Mat E 272
Fall 2001 – Midterm Review
Tuesday October 9, 2001

Homework assignments:

- **Set # 3 is being returned today and will be discussed in class**
- **Set #4 is due one week from today (October 16)**

  (the 3 graded problems are identified (7.5, 7.17, and 7.33) These only require a short answer; please do these before the midterm on Thursday)

- **Set # 5 will be due October 23; the problems will be posted on the web by the end of this week**

Reading assignments:

- **Week 8: we will discuss fatigue and failure first (Tuesday October 16) so read Chapter 8 (excluding 8.10)**
- **Chapter 9 (phase diagrams) will be discussed Thursday October 18 and continuing on Tuesday October 23.**

Chapter 2:

Metals: Materials characterized by high density of de-localized electrons (metallic bonding)
Examples: Cu, Zn, Fe, Ti, Ag, Pt, brass, steel, monel,…

Ceramics: Materials characterized by covalent &/or ionic bonding
Examples: silica (quartz), alumina, silicon carbide

Polymers: Organic materials, generally consisting of covalently-bonded hydrocarbons
Examples: nylon, polystyrene, polyethylene, polyester

Composites: Materials consisting of more than one distinct phase or component
- engineered for specific applications (high strength – low density, high strength – high conductivity, etc.)
- usually strong (by design) (fiberglass: glass fibers → strength and polymer matrix → formability)

Semiconductors: Materials characterized by electronic conduction intermediate between metals and ceramics (e.g., Si, Ge, GaAs, InP)

Chemical bonding:

Electronegativity – the tendency for an atom to accept an electron

high electronegativity → strong tendency to accept an electron (i.e., Group VIIA: F, Cl)

low electronegativity (called "electropositive") → strong tendency to give up an electron, i.e., Group IA: Li, Na, K)

the difference in electronegativity between two atoms determines the resulting electron distribution and the type of bond

Equilibrium separation between atoms:

ASYMMETRY of the potential vs. distance curve is due to differing relative strengths of the attractive and repulsive forces

THIS IS THE REASON FOR THERMAL EXPANSION

(slope of force vs. distance curve at equilibrium separation = modulus of elasticity)

Bonding energy: Minimum of the potential vs. distance curve
Indicates how much energy must be supplied to completely disassociate the two atoms
Depth of the potential well indicates bonding strength
Deep well → strongly bonded
Shallow well → weakly bonded

Bonding types

Primary

1. **Ionic**: **Electron transfer from one atom (cation) to the other (anion)**
More likely between atoms with large electronegativity differences
Typically found between metal and non-metal atoms:

NaCl, KF, CsBr, MgO

Charge transfer results in electrostatic attraction between cations and anions:

Typical characteristics of ionically-bonded materials:
- High melting temperature
- Hard
- Brittle
- Insulator (electrical and thermal)

2. **Covalent**: **electron sharing between atoms**

highly directional
- fixed orientation of the atoms

Shared electrons may be considered to belong to each atom
- Each atom tries to achieve a more stable orbital filling configuration

Found in such diverse materials as diamond, silicon, SiC, GaAs, H_2O, & many organic compounds (CH_4, HNO_3, HF)

- MOST MATERIALS ARE NEITHER 100% IONIC NOR 100% COVALENT

3. **Metallic**: **Ion cores are held together by electrostatic attraction with a "sea" of free electrons**

More likely between atoms with large electronegativity differences
Valence electrons are not bound to any specific atom…
"free" to drift throughout the material (subject to local and external electromagnetic fields)

Secondary bonding (~ 10 kJ/mole or 0.1 eV/atom)

Van der Waals

charge polarization (dipoles)
Thermal vibration fluctuations can disrupt charge symmetry
The presence of one dipole can induce a dipole in an adjacent molecule (or atom) and so on.

Permanent diploes: called POLAR molecules

Examples: water, ammonia, hydrogen fluoride

Chapter 3: Crystal Structure, Directions, and Planes

Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons.

Crystal structure pertains to the arrangement of atoms in the crystalline solid material.

Crystal = point lattice (framework or basis) + atoms

A unit cell is the smallest entity that exhibits the chemical and crystallographic properties of the material.

the length of each unit cell axis is called a lattice parameter

In cubic systems, all three orthogonal lattice parameters are equal

Lattice parameters are typically on the order of a few Angstroms (or a few tenths of a nanometer)

atoms per unit cell:

The number of atoms/unit cell is an important quantity and determines many physical properties (thermal conductivity)

In general, the number of atoms/unit cell, N, is given by

$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$, where N_i = # interior atoms, N_f = # face atoms, N_c= # corner atoms

there are 7 distinct crystal systems and 14 Bravais lattice types:

Crystal system	Types of possible lattice arrangements
Cubic	SC, BCC, FCC
Hexagonal	HCP
Tetragonal	Simple, body-centered
Orthorhombic	Simple, base-centered, body-centered, face-centered
Rhombohedral	Simple
Monoclinic	Simple, base-centered
Triclinic	Simple

Atomic Packing Factor (APF or APE) = $\frac{total\ "sphere"\ volume}{total\_unit\_cell\_volume}$

APF for common crystal systems:

BCC → 0.68
FCC, HCP → 0.75

Crystallographic directions:

Crystal directions are specified by a set of three integers called indicies $(n_1\ n_2\ n_3)$

Each index represents the component of the directional vector with respect to a coordinate system appropriate for the particular lattice.

Suppose the origin of the directional vector does not coincide with the origin of the coordinate system?

In a cubic unit cell, simply choose another corner

General approach:

1) **Projections of vector on unit cell axes**
2) **Projections in terms of unit cell parameters a, b, c (fractional values)**
3) **Reduction of projections to integers**
4) **Enclosure [ ]**

Note: reciprocals are NOT involved with directions

Crystallographic planes:

General procedure for specifying **crystallographic planes**:

1. **If the plane passes through the origin, either select another (parallel and equivalent) plane OR choose another (and equivalent) origin.** Usually, it is easier to select another origin, which is generally another corner of the unit cell.
2. The plane either intercepts each axis or is parallel to one or two of them. **Determine the fractional intercept along each axis in term of the lattice parameters a, b, and c (note that if the plane is parallel to an axis, the intercept is infinity, ∞)**

3. **Take the inverse (reciprocal) of each intercept**. For this purpose, the inverse of infinity is zero.
4. **Multiply each number by a common factor to reduce to the smallest set of integers**.
5. **Enclose the resulting set of number in parentheses**: e.g., (001)

[ ] → direction

< > → family of equivalent directions

( ) → plane

{ } → family of equivalent planes

Close-packed directions:

Crystallographic directions corresponding to highest linear packing density
BCC: body diagonals
FCC: face diagonals

C-P directions correspond to direction of slip

Close-packed planes:

Crystallographic planes corresponding to highest areal packing density
Interplanar separation is greatest for C-P planes
Close-packed planes in FCC metals are {111}:

Chapter 4 Imperfections in Solids

Examples of "defects:"

- addition of C to Fe to make steel
- addition of Cu to Ni to make thermocouple wires
- addition of Ge to Si to make thermoelectric materials
- addition of Cr to Fe for corrosion resistance
- introduction of grain boundaries to strengthen materials

In general, a defect simply refers to a disruption in the crystalline order of an otherwise periodic material.

1) one-dimensional (point)

vacancy → $N_v = N_o \exp\left(-\frac{Q}{kT}\right)$ **where Q is generally on the order of ~1 eV/atom**

The quantity $\left[\frac{N_v}{N_o}\right]$ **is just the fraction of vacant lattice sites.**

exp(-Q/kT) is a strong function of temperature

self-interstitial → an atom from the crystal that crowds its way into an otherwise empty void between atoms

impurity → addition of an atom of a different species than the "host" or matrix

Alloys – other types of atoms are deliberately added to give the material certain properties

- **May or may not result in the same crystal structure**
- **May or may not result in secondary phases**

solid solution

- **A homogeneous distribution of two or more elements.**
- **"solute" atoms are added without altering the crystal structure or resulting in formation of a new phase.**
- **Solid solution is a particular type of alloy**
- **Two types: substitutional and interstitial**

There are very specific rules that govern the extent to which solid solutions can form:

General guidelines for predicting solid solubility between any two elements:

For appreciable solubility to occur the following factors must be true:

- **Atomic size factor**
  the difference in atomic radii between the two atoms must be ≤ ± 15%
- **Electronegativity**
  the difference in electronegativity between the two atoms must be ≤ ± 0.4
- **Crystal structure**
  The crystal structure of each element must be the same
- **Valence**
  For a given solvent, a solute with a higher valency is more likely to be soluble than one of lower valency, all other factors being equal.

Composition and conversion between weight and atomic percent:

Mixtures (i.e., composites) or alloys of two (or more) elements, are quantitatively described in terms of composition, either by weight percent or by atomic percent.

2) two-dimensional (linear)

Most common types of linear defect are dislocations, grain boundaries, twins, and external surfaces.

Dislocations: an extra half-plane of atoms in a crystal:

- Dislocations result from solidification from the melt, from mechanical work (e.g., rolling, swaging, drawing, compressive impact, tensile or shear stress), or from thermal stresses

- **Dislocation motion is the primary mechanism responsible for the strength and ductility behavior of metals**

- From estimates of binding energy and atomic density, one can calculate the theoretical strength of a metal

  Result: observed strength <<< theoretical strength

  Why the difference? Because the large-scale motion of atoms during deformation is due to dislocation motion in a process called slip

  shear stresses cause atoms to slip by one atomic spacing

- Slip = movement of dislocations under the action of an applied stress
- Slip planes are close-packed planes / slip occurs in close-packed directions
- **Dislocations are not thermally stable**

External surfaces

- atoms are in a high energy state
- surface energy expressed in J/m^3
- materials try to minimize surface energy

Grain boundaries

- interfacial region separating single crystalline volumes
- usually only a few atoms wide
- higher energy than bulk, but lower energy than external surface
- many physical properties are determined by *grain size*

Twin boundaries:

- A disruption in the atomic stacking sequence
- Results in a "mirror plane" symmetry:
- Twins are formed during mechanical shear stresses (mostly BCC and HCP metals) and during heat treatments (annealing twins – mostly in FCC metals)

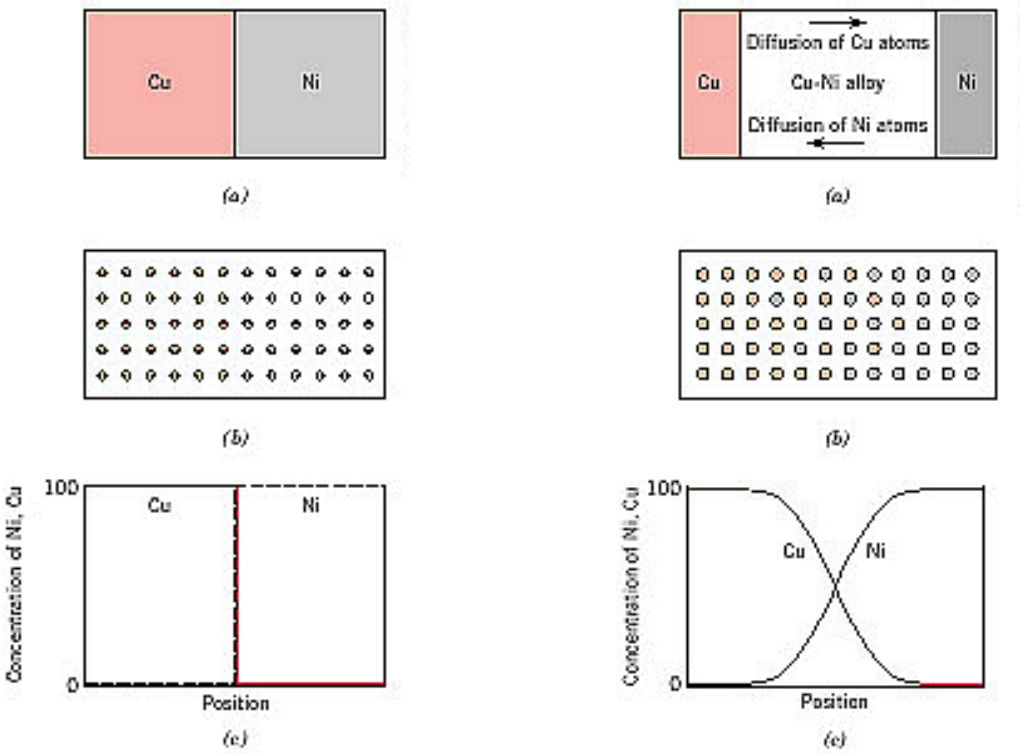
3) three-dimensional (volumetric) defects

- second phase inclusions
- porosity

- cracks

Chapter 5: Fundamentals of Diffusion

Diffusion: Transport in a solid, liquid, or gas driven by a concentration gradient (or, in the case of mass transport, a chemical potential gradient).



- The process of substitutional diffusion requires the presence of *vacancies*
- Factors that affect solid state diffusion:
  - Diffusion occurs at a higher rate…
    - at higher temperatures
    - with smaller atoms
    - in lower melting point host material
    - in lower packing density host material
    - in grain boundaries

- Steady state diffusion is described in terms of a flux and a concentration gradient:

  (steady state means the concentration gradient does not change with time, or that the flux into a unit area is equal to the flux leaving the area – no accumulation or loss)

  Flux = number (or mass) of atoms passing through an area per unit time

  Two examples of units of flux:: $\frac{atoms}{cm^2 \cdot \sec}$ **or** $\frac{grams}{cm^2 \cdot \sec}$

  flux $\propto$ concentration gradient : $J \propto \frac{\Delta C}{\Delta x}$

  or, $J = D\frac{dC}{dx}$

  where the constant of proportionality (D) is called the diffusion coefficient:

  $$D = D_o e^{-\frac{q_d}{kT}}$$

  2 primary mechanisms that affect flux:

  - **temperature (via diffusion coefficient)**
  - **slope of concentration gradient**

- We usually don't have steady state; more often, the concentration versus position curve changes with time (non-steady state)

  In this case, we must use another relationship → Fick's second law: $\frac{dC}{dt} = D\frac{d^2C}{dx^2}$, which describes diffusion in cases where the concentration profile changes with time

- **Solution to Fick's 2nd law:**

$$\frac{C_x - C_o}{C_s - C_o} = 1 - erf\left\{\frac{x}{2\sqrt{Dt}}\right\}$$

C_x = carbon concentration at any point "x" in the steel during diffusion,
C_o = initial (uniform) carbon concentration in the steel (at t = 0),
C_s = surface concentration of carbon during diffusion

erf{} = "error" function: $-1 < \text{erf}(x) < 1$

The assumption that $\text{erf}(x) \cong x$ isn't unreasonable for $x < 0.7$. In situations where $x > 0.7$ or where $\text{erf}(x) > 0.65$, you should really use the correct value:

Table 5.1 Tabulation of Error Function Values

z	$erf(z)$	z	$erf(z)$	z	$erf(z)$
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

- Important example: **carburization** (be familiar with examples)

$$\frac{C_x - C_o}{C_s - C_o} = 1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

- You should be comfortable working with and solving this equation for quantities like time, position, and composition.
- Make sure you review the examples in class and in the text
- Interpolation isn't required for this class but if the value of the argument > 0.7, you should be able to look at the erf table and estimate a reasonable value for the function.

Chapter 6: Introduction to Mechanical Properties of Metals

- **The quantity $\frac{\Delta l}{l_o} = \frac{l - l_o}{l_o}$ is defined as the strain, ε,**

where l = instantaneous length
l_o = initial length

- strain can also be reported as a percentage
- Strain is a dimensionless quantity (or, can be reported as m/m or in./in.)

- **The quantity (F/A) is defined as the stress, σ,**

where F is the load (pounds, N)
A is the cross sectional area:

  - **If use A_o (initial area) → engineering stress**
  - **If use A (instantaneous area) → true stress**
  - **Engineering stress is more commonly used but can lead to misinterpretation of σ - ε curves.**

- Elastic response:

In the elastic regime, the deformation is completely reversible, and we can write

$$\frac{F}{A_o} = E\frac{\Delta l}{l_o}$$

-or-

σ = E ε

The constant of proportionality, ***Young's modulus or modulus of elasticity***, is a measure of the material's stiffness.

$$\sigma = E\varepsilon = E\left(\frac{\Delta l}{l_o}\right) \quad \text{so} \quad \Delta l = \frac{\sigma l_o}{E}$$ **(elongation)**

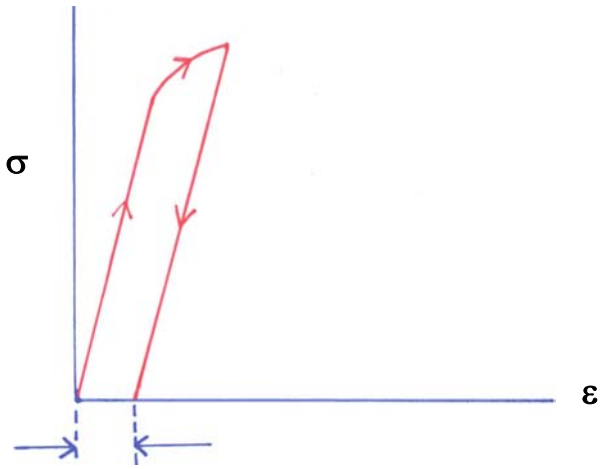
- **Poisson's ratio**:

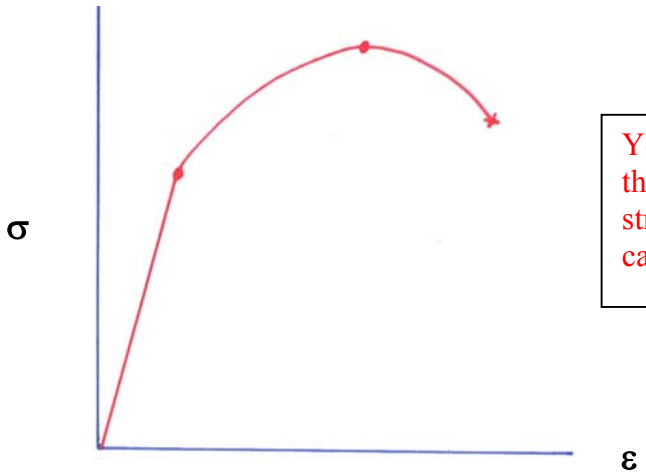
  The ratio of lateral (ε_x, ε_y) to axial (ε_z) strain is known as Poisson's ratio:

$$\nu = -\frac{\varepsilon_x}{\varepsilon_z} = -\frac{\varepsilon_y}{\varepsilon_z}$$

- **Plastic deformation:**

  Plastic ⇒ permanent (or non-recoverable) deformation





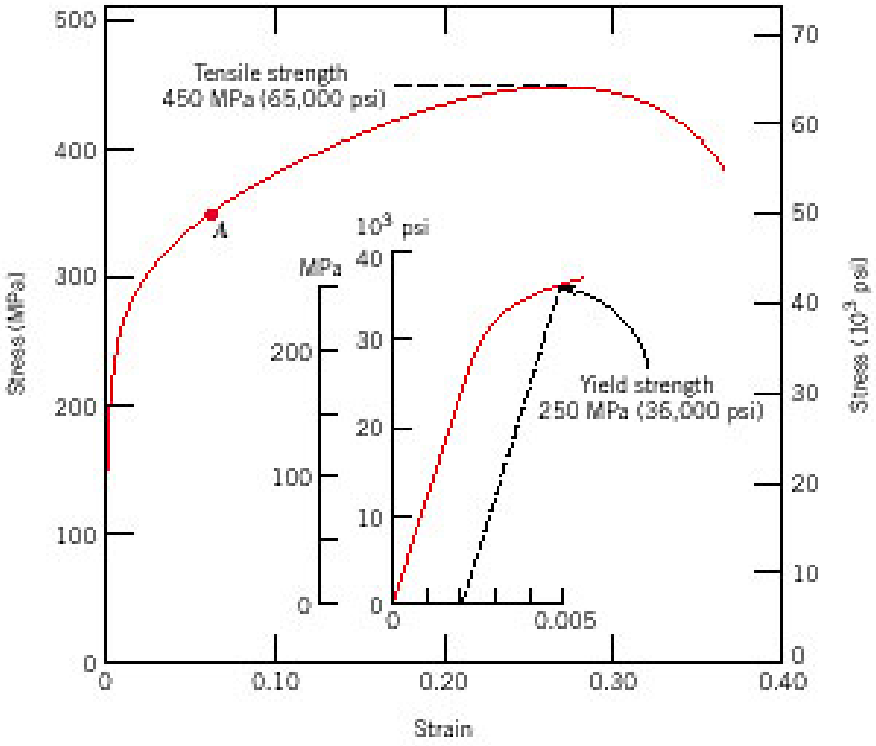
You should know what the key points on the stress – strain curve are called.

In ductile metals, the σ-ε curve eventually turns down after reaching the ultimate tensile strength (UTS). This does NOT mean that the material is becoming weaker.

Why? The gauge area decreases during plastic deformation due to necking.

- Since the actual cross-sectional area is reduced, use of the initial area gives a value for stress that is too high by the ratio (A_o/A)
- True (breaking or fracture) strength > tensile strength (but the engineering σ-ε diagram does not show this.

- Be able to work with a typical σ - ε curve such as the following
  - Know how to calculate elastic modulus ($E = slope = \frac{\Delta\sigma}{\Delta\varepsilon} = \frac{\sigma_2 - \sigma_1}{\varepsilon_2 - \varepsilon_1}$), maximum loading, elongation



Other important mechanical properties:

- Ductility
- Toughness
- Hardness

Ductility:

- Ductility is a measure of how much strain a given stress produces.

Percent elongation:

$$\%EL = \left(\frac{l_f - l_o}{l_o} \right) x100$$

where l_o is the initial gauge length
l_f is the final gauge length at fracture

Since the magnitude of %EL depends on gauge length, you should specify l_o as well.

Percent reduction in area:

$$\%RA = \left(\frac{A_o - A_f}{A_o} \right) x100$$

where A_o is the initial cross sectional area (in the gauge section)
A_f is the final cross sectional area at fracture

Toughness:

- the amount of energy a material can absorb energy up to fracture.
- The units are energy per unit volume of material: J/m^3
- Toughness requires both strength and ductility.

Hardness:

- the resistance to a localized applied plastic deformation.
- **Mohs scale: relative ability of one material to scratch another**

- Indentation methods are now commonly used:
    - Brinell
    - Vickers
    - Knoop
    - Rockwell
- These all relate either depth or area of indentation to hardness

Chapter 7: Dislocations and Strengthening

- **dislocation motion and interaction is the primary mechanism responsible for plastic deformation in metals.**

- **The presence of the dislocation results in local strain because the natural (equilibrium) spacing of the lattice is disrupted or distorted.**

- Plastic deformation corresponds to the motion of large numbers of dislocations along their respective slip planes.

- **Slip only occurs in close-packed planes and only in close-packed directions.**

    - **the movement of the dislocation requires the breaking (and formation) of only one set of bonds per step.**

- The motion of edge or screw dislocations under the action of an applied shear stress causes one atomic plane to slide over another, resulting in permanent (plastic) deformation.

- Dislocations are produced by :
    - solidification from the melt,
    - mechanical work (e.g., rolling, swaging, drawing, compressive impact, tensile or shear stress), or
    - thermal stresses

- As a metal is plastically deformed:
    - the density of dislocations increases
    - they interact with each other.
        - This interaction is responsible for the observed increase in strength
        - The movement of these dislocations is what enables plastic flow (or slip) to occur in materials

- Dislocations move in close-packed directions within close-packed planes.
- **The combination of C-P plane (the slip plane) and C-P direction (the slip direction) is called a slip system.**

- The more slip systems available, the easier it is for dislocations to move, which is why (on the average) FCC and BCC metals are more ductile than HCP metals.
- For any given tensile axis, there is a greater probability in FCC and BCC metals that some slip systems are favorably oriented for slip to occur.

- Resolved shear stress
    - the magnitude of the shear component is responsible for slip in any given plane.
    - The larger the shear component, the more likely slip will occur in that plane.
    - plastic deformation occurs when $\tau_r = \tau_{CRSS}$
    - τ_{CRSS} is a material property that determines the onset of plastic deformation.

Methods of Strengthening in Metals:

1) **Grain boundaries act as a barrier to dislocation motion**.

- $\sigma_y = \sigma_o + k_y d^{-\frac{1}{2}}$
    - more energy is required for a dislocation to cross grain boundaries, especially if high-angle

2) Plastic deformation (strain- or work-hardening)

- Dislocation motion is impaired by strain fields within a crystal.
    - An increase in dislocation density ⇒ increase in number of repulsive strain fields throughout the crystal ⇒ dislocation movement is hindered.
    - increasing dislocation density increases strength

3) Solid solution strengthening

- a lattice strain results from the substitution of a different atom onto a given lattice site.
    - Tensile in the case of smaller solutes
    - Compressive in the case of larger solutes
- Lattice strain fields resulting from substitutional alloying interact with the dislocation strain fields and impede dislocation movement.
    - Solute atoms tend to diffuse to the core of dislocations

- smaller atoms tend to occupy sites within the compressive strain field above the slip plane.
- larger atoms tend to occupy sites within the tensile strain field below the slip plane

- **Ceramics, as a rule, do not exhibit plastic deformation**

  - few, if any, active slip systems
  - interplanar sliding is not energetically favorable because of the distinct charge distribution of the ions:

    - If any plane tries to slip over an adjacent plane, ions of the same charge would be brought closer together (electrostatic repulsion)
    - Thus ceramics tend to be intrinsically strong but not very ductile

Recovery:

- **Reduction in lattice strains by heat treatment**
- Recovery does not completely remove all lattice strains
  - Can be useful in dissipating localized high stress regions that could lead to stress-corrosion problems.

Recrystallization:

- **At sufficiently high temperatures, heavily cold-worked regions produce nuclei of new, stress-free grains.**
  - Mechanical properties of recrystallized metals are restored to their pre-cold worked state (weaker but more ductile).

  - Recrystallization depends on both time and temperature.

    - Metals are classified by their **recrystallization temperature**

      - (temperature at which recrystallization just reaches completion in 1 hour)

      - Rule-of-thumb: recrystallization temperature generally ranges from 33% to 50% of the absolute melting temperature.

    - Note that the recrystallization temperature for Pb, Sn, and Zn is below room temperature. This means that these metals will not work-harden at room temperature.

      - These materials continuously recrystallize during plastic deformation (i.e., they do not work-harden)

Grain Growth:

- **There exists a thermodynamic driving force to reduce excess grain boundary energy**
  - This process is called **grain growth**
- Grain growth is a diffusional process (which means that it has an explicit temperature dependence)
- Grain growth proceeds by the diffusion of atoms across grain boundaries:
- Large grains grow at the expense of small grains
  - The direction of grain growth is always towards the center of curvature