

## SI Prefixes

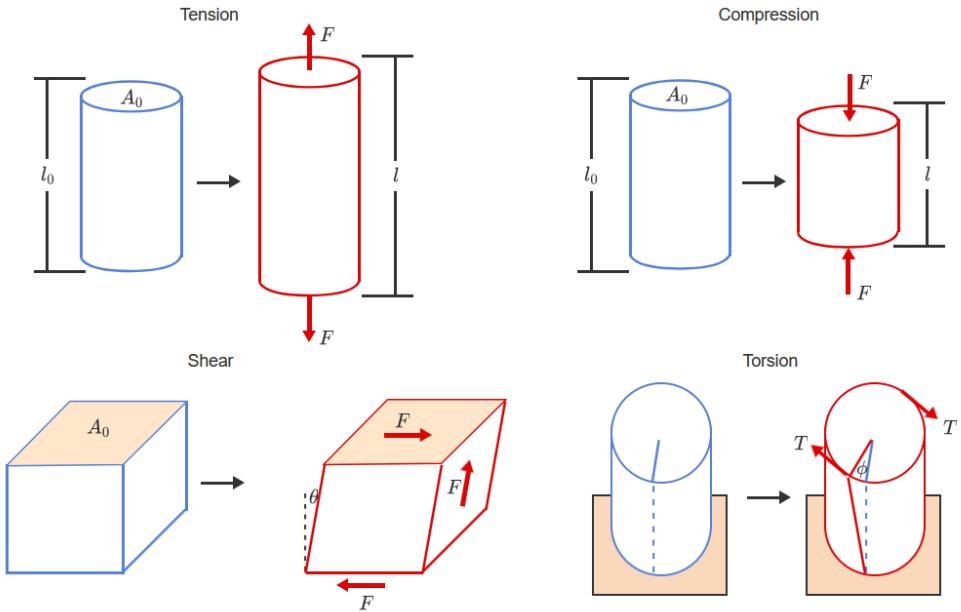
femto (f)	$= 10^{-15}$
pico (p)	$= 10^{-12}$
nano (n)	$= 10^{-9}$
micro ( $\mu$ )	$= 10^{-6}$
milli (m)	$= 10^{-3}$
centi (c)	$= 10^{-2}$
deci (d)	$= 10^{-1}$
deca (da)	$= 10^1$
hecto (h)	$= 10^2$
kilo (k)	$= 10^3$
mega (M)	$= 10^6$
giga (G)	$= 10^9$
tera (T)	$= 10^{12}$
peta (P)	$= 10^{15}$

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)

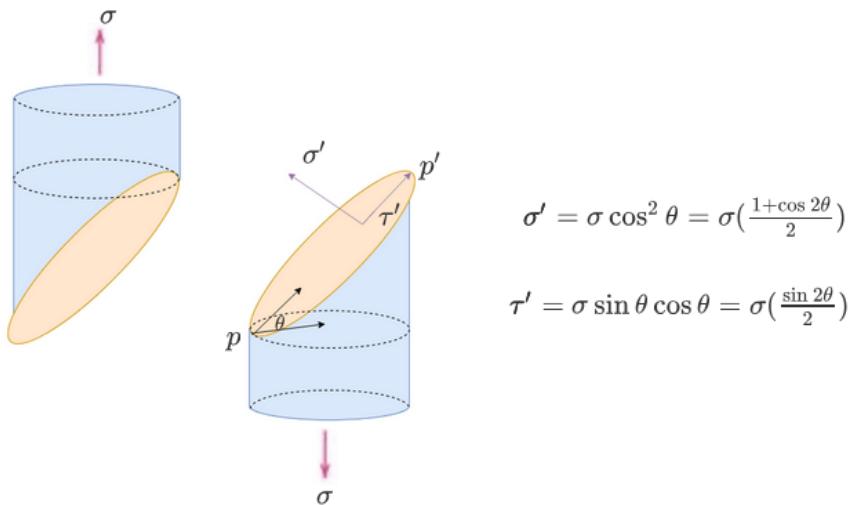
Tensile and Compression Strain

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

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

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

Shear

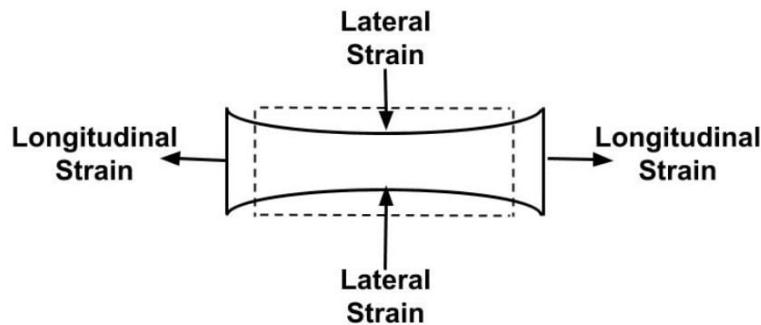
$$\tau = G\gamma \quad (G \text{ is the shear modulus})$$

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  $\Rightarrow$  higher E)

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

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

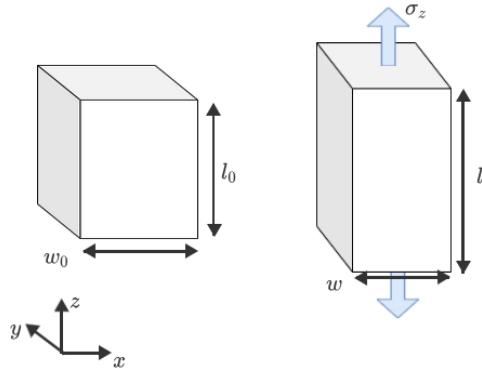
## Poisson's Ratio



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

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  $\sigma_z$ ,  $\epsilon_x = \epsilon_y$

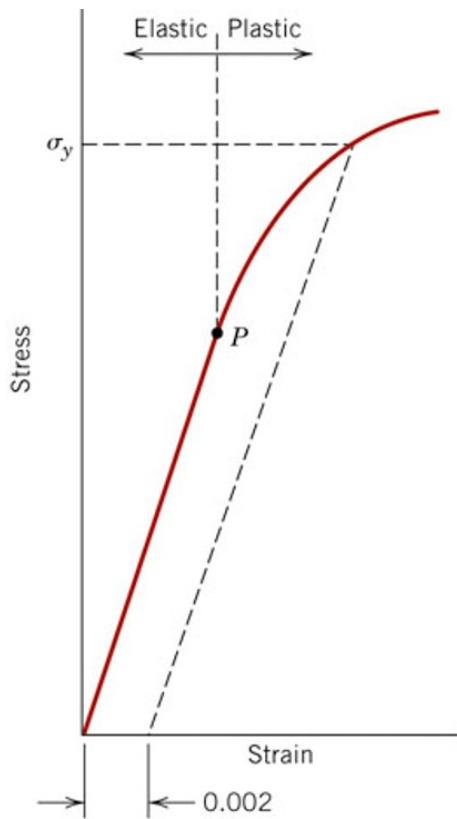
$$\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$$

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

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

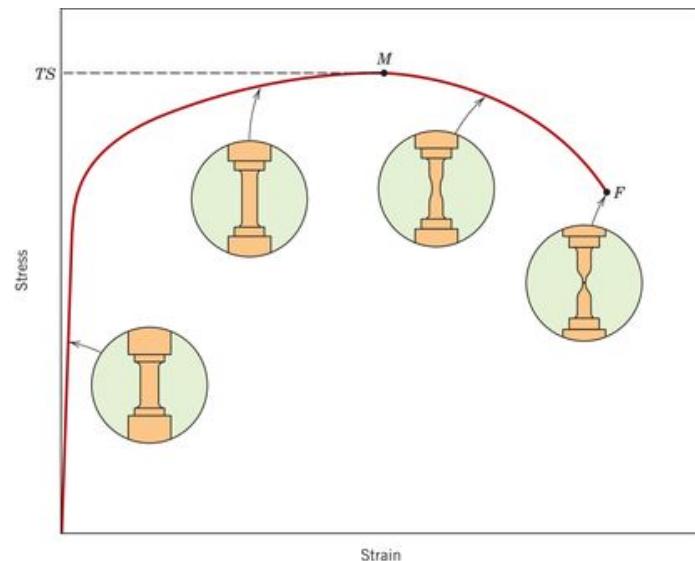
Note: Some materials (like foams) expand under tension so they have a negative Poisson's ratio, these materials are called **auxetics**.

# 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

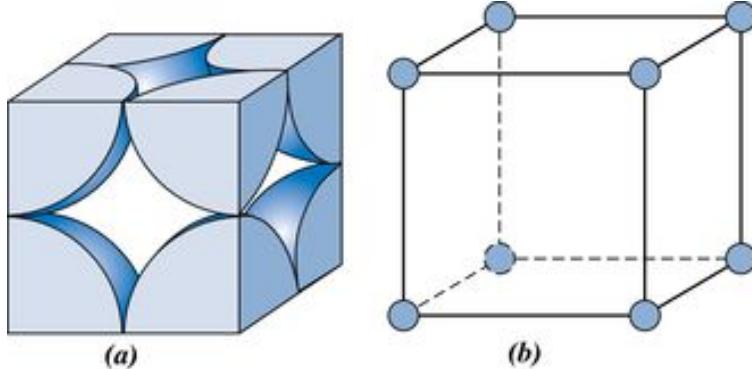
$$PF = \frac{\text{Total Cross Sectional Area of Atoms}}{\text{Total Area of Plane}}$$

## 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

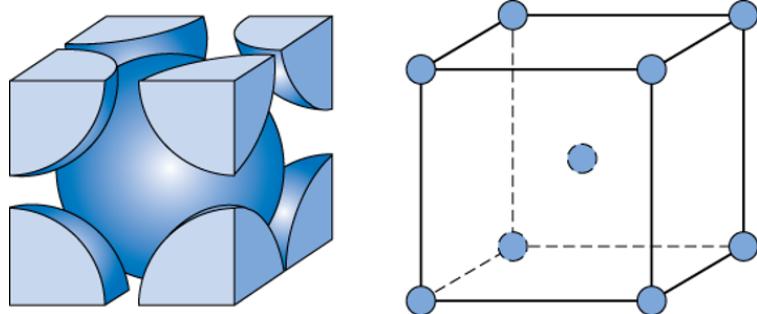


$$2R = a$$

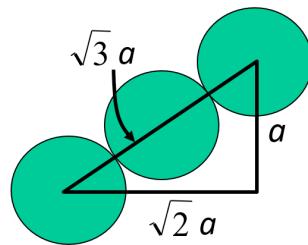
$$APF = \frac{(\# \text{ atoms})(\text{volume/atom})}{(\text{volume/unit cell})}$$

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

## Body Centered Cubic



Triangle formed along the main diagonal and face diagonal

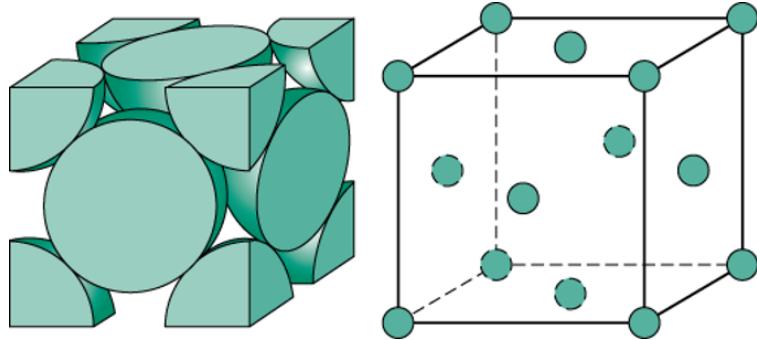


$$4R = \sqrt{3}a$$

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

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

## Face Centered Cubic



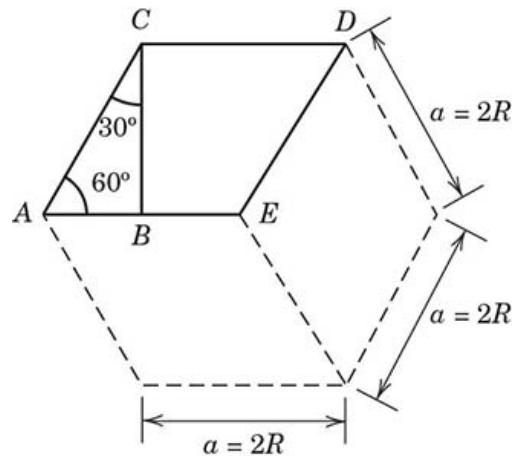
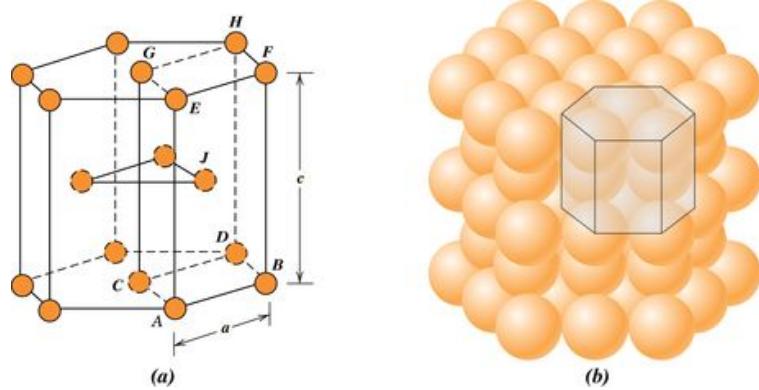
Along the face diagonal:

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

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

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

## 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:

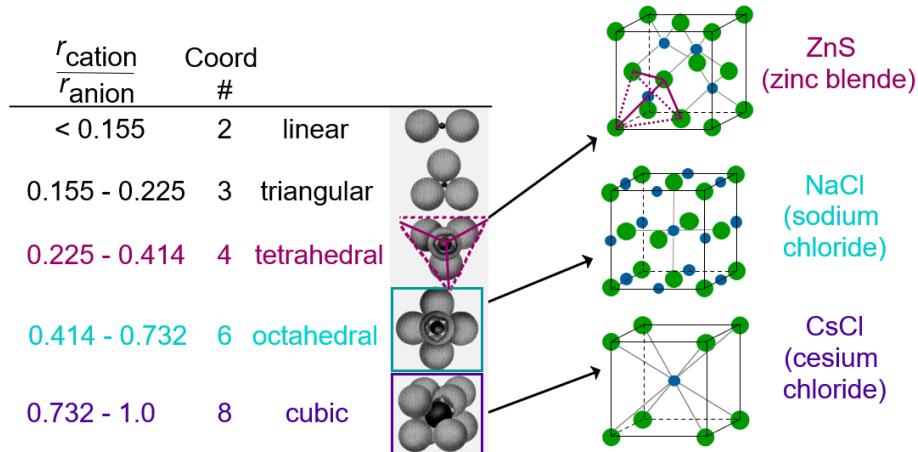
- n = # of atoms in unit cell
- A = atomic weight
- $V_c$  = volume of unit cell
- $N_a$  = Avogadro's number ( $6.022 \times 10^{23}$  atoms/mol)

## 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



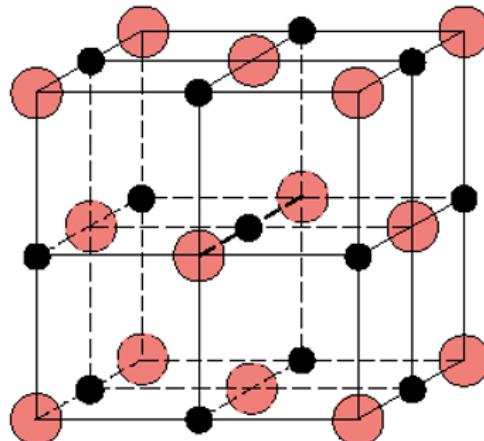
## Theoretical Density for Ceramics

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

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

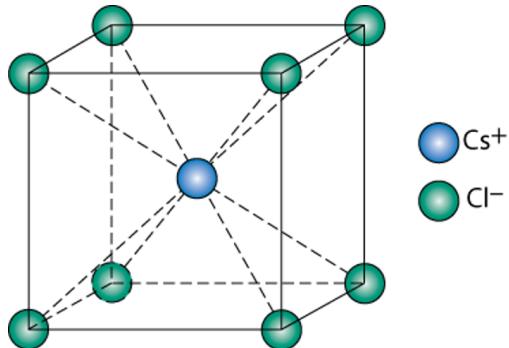


Note: Cations prefer octahedral sites (in black)

Along the edges:

$$2R_A + 2R_C = a$$

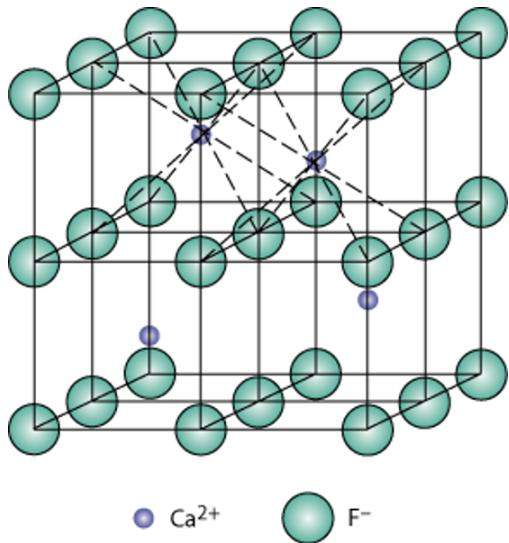
## AX Crystal Structure (Cesium Chloride)



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

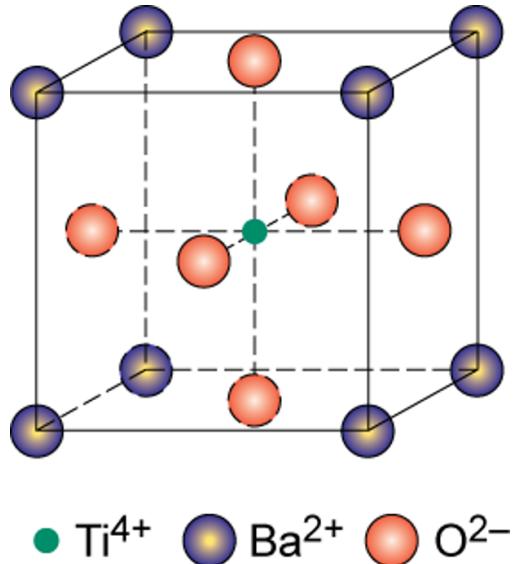
$$2R_A + 2R_C = \sqrt{3}a$$

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



Note: Cations prefer cubic sites (Body Center, in blue)  
There are half as many  $\text{Ca}^{2+}$  as  $\text{F}^-$  (for  $\text{CaF}_2$ )

## $\text{ABX}_3$ 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

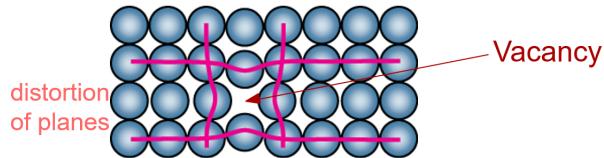
$$LD = \frac{\text{Number of atom centered on line}}{\text{Unit length of direction vector}}$$

### Planer Density

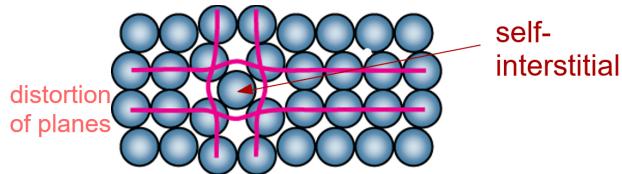
$$PD = \frac{\text{Number of atoms centered on plane}}{\text{Area of plane}}$$

# Point Defects

- Vacancies: Missing atoms in the lattice



- Interstitials: Extra atoms positioned between lattice sites



## Equilibrium Concentration of Vacancies

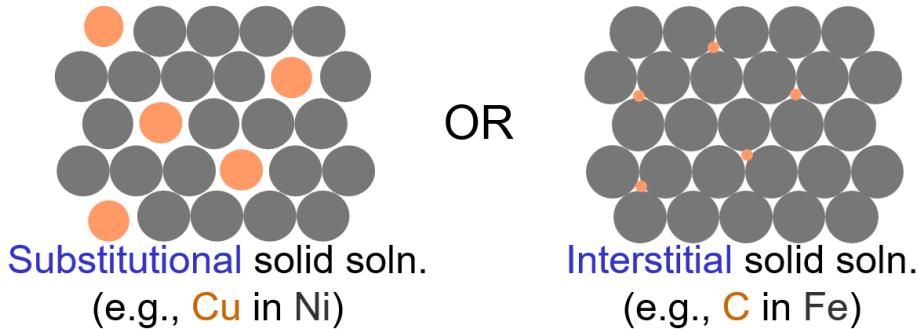
$$N_v = N e^{\left(\frac{-Q_v}{kT}\right)}$$

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:



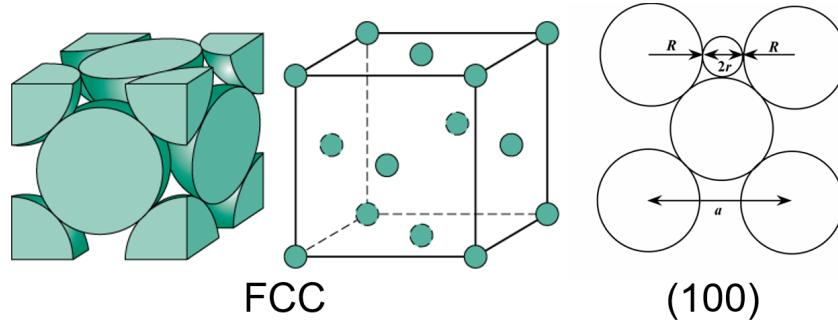
## Hume-Rothery rule

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

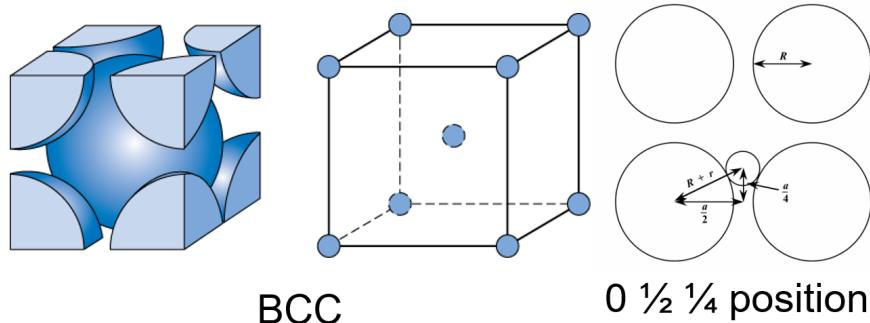


$$2r + 2R = a$$

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

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

BCC



BCC

$0 \frac{1}{2} \frac{1}{4}$  position

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

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

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

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

$$r = 0.291R$$

## 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%

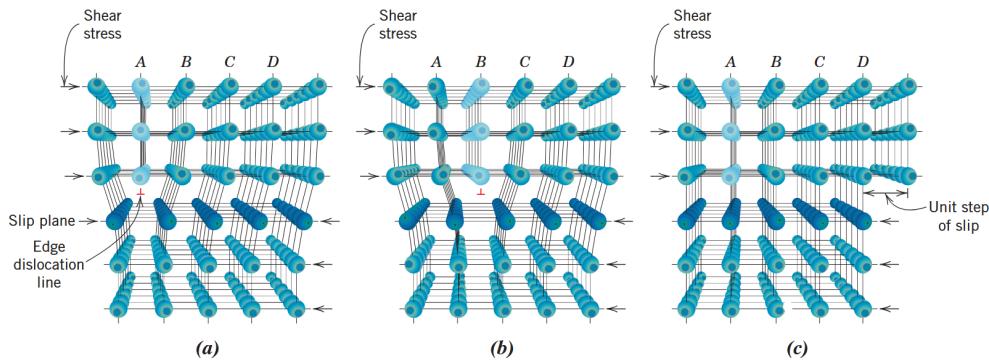
$$C'_1 = \frac{C_1 A_2}{C_1 A_2 + C_2 A_1} \times 100$$

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

# Line Defects

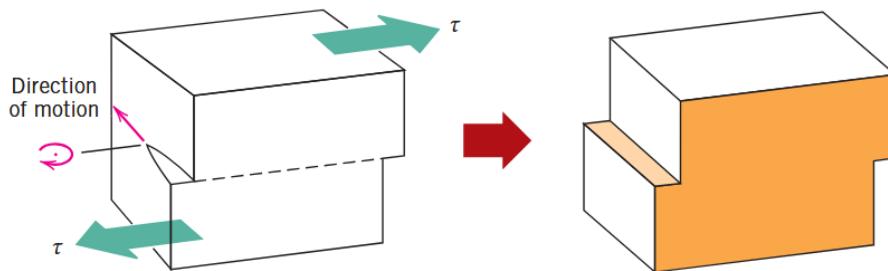
Dislocations are line defects. It occurs when there is slipping between crystal planes when dislocations move and they cause permanent (plastic) deformation. There are two main types:

- 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.

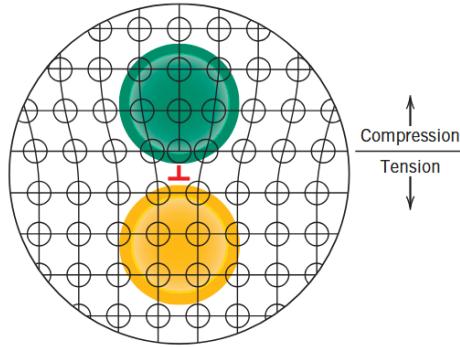
Plastic deformation occurs due to many dislocations. The process by which plastic deformation is produced by dislocation motion is termed **slip**; the crystallographic plane along which the dislocation line traverses is the **slip plane**.

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

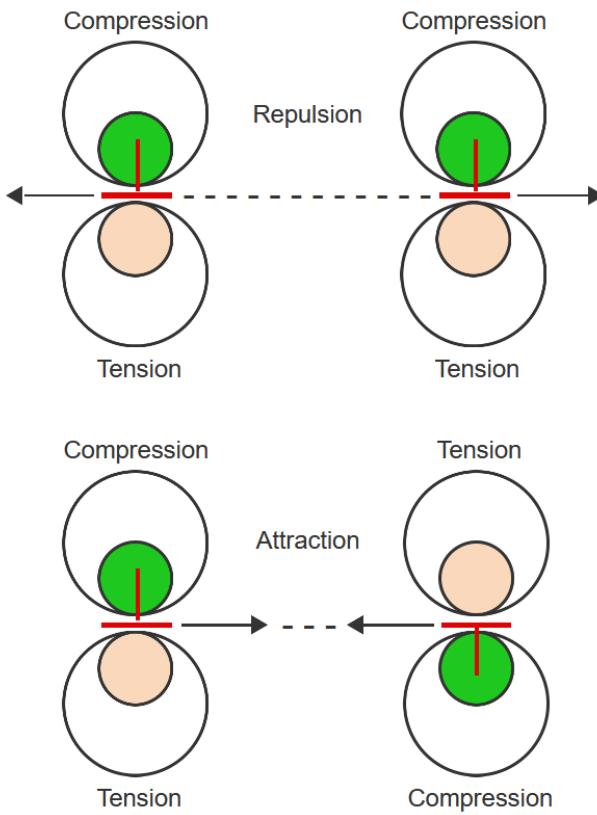
## Characteristics of dislocations

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.

# Slip Systems

The preferred slip plane and slip direction are those with the densest atomic packing (highest planer density) and highest linear density respectively. The combination of slip plane and slip direction is called a **slip system**.

Ex: FCC  $\{111\}\langle110\rangle$  slip system

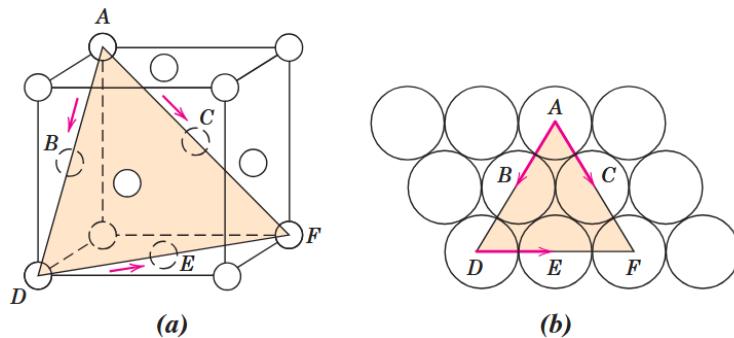


Table of Slip Systems

Metals	Slip Plane	Slip Direction	Number of Slip Systems
<b>Face-Centered Cubic</b>			
Cu, Al, Ni, Ag, Au	$\{111\}$	$\langle110\rangle$	12
<b>Body-Centered Cubic</b>			
$\alpha$ -Fe, W, Mo	$\{110\}$	$\langle111\rangle$	12
$\alpha$ -Fe, W	$\{211\}$	$\langle111\rangle$	12
$\alpha$ -Fe, K	$\{321\}$	$\langle111\rangle$	24
<b>Hexagonal Close-Packed</b>			
Cd, Zn, Mg, Ti, Be	$\{0001\}$	$\langle11\bar{2}0\rangle$	3
Ti, Mg, Zr	$\{10\bar{1}0\}$	$\langle11\bar{2}0\rangle$	3
Ti, Mg	$\{10\bar{1}1\}$	$\langle11\bar{2}0\rangle$	6

Note: More slip systems = more ductile material

The **Burgers vector** has the same direction as the dislocation motion (slip direction) and its magnitude is equal to the interatomic spacing in that direction (unit slip distance). Ex: Burgers vector for FCC and BCC

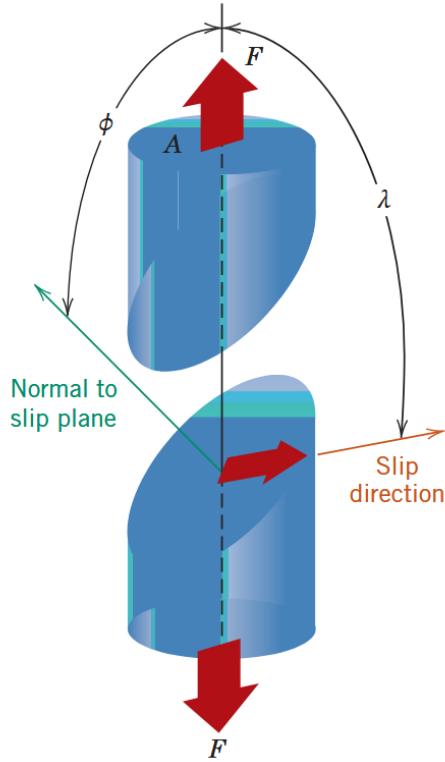
$$\vec{b}_{FCC} = \frac{a}{2}\langle110\rangle$$

$$\vec{b}_{BCC} = \frac{a}{2}\langle111\rangle$$

## Slip in single crystals

For an applied shear stress  $\sigma$ , the resolved shear stress represents the magnitude of the shear stress acting on the slip plane in the slip direction. It is given by:

$$\tau_R = \sigma \cos \phi \cos \lambda$$



A metal single crystal has a number of different slip systems, each with its own value of resolved shear stresses. However, there will be one slip system with the maximum resolved shear stress, denoted  $\tau_R(\max)$ .

$$\tau_R(\max) = \sigma (\cos \phi \cos \lambda)_{\max}$$

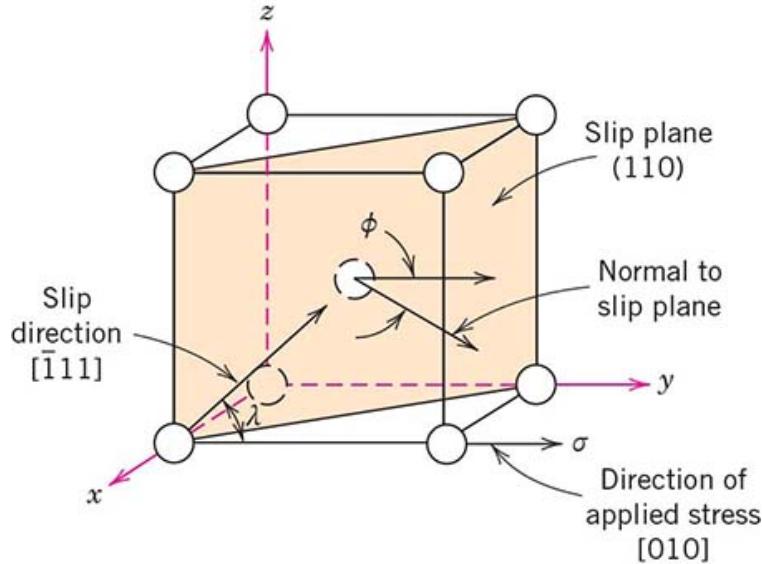
In this slip system with the maximum resolved shear stress, slip occurs when the resolved shear stress reaches a critical value (the critical resolved shear stress,  $\tau_{CRSS}$ ). This is the minimum shear stress required to initiate slip and thus determines when yielding will begin (when  $\tau_R(\max) = \tau_{CRSS}$ ).

$$\sigma_y = \frac{\tau_{CRSS}}{(\cos \phi \cos \lambda)_{\max}} \quad (\text{yield stress})$$

This yield stress is minimized when  $\phi = \lambda = 45^\circ$ , maximizing  $\cos \phi \cos \lambda = 0.5$ . Thus

$$\sigma_{y,\min} = 2\tau_{CRSS}$$

Ex: Consider a single crystal of BCC iron oriented such that a tensile stress is applied along a [010] direction. Compute the resolved shear stress along a (110) plane and in a [1̄11] direction when a tensile stress of 52 MPa (7500 psi) is applied.



Recall that we can find the angle by using the projection:

$$\cos \theta = \frac{\vec{a} \cdot \vec{b}}{|\vec{a}| |\vec{b}|}$$

Where:

- Applied tensile direction [010]  $\Rightarrow \vec{l} = (0, 1, 0)$
- Slip plane (110)  $\Rightarrow \vec{n} = (1, 1, 0)$  (normal vector to plane)
- Slip direction [1̄11]  $\Rightarrow \vec{d} = (-1, 1, 1)$

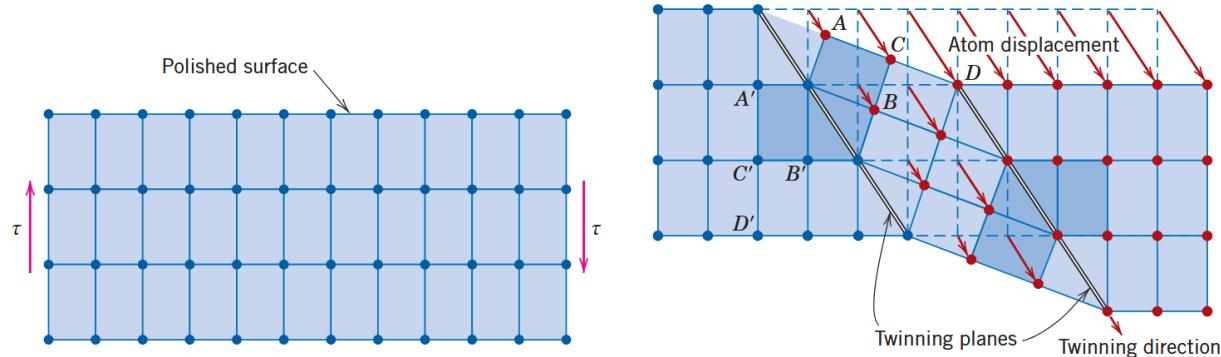
Thus,

$$\begin{aligned} \phi &= \cos^{-1} \left( \frac{\vec{n} \cdot \vec{l}}{|\vec{n}| |\vec{l}|} \right) & \lambda &= \cos^{-1} \left( \frac{\vec{d} \cdot \vec{l}}{|\vec{d}| |\vec{l}|} \right) \\ &= \cos^{-1} \left( \frac{(1, 1, 0) \cdot (0, 1, 0)}{\sqrt{1^2 + 1^2 + 0^2} \sqrt{0^2 + 1^2 + 0^2}} \right) & &= \cos^{-1} \left( \frac{(-1, 1, 1) \cdot (0, 1, 0)}{\sqrt{(-1)^2 + 1^2 + 1^2} \sqrt{0^2 + 1^2 + 0^2}} \right) \\ &= \cos^{-1} \left( \frac{1}{\sqrt{2}} \right) = 45^\circ & &= \cos^{-1} \left( \frac{1}{\sqrt{3}} \right) = 54.74^\circ \end{aligned}$$

$$\tau_R = (52 \text{ MPa}) \cos(45^\circ) \cos(54.74^\circ) = 21.3 \text{ MPa}$$

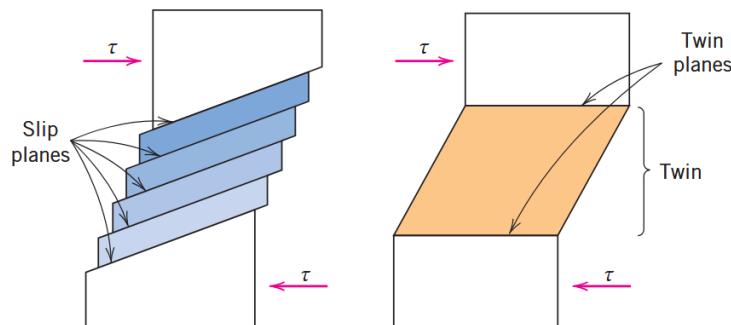
# Deformation by Twinning

In addition to slip, plastic deformation in some metallic materials can occur by the formation of mechanical twins, or twinning. Twinning occurs when a shear force produces atomic displacements such that on one side of a plane (the twin boundary), atoms are located in mirror-image positions of atoms on the other side.



Twinning is different from slip in several ways:

- Twinning produces a reorientation of the crystal lattice, where slip crystallographic orientation is the same before and after deformation
- Slip occurs in distinct atomic spacing multiples, whereas the atomic displacement for twinning is less than the interatomic separation.



Mechanical twinning occurs in metals with BCC and HCP crystal structures at low temps and high rates of loading where there are fewer slip systems. Twinning is important because it may place new slip systems in orientations that are favorable relative to the stress axis such that the slip process can now take place.

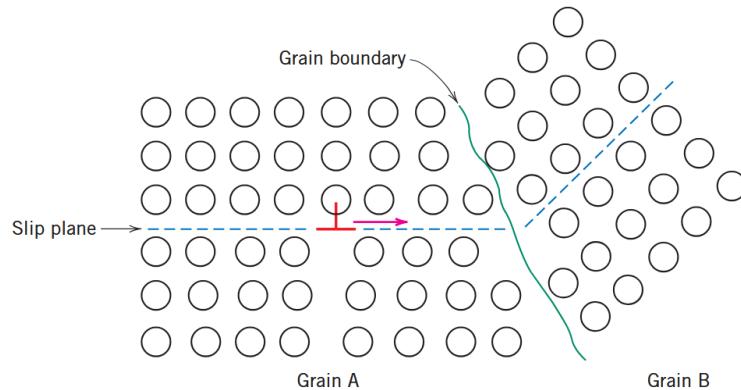
## Strengthening by grain size reduction

The strength and hardness of metals depend on how easily dislocations can move. Plastic deformation occurs through dislocation motion, so if dislocations move freely, the metal is soft and weak. If their motion is restricted, more force is needed to deform the metal, making it harder and stronger. Thus, nearly all strengthening methods work by hindering dislocation movement.

Grain size affects a metal's mechanical properties because grain boundaries hinder dislocation motion. When a dislocation moves from one grain to another, it encounters two obstacles:

- The change in crystal orientation makes it harder for the dislocation to continue moving.
- The atomic disorder at the grain boundary disrupts slip-plane continuity.

As a result, smaller grains (more boundaries) strengthen the metal by restricting dislocation motion.



The relationship between yield strength and grain size is given by the **Hall-Petch equation**:

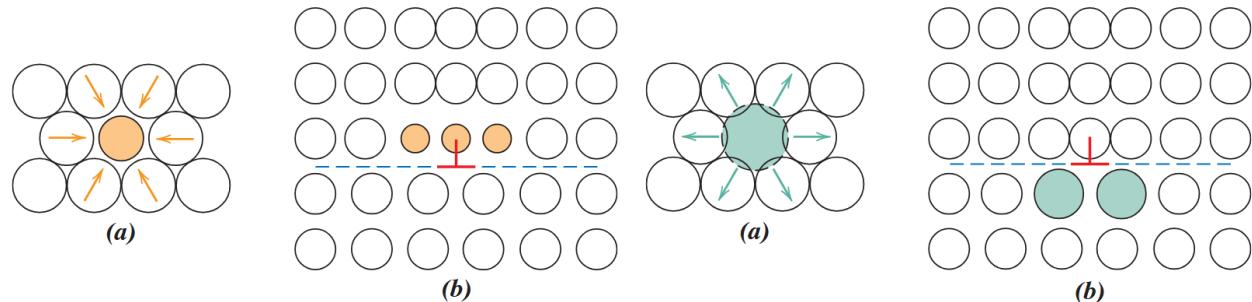
$$\sigma_y = \sigma_o + k_y d^{-1/2}$$

Where:

- $\sigma_y$  = yield stress
- $\sigma_o$  = friction stress (stress required to move dislocations, a material constant)
- $k_y$  = strengthening coefficient (a material constant)
- $d$  = average grain diameter

## Solid-solution strengthening

By creating alloys with impurity atoms in either a substitutional or interstitial solid solution, the strength of a metal can be increased. This process is called **solid-solution strengthening**. High-purity metals are almost always softer and weaker than alloys composed of the same base metal. This is because the impurity atoms impose lattice strains that hinder dislocation motion.



## Strain hardening

**Strain hardening** is the phenomenon by which a ductile metal becomes harder and stronger as it is plastically deformed. Sometimes it is also called work hardening, or **cold working**.

We can define the amount of plastic deformation as **percent cold work** instead of strain:

$$\%CW = \frac{A_o - A_d}{A_o} \times 100$$

Where:

- $A_o$  = original cross-sectional area
- $A_d$  = cross-sectional area after deformation

## Recovery

When a polycrystalline metal is plastically deformed at low temperatures, its grains change shape, dislocation density increases, and it undergoes strain hardening. Some deformation energy is stored as strain energy, and properties such as electrical conductivity and corrosion resistance may change.

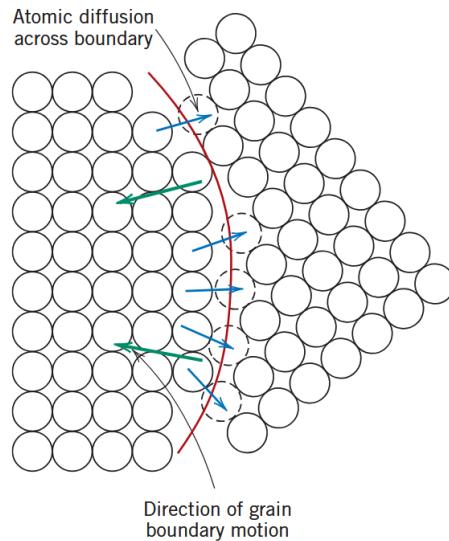
These effects can be reversed by **annealing**, a heat treatment involving **recovery** and **recrystallization** (sometimes followed by grain growth). During **recovery**, atomic diffusion allows dislocations to rearrange and reduce internal strain energy without external stress. This lowers dislocation density and restores properties such as electrical and thermal conductivity to their original states.

# Recrystallization

**Recrystallization** replaces deformed grains with new, strain-free, equiaxed ones that have low dislocation density. This process, driven by stored strain energy, restores the metal's softness and ductility. It depends on time and temperature; the **recrystallization temperature** (temp for completion in 1 h) is typically  $0.3\text{--}0.5 T_m$  for metals and up to  $0.7 T_m$  for alloys ( $T_m$  is the melting temperature). Greater cold work lowers this temperature, while impurities raise it by slowing grain boundary motion.

# Grain Growth

**Grain growth** occurs when strain-free grains enlarge at elevated temperatures, even without prior recovery or recrystallization. As grain boundaries migrate, large grains grow at the expense of smaller ones, reducing total boundary area and energy. The driving force is the decrease in grain boundary energy, and boundary motion occurs through short-range atomic diffusion.



The grain diameter varies with time according to the relationship:

$$d^n - d_o^n = Kt$$

Where:

- $d$  = grain diameter at time  $t$
- $d_o$  = initial grain diameter
- $n$  = grain growth exponent (typically 2)
- $K$  = temperature-dependent rate constant