SI Prefixes

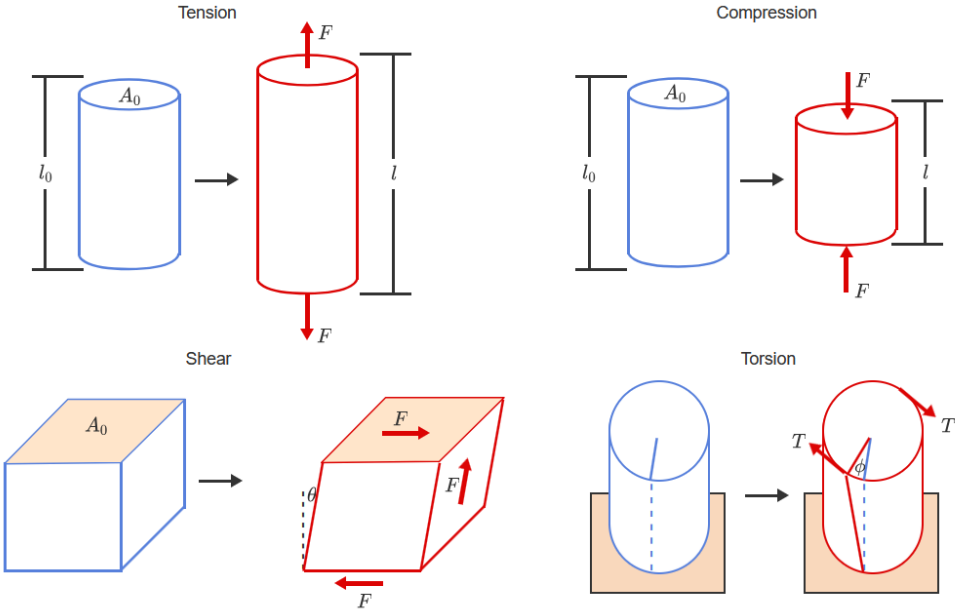
$$\begin{aligned}
\text{femto (f)} &= 10^{-15} \\
\text{pico (p)} &= 10^{-12} \\
\text{nano (n)} &= 10^{-9} \\
\text{micro } (\mu) &= 10^{-6} \\
\text{milli (m)} &= 10^{-3} \\
\text{centi (c)} &= 10^{-2} \\
\text{deci (d)} &= 10^{-1} \\
\text{deca (da)} &= 10^{1} \\
\text{hecto (h)} &= 10^{2} \\
\text{kilo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

Note: $1\text{Angstrom}\,(\text{Å}) = 10^{-10}$ 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)

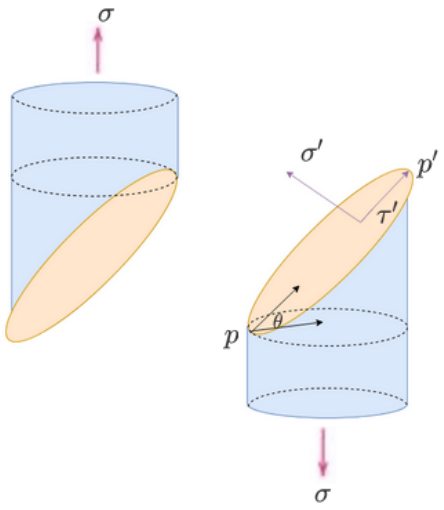
Tensile and Compression Strain

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

Shear Strain

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

Normal and Shear Stress Along an Angled Plane



$$\sigma' = \sigma \cos^2\theta = \sigma\left(\frac{1+\cos 2\theta}{2}\right)$$

$$\tau' = \sigma \sin\theta \cos\theta = \sigma\left(\frac{\sin 2\theta}{2}\right)$$

Elastic Deformation

Relationship Between Stress and Strain

Tensile and Compression

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

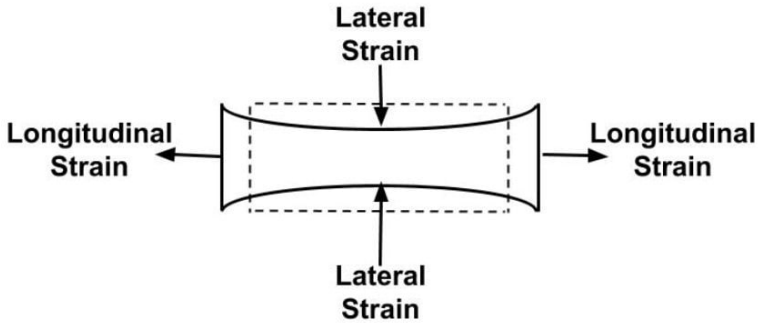
Shear

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

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

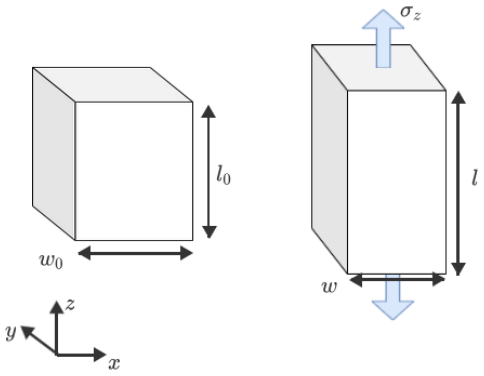
Poisson's Ratio



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

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 σ_z, $\epsilon_x = \epsilon_y$

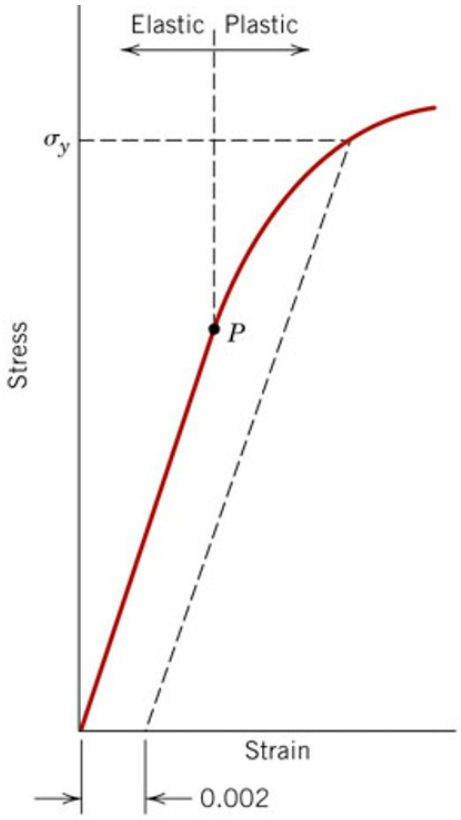
$$\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$$

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

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

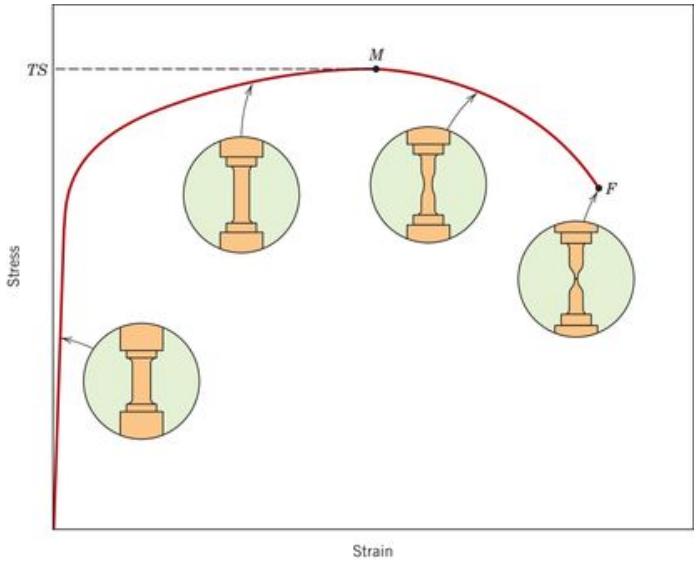
Note: Some materials (like foams) expand under tension so they have a negative Poisson's ratio, these materials are called **auxetics**.

Plastic Deformation



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

Yield Stress (σ_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

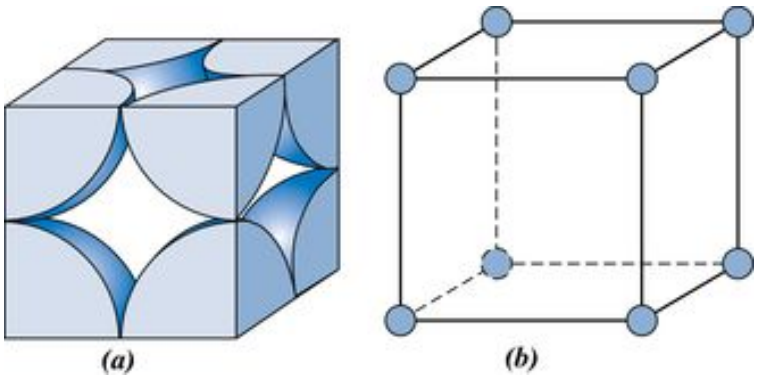
$$PF = \frac{\text{Total Cross Sectional Area of Atoms}}{\text{Total Area of Plane}}$$

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

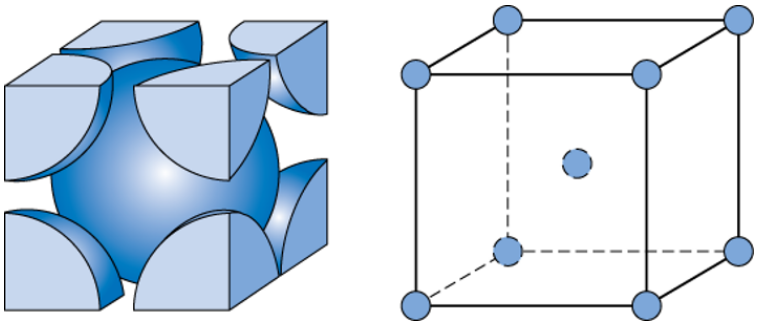


$$2R = a$$

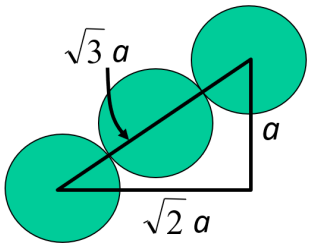
$$APF = \frac{(\#\text{ atoms})(\text{volume/atom})}{(\text{volume/unit cell})}$$

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

Body Centered Cubic



Triangle formed along the main diagonal and face diagonal

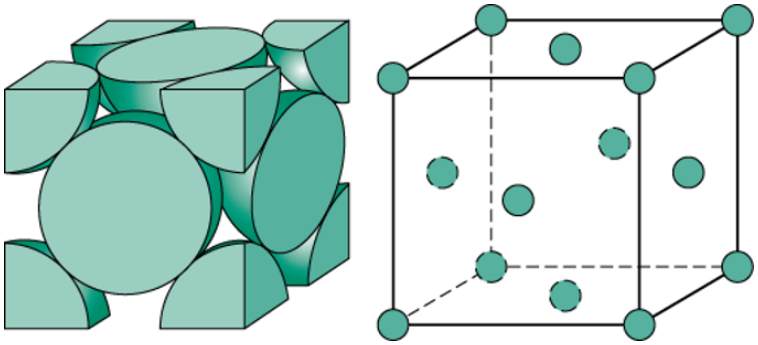


$$4R = \sqrt{3}a$$

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

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

Face Centered Cubic



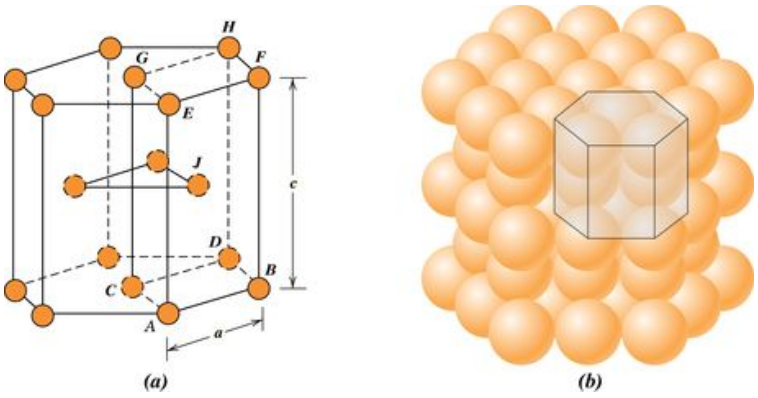
Along the face diagonal:

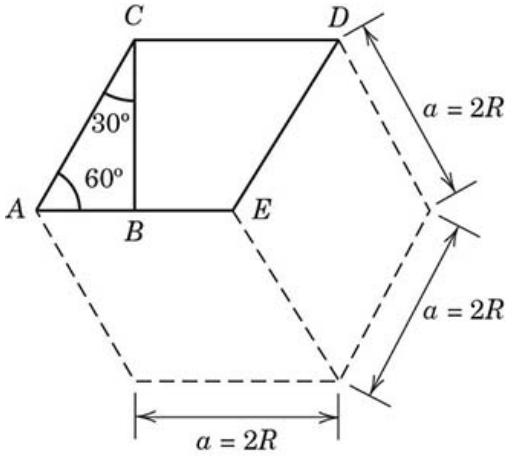
$$4R = \sqrt{2}a$$

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

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

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:

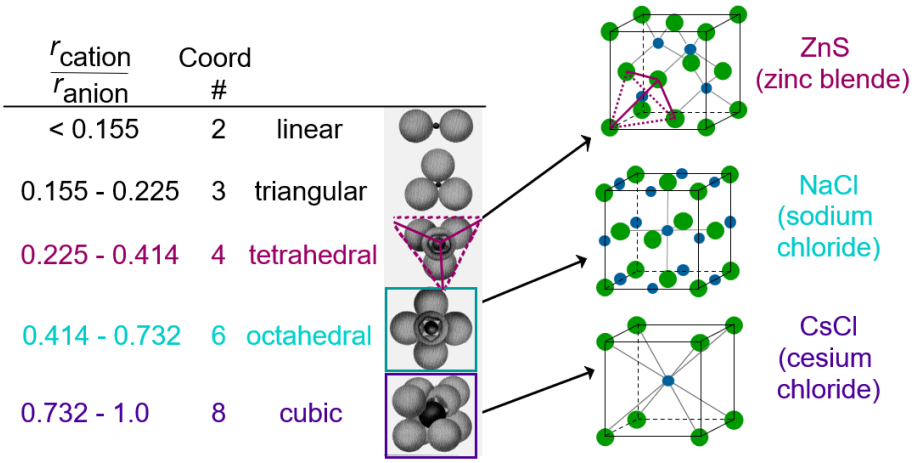
- n = # of atoms in unit cell
- A = atomic weight
- V_c = volume of unit cell
- N_a = Avogadro's number (6.022×10^{23} atoms/mol)

Ceramic Crystal Structures

Factors that determine crystal structure:

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

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



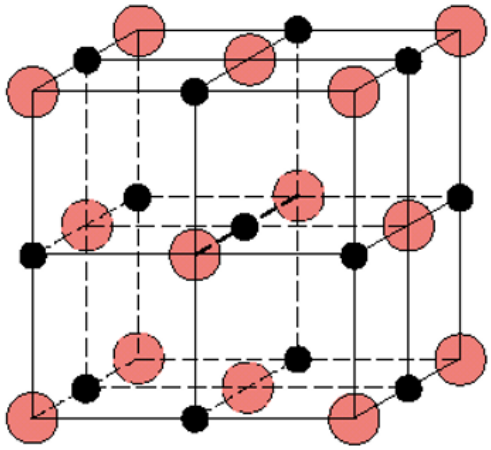
Theoretical Density for Ceramics

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

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 (6.022×10^{23} atoms/mol)

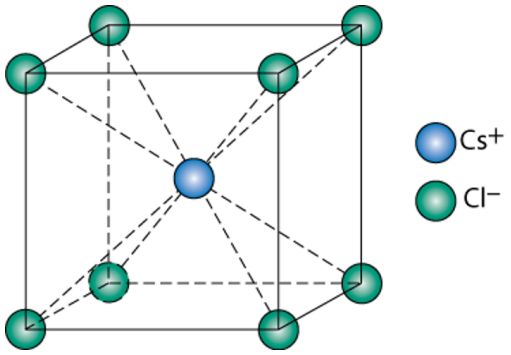
Rock Salt Structure



Note: Cations prefer octahedral sites (in black)
Along the edges:

$$2R_A + 2R_C = a$$

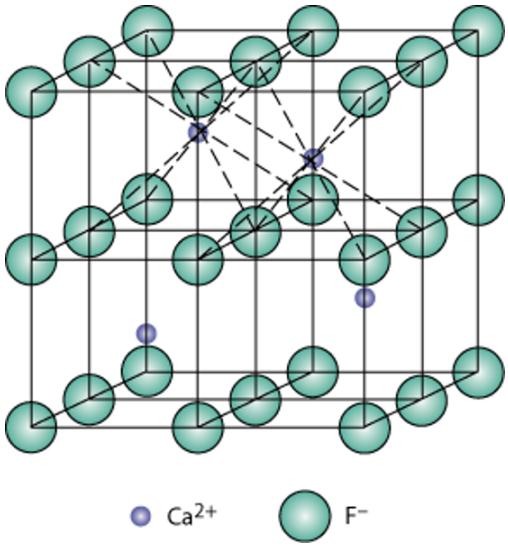
AX Crystal Structure (Cesium Chloride)



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

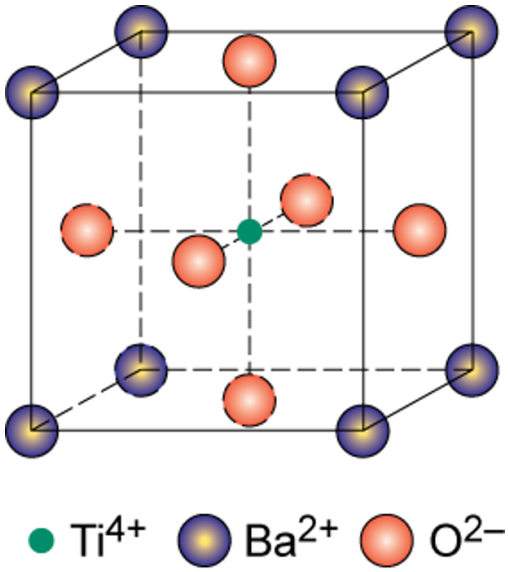
$$2R_A + 2R_C = \sqrt{3}a$$

AX_2 Crystal Structures (Flourite)



Note: Cations prefer cubic sites (Body Center, in blue)
There are half as many Ca^{2+} as F^- (for CaF_2)

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 reciprocols 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

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

Dislocations and Strengthening Mechanisms

Basic Concepts

Types of dislocations