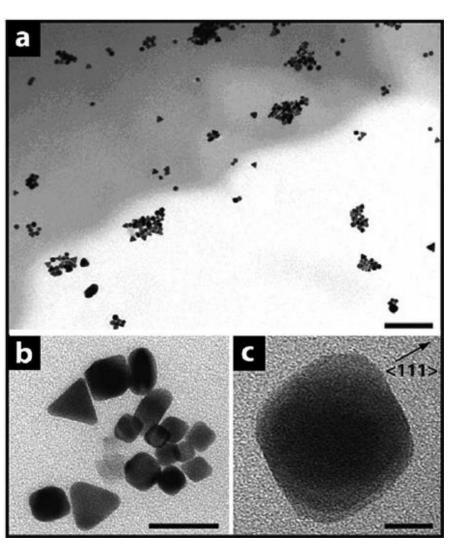
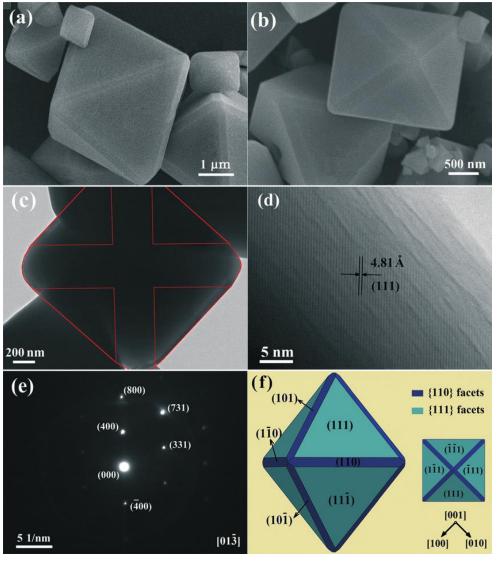
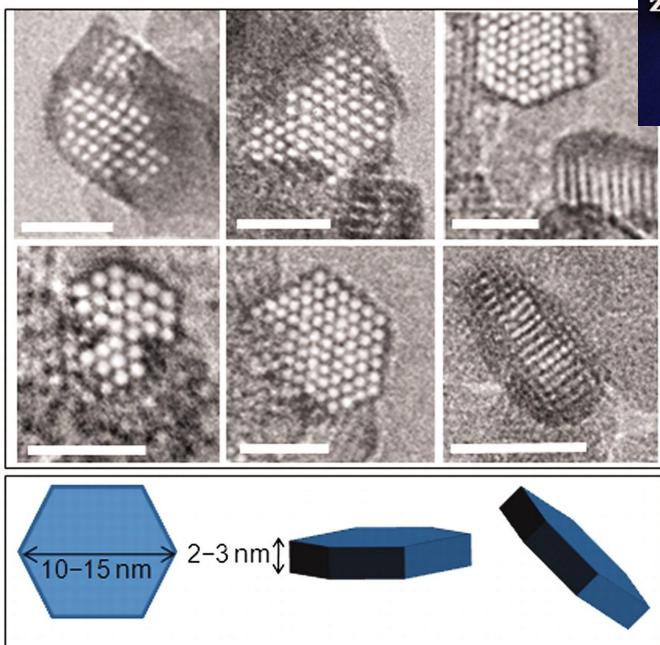
Crystallography











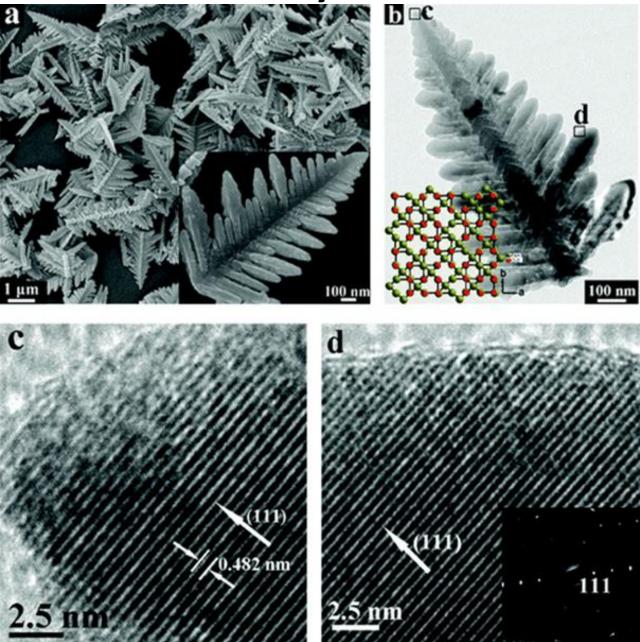




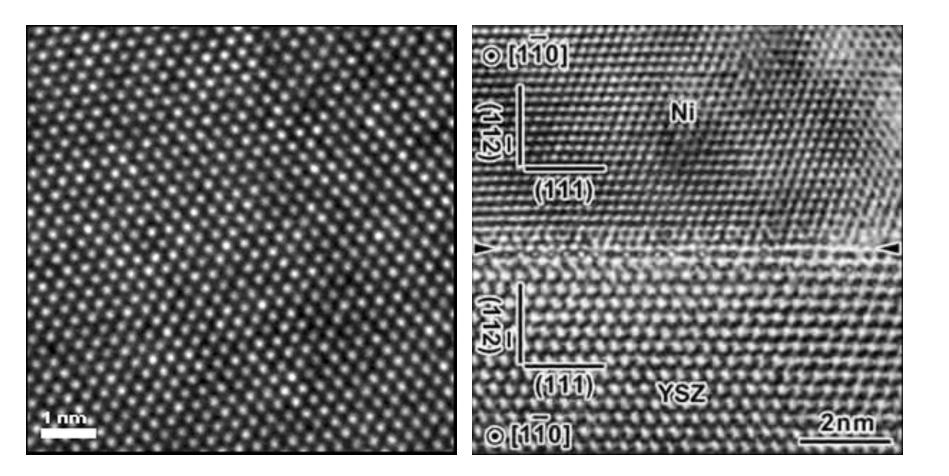
Snow flakes



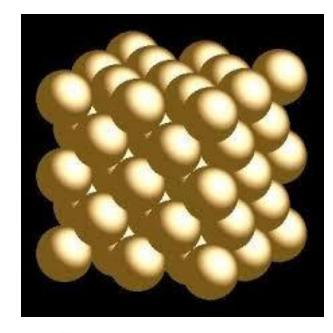
Metal Crystals

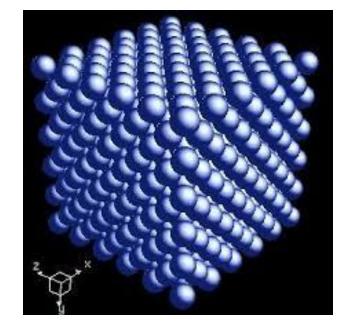


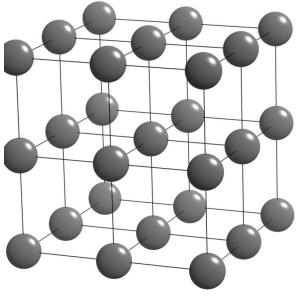
Periodicity of atoms

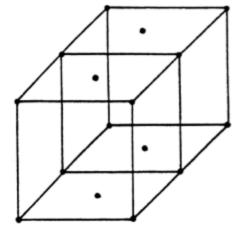


Atoms/crystals representation

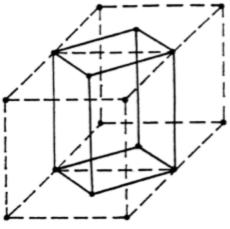








two adjacent base-centered unit cells



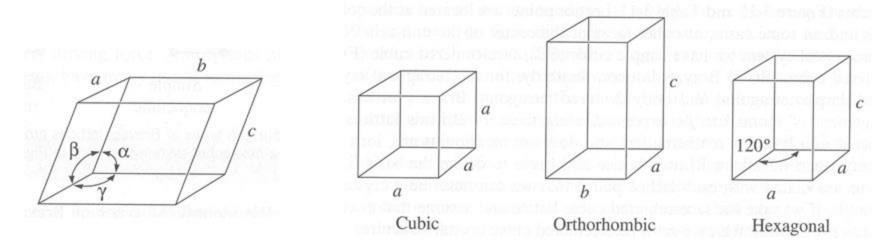
a simple tetragonal unit cell

- Crystallography is that branch of science in which the internal structure of crystals, their properties, external or internal symmetries of crystals are studied.
- Various terms associated with crystallography are:
- Crystal is a solid whose constituent atoms or molecules are arranged in a systematic geometric pattern
- Structure implies the arrangement and disposition of atoms within a crystal

- The atoms arrange themselves in distinct pattern in space called a space lattice
- Unit cell is the smallest group of atoms possessing the symmetry of the crystal
- The layers of atoms or the planes along which atoms are arranged are known as **atomic** or crystallographic planes
- Characteristic intercepts and interfacial angles of crystal constitute the lattice parameters of a cell

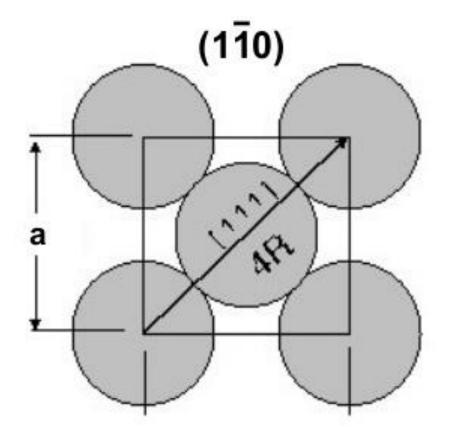
Lattice Parameters

- The lattice parameters describe the size and shape of the unit cell.
- There are three lengths, a, b, and c that describe the cell's edges.
- There are three angles, alpha, beta, and gamma, that describe the three angles between the adjacent cell axes.



Lattice parameters and their use to describe crystal systems.

Lattice Parameters & Atomic Radii



Body Centered Cubic (BCC)

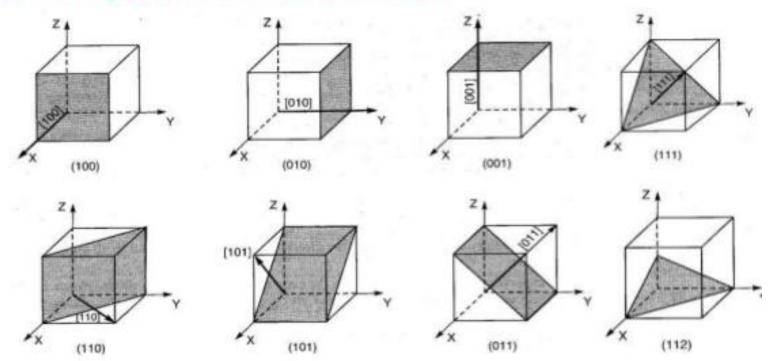
$$a = \frac{4R}{\sqrt{3}}$$

Common BCC Metals

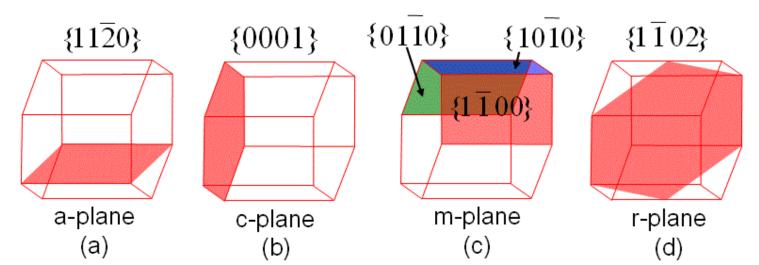
- Chromium
- Iron (α)
- Molybdenum
- Tantalum
- Tungsten

- Miller indices is a system of notation for designating crystallographic planes and directions
- Atomic Packing Factor is the ratio of volume of atoms per unit cell to the total volume occupied by the unit cell
- Coordinate no. is the number of nearest atoms directly surrounding a given atom in a crystal
 i.e., nearest neighbours to an atom in a crystal

Some important Planes of a Cube:

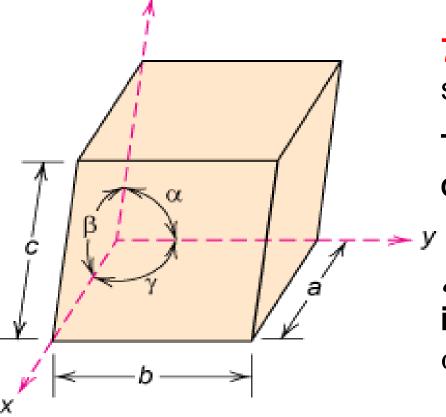


Important planes of Hexagonal Crystals



Crystal Systems

Unit cell: basic building block of the crystal



7 crystal systems of varying symmetry are known

These systems are built by changing the lattice parameters:

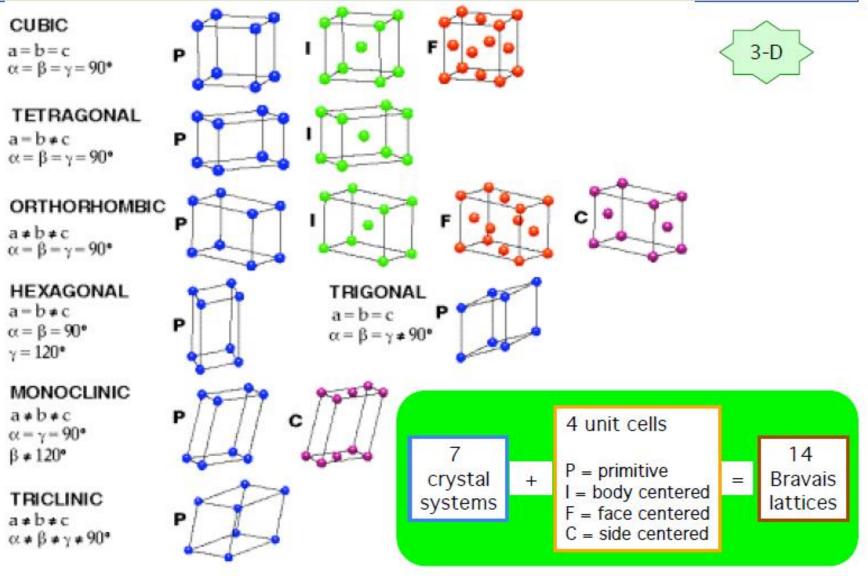
a, b, and *c* are the characteristic **intercepts**

 α , β , and γ are interfacial **angles**

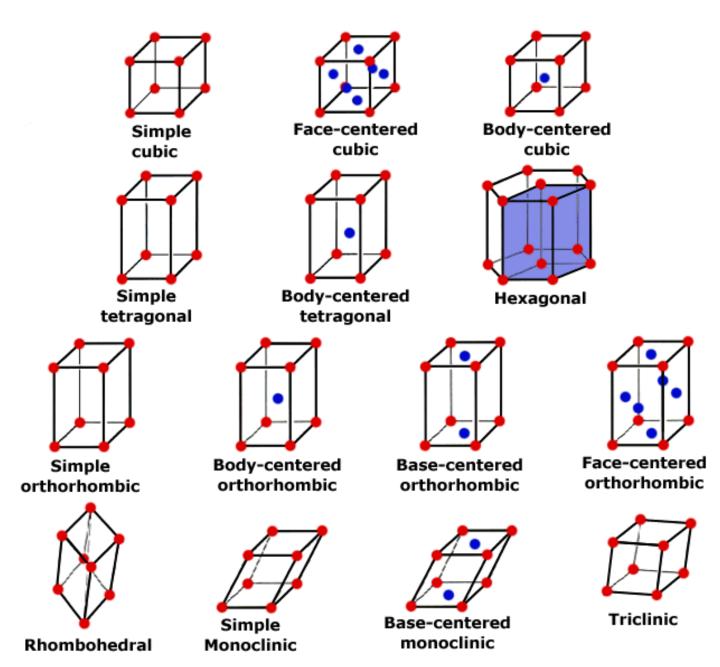
Fig. 3.4, Callister 7e.

3-D Bravais lattices

Paolo Fornasini Univ. Trento



Bravais Lattices

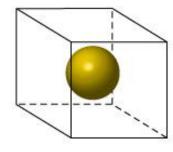


Parameter that characterises the crystal structure

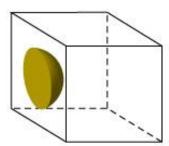
- Lattice parameters
- Atoms per unit cell
- Coordination number- no. of nearest neighbouring atoms
- Atomic packing factor =

 (Volume occupied by atoms in the unit cell)/
 (Volume of unit cell)

Atoms in unit cell



1





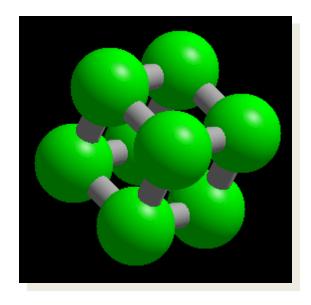


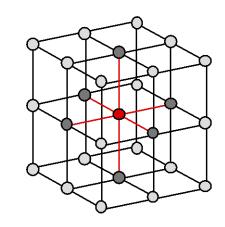
1/8

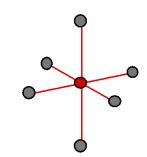
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Simple Cubic Structure (SC)

- 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

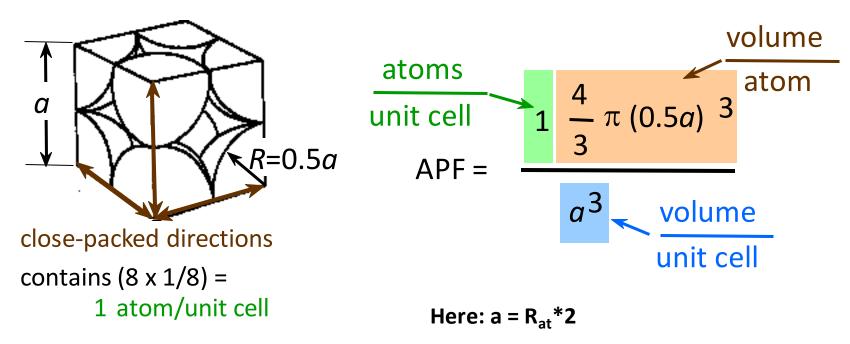
Atomic Packing Factor (APF)

APF = Volume of atoms in unit cell*

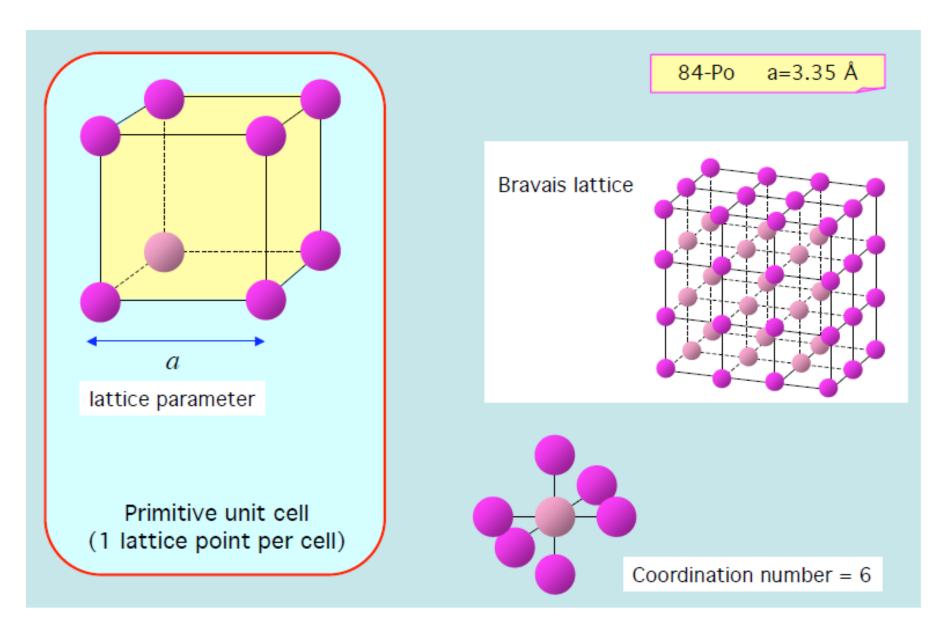
Volume of unit cell

*assume hard spheres

• APF for a simple cubic structure = 0.52

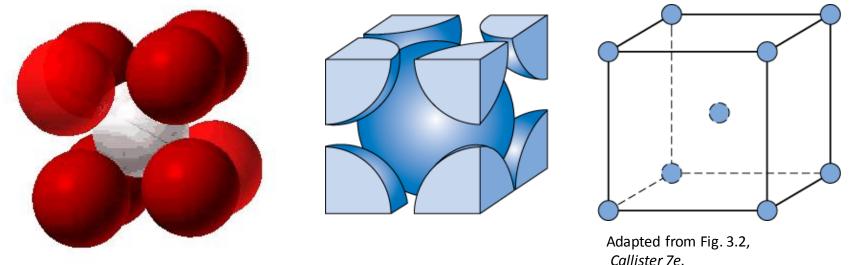


Where R_{at} is the atomic radius



Body Centered Cubic Structure (BCC)

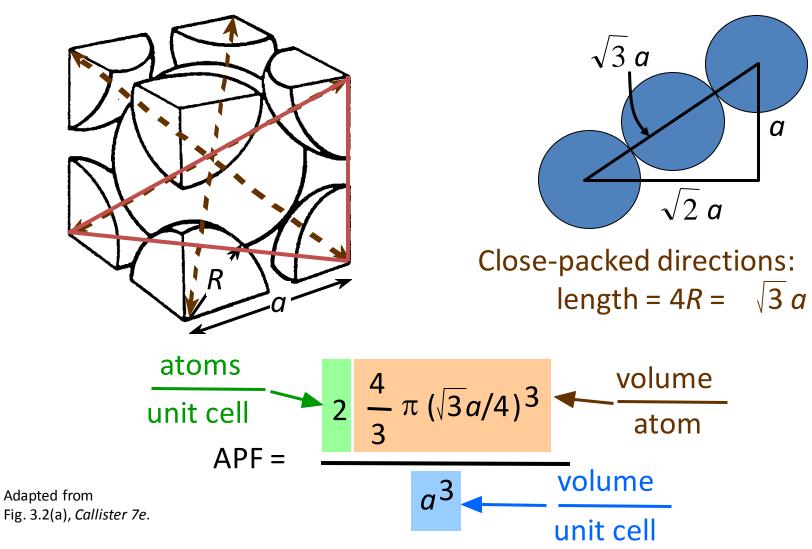
- Atoms touch each other along *cube diagonals within a unit cell*.
- --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.
 - ex: Cr, W, Fe (α), Tantalum, Molybdenum



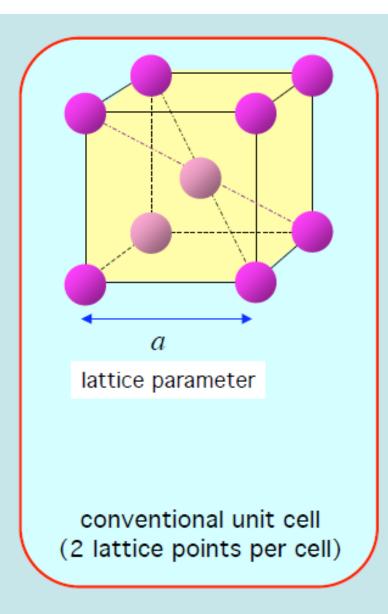
• Coordination # = 8

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

Atomic Packing Factor: BCC



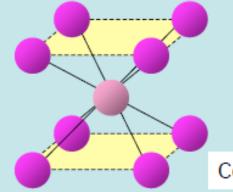
• APF for a body-centered cubic structure = 0.68



24-Cr a=2.88 Å 26-Fe a=2.87 Å 42-Mo a=3.15 Å

Bravais lattice



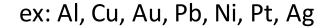


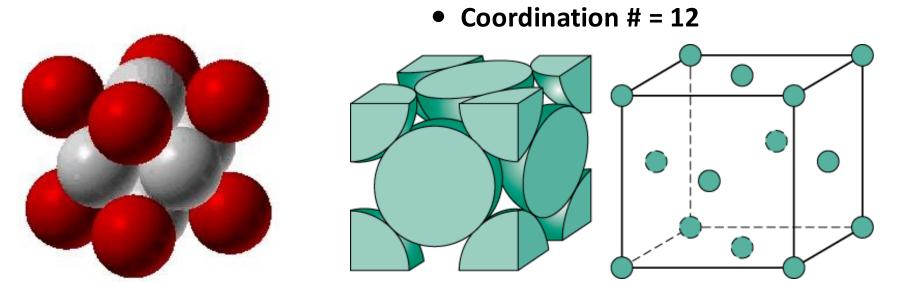
Coordination number = 8

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.



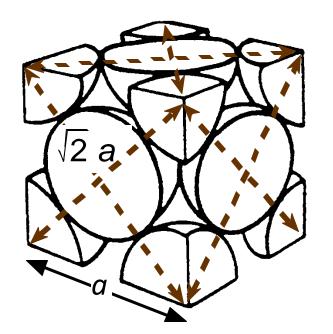


Adapted from Fig. 3.1, Callister 7e.

4 atoms/unit cell: (6 face x ½) + (8 corners x 1/8)

Atomic Packing Factor: FCC

• APF for a face-centered cubic structure = 0.74

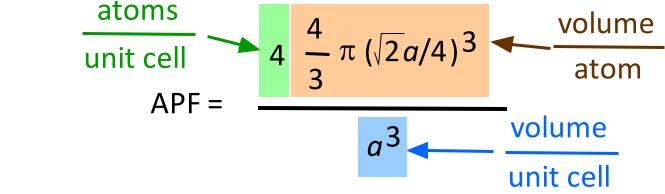


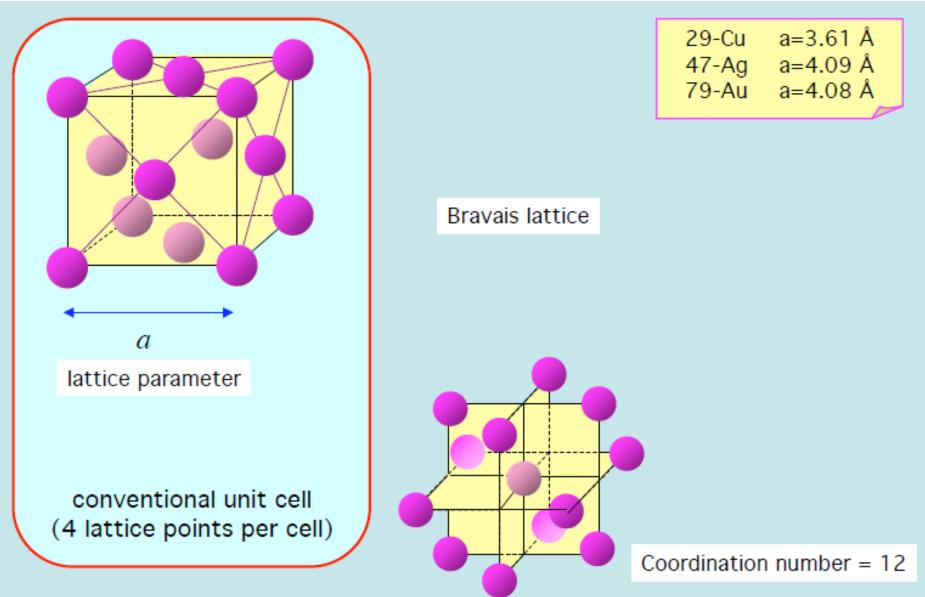
Adapted from

Fig. 3.1(a),

Callister 7e.

The maximum achievable APF! Close-packed directions: $length = 4R = \sqrt{2} a$ $(a = 2\sqrt{2}R)$ Unit cell contains: $6 \times 1/2 + 8 \times 1/8$ = 4 atoms/unit cell

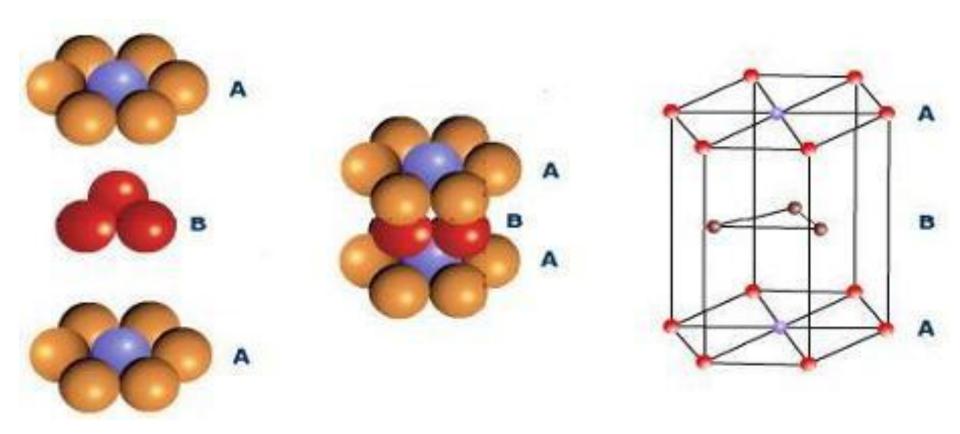


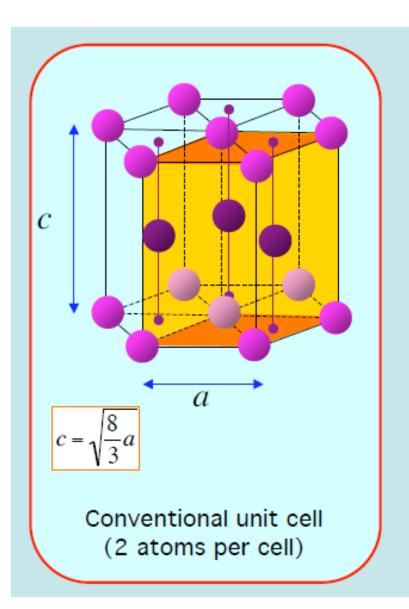


Hexagonal close packed (HCP)

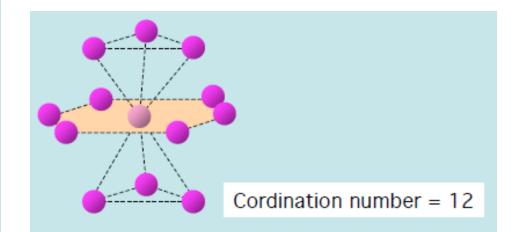
- A hexagonal close packed structure has
 - One atom at each corner of the hexagon
 - One atom at the centre of two hexagonal faces (Basal planes)
 - One atom at the centre of the line connecting the perpendiculars in case of three rhombuses which combine and form the hexagonal close packed structure
- Atomic Packing Factor = 0.74
- Eg.: Zn, Cd, Be, Mg

Hexagonal close packed (HCP)





4-Be a=2.29 Å 12-Mg a=3.21 Å 48-Cd a=2.98 Å



Properties of crystalline solids:

➤These solids have a particular three dimensional geometrical structure.

➤The arrangement order of the ions in crystalline solids is of long order.

➤The strength of all the bonds between different ions, molecules and atoms is equal.

 \geq 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.

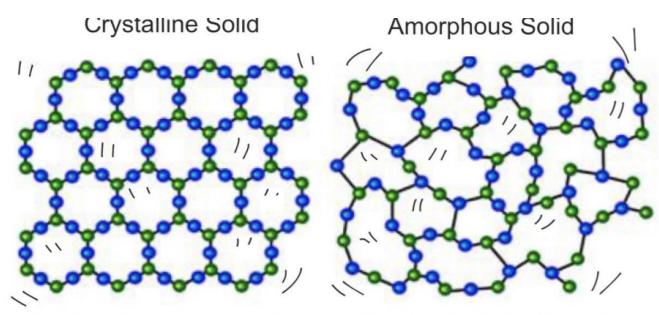
Properties of Amorphous solids:

> The strength of different bonds is different in amorphous solids.

>There is no regularity in the external structure of amorphous solids.

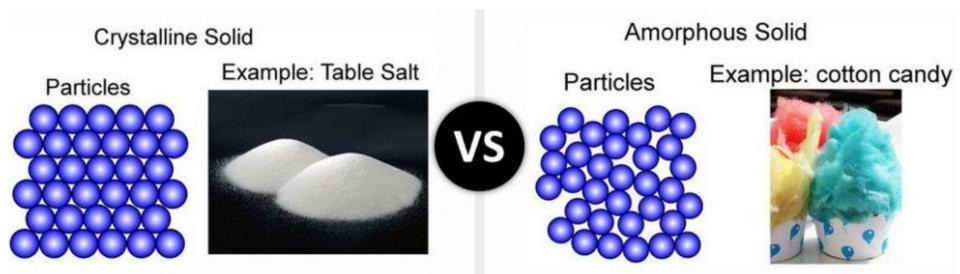
➢On the other hand, amorphous solids don't have sharp melting point. This is due to the variable strength of bonds present between the molecules, ions or atoms. So, bonds having low strength on heating break at once. But the strong bonds take some time to break. This is the reason that the amorphous 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.



Atoms vibrate in place in a fixed pattern

Atoms vibrate in place in more random arrangements



Miller Indices

>Miller indices is a system of notation

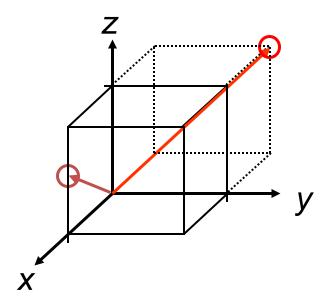
for designating crystallographic planes

and directions of planes

Miller indices of a direction

- ➤ A crystallographic direction is defined as a line or vector between two points. Following are the steps for determination of the Miller indices of a direction
 - 1. Determinate the co-ordinates of two points that lie on the direction, usually a right handed coordinate system
 - 2. Subtract the co-ordinates of tail point from those of the head point and express the same in terms of the unit cell dimensions
 - 3. Multiply or divide these numbers by a common factor to reduce them to the smallest integers
 - 4. The three indices are enclosed in square brackets as [*uvw*]. A negative integer is represented with a bar over the number

Crystallographic Directions



Ex 1: 1, 0, $\frac{1}{2}$ & 0,0,0 => (1,0, $\frac{1}{2}$) - (0, 0, 0) => 1,0, $\frac{1}{2}$ => 2,0,1

=> [201]

Ex 2:(-1, 1, 1) & (0,0,0) => (-1, 1, 1) - (0, 0, 0) => -1, 1, 1

=> [111] where 'overbar' represents a negative index

Points to be noted about the use of miller indices for direction

- As the directions are vectors, a direction and its negative are not identical. The directions [110] & [1 10] represent the same line but opposite directions
- A direction and its multiple are identical; [120] & [240] represent same direction
- In any crystal system, there are certain groups of directions which are equivalent and are called family of directions. In cubic system corresponding to [100] direction a family of equivalent directions are obtained by interchanging the positions and signs of indices. The index when enclosed in angle brackets represent a family.
- <100> = [100], [010], [001], [100], [010], [001]

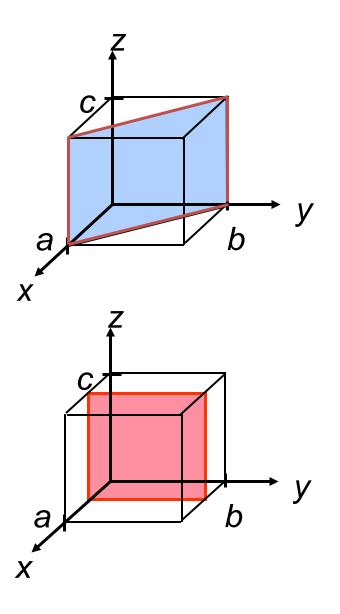
Miller indices of planes

Procedure for determining miller indices of planes

- 1. If the plane passes through the origin of co-ordinate system, the origin must be moved to another corner of unit cell
- 2. Identify the points at which the plane intercepts the x,y,z axes and express the intercepts in terms of the lattice parameters
- 3. Take reciprocals of these numbers. Intercept for a plane parallel to an axis to be taken as infinity with reciprocal equal to zero
- 4. Change these numbers to a set of smallest integers by multiplication or division by a common factor
- 5. Enclose the integer indices within parentheses (hkl)

Crystallographic Planes

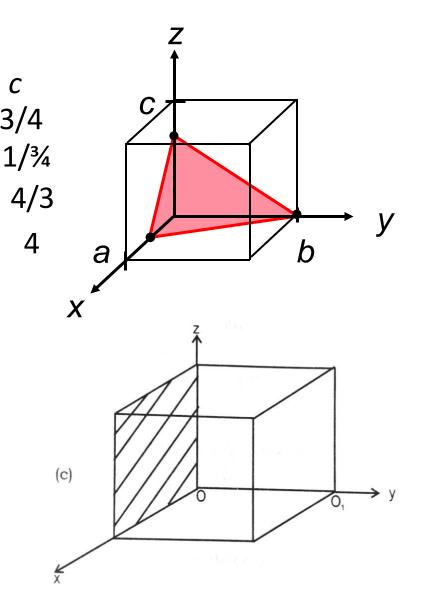
<u>example</u>		а	b	С
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110))	
<u>exar</u>	nple	а	b	С
<u>exar</u> 1.	<u>nple</u> Intercepts	а 1/2	$b \\ \infty$	с ∞
			~	-
1.	Intercepts	1/2	~	00
1.	Intercepts	1/2 1/½	∞ 1/∞	∞ 1/∞



Crystallographic Planes

<u>example</u> b a 1/2 1 3/4 Intercepts 1. Reciprocals 1/1/2 1/1 1/3/4 2. 2 1 Reduction 3. 6 3 (634)Miller Indices 4.

Origin to be moved from O to O₁ 1. $x = \infty, y = -1, z = \infty$ 2. $\frac{1}{x} = 0, \frac{1}{y} = -1, \frac{1}{z} = 0$ 3. No fractions to clear 4. $(0\overline{1}0)$

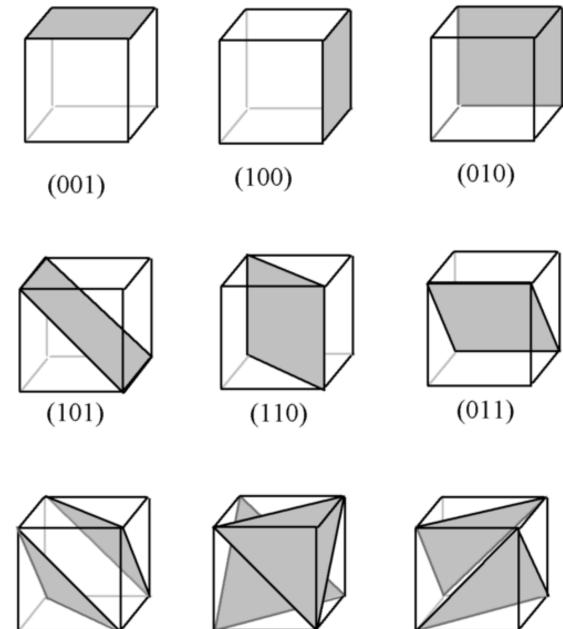


- Important aspects
 - Planes and their negatives are identical; (010) = (010)
 i.e a plane located at the same distance on the other side of origin
 - Planes and their multiples are not identical

Family of planes {110}

- In cubic system a plane and a direction having the same indices are perpendicular to each other. Hence the direction [110] is perpendicular to the plane (110) in a cubic unit cell.
- Parallel planes have the same Miller indices. Distance between two adjacent parallel planes with same Miller index (hkl) is called interplanar spacing. Interplanar spacing in cubic crystals is given by

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$



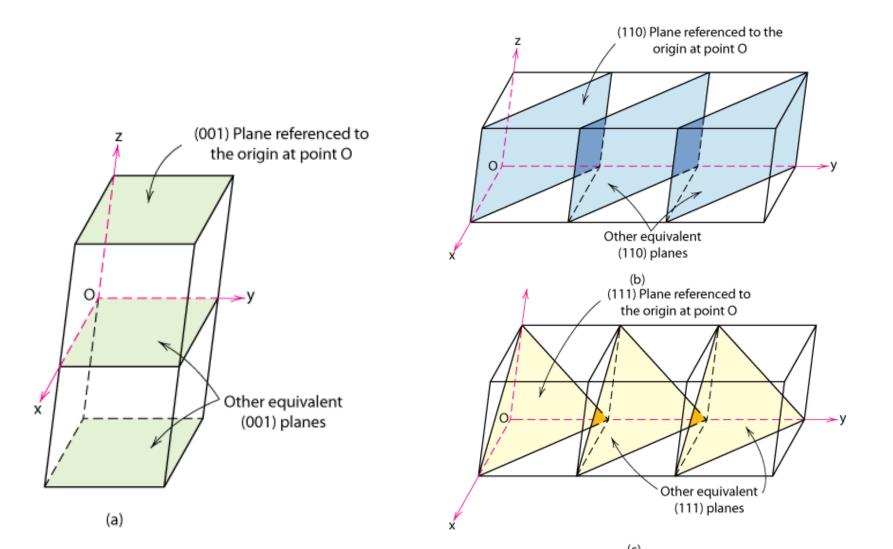
(111)

(111)

(111)

Family of Planes {*hkl*}

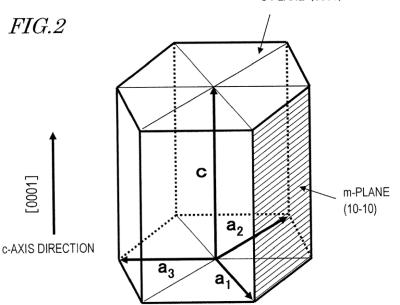
Ex: $\{100\} = (100), (010), (001), (\overline{1}00), (0\overline{1}0), (00\overline{1})$



Miller Bravais Indices

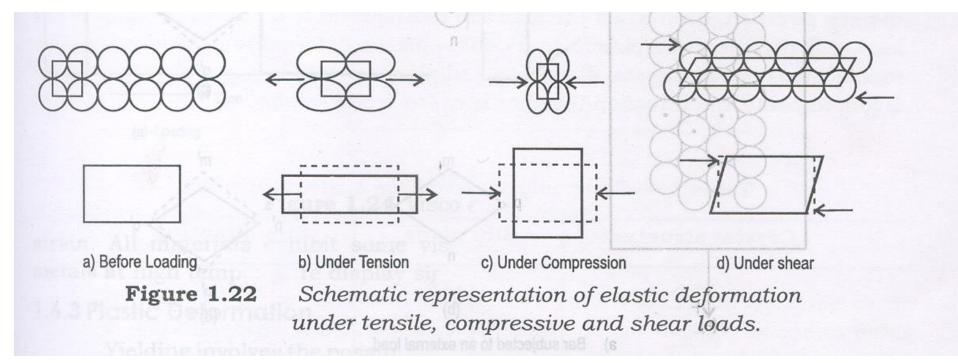
Planes and directions in hexagonal crystals are defined in terms of indices containing four digits instead of three. Theses are known as Miller Bravais Indices

➤ The four indices are designated as (h k i l) such that h+k=-i



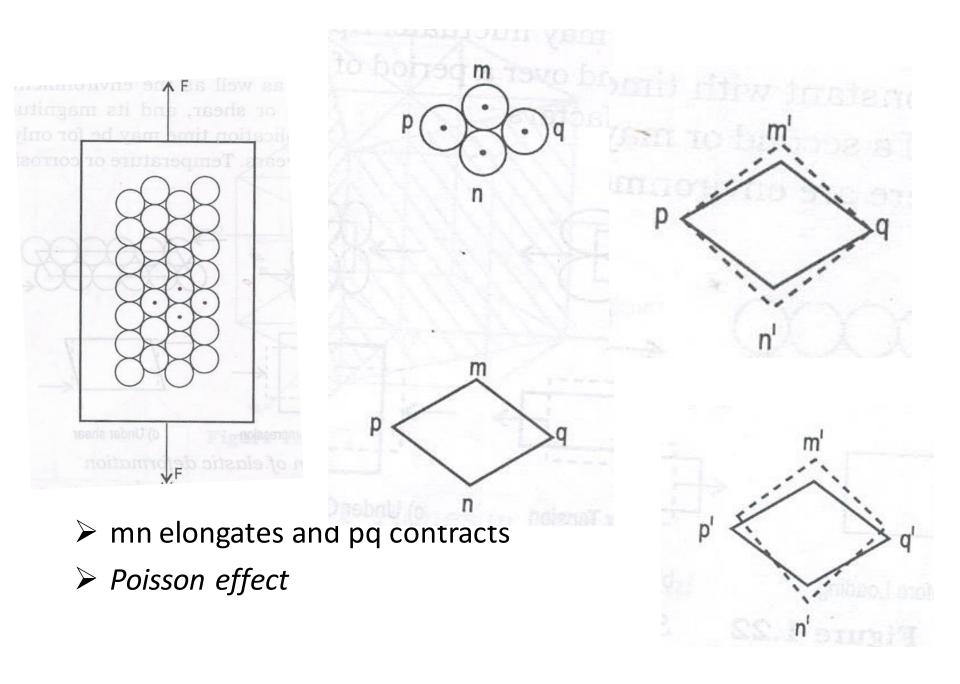
Deformation of Metals

- Deformation change in shape that take place in a material when subjected to an external force or load.
- Elastic (temporary) and plastic (permanent) deformation.
- Both take place due to adjustments or displacement in atomic arrangement.
- Applied load may be tensile, compressive or shear (constant or fluctuating)
- > Application time fraction of second or a period of years
- Environmental factors- temperature or corrosive atmosphere



Elastic deformation

- When a material is subjected to an applied force, atoms within the crystal are displaced from their normal positions of equilibrium deformation.
- This displacement will be just enough to develop attractive forces between the atoms to balance the applied load.
- > Elastic deformation in a solid bar (loaded axially in tension)
- Elastic deformation Displacement of atoms is by small amount removal of load allows atoms to return to their normal equilibrium positions – ie, REVERSIBLE



As the applied load increases and atoms are displaced further apart – end of elastic range

Deformation is no longer a simple separation of atoms

- inelastic

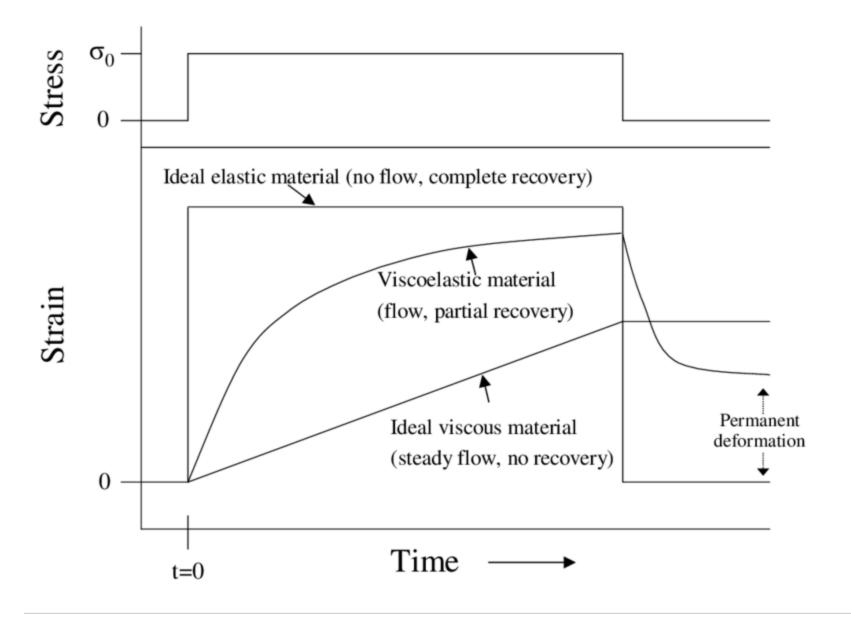
> Two possible ways by which elastic stage ends:

- by yielding
- by fracture
- BRITTLE —elastic range followed by fracture

Anelastic and Viscoelastic Behaviour

- > Elastic strain disappears as the applied load is removed.
- When a metal is strained plastically and when load is released elastic strain will recover immediately.
- However the strain remaining is not completely plastic strain
- Depending upon the metal and the temperature a small amount of plastic strain will disappear with time.
- This time dependent elastic behaviour is called *anelasticity* (very small in metals; neglected)

- A similar time dependent behaviour exhibited by some polymeric materials, wood and human tissue is called *viscoelasticity*
- It is the property of materials that exhibit both viscous and elastic characteristics.
- Elasticity is the result of stretching of atomic bonds along crystallographic planes in an ordered solid.
- Viscosity is the result of the diffusion of atoms or molecules inside an amorphous material
- Viscoelastic materials have elements of both these properties and exhibit time dependent strain...



Plastic Deformation

- Due to yielding, some of the atoms move to new equilibrium positions
- Atoms form new bonds in their new positions; hence material is not weakened and do not return to original positions
- > Thus the deformation is inelastic or irrecoverable
- Such a deformation is permanent, known as plastic deformation.
- > Two common mechanisms:
 - by Slip
 - > by **Twinning**...

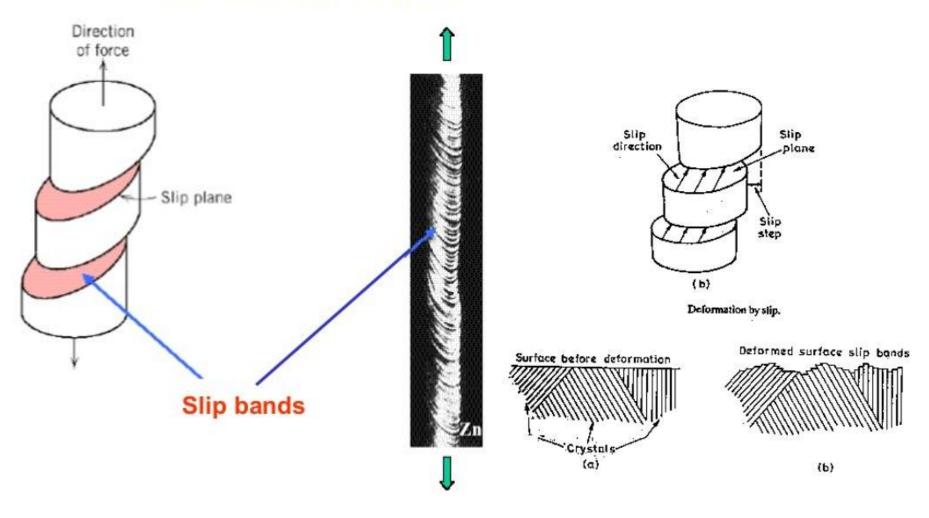
Plastic Deformation by Slip

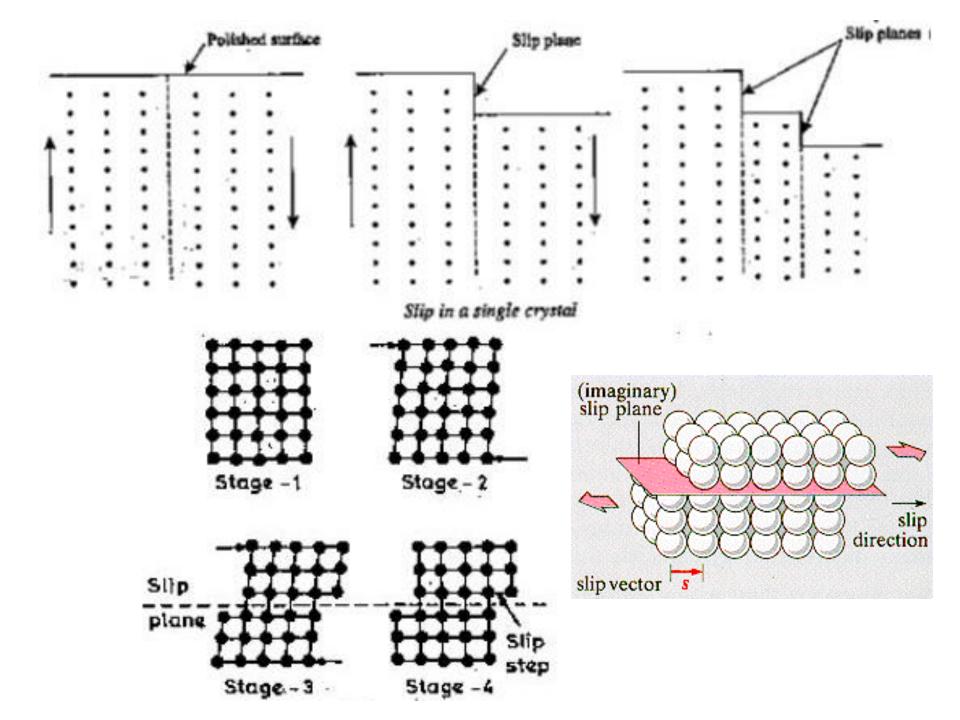


Metals are significantly weaker in shear

- Under the influence of a shear force atoms move relative to each other on certain planes from one position of equilibrium to another causing a permanent deformation
- Some atoms slip past the other atoms on a certain plane in a certain direction. This process is called slip
- > SLIP PLANE: the plane on which slip takes place
- > SLIP DIRECTION: directions along which atoms move
- Slip system: set of favoured plane and direction

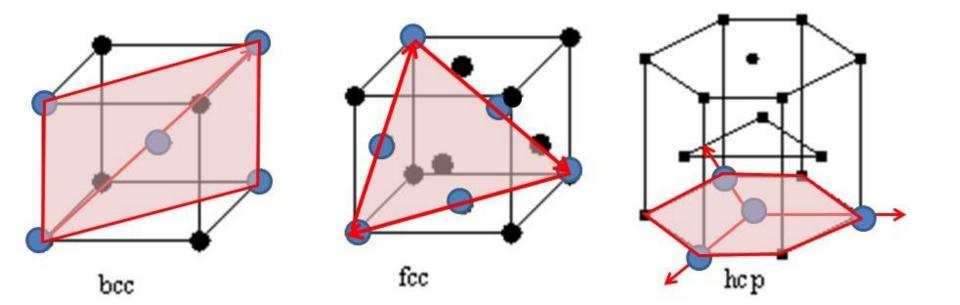
Slip in a Single Crystal





Commonly observed slip systems in Metals

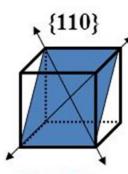
Crystal Structure	Slip Plane	Slip Direction
FCC	{111}	< 1 1 0 >
BCC	{110}	< 1 1 1 >
НСР	{0001}	< 1 1 2 0 >



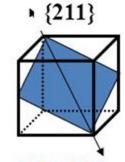
Slip system	Slip plane	Burgers vector	Schmid factor
1	(111)	[011]	0.816
2	(111)	[011]	0.816
3	$(\bar{1}\bar{1}1)$	[011]	0.816
4	$(1\bar{1}1)$	[011]	0.816
5	(111)	[101]	0.408
6	$(\bar{1}\bar{1}1)$	[101]	0.408
7	(111)	[101]	0.408
8	$(1\bar{1}1)$	[10]	0.408
9	(111)	[110]	0.408
10	$(1\bar{1}1)$	[110]	0.408
11	$(\overline{1}\overline{1}1)$	[110]	0.408
12	(111)	[110]	0.408

Slip systems in crystals

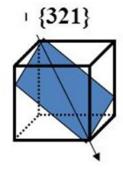
• BCC



 α Fe, Mo, W, β brass

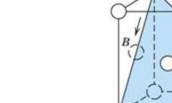


αFe, Mo, W, Na

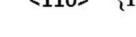


 α Fe, K



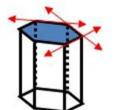


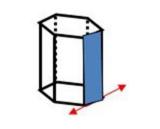
(110) (111)



<110> {111}







 $\Theta_{\underline{E}}$

U.

<11-20>(10-11)

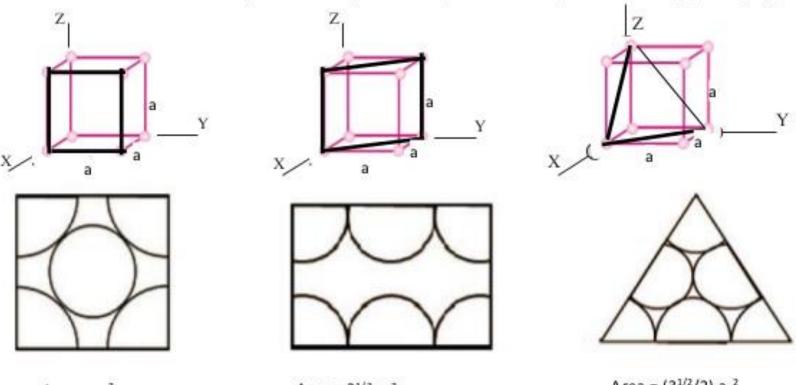
<11-20>(10-10)

<11-20>{0001}

Planar Packing Density of Atoms – FCC

Planar packing density - number atoms within plane / unit area of plane Count fractions of circle area on plane only when atom centers sit exactly on plane Ex.- For FCC give planar packing density on (100); (110); (111)

Label dimensions of areas shown, fill in atoms, calculate planar density in terms of a₀ (atoms/a₀²).



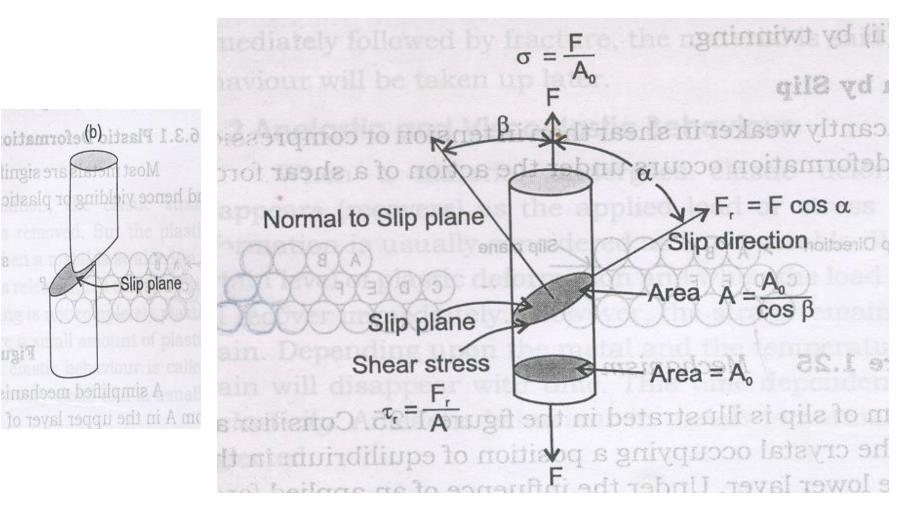
 $Area = a_0^2$

Area = $2^{1/2} a_0^2$

Area = $(3^{1/2}/2) a_0^2$

а

Schmid's law



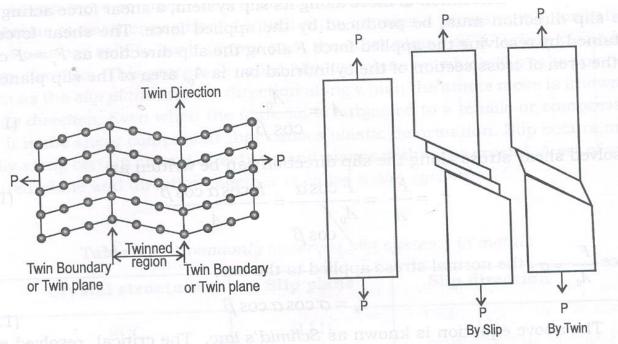
Shear Force, $F_r = F \cos \alpha$ Area of slip plane, $A = A_0$ $\cos \beta$

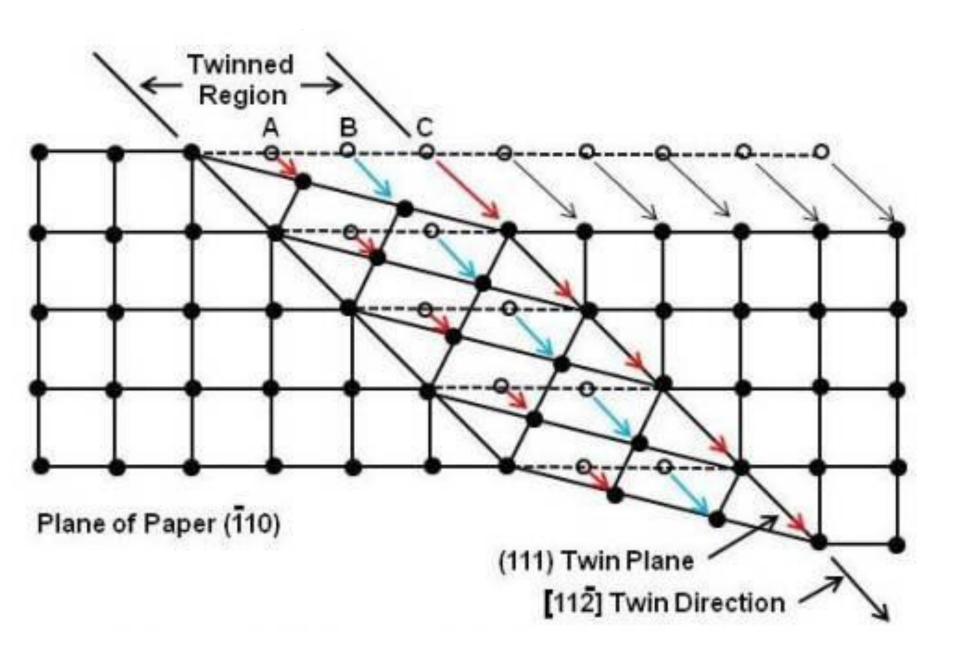
Resolved shear stress,
$$\tau_r = \frac{F_r}{A}$$

$$= \frac{F \cos \alpha \cos \beta}{A_0}$$
$$\tau_r = \sigma \cos \alpha \cos \beta \quad (Schmid's Law)$$

 F/A_0 $_{=}\sigma$, the normal stress applied to the bar

Plastic Deformation by Twinning

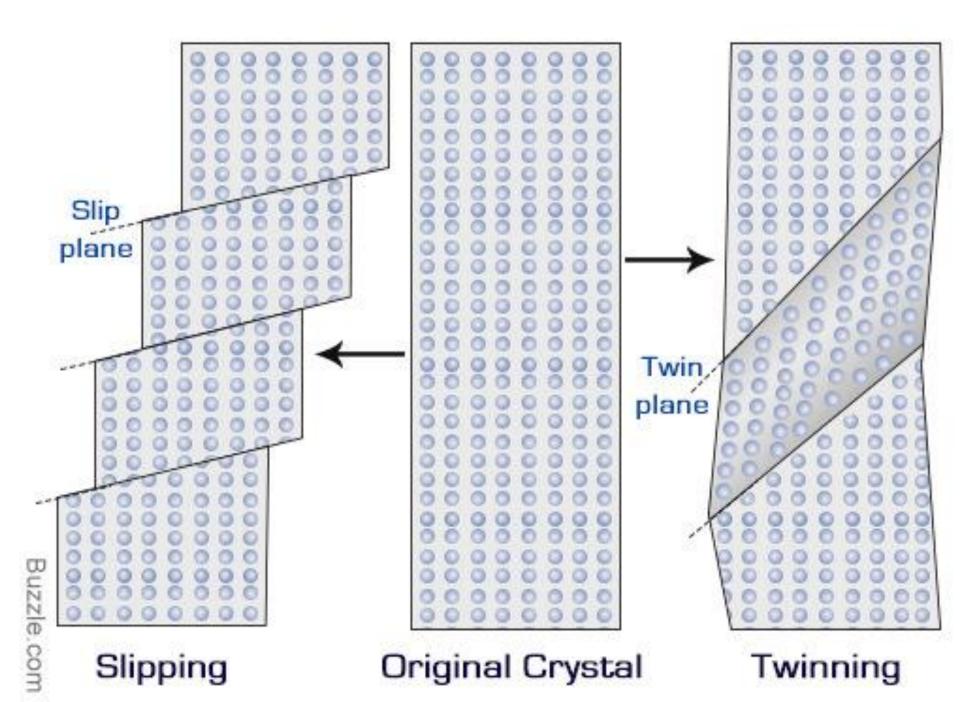




Plastic Deformation by Twinning

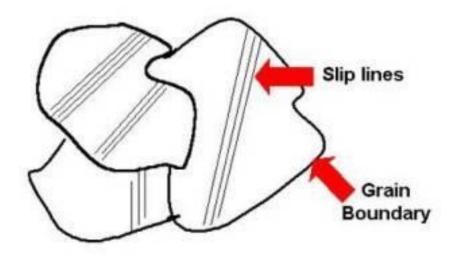
- In certain materials, when a shear stress is applied, planes of atoms in the lattice move parallel to a specific plane so that the lattice is divided into two symmetrical parts which are differently oriented. This phenomenon is known as Twinning
- Twinning plane: the planes parallel to which atomic movement has taken place
- Twinned region: differently oriented region within the crystal and the twinning planes
- > Twinning is produced suddenly and is accompanied with sound

- In both slip and twinning, lattice is sheared
- In slip, shear is uniformly distributed over a volume rather than localised on a discrete no of slip planes
- Twinning atoms move only a fraction of interatomic distance relative to each other
- The amount of movement of each plane of atoms in the twinned region is proportional to its distance from the twinning plane – Mirror image
- > Twinning is common in HCP crystals.
- During twinning the lattice over the twinned regions may get favourably oriented for slip w.r.t the applied load.
- Thus under certain conditions a twinned metal can be more easily deformed by slip

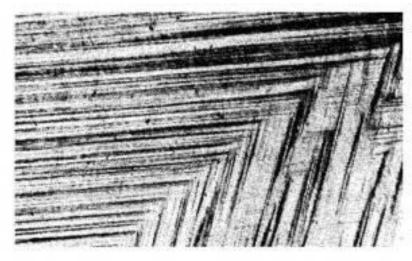


Slip	Twinning
Slip involves sliding movement of atoms on slip planes.	Twinning involves displacive movement of atoms relative to each other on many planes.
Orientation of crystals above and below slip plane before and after slip is the same.	Orientation on either side of the twinning plane are different. Twinned region is the mirror image of the original lattice.
Atomic movements are of one or more atomic spacing.	Atomic movements are a fraction of atomic spacing.
Through microscope slip appears as thin lines.	Twinning appears as broad lines or bands.
Slip is initiated even at lower stress values.	Twinning requires higher stresses.
A minimum value of stress called critical shear stress is required for slip to take place.	For twinning there is no such minimum value.
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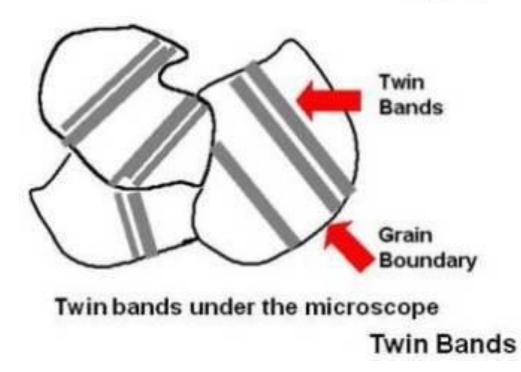
Slip	Twinning
Observed in all types of crystal lattices	More significant in HCP crystals.
Steps formed by slip are visible only on the surface. If steps are removed by polishing, no evidence remains.	
Slip lines may be present in even or odd numbers.	Twin lines always occur in pairs.



Slip appears as thin lines under the microscope Slip Lines

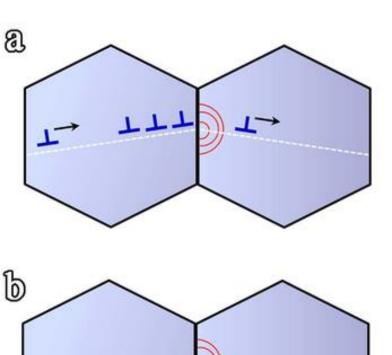


Slip lines in copper

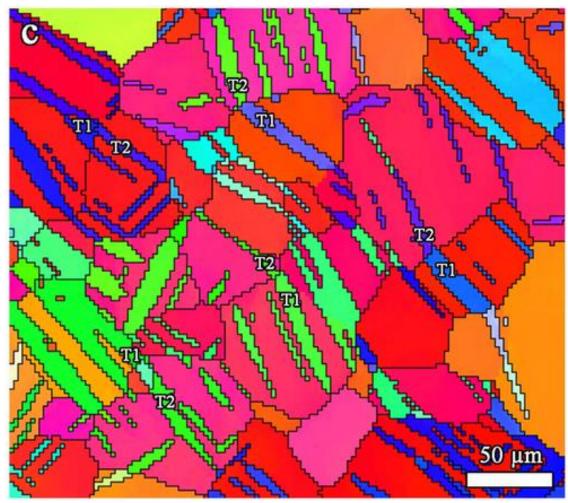




Twin bands in zinc



M



Brittleness of BCC, HCP and ductility of FCC

- When stressed some materials undergo extensive plastic deformation Ductile
- Some break up suddenly with very less or no plastic deformation Brittle
- > In crystalline materials dominant mode of plastic deformation is

slip – dependant on available no: of slip systems

Slip occurs easily on <u>planes and in directions</u> of maximum atomic density – easy slip systems > In FCC, $\{111\}$ and < 110 > have max: atomic density -12

easy slip systems available

Atleast one slip system oriented in a favourable position for slip to take place

Hence slip and thereby plastic deformation is initiated easily in FCC crystals

> Materials having FCC structure are therefore ductile in nature

- BCC crystals also have 12 easy slip systems with { 1 1 0 } and < 1 1 1 >
- However the { 1 1 0 } planes of BCC have lesser atomic density compared to the { 1 1 1 } planes of FCC
- Therefore stress required is high in BCC
- So BCC materials are less ductile (plastic) compared to FCC
- In HCP, basal planes { 0 0 0 1 } and < 1 1⁻² 0 > have maximum atomic density
- > Only 3 easy slip systems are available in HCP
- Hence HCP materials are normally brittle
- "Less common slip systems" are also available in these crystals
- Become operative at higher stresses or at higher temperatures.

Correlation of slip system with slip in metals

- The value of critical stress varies from material to material depending upon the strength of interatomic bond
- Within a material the value varies with the slip system depending upon the atomic density on the slip plane and in the slip direction
- Hence for a given material critical stress values are different for different slip systems

$$T_r = \sigma \cos \alpha \cos \beta$$

value of τ_r depends on:

value of applied stress, σ

The angles α and β

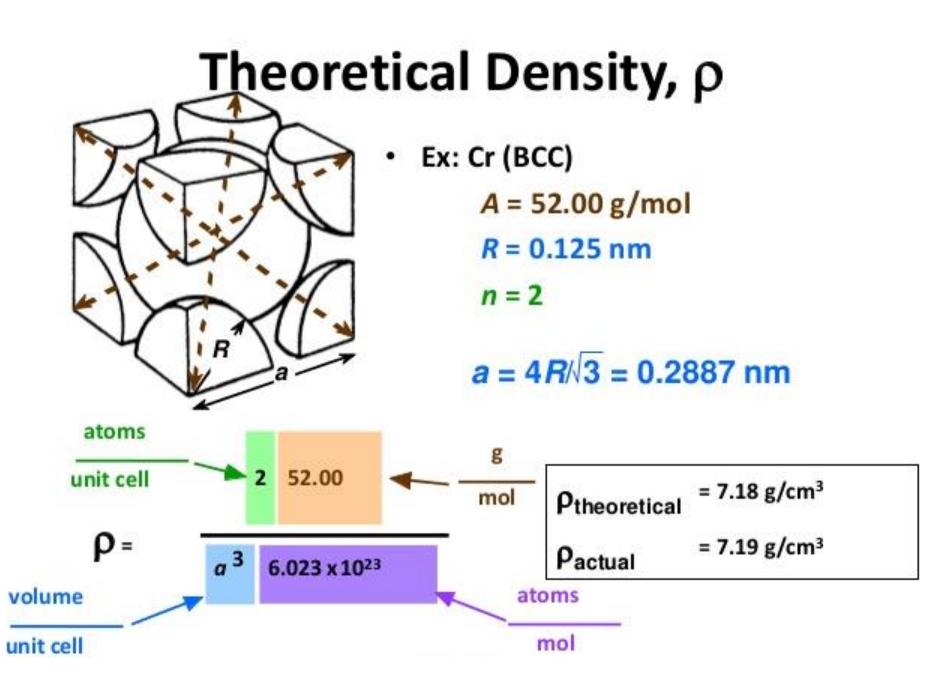
- For a given direction of the applied stress some slip systems will be favourably oriented for slip to be initiated
- On such a plane slip will take place when the value of resolved shear stress equals the value of critical resolved shear stress for that slip system
- As applied stress is increased from zero deformation will be initiated on that slip plane and along that slip direction for which resolved shear stress is maximum and so reaches critical value first.
- > Thus it is seen that slip and thereby plastic deformation within crystal structures is dependent on type of slip systems and their orientation with

the direction of **applied stress**

Theoretical Density, p

Density = ρ = $\frac{Mass of Atoms in UnitCell}{Total Volume of UnitCell}$ $\rho = \frac{n A}{V_c N_A}$

where n = number of atoms/unit cell A = atomic weight V_c = Volume of unit cell = a³ for cubic N_A = Avogadro's number = 6.023 x 10²³ atoms/mol



- Radius ratio
- $\frac{r_c}{r_a}$
- r_c = radius of cation
- $r \square a$ = radius of anion