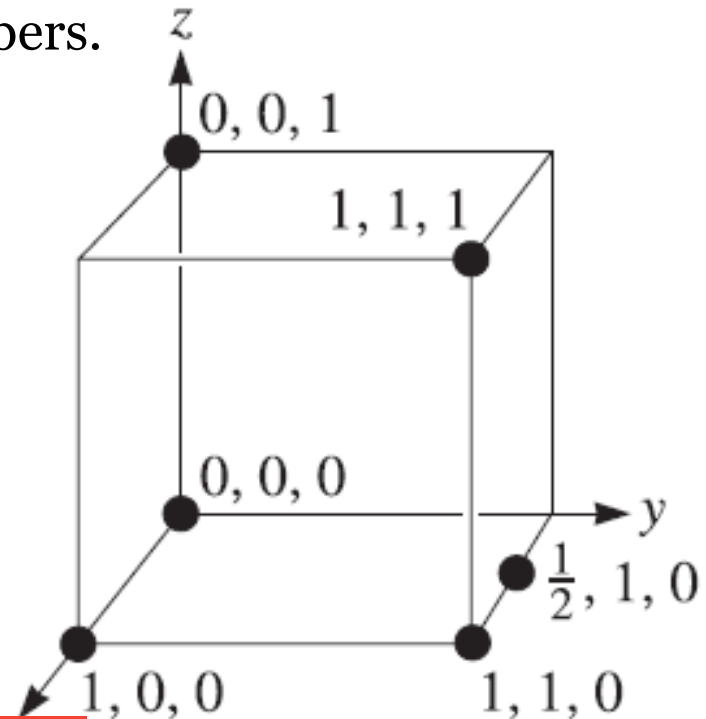
Directions in the Unit Cell (Miller Indices)

- **Miller indices** for directions are the shorthand notation used to describe these directions. The procedure for finding the Miller indices for directions is as follows:

- 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.

- Enclose the numbers in square brackets [ ]. If a negative sign is produced, represent the negative sign with a bar over the number.

Miller Indices for directions

- Determine the Miller indices of directions *A, B, and C*
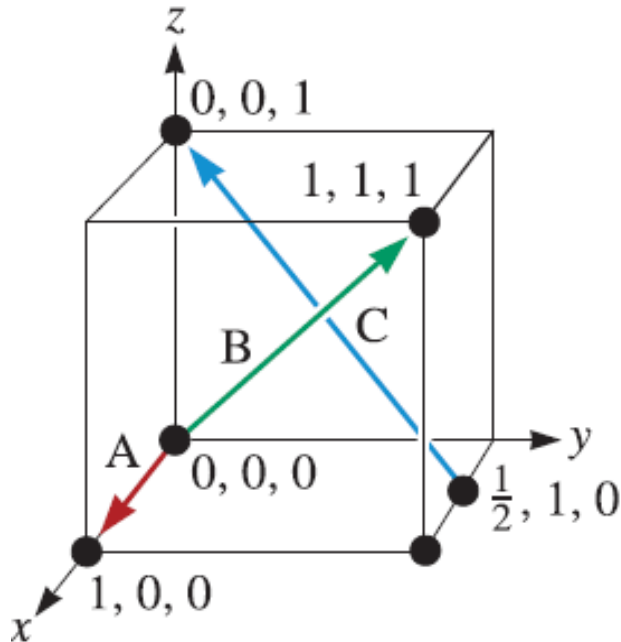
Direction A

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

- Because directions are vectors, a direction and its negative are not identical; [100] is not equal to [100]. They represent the same line, but opposite directions.

- A direction and its multiple are *identical; [100] is the same direction as [200].*

- Certain groups of directions are *equivalent; they have their particular indices* because of the way we construct the coordinates.

- a [100] direction is a [010] direction if we redefine the coordinate system. The groups of equivalent directions can be said as **directions of a form or family. The special brackets <> are used to indicate this collection of** directions. All of the directions of the form 110 are

$$\langle 110 \rangle = \begin{cases} [110] \, [\bar{1}\,\bar{1}0 \\ [101] \, [\bar{1}0\,\bar{1} \\ [011] \, [0\bar{1}\,\bar{1} \\ [1\,\bar{1}0] \, [\bar{1}\,10 \\ [10\bar{1}] \, [\bar{1}\,01 \\ [01\,\bar{1}] \, [0\bar{1}\,1 \end{cases}$$

- We expect a material to have the same properties in each of these twelve directions of the form 110 .

Interplanar spacing

- The distance between two adjacent parallel planes of atoms with the same Miller indices is called the **interplanar spacing (d_{hkl}).**

- *The **interplanar spacing** in cubic materials is given by the general equation,*

$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$

where a_o *is the lattice parameter and h, k, and l represent the Miller indices of the adjacent* planes being considered.

Problem:

The lattice constant for a unit cell of aluminum is 4.031Å Calculate the interplanar space of (2 1 1) plane.

a = 4.031 Å

(h k l) = (2 1 1)

Interplanar spacing

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{4.031 \times 10^{-10}}{\sqrt{2^2 + 1^2 + 1^2}}$$

∴ d = 1.6456 Å

Problem

Find the perpendicular distance between the two planes indicated by the Miller indices (1 2 1) and (2 1 2) in a unit cell of a cubic lattice with a lattice constant parameter 'a'.

● We know the perpendicular distance between the origin and the plane is (1 2 1) and the perpendicular distance between the origin and the plane (2 1 2),

$$d_1 = \frac{a}{\sqrt{h_1^2 + k_1^2 + l_1^2}} = \frac{a}{\sqrt{1^2 + 2^2 + 1^2}} = \frac{a}{\sqrt{6}}$$

$$d_2 = \frac{a}{\sqrt{h_2^2 + k_2^2 + l_2^2}} = \frac{a}{\sqrt{2^2 + 1^2 + 2^2}} = \frac{a}{\sqrt{9}} = \frac{a}{3}$$

The perpendicular distance between the planes (1 2 1) and (2 1 2) are,

$$d = d_1 - d_2 = \frac{a}{\sqrt{6}} - \frac{a}{3} = \frac{3a - \sqrt{6}a}{3\sqrt{6}} = \frac{a(3 - \sqrt{6})}{3\sqrt{6}}$$

(or) d = 0.0749 a.

Miller Indices for Planes

- Miller indices are used as a shorthand notation to identify these important planes, as described in the following procedure.

1. Identify the points at which the plane intercepts the *x, y, and z coordinates in* terms of the number of lattice parameters. If the plane passes through the origin, the origin of the coordinate system must be moved to that of an adjacent unit cell.

2. Take reciprocals of these intercepts.

3. Clear fractions but do not reduce to lowest integers.

4. Enclose the resulting numbers in parentheses (). Again, negative numbers should be written with a bar over the number.

Plane A

1. $x = 1, y = 1, z = 1$

2. $\dfrac{1}{x} = 1, \dfrac{1}{y} = 1, \dfrac{1}{z} = 1$

3. No fractions to clear

4. (111)

Plane B

1. The plane never intercepts the z axis, so $x = 1$, $y = 2$, and $z = \infty$

2. $\dfrac{1}{x} = 1, \dfrac{1}{y} = \dfrac{1}{2}, \dfrac{1}{z} = 0$

3. Clear fractions: $\dfrac{1}{x} = 2, \dfrac{1}{y} = 1, \dfrac{1}{z} = 0$

4. (210)

Plane C

1. We must move the origin, since the plane passes through 0, 0, 0. Let's move the origin one lattice parameter in the y-direction. Then, $x = \infty$, $y = -1$, and $z = \infty$.

2. $\dfrac{1}{x} = 0, \dfrac{1}{y} = -1, \dfrac{1}{z} = 0$

3. No fractions to clear.

4. $(0\bar{1}0)$
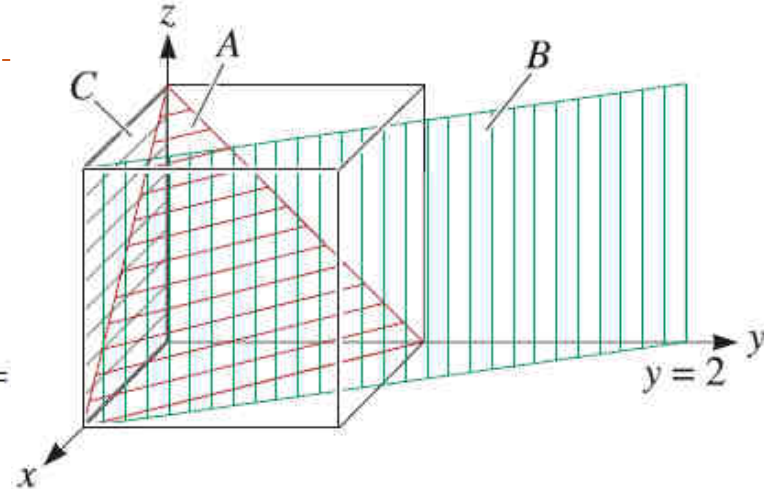
Family of planes

- In each unit cell, **planes of a form or family represent groups of equivalent planes** that have their particular indices because of the orientation of the coordinates.

- We represent these groups of similar planes with the notation {}. The planes of the form {110} in cubic systems are

$$\{110\}\begin{cases}(110)\\(101)\\(011)\\(1\bar{1}0)\\(10\bar{1})\\(01\bar{1})\end{cases}$$

- In cubic systems, a direction that has the same indices as a plane is perpendicular to that plane.

- Planes and their negatives are identical (this was not the case for directions) because they are parallel.

- Planes and their multiples are not identical. (Planar density)

Miller Indices for Hexagonal Unit Cells

- The coordinate system uses four axes instead of three, with the a_3 axis being redundant. The axes a_1, a_2, and a_3 lie in a *plane that is perpendicular to the fourth* axis.

- The procedure for finding the indices of planes is exactly the same for cubic system, but four intercepts are required, giving indices of the form (*hkil*).

$[100] = [2\bar{1}\bar{1}0]$

$[110] = [11\bar{2}0]$

$[010] = [\bar{1}2\bar{1}0]$
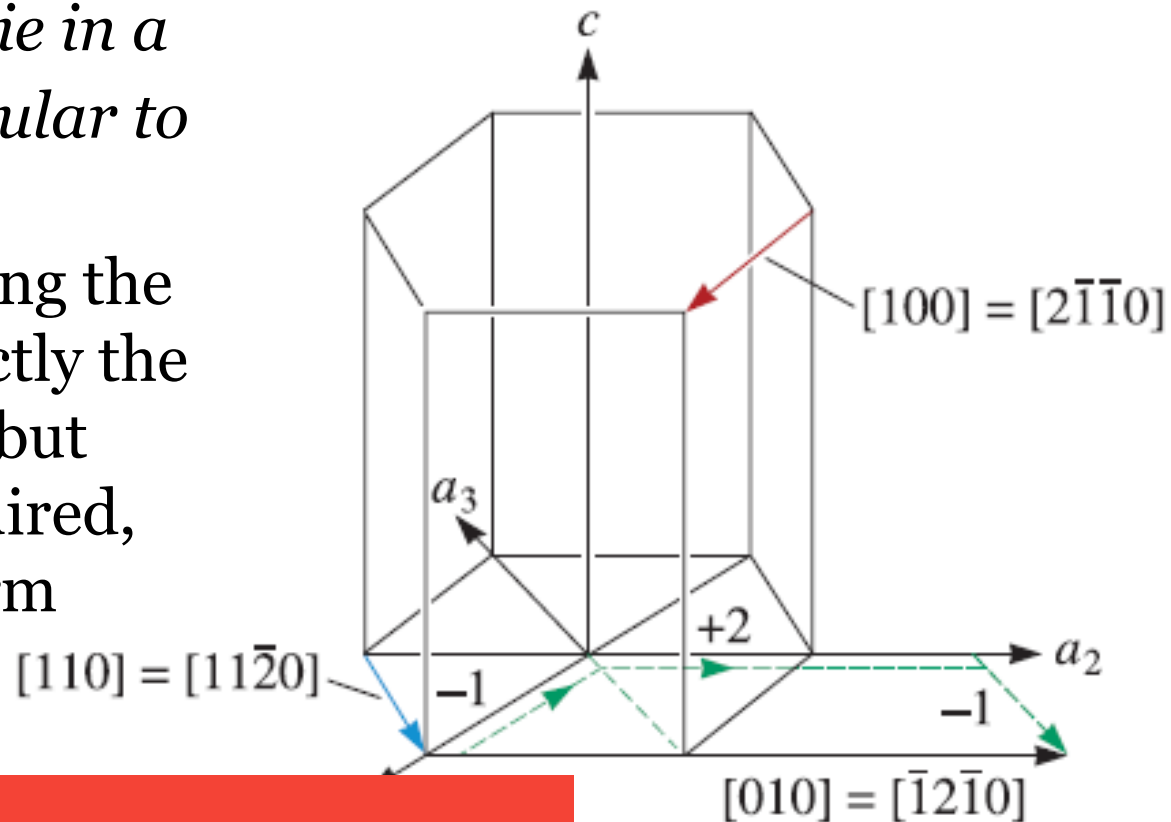
Construction of Directions and Planes To construct a direction

Draw (a) the [1$\bar{2}$1] direction and (b) the ($\bar{2}$10) plane in a cubic unit cell.
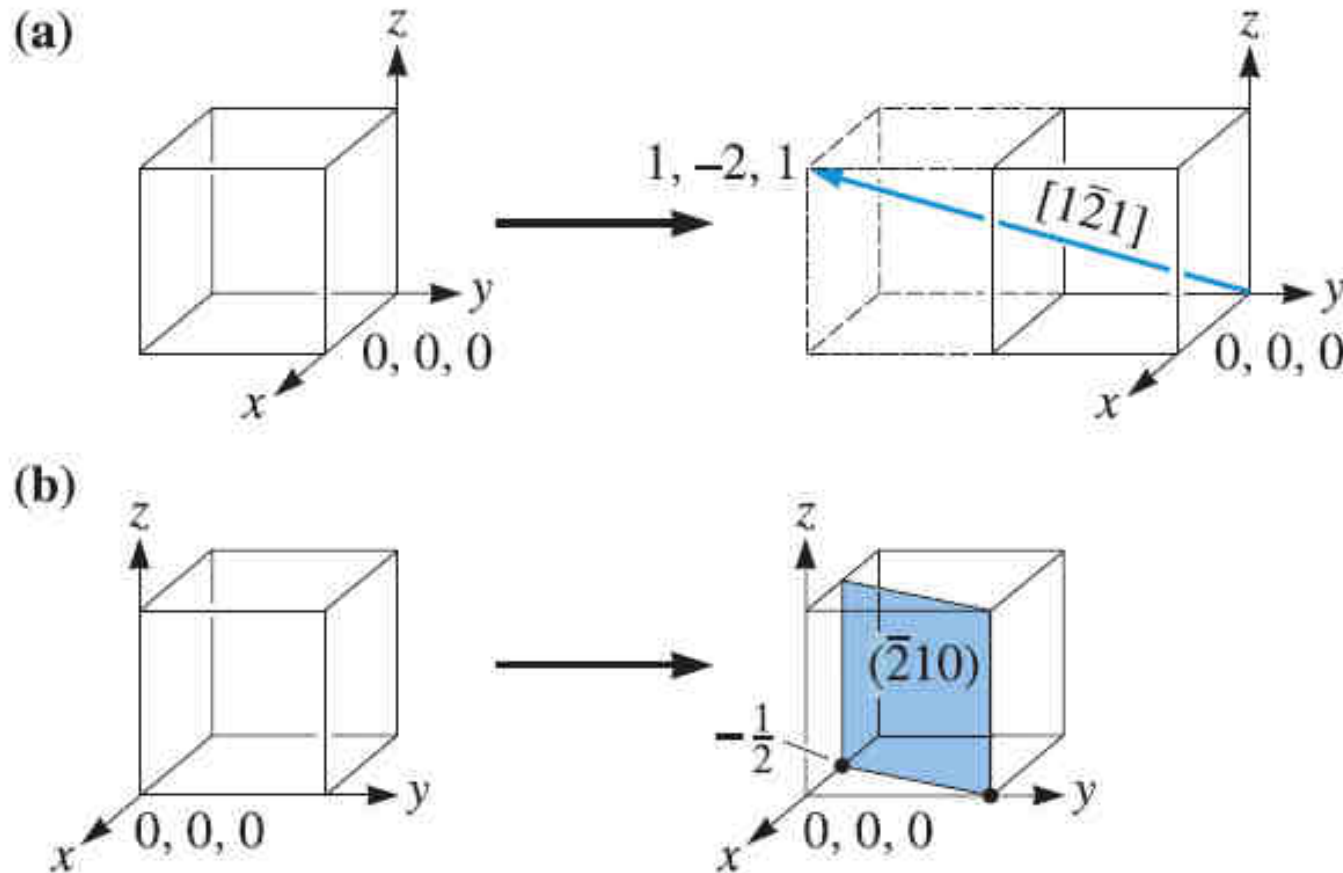
Plastic Deformation

- The level of stress needed to initiate plastic deformation is known as the "yield strength."
- The plastic deformation of metals is primarily the result of the propagation of dislocations.
- The propagation of dislocation is called **Slip**

Stress *vs* strain curve

- Up to Proportional limit
  stress $\propto$ strain
- Up to elastic limit the material deforms elastically.
- Yield point is the point at which plastic to elastic transition occurs.

Actual Rupture Strength

U – Ultimate Strength

Stress, σ

R – Rupture Strength

Y – Yield Point

E – Elastic Limit

P – Proportional Limit

Strain, ε
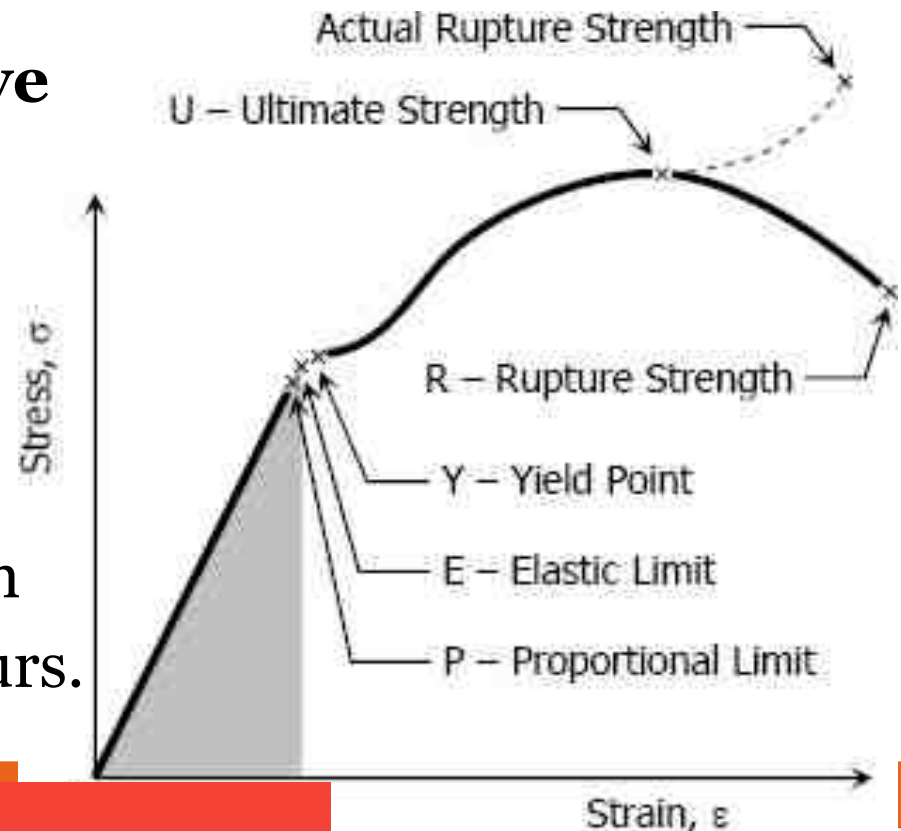
Slip

- A plane that contains both the dislocation line and the Burgers vector is known as a **slip plane,** over which the dislocation moves.

- When a sufficiently large shear stress acting parallel to the Burgers vector is applied to a crystal containing a dislocation, the dislocation can move through a process known as **slip.**
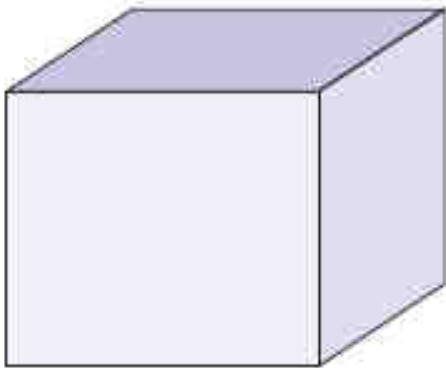
Extra half plane of atoms
In perfect crystal

Perfect crystal
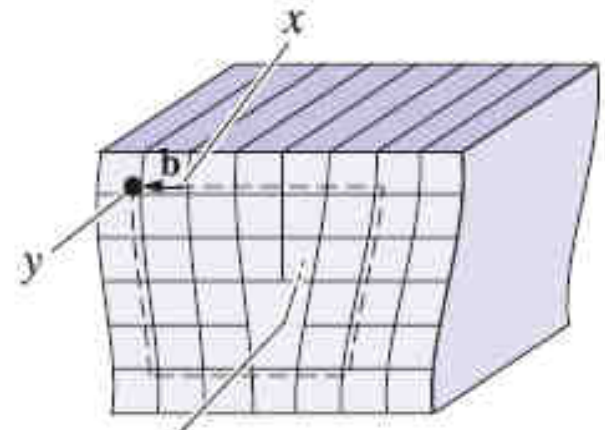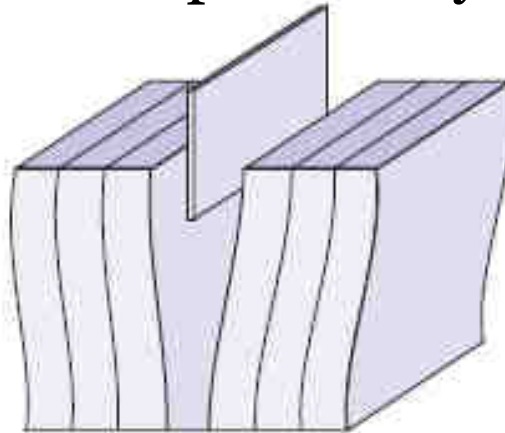
Edge dislocation

Movement of dislocation-slip
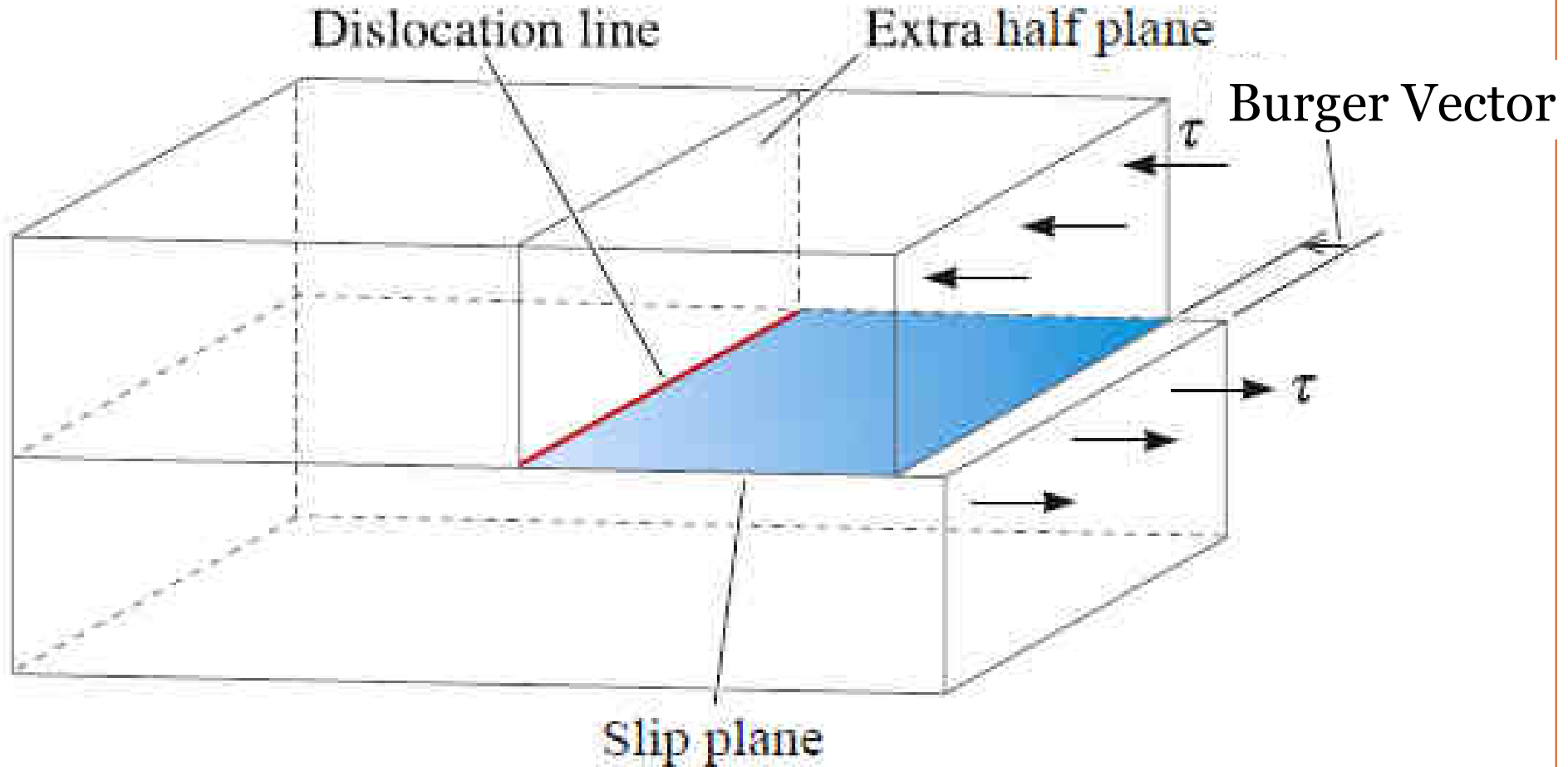
Slip-dislocation movement during plastic deformation
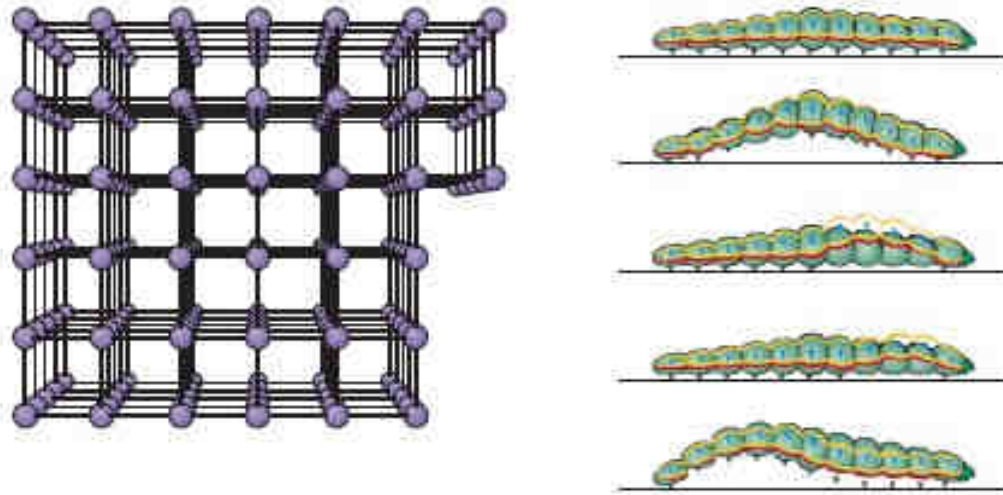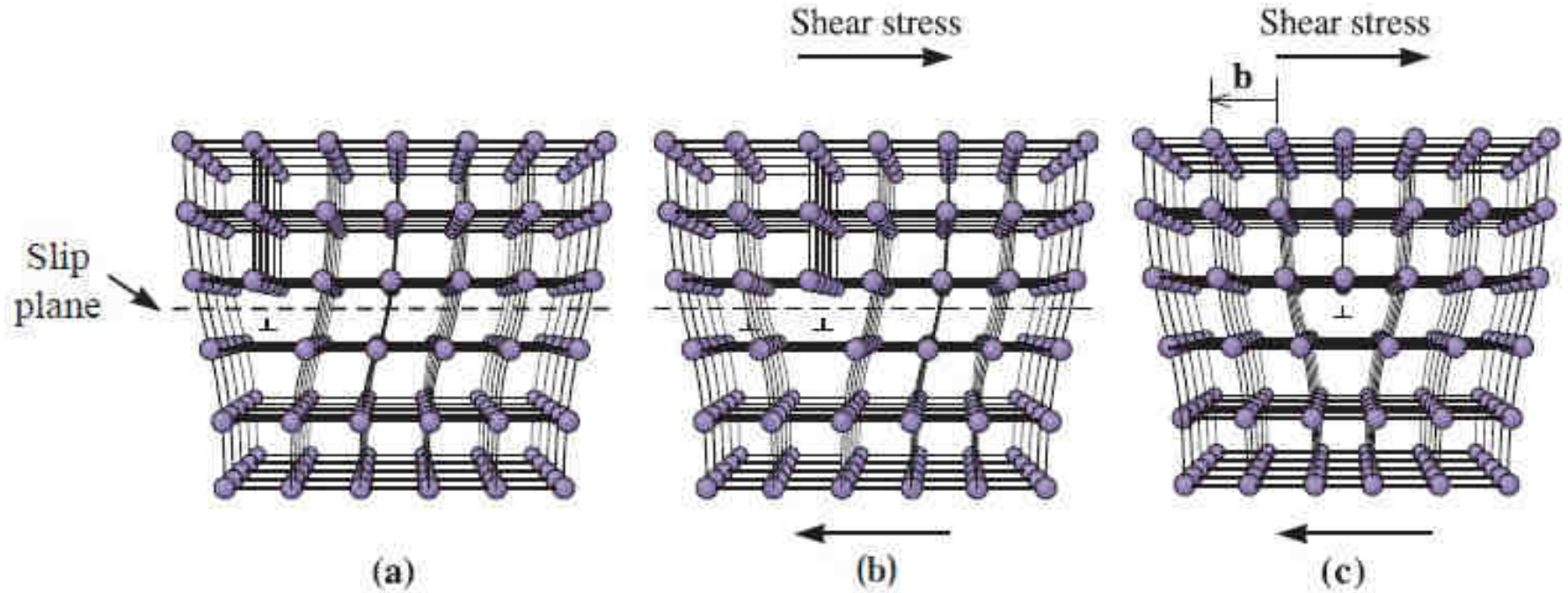
Slip System

- Dislocations do not move easily on all crystallographic planes of atoms and in all crystallographic directions.

- Ordinarily there is a preferred plane, and in that plane itself there are specific directions along which dislocation motion occurs.

- This plane is called the ***slip plane***; *it follows that the direction of movement is* called the ***slip direction***.

- *Combination of the slip plane and the slip direction is* termed the **slip system.**

- The slip system depends on the crystal structure of the metal and is such that the atomic distortion that accompanies the motion of a dislocation is a minimum.

- For a particular crystal structure, the slip plane is the plane that has the most dense atomic packing—that is, has the greatest **planar density**. The slip direction corresponds to the direction, in this plane, that is most closely packed with atoms—that is, has the highest **linear density**

Slip and Close Packing

- Slip planes are normally close-packed planes
- Slip directions are normally close-packed directions
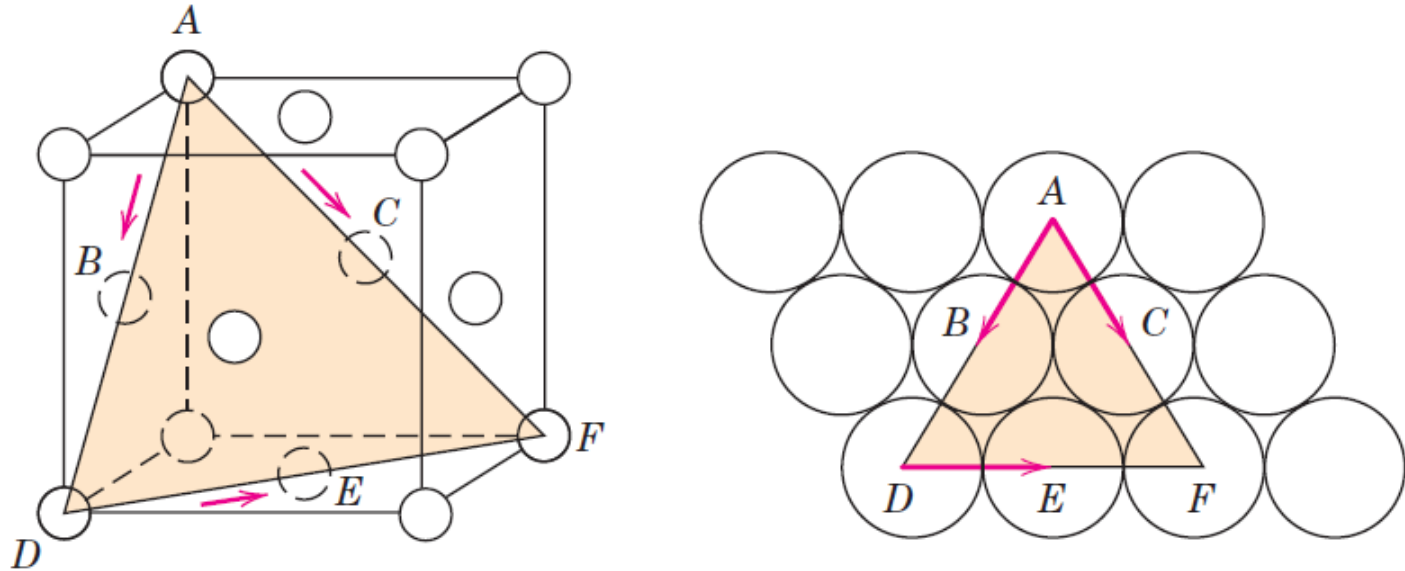
Figure shows (*a*) *A {111}* slip system shown within an FCC unit cell. (*b*) *The (111) plane* from (*a*) *and three <110>* slip directions (as indicated by arrows) within that plane comprise possible slip systems.

Recall for FCC, close-packed planes are {111} Close-packed directions are <110>

Close-Packed Planes and Directions in HCP

- In close-packed directions atoms are in continuous contact. The Miller indices to these close-packed directions.

- Only the basal planes—(0001) and (0002) are close-packed.

TABLE 3-5 ■ *Close-packed planes and directions*

Structure	Directions	Planes
SC	$\langle 100 \rangle$	None
BCC	$\langle 111 \rangle$	None
FCC	$\langle 110 \rangle$	$\{111\}$
HCP	$\langle 100 \rangle$, $\langle 110 \rangle$ or $\langle 11\bar{2}0 \rangle$	(0001), (0002)

- In FCC and HCP unit cells there is at least one set of close-packed planes in each.

- In HCP, hexagonal arrangement of atoms is produced in two dimensions.

- The close-packed planes are easy to find in the HCP unit cell; they are the (0001) and (0002) planes of the HCP structure and are given the special name **basal planes.**

- The center atom in a basal plane touches six other atoms in the same plane. Three atoms in a lower plane and three atoms in an upper plane also touch the same atom. The coordination number is twelve.

Close packing in FCC

- In the FCC structure, close-packed planes are of the form {111} When parallel (111) planes are stacked, atoms in plane *B fit over valleys in plane A and* atoms in plane *C fit over valleys in both planes A and B. The fourth plane fits directly over* atoms in plane *A.*

- *Consequently, a stacking sequence . . . ABCABCABC . . . is produced*

- using the (111) plane. Again, we find that each atom has a coordination number of twelve.

- Unlike the HCP unit cell, there are four sets of nonparallel close-packed planes— $(111), (11\bar{1}), (1\bar{1}1), \text{and } (\bar{1}11)$ —in the FCC cell. This difference between the FCC and HCP unit cells—the presence or absence of intersecting close-packed planes—affects the mechanical behavior of metals with these structures.

Twinning

- **Crystal twinning** occurs when two separate crystals share some of the same crystal lattice points in a symmetrical manner.

- A *twin boundary is a special type of grain boundary across which there is a specific* mirror lattice symmetry; that is, atoms on one side of the boundary are located in mirror-image positions of the atoms on the other side
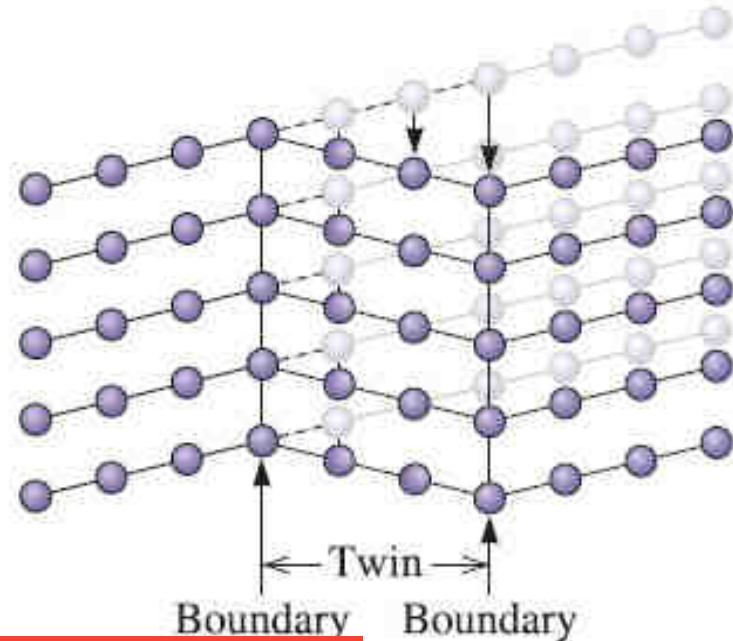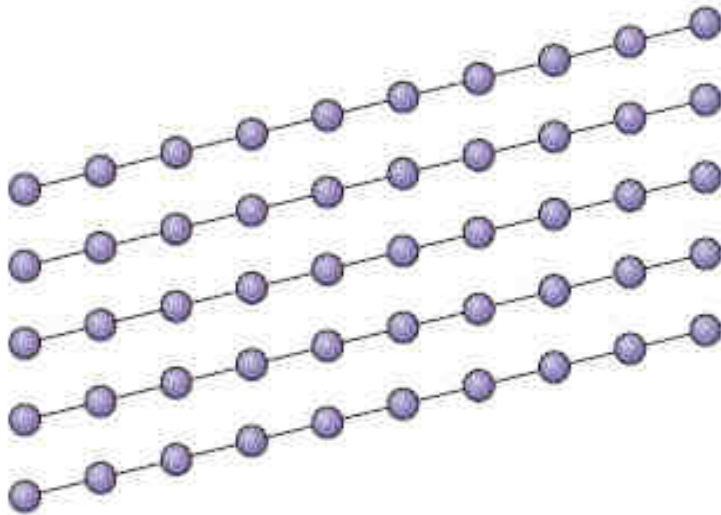
Schmid's Law

- One can understand the differences in behavior of metals that have different crystal structures by examining the force required to initiate the slip process.
- Suppose a unidirectional force F is applied *to a cylinder of metal that is a single crystal, We can* orient the slip plane and slip direction to the applied force by defining the angles λ and ϕ.
  - λ is the angle between the slip direction and the applied force
  - ϕ is the angle between the normal to the slip plane and the applied force.

Schmid's Law
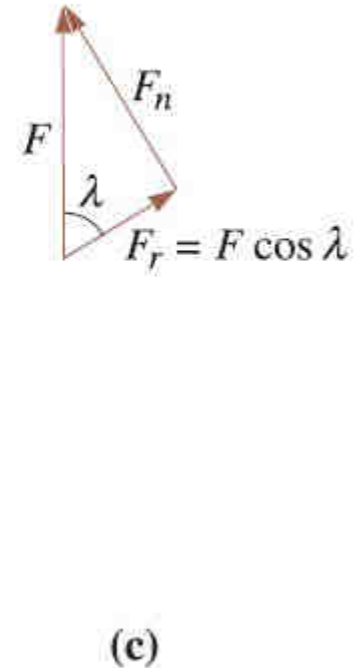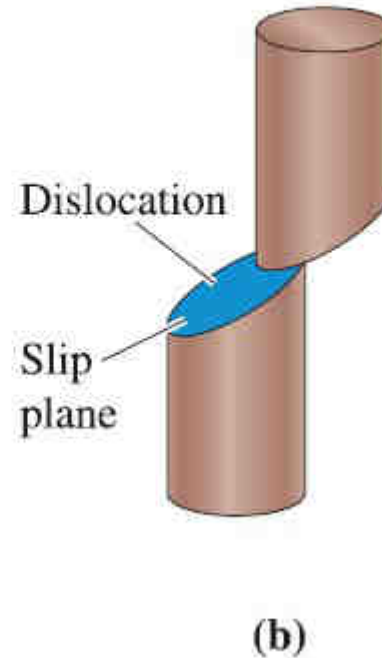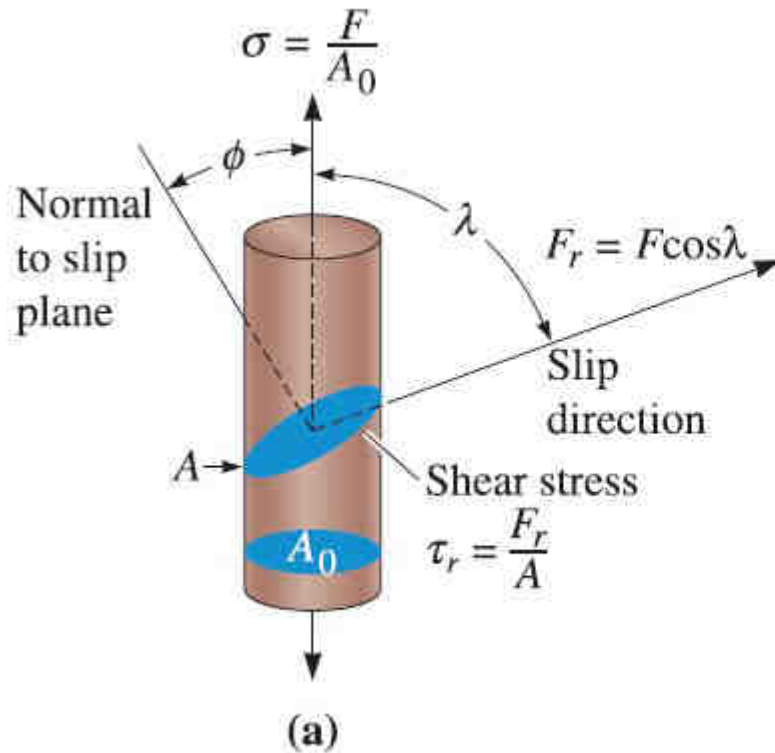
(a) A resolved shear stress *t is produced on a slip system. [Note: ($\phi+\lambda$) does not have to equal 90°.]* (b) Movement of dislocations on the slip system deforms the material. (c) Resolving the force.

- In order for the dislocation to move in its slip system, a shear force acting in the slip direction must be produced by the applied force.

Schmid's law

- This resolved shear force *F_r* *is given by*

$$F_r = F \cos \lambda$$

- If we divide the equation by the area of the slip plane,

$$A = A_o/cos\phi$$

The following equation known as **Schmid's law:**

$$\tau_r = \sigma \cos\phi \cos\lambda$$

Where:

$$\tau_r = \frac{F_r}{A} = \text{resolved shear } stress \text{ in the slip direction}$$

and

$$\sigma = \frac{F}{A_0} = \text{normal } stress \text{ applied to the cylinder}$$

Critical resolved shear stress

- The **critical resolved shear stress** τ_{crss} is the shear stress required for slip to occur.

- Thus slip occurs, causing the metal to plastically deform, when the *applied stress σ produces* a *resolved shear stress (τ_r) that equals the critical resolved shear stress:*

$$\tau_r = \tau_{crss}$$

- The magnitude of the applied stress required to initiate yielding (i.e., the yield strength σ_y) is

$$\sigma_y = \frac{\tau_{crss}}{(\cos\phi \cos\lambda)_{max}}$$

- The minimum stress necessary to introduce yielding occurs when a single crystal is oriented such that

$$\sigma_y = 2\tau_{crss}$$

Problem

- Design a rod composed of a single crystal of pure aluminum, which has a critical resolved shear stress of 148 psi. The rod is oriented in such a manner that, when an axial stress of 500 psi is applied, the rod deforms by slip in a 45° direction to the axis of the rod and actuates a sensor that detects the overload.

Dislocations begin to move when the resolved shear stress τ_r equals the critical resolved shear stress, 148 psi. From Schmid's law:

$$\tau_r = \sigma \cos \lambda \cos \phi \text{ or}$$

$$148\,\text{psi} = (500\,\text{psi}) \cos \lambda \cos \phi$$

Because we wish slip to occur at a 45° angle to the axis of the rod, $\lambda = 45°$, and

$$\cos \phi = \frac{148}{500 \cos 45°} = 0.4186$$

$$\phi = 65.3°$$

Therefore, we must produce a rod that is oriented such that $\lambda = 45°$ and $\phi = 65.3°$.

We might do this by a solidification process. We could orient a seed crystal of solid aluminum at the bottom of a mold. Liquid aluminum could be introduced into the mold. The liquid solidifies at the seed crystal, and a single crystal rod of the proper orientation is prod

Number of Slip Systems in close packing

- If at least one slip system is oriented to give the angles and near 45°, then τ_r *equals* τ_{crss} at low applied stresses.

- Ideal HCP metals possess only one set of parallel close-packed planes, the (0001) planes, and three close-packed directions, giving three slip systems.

- Consequently, the probability of the close-packed planes and directions being oriented with and near 45° is very low.

- The HCP crystal may fail in a brittle manner without a significant amount of slip; however, in HCP metals with a low *c/a ratio, or when* HCP metals are properly alloyed, or when the temperature is increased, other slip systems become active, making these metals less brittle than expected.

- FCC metals contain four nonparallel close-packed planes of the form {111} and three close-packed directions of the form 110 within each plane, giving a total of twelve slip systems.

- At least one slip system is favorably oriented for slip to occur at low applied stresses, permitting FCC metals to have high ductilities.

- **FCC slip** occurs on close-packed **planes** in close-packed directions. There are 4 octahedral **planes**, (111), (111), (111), and (111), six <110> directions, each one common to two octahedral **planes**, giving **12 slip systems**.

- Finally, BCC metals have as many as 48 slip systems that are **nearly close-packed**.

- Several slip systems are always properly oriented for slip to occur, allowing BCC metals to have ductility.

- BCC which is not a closed pack system, does not has a predominant atomic density. Therefore total 3 family of planes acts as the slip planes and neither of them is a dominant and hence has a total of 48 slip system .

- Some bcc materials (e.g. α-Fe) can contain up to 48 slip systems. There are six slip planes of type {**110**}, each with two <**111**> directions (12 systems). There are 24 {123} and 12 {112} planes each with one <**111**> direction (36 systems, for a total of 48).

Why FCC metals are ductile than BCC metals and HCP metals

- In ductility, the material will be deformed and as a result of which the dislocation present inside them will also travel.

- but slip (movement /travel of dislocation) happens in close packed planes and directions, which are called as **slip planes** and **slip directions.**

- In FCC the atoms are closed pack and has a predominant **slip system** (12) and hence the slip can travel easily inside it and the material can be deformed easily as a result it will be more ductile

- While incase of BCC the dislocation cannot travel with such an ease, since there is no close packed planes but nearly close packed planes making 48 slip systems, which are not dominent.

- In HCP system only 3 predominant slip systems are present.

- And hence we can conclude that the FCC structure has more ductility than BCC and BCC has more ductility in HCP structures.

Plastic deformation in metals

- Deformation and slip in polycrystalline materials is somewhat more complex because of the random crystallographic orientations of the numerous grains, the direction of slip varies from one grain to another. For each, dislocation motion occurs along the slip system that has the most favorable orientation, as defined above.

- Gross plastic deformation of a polycrystalline specimen corresponds to the comparable distortion of the individual grains by means of slip.

- During deformation, mechanical integrity and coherency are maintained along the grain boundaries; that is, 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.

- Before deformation the grains are equiaxed, or have approximately the same dimension in all directions.

- For this particular deformation, the grains become elongated along the direction in which the specimen was extended.

- Polycrystalline metals are stronger than their single-crystal equivalents, which means that greater stresses are required to initiate slip and the attendant yielding.

- This is, to a large degree, also a result of geometrical constraints that are imposed on the grains during deformation. Even though a single grain may be favorably oriented with the applied stress for slip, it cannot deform until the adjacent and less favorably oriented grains are capable of slip also; this requires a higher applied stress level.