

## SI Prefixes

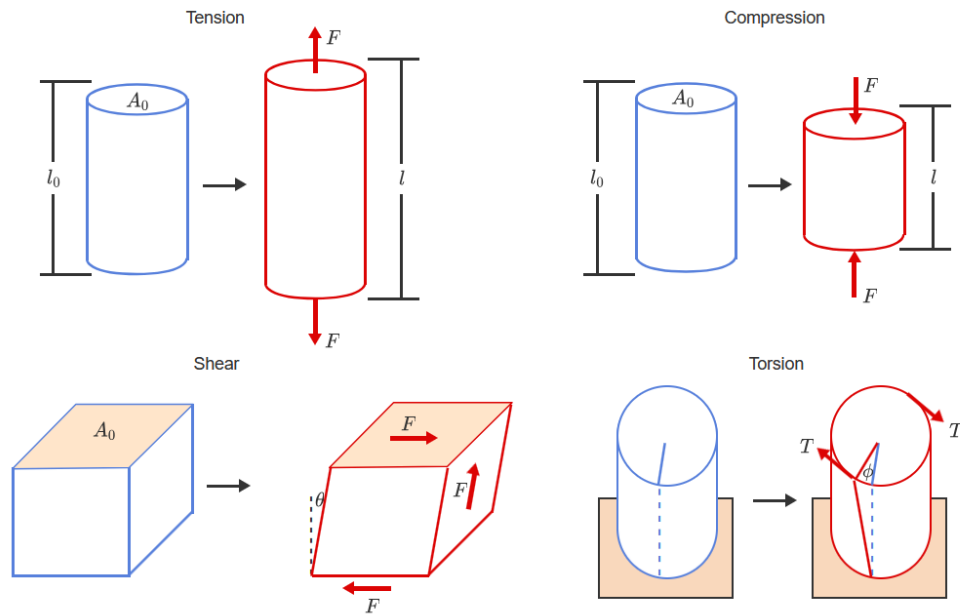
femto (f)	$= 10^{-15}$
pico (p)	$= 10^{-12}$
nano (n)	$= 10^{-9}$
micro ( $\mu$ )	$= 10^{-6}$
milli (m)	$= 10^{-3}$
centi (c)	$= 10^{-2}$
deci (d)	$= 10^{-1}$
deca (da)	$= 10^1$
hecto (h)	$= 10^2$
kilo (k)	$= 10^3$
mega (M)	$= 10^6$
giga (G)	$= 10^9$
tera (T)	$= 10^{12}$
peta (P)	$= 10^{15}$

Note: 1Angstrom ( $\text{\AA}$ )  $= 10^{-10}$  m

# Mechanical Properties

## Stress and Strain

### Types of loading



## Stress (Force Normalized by Area)

Tensile and Compression Stress

$$\sigma = \frac{F}{A_o} \quad (\text{in units of pressure})$$

Shear Stress

$$\tau = \frac{F}{A_o}$$

## Strain (Displacement Normalized by Original Length)

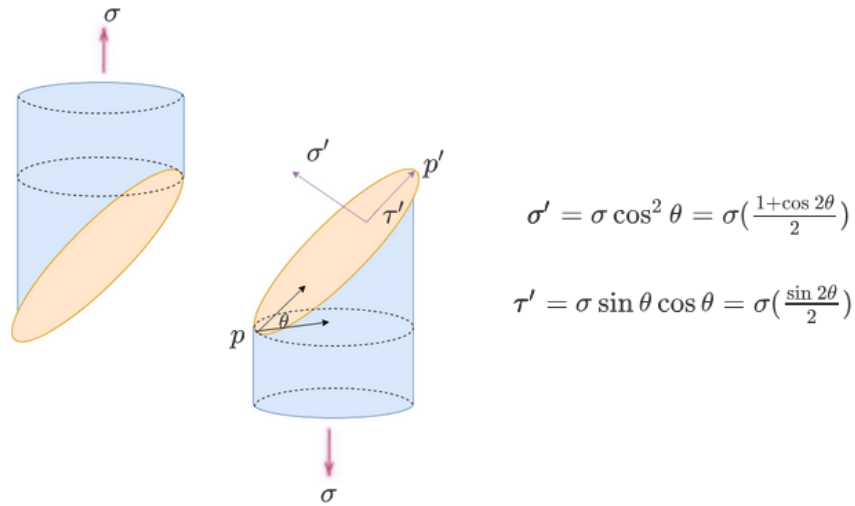
Tensile and Compression Strain

$$\epsilon = \frac{l - l_0}{l_0}$$

Shear Strain

$$\gamma = \tan \theta \quad (\theta \text{ is the shear angle})$$

## Normal and Shear Stress Along an Angled Plane



# Elastic Deformation

## Relationship Between Stress and Strain

Tensile and Compression

$$\sigma = E\epsilon \quad (E \text{ (GPa or psi) is the modulus of elasticity})$$

Shear

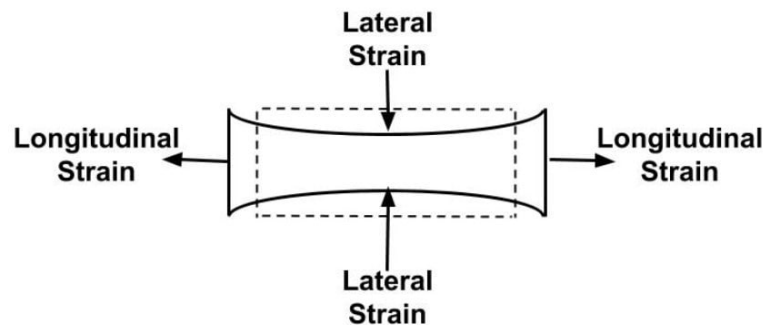
$$\tau = G\gamma \quad (G \text{ is the shear modulus})$$

Note: The modulus of elasticity (Young's modulus) is the slope of the stress - strain plot. (It describes a material's resistance to elastic deformation. Stiffer  $\implies$  higher E)

**Anelasticity:** time dependent elastic strain, where deformation and recovery is not instantaneous.

**Viscoelastic behavior:** materials (such as polymers) with significant anelasticity

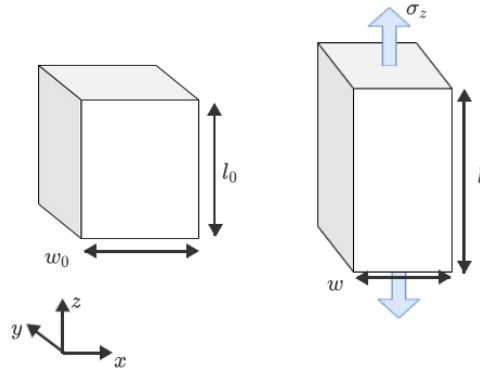
## Poisson's Ratio



$$\nu = -\frac{\epsilon_{\text{lateral}}}{\epsilon_{\text{longitudinal}}}$$

Note: Lateral is perpendicular to the direction of loading and longitudinal is along the direction of loading

Example: Rectangular prism



If the applied stress is uniaxial (only along 1 axis) and the material is isotropic (constant properties regardless of direction), then for a  $\sigma_z$ ,  $\epsilon_x = \epsilon_y$

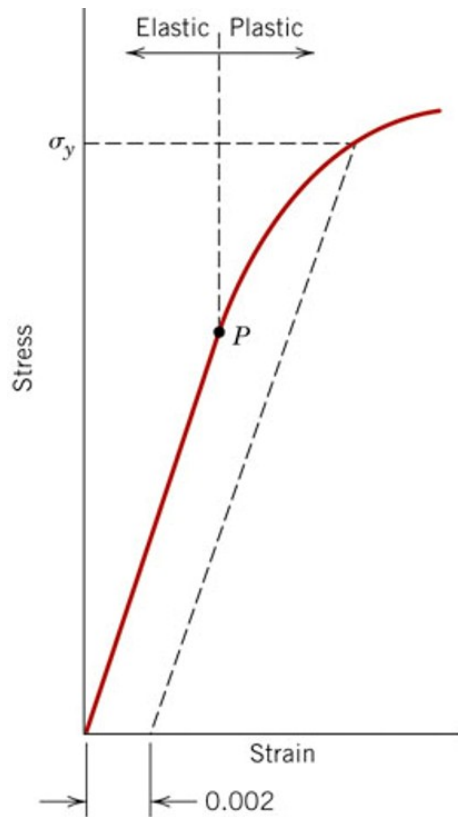
$$\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$$

**Relating modulus of elasticity, shear modulus and Poisson's ratio**

$$E = 2G(1 + \nu)$$

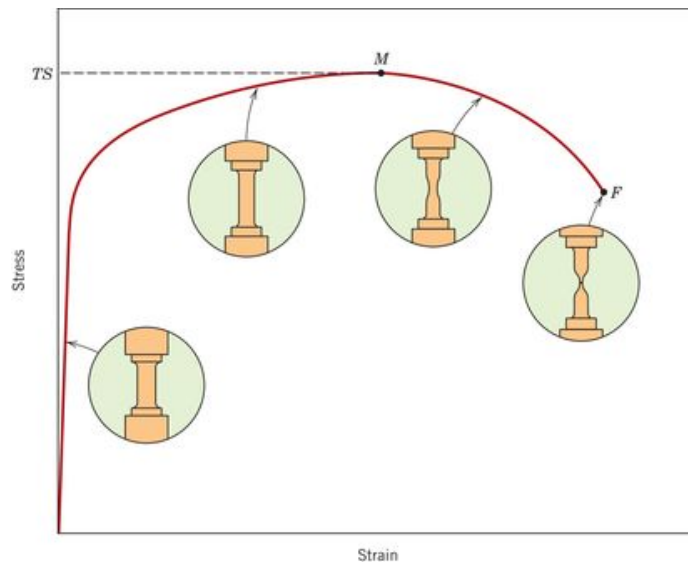
Note: Some materials (like foams) expand under tension so they have a negative Poisson's ratio, these materials are called **auxetics**.

# Plastic Deformation



Point P is the **Proportional Limit** where the exact departure from linearity occurs and deformation becomes permanent.

**Yield Stress ( $\sigma_y$ ):** stress at which noticeable strain has occurred (0.002)



**Tensile Strength:** Stress at the maximum point on the stress - strain plot. After this point, necking occurs and all deformation is focused at the neck until fracture (point F)

## Ductility

As % elongation:

$$\%EL = \frac{l_f - l_0}{l_0} \times 100$$

As % reduction in area

$$\%RA = \frac{A_0 - A_f}{A_0} \times 100$$

$l_f$  and  $A_f$  are length and cross sectional area of sample at fracture respectively.

**Resilience:** capacity of a material to absorb energy when it is deformed elastically and unloaded (similar to spring potential energy)

## Modulus of Resilience

$$U_r = \int_0^{\epsilon_{yield}} \sigma d\epsilon$$

Area under the stress - strain plot from 0 to yield point

Assuming a linear elastic region:

$$U_r = \frac{1}{2} \sigma_y \epsilon_y$$

# Crystal Structures

## Atomic Packing Factor

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

## Packing Fraction

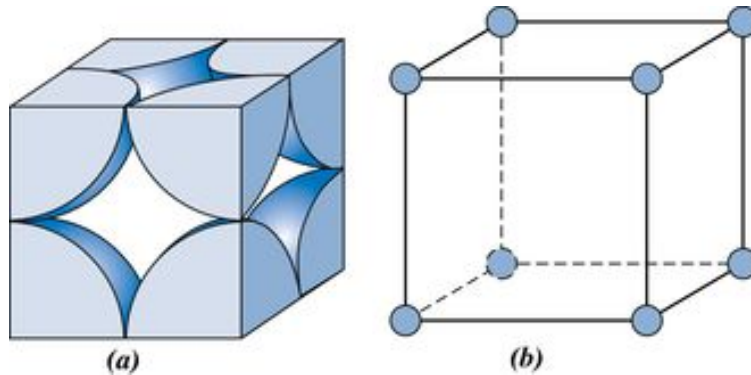
$$PF = \frac{\text{Total Cross Sectional Area of Atoms}}{\text{Total Area of Plane}}$$

## Number of Atoms per Unit Cell

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

$N_i$  are interior atoms,  $N_f$  are face atoms and  $N_c$  are corner atoms

## Simple Cubic



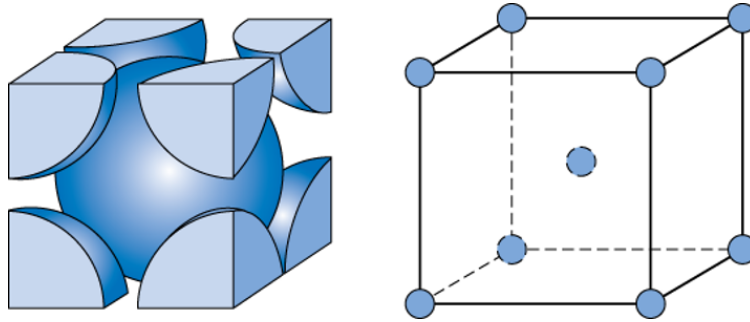
$$2R = a$$

$$APF = \frac{(\# \text{ atoms})(\text{volume/atom})}{(\text{volume/unit cell})}$$

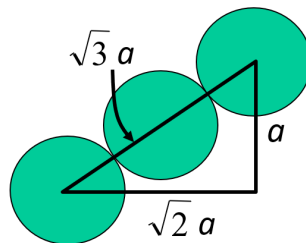
$$APF = \frac{(1)(\frac{4}{3}\pi(a/2)^3)}{a^3}$$



# Body Centered Cubic



Triangle formed along the main diagonal and face diagonal

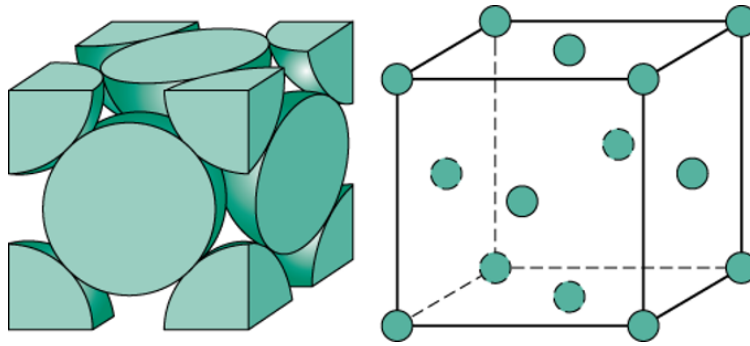


$$4R = \sqrt{3}a$$

$$APF = \frac{(\# \text{ atoms})(\text{volume/atom})}{(\text{volume/unit cell})}$$

$$APF = \frac{(2)(\frac{4}{3}\pi(\frac{\sqrt{3}}{4}a)^3)}{a^3}$$

## Face Centered Cubic



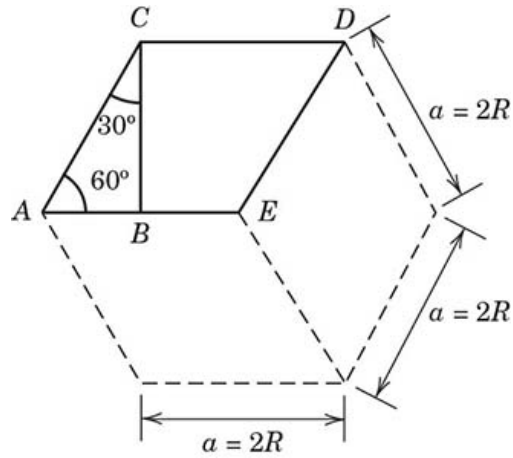
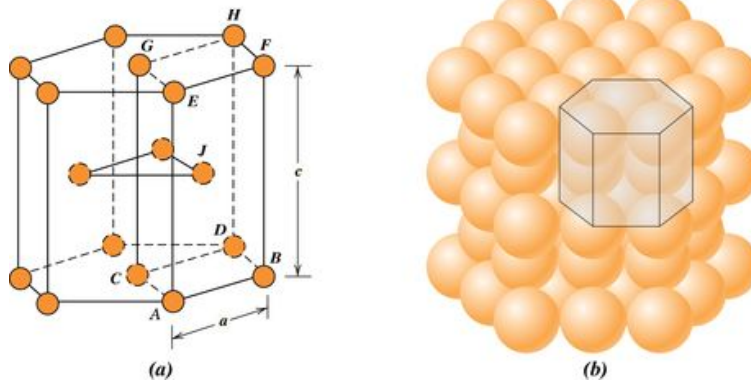
Along the face diagonal:

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

$$APF = \frac{(\# \text{ atoms})(\text{volume/atom})}{(\text{volume/unit cell})}$$

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

# Hexagonal Close Packed



Area of base hexagon is 3 parallelograms or 6 equilateral triangles:

$$\text{Area} = \frac{3a^2\sqrt{3}}{2}$$

Given height  $c$ :

$$\text{Volume of unit cell} = \frac{3a^3\sqrt{3}}{2}$$

# Theoretical Density for Crystals

$$\rho = \frac{(\text{atoms/unit cell})(\text{g/mol})}{(\text{vol/unit cell})(\text{atoms/mol})} = (\text{g/vol})$$

$$\rho = \frac{nA}{V_c N_A}$$

Where:

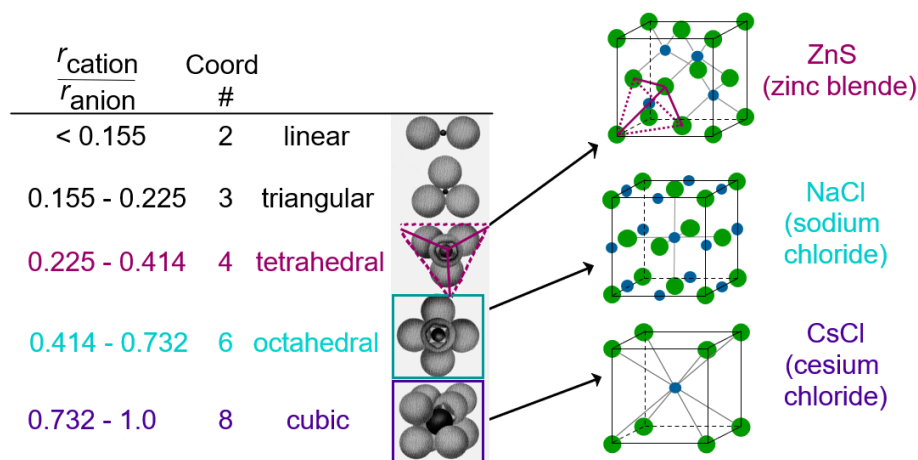
- $n$  = # of atoms in unit cell
- $A$  = atomic weight
- $V_c$  = volume of unit cell
- $N_a$  = Avogadro's number ( $6.022 \times 10^{23}$  atoms/mol)

## Ceramic Crystal Structures

Factors that determine crystal structure:

- Relative sizes of ions ( $\frac{r_{\text{cation}}}{r_{\text{anion}}}$ )
- Maintenance of charge neutrality (Net charge in ceramic is zero)

Note: As  $\frac{r_{\text{cation}}}{r_{\text{anion}}}$  increases, so does coordination number



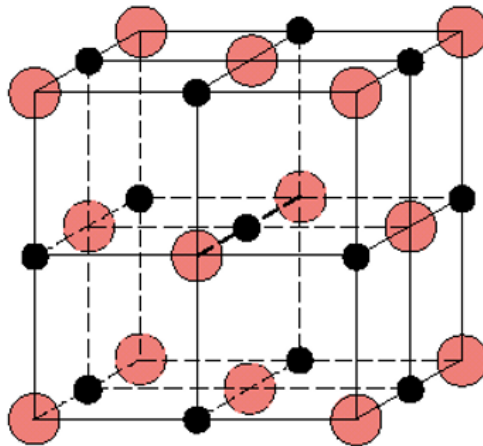
## Theoretical Density for Ceramics

$$\rho = \frac{n'(\sum A_C + \sum A_A)}{V_c N_A}$$

Where:

- $n' = \#$  of Atoms per unit cell (For AX structures, this is equal for cations and anions)
- $\sum A_A =$  sum of cation molar mass
- $\sum A_C =$  sum of anion molar mass
- $V_c =$  volume of unit cell
- $N_A =$  Avogadro's number ( $6.022 \times 10^{23}$  atoms/mol)

## Rock Salt Structure

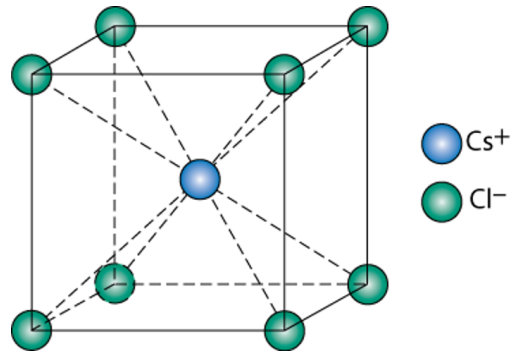


Note: Cations prefer octahedral sites (in black)

Along the edges:

$$2R_A + 2R_C = a$$

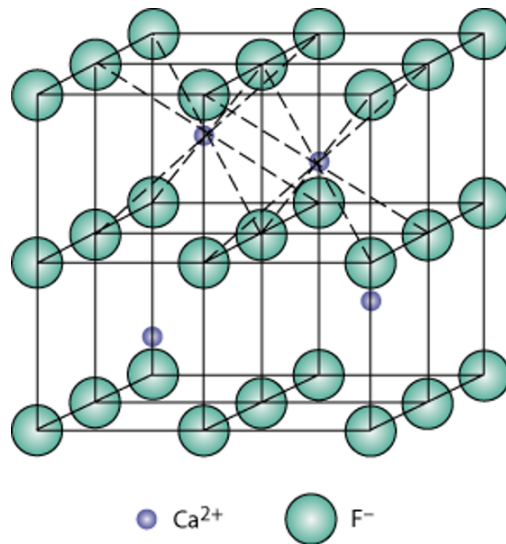
## AX Crystal Structure (Cesium Chloride)



Note: Cations prefer cubic sites (Body Center, in blue)  
Across the main diagonal:

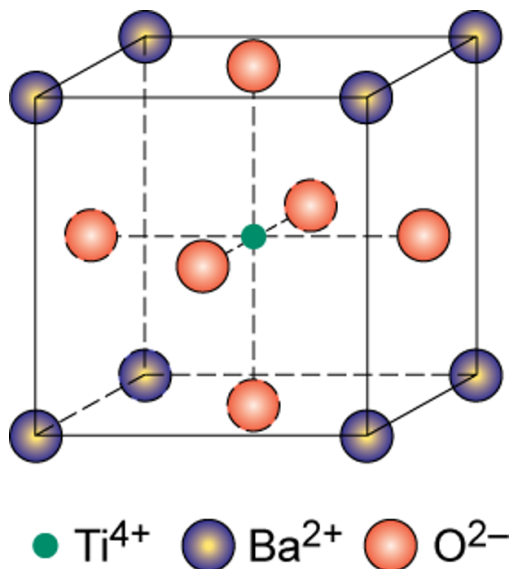
$$2R_A + 2R_C = \sqrt{3}a$$

## AX<sub>2</sub> Crystal Structures (Flourite)



Note: Cations prefer cubic sites (Body Center, in blue)  
There are half as many Ca<sup>2+</sup> as F<sup>-</sup> (for CaF<sub>2</sub>)

## ABX<sub>3</sub> Crystal Structure (Perovskite)



## Point Coordinates

To find the coordinate indices (q,r,s), find the cartesian coordinates and divide by the corresponding lattice parameter

$$(q, r, s) = \left( \frac{x}{a}, \frac{y}{b}, \frac{z}{c} \right)$$

## Crystallographic Directions

How to define:

- Position vector to pass through origin
- Read off projections onto coordinate axes in terms of lattice parameters (a,b,c)
- Multiply through by common denominator
- Enclose in square brackets without commas, negatives go on top (ex:  $[\bar{1}23]$ )

How to read  $[123]$ :

- Divide by the common denominator used previously (say 6)
- Vector in cartesian:  $(1/6, 1/3, 1/2)$

# Crystallographic Planes

How to define with Miller indices:

- Define any origin
- Read intercepts of the plane with the coordinate axes in terms of lattice parameters (a,b,c)
- Take reciprocals of intercepts
- Enclose in parenthesis without commas, negatives go on top (ex:  $(\bar{1}23)$ )

How to read:

- Take reciprocals of plane to identify intercepts

## Linear and Planer Density

**Linear Density**

$$LD = \frac{\text{Number of atom centered on line}}{\text{Unit length of direction vector}}$$

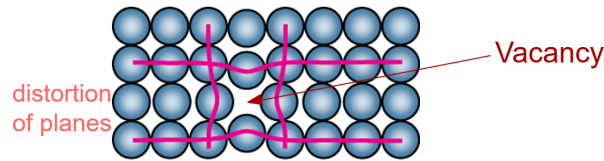
**Planer Density**

$$PD = \frac{\text{Number of atoms centered on plane}}{\text{Area of plane}}$$

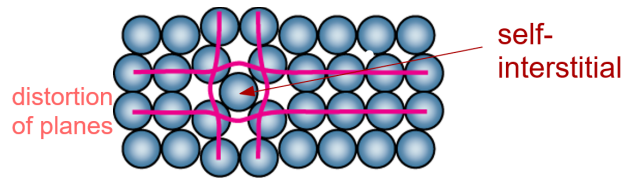


# Point Defects

- Vacancies: Missing atoms in the lattice



- Interstitials: Extra atoms positioned between lattice sites



## Equilibrium Concentration of Vacancies

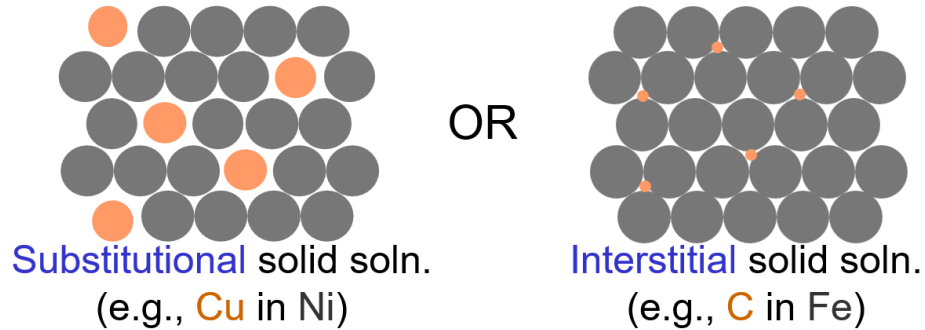
$$N_v = N e^{\left(\frac{-Q_v}{kT}\right)}$$

Where:

- $N_v$  = number of vacancies
- $N$  = total number of atomic sites (each lattice site can be occupied by an atom or be a vacancy)
- $Q_v$  = activation energy required to form a vacancy (J or eV)
- $k$  = Boltzmann's constant ( $8.617 \times 10^{-5}$  eV/atom-K)
- $T$  = temperature (K)

# Alloys

Alloys are solid solutions of an impurity element (solute) dissolved in a base element (solvent). There are two types:



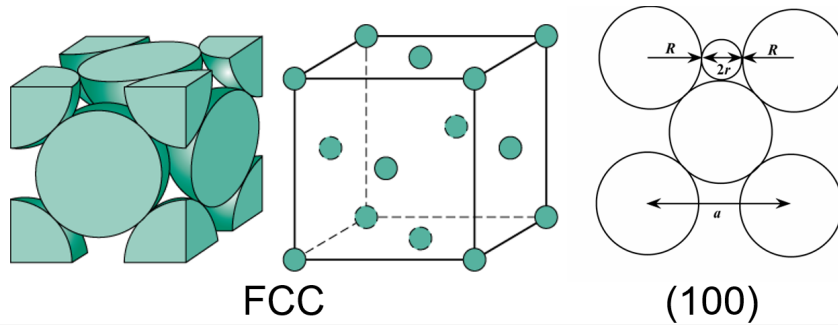
## Hume-Rothery rule

Conditions for forming a solid solution:

- Atomic radii must be within 15% of each other ( $\Delta r < 0.15\%$ )
- Electronegativity values must be similar (ie. Close together on the periodic table)
- Crystal structures of solvent and solute must be the same (for pure metals)
- Valencies should be similar (All else being equal, a metal will have a greater tendency to dissolve a metal of higher valency than one of lower valency)

## Maximum Radius for an Interstitial Impurity

### FCC

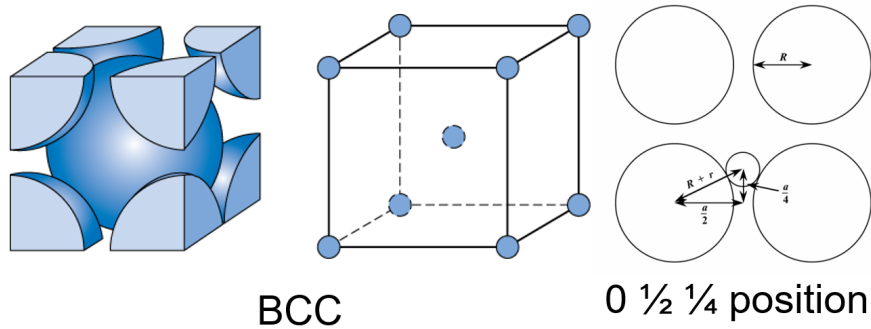


$$2r + 2R = a$$

$$r = \frac{a - 2R}{2}$$

$$r = \frac{2R\sqrt{2} - 2R}{2} = 0.41R$$

### BCC



$$\left(\frac{a}{2}\right)^2 + \left(\frac{a}{4}\right)^2 = (R + r)^2$$

$$\left(\frac{4R}{2\sqrt{3}}\right)^2 + \left(\frac{4R}{4\sqrt{3}}\right)^2 = R^2 + 2Rr + r^2$$

$$r^2 + 2Rr - 0.667R^2 = 0$$

$$\Rightarrow r = \frac{-2R \pm \sqrt{(2R)^2 - 4(1)(-0.667R^2)}}{2(1)}$$

$$r = 0.291R$$

# Specification of composition

## Weight Percent

$$C_1 = \frac{m_1}{m_1 + m_2} \times 100$$

Where

- $C_1$  = weight percent of element 1
- $m_1$  = mass of element 1
- $m_2$  = mass of element 2

## Atomic Percent

$$C'_1 = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100$$

Where

- $C'_1$  = atomic percent of element 1
- $n_{m1}$  = number of moles of element 1
- $n_{m2}$  = number of moles of element 2

Note:

$$n_{m1} = \frac{m_1(\text{grams})}{A_1(\text{g/mol})}$$

## Conversion between wt% and at%

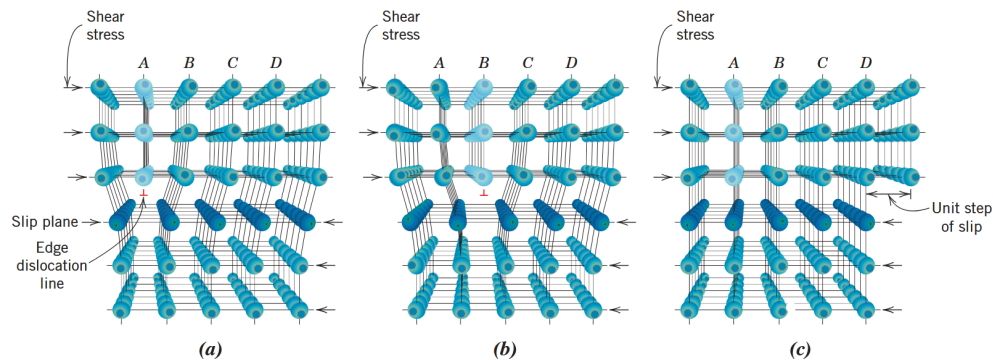
$$C'_1 = \frac{C_1 A_2}{C_1 A_2 + C_2 A_1} \times 100$$

Where  $A_1$  and  $A_2$  are the atomic weights of elements 1 and 2 respectively

# Line Defects

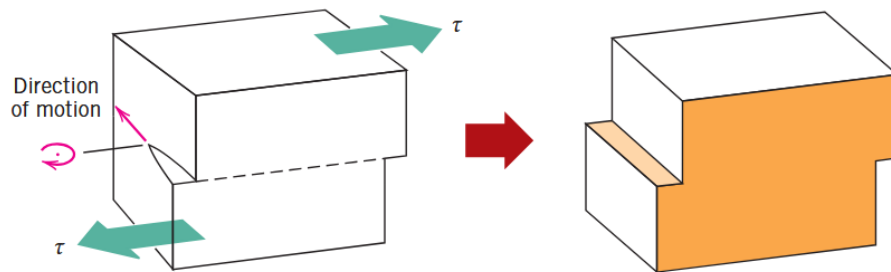
Dislocations are line defects. It occurs when there is slipping between crystal planes when dislocations move and they cause permanent (plastic) deformation. There are two main types:

- **Edge Dislocation**



This occurs when an extra half plane of atoms is inserted in a crystal and moves when shear stress is applied. The direction of movement is parallel to the applied shear stress.

- **Screw Dislocation**



The direction of movement is perpendicular to the applied shear stress.

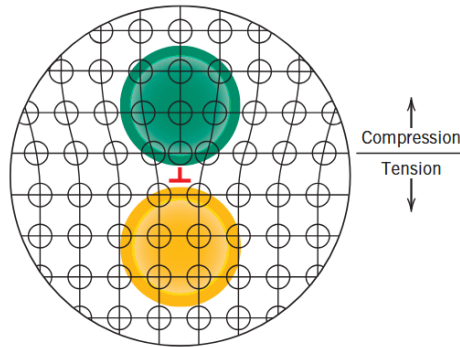
Plastic deformation occurs due to many dislocations. The process by which plastic deformation is produced by dislocation motion is termed **slip**; the crystallographic plane along which the dislocation line traverses is the **slip plane**.

All metals and alloys contain dislocations formed during solidification. The **solidification density** is the number of dislocations per unit volume in a material.

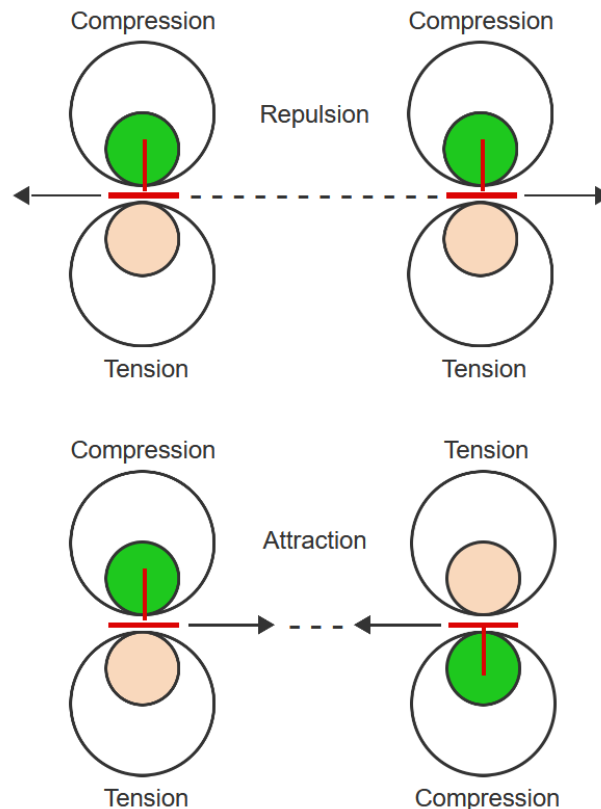
## Characteristics of dislocations

Due to the presence of an extra half plane of atoms, there exists regions of compressive, tensile, and shear **lattice strains** around the dislocation line.

Ex:



These lattice strains interact in the following ways:



The attractive forces will result in the half planes merging into a complete plane, eliminating the dislocation. The repulsive forces will make it more difficult for dislocations to move. The number of dislocations increases dramatically during plastic deformation because of multiplication of existing dislocations, grain boundaries, internal defects, and surface irregularities.