MSE 160 Lecture Notes

Hei Shing Cheung

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The up-to-date version of this document can be found at `https://github.com/HaysonC/skulenotes`

> *"In this class we are mostly understanding solids"*
> - Prof. SCOTT RAMSAY

1 Mechanical Behavior

Classes of Materials   In this class, we look at three classes of materials (non-exhaustive):

- **Metal** held together with metallic bonds, typically **ductile** and **conductive**.

- **Ceramics** (often metal oxides [excp: diamond]) held together via covalent & ionic bonds, typically **brittle** and **insulating**.

- **Polymers** Molecules (often hydrocarbons) typically **ductile** and **insulating**

Engineering Stress   For normal stress, we know that:

$$\sigma = \frac{F}{A_0} \tag{1}$$

Engineering Strein   Also:

$$\epsilon = \frac{\Delta l}{l_0} \tag{2}$$

Young's Moduclus   For elastic deformation, E, is given, by Hooke's Law, as follows:

$$\sigma = E\epsilon \tag{3}$$

Tensile Test   We apply force as to the ends of a dogbone-sample, with l_0 being the gauge length and A_0 being the area of the cross-section at the middle.

Tensile Strein   Maximum tensile strain on the engineeging stress-strain curve.

1.1 Understanding Elastic Properties in terms of Atomic Configuration

Atomic Configuration We can understand the elastic properties of a material by looking at the atomic configuration. Skemetically, we can represent the atomic configuration as a spring system:

1. **Intial - Before Loading** Atoms are in equilibrium, with the interatomic forces being balanced.

2. **Loading** We apply a force to the material, causing the atoms to move from their equilibrium positions. The bond stretches and the atoms move further apart.

3. **Unloading** We remove the force, causing the atoms to return to their equilibrium positions.

Atom Positions Elastic modulus is dependent on the atomic interatomic bonding force. Thus, The elastic modulus is prootionaly to the slope of the interatomic force-seperation curve.

Force-Seperation Curve The force-seperation curve is a plot of the force between two atoms as a function of the distance between them. The slope of the curve is proportional to the elastic modulus near the equilibrium position.
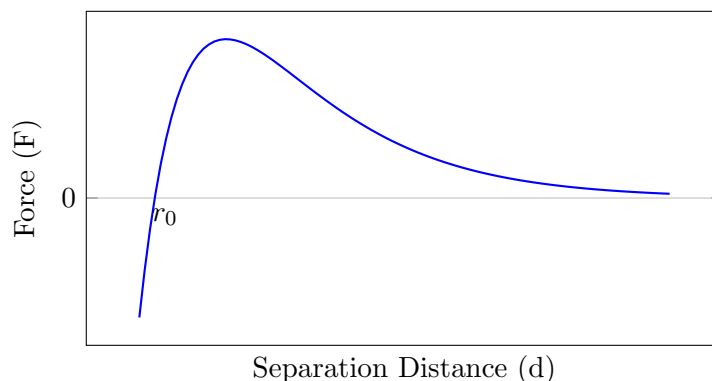

Figure 1: Force-Separation Curve (Lennard-Jones Force)

$$E \propto \left. \frac{dF}{dr} \right|_{r_0} \tag{4}$$

Definiton 1.1.1 (Equilibrium interatomic seperation distance)**.** The equilibrium interatomic seperation distance, r_0, is the distance between two atoms at which the interatomic force is zero. This is due to the interatomic forces being the sum of attractive and repulsive forces.

Elastic Modulus Thus, strongly bonded materials have a higher elastic modulus and the slope of the force-seperation curve is steeper at r_0.

1.2 Understanding Other Properties in terms of Atomic Configuration

Potential Energy-Separation Curve The potential energy-seperation curve is a plot of the potential energy between two atoms as a function of the distance between them. The potential energy is the area under the force-seperation curve.

Depth of the Minimum Energy Well The depth of the minimum energy well, E_0, is the energy required to break the bond between two atoms. This is the energy required to move the atoms from the equilibrium position to infinity. It is proportional to the melting temperature of the material.
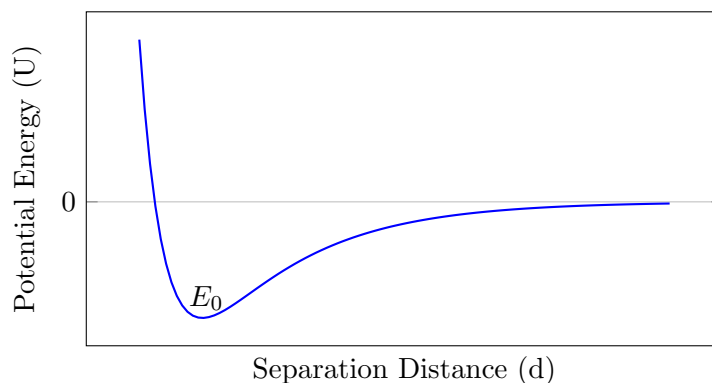

Figure 2: Potential Energy-Separation Curve

Coefficient of Thermal Expansion The coefficient of thermal expansion, α, is the fractional change in length per degree change in temperature.

Depth of Potential Energy Curve The deeper the potential energy curve, the higher the melting temperature and more symetric the curve near E_0. This would give the follwoing three properties:

1. **Higher Melting Temperature** The higher the melting temperature, the deeper the potential energy curve.

2. **Higher Elastic Modulus** The steeper the slope of the force-seperation curve at r_0, the higher the elastic modulus.

3. **Lower Coefficient of Thermal Expansion** The more symetric the potential energy curve near E_0, the lower the coefficient of thermal expansion.

1.3 Shear and Tensile Stress

1.3.1 Shear

Shear Stress   Shear stress is the force per unit area acting parallel to the surface. It is given by:

$$\tau = \frac{F}{A_0} \tag{5}$$

Shear Strain   Shear strain is the change in angle between two lines originally perpendicular to each other. It is given by:

$$\gamma = \frac{\Delta l}{l_0} \approx \tan\theta \approx \theta = \frac{\pi}{2} - \phi \tag{6}$$

Shear Modulus   The shear modulus, G, is the ratio of shear stress to shear strain. It is given by:

$$\tau = G\gamma \tag{7}$$

Relationship between Shear and Tensile Modulus   The shear modulus is related to the tensile modulus by the following equation:

$$G = \frac{E}{2(1+\nu)} \tag{8}$$

where ν is the Poisson's ratio.

Poisson's Ratio   Poisson's ratio, ν, is the ratio of lateral strain to axial strain. It is given by:

$$\nu = -\frac{\epsilon_{\text{lat}}}{\epsilon_{\text{axial}}} \tag{9}$$

1.4 Testing

Definiton 1.4.1 (Gauge Length)**.** The gauge length, l_0, is the length of the sample over which the strain is measured.

Definiton 1.4.2 (Reduced Section)**.** The reduced section is the part of the sample where the cross-sectional area is reduced to a smaller value.

Gauge length is always no longer than the reduced section. The reduced section is where the sample will likely break.

Testing Ceremics   In relation to tensile testing, ceramics have the following properties:

- **Brittle** Ceramics are brittle and will break suddenly.

- **High Strength** Ceramics have high strength and thus difficult to machine the sample.

- **Sample Alignment** The sample must be aligned properly to test for pure tension. Unlike metals and polymers, which are self-aligning.

- **Fracture** Ceramics will fracture while still off-axis. Hence, there would be a large shear component.

Thus, we often approxiate tensile behaviour with a point loading on a horizontal beam, with two point support (3 point bending test). Peak stress is given by:

$$\sigma_{\text{peak}} = \frac{3FL}{2bd^2} \tag{10}$$

, where:

- L (span) is the distance between the two supports.

- b is the width of the sample

- d is the thickness/depth of the sample

2   Seleection of Materials

2.1   Material Performance

Example 2.1.1 (Aircraft Wing Spar)**.** The aircraft wing spar is beam (loaded in bending) that supports the wing. The spar is made of a material with the objective of minimize mass under the following constraints:

- **Deflection** There is a maximum allowable deflection of the wing.

- There is more..., but for this example, we will only consider the deflection.

The material selection solve for a **light stiff beam**.

Mass   The mass of the beam is given by:

$$m = \rho V = \rho A L$$

Deflection   The deflection of the beam is given by:

$$\delta = \frac{FL^3}{48EI} \tag{11}$$

For a beam with a rectangular cross-section, we have:

$$\delta = \frac{FL^3}{48E} \cdot \frac{12}{bh^3} = \frac{FL^3}{4Ebh^3}$$

We can set b proportional to h:

$$\delta = \frac{FL^3}{cE} \cdot \frac{1}{A^2}, \quad \text{for some constant } c$$

We can then isolate for A, the free variable, and minimize the mass via the objective equation $m = \rho AL$:

$$A = \sqrt{\frac{FL^3}{cE\delta}}$$

$$m = \rho L \sqrt{\frac{FL^3}{cE\delta}} = \rho L \sqrt{\frac{FL^3}{cE\delta}}$$

Arrange into the form (functional)(geometric)(material):

$$m = \left(\frac{F}{c\delta}\right)^{\frac{1}{2}} \cdot \left(L^{\frac{5}{2}}\right) \cdot \left(\frac{\rho}{E^{\frac{1}{2}}}\right)$$

Material Peformance Index   The material performance index is given by:

$$\text{Material Performance Index (MSI)} = \frac{E^{\frac{1}{2}}}{\rho} \tag{12}$$

MPI Graph   We plot $\log E$ against $\log \rho$ to get the MPI graph.

Tempered Glass   Temperglass are made to resist tension. It is done by applying a compressive stress to the surface of the glass. This is done by cooling the surface of the glass faster than the core or chemically treating the surface.

2.2   Density

Density   The density of a material is given by:

$$\rho = \frac{m}{V} \tag{13}$$

Archimedes' Principle The buoyant force on an object is equal to the weight of the fluid displaced by the object. Derive from that, we have:

$$\rho = \frac{m}{V} = \frac{m_{\text{object}}}{m_{\text{object}} - m_{\text{object in fluid}}} \tag{14}$$

3 Atomic Structures

3.1 General Definitions

Ordered structures We have the following three orders:

1. **Long Range Order (LRO)** Atoms are arranged in a well-defined pattern over long distances in repeating units.
   (Example) Diamonds, some polymers, most metals, many ceramics, graphite, quartz, etc.

2. **Short Range Order (SRO)** Periodic arrangement of atoms over a few atomic or molecular spacings.
   (Example) Most polymers, glasses, amorphous materials, etc.

3. **No Order (NO)** Atoms are randomly arranged.
   (Example) Ideal gases, etc.

Describing Crystal Structures We can describe crystal structures by the following:

- **Unit Cell** The smallest repeating unit of a crystal structure that could be used to represent the entire crystal.

- **Lattice** The repeating arrangement of points that repersent the positions of atoms in the unit cell.
  (Example) Simple Cubic, Body-Centered Cubic, Face-Centered Cubic, etc.

- **Lattice Plus Basis** *Not required for this course*

Theortical Density of Metals The theoretical density of metals is given by:

$$\rho = \frac{nM}{V_c N_A} \tag{15}$$

, where:

- n is the number of atoms in the unit cell.

- M is the atomic mass of the element (amu = g/mol).

- V_c is the volume of the unit cell.

- N_A is Avogadro's number ($6.022 \times 10^{23} \text{mol}^{-1}$)

3.2   Describing Basic Unit Cells

Definiton 3.2.1 (Coordination Number (CN))**.** The coordination number is the number of nearest neighbors an atom has in a crystal structure.

Definiton 3.2.2 (Atomic Packing Factor (APF))**.** The atomic packing factor is the fraction of the volume of the unit cell that is occupied by hard spheres. It is given by:

$$\text{APF} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}} \tag{16}$$

Simple Cubic (SC)   The simple cubic structure has the following properties:

- **Centers of atoms** Located at the eight corners of a cube

- **Rare Packing Density** Due to low packing density (only known example: Polonium, Po)

- **Close-packed directions** As cube edges.

- **Coordination Number** Number of nearest neighbor: 6

Face-Centered Cubic (FCC)   The face-centered cubic structure has an atom on the centre of each face of the cube. It has the following properties:

- **Ductile** and **Malleable** due to the close-packed planes. Common examples include: $\text{Al}, \text{Cu}, \text{Au}, \text{Ag}$.

- **Coordination Number** Number of nearest neighbor: 12

- **Close-packed directions** As cube diagonals.

- **Theortical Density** The theoretical density of FCC is derived from Equation (15):

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

With $n = 4$ (8 corners $\times \frac{1}{8}$ atom each + 6 faces $\times \frac{1}{2}$ atom each) and $V_c = a^3$ (where a is the **lattice parameter**):

$$\rho_{\text{FCC}} = \frac{4M}{a^3 N_A}$$

We can then obtain a via the relationship between the atomic radius, r, and the lattice parameter via the geometry on the close-packed direction (face diagonal):

$$a = 2\sqrt{2}r$$

Substitute a back into the equation:

$$\rho_{\text{FCC}} = \frac{4M}{(2\sqrt{2}r)^3 N_A} = \frac{4M}{16\sqrt{2}r^3 N_A}$$
$$= \frac{M}{4\sqrt{2}r^3 N_A} \tag{17}$$

- **Atomic Packing Factor** The atomic packing factor of FCC is given by:

$$\mathrm{APF_{FCC}} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{4 \times \frac{4}{3}\pi r^3}{a^3} = \frac{4 \times \frac{4}{3}\pi r^3}{(2\sqrt{2}r)^3} = \frac{\pi}{6\sqrt{2}} = \mathbf{0.74} \qquad (18)$$

This is the highest possible packing factor for spheres. Thus, no other structure can have a higher packing factor.

- **Stacking** The FCC structure can be thought of as stacking close-packed planes. The stacking sequence is ABCABC... (where A, B, and C describe the orientation hexagonal close-packed planes).

Hexagonal Close-Packed (HCP) The hexagonal close-packed structure is **crytal structure** by stacking close-packed hexagonal planes. It has the following properties:

- **Coordination Number** Number of nearest neighbor: 12

- **Close-packed directions** As cube diagonals.

- **Theortical Density** The theoretical density of HCP is derived from Equation (15):

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

With $n = 6$ (12 corners $\times \frac{1}{6}$ atom each) and $V_c = a^3$:

$$\rho_{\mathrm{HCP}} = \frac{6M}{a^3 N_A} \qquad (19)$$

- **Atomic Packing Factor** The atomic packing factor of HCP is given by:

$$\mathrm{APF_{HCP}} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{6 \times \frac{4}{3}\pi r^3}{a^3} = \frac{6 \times \frac{4}{3}\pi r^3}{a^3} = \mathbf{0.74} \qquad (20)$$

- **Stacking** The HCP structure can be thought of as stacking close-packed planes. The stacking sequence is ABAB...

Example 3.2.3 (Density of Aluminum)**.** Given that the atomic radius of aluminum is $r = 143$ pm and the atomic mass is $M = 26.98$ g/mol, we can calculate the density of aluminum with FCC structure. We have:

$$\rho_{\mathrm{Al}} = \frac{M}{4\sqrt{2}r^3 N_A} = \frac{26.98}{4\sqrt{2} \times (143 \times 10^{-12})^3 \times 6.022 \times 10^{23}}$$

$$= \frac{26.98}{4\sqrt{2} \times (143 \times 10^{-12})^3 \times 6.022 \times 10^{23}} = 2.7 \text{ g/cm}^3$$

Body-Centered Cubic (BCC) The body-centered cubic structure has an atom at the centre of the cube. It has the following properties:

1. **Coordination Number** Number of nearest neighbor: 8

2. **Atomic Packing Factor** The atomic packing factor of BCC is given by:

$$\text{APF}_{\text{BCC}} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{2 \times \frac{4}{3}\pi r^3}{a^3} = \frac{2 \times \frac{4}{3}\pi r^3}{(4r/\sqrt{3})^3} = \mathbf{0.68} \tag{21}$$

3. **Close Packed Directions** As cube diagonals.

4. **Theortical Density** The theoretical density of BCC is derived from Equation (15):

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

With $n = 2$ (8 corners $\times \frac{1}{8}$ atom each + 1 center atom) and $V_c = a^3$:

$$\rho_{\text{BCC}} = \frac{2M}{a^3 N_A} \tag{22}$$

5. **Stacking** The BCC structure can be thought of as stacking close-packed planes. The stacking sequence is ABAB...

4 Geometric Properties of Crystals

4.1 Crystallographic Directions and Planes

Point Coordinates A lattice positon in a unit cell is determined as fractional multiples of the unit cell edge lengths a, b, and c. (Defining the origin at one corner of the unit cell and $a = b = c = \mathbf{1}$)

Crystallographic Directions A crystallographic direction is a line between two points in a crystal. It is denoted by square brackets, $[uvw]$. The direction is determined from the "tail" to the "head" of the vector. Also:

1. It **shall not** include commas; and

2. It **shall be reduced** to the smallest integers; and

3. Negative signs are represented by a bar over the number.

Example 4.1.1. The crystallographic direction from $(0, 0, 0)$ to $(-1, 0, 1/2)$ is $[\bar{2}01]$.

Family of Directions A family of directions is a set of directions that are parallel to each other. It is denoted by $< uvw >$.

Example 4.1.2. The family of directions $< 100 >$ is the set of directions $[100]$, $[010]$, $[001]$, $[\bar{1}00]$, $[0\bar{1}0]$, and $[00\bar{1}]$.

Angle between Directions The angle between two directions in a **cubic** crystal is given by:

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}} \tag{23}$$

, which is simply the normalized dot product of the two vectors.

Crystallographic Planes A crystallographic plane is a set of parallel planes in a crystal. It is denoted by (hkl). The plane is determined by the intercepts on the x, y, and z axes.

Generally, we find the intercepts by finding the points where the plane intersects the axes. We then take the reciprocals of the intercepts and multiply by the smallest integer to get the Miller Indices.

Family of Planes A family of planes is a set of planes that are parallel to each other. It is denoted by $\{hkl\}$.

Distance between Planes The distance between two planes with miller indices $(h_1 k_1 l_1)$ and $(h_2 k_2 l_2)$ is given by:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{24}$$

, where a is the lattice parameter.

4.2 X-Ray Diffraction

The diffraction pattern is used to determine the crystal structure. By measuring the n$^{\text{th}}$ order peak angle θ_c and the wavelength of the X-ray, we can determine the distance between planes:

$$2d \sin \theta = n\lambda$$
$$d = \frac{n\lambda}{2 \sin \theta_c} \tag{25}$$

Thus, we could determine the lattice parameter a by the following equation:

$$a = \frac{n\lambda}{2 \sin \theta_c}\sqrt{h^2 + k^2 + l^2} \tag{26}$$

4.3 Geometrcally Ideal Crystal Structures

Coordination Number and Ratio The coordination number increases with $\frac{r_{\text{cation}}}{r_{\text{anion}}}$ (The ionic radii ratio). It relates to coordination number as follows:

Ionic Radii Ratio	Coord. Number	Name
< 0.155	2	Linear
0.155 - 0.225	3	Trigonal Planar
0.225 - 0.414	4	Tetrahedral
0.414 - 0.732	6	Octahedral
0.732 - 1.0	8	Cubic

Table 1: Coordination Number and Ionic Radii

Definiton 4.3.1 (AX Type)**.** The AX type is a crystal structure where the cation and anion are of the same ratio.

Example 4.3.2 (AX Type: NaCl rock salt)**.** The NaCl structure is an AX type structure. The cation and anion are of the same ratio. Soldium (Cation) has radius $r_{\text{Na}} = 0.102$ nm and Chlorine (Anion) has radius $r_{\text{Cl}} = 0.181$ nm. The ratio is:

$$\frac{r_{\text{cation}}}{r_{\text{anion}}} = \frac{0.102}{0.181} = 0.56$$

Thus, the coordination number is 6.
Additionally, we could calculate its theoretical density. It has 4 cation and 4 anion in the unit cell. The volume of the unit cell is a^3, and it follows a FCC structure. Thus, the density is:

$$
\begin{aligned}
\rho &= \frac{4M_{\text{Na}} + 4M_{\text{Cl}}}{a^3 N_A} = \frac{4(22.99) + 4(35.45)}{a^3 N_A} \\
&= \frac{4(22.99) + 4(35.45)}{(2\sqrt{2}r_{\text{Na}})^3 N_A} = \frac{4(22.99) + 4(35.45)}{(2\sqrt{2} \times 0.102)^3 N_A} \\
&= \frac{4(22.99) + 4(35.45)}{(2\sqrt{2} \times 0.102)^3 N_A} = 2.16 \text{ g/cm}^3
\end{aligned}
$$

Example 4.3.3 (AX Type: ZnS, Zinc Blende)**.** The ZnS structure is an AX type structure. It has a FCC structure with CN = 4. The radius of Zinc (Cation) is $r_{\text{Zn}} = 0.074$ nm and the radius of Sulfur (Anion) is $r_{\text{S}} = 0.184$ nm. The ratio is:

$$\frac{r_{\text{cation}}}{r_{\text{anion}}} = \frac{0.074}{0.184} = 0.40$$

Example 4.3.4 (AX_2 Type: CaF_2)**.** The CaF_2 structure is an AX_2 type structure. It has a FCC structure with CN = 8. The radius of Calcium (Cation) is $r_{\text{Ca}} = 0.099$ nm and the radius of Fluorine (Anion) is $r_{\text{F}} = 0.133$ nm. The ratio is:

$$\frac{r_{\text{cation}}}{r_{\text{anion}}} = \frac{0.099}{0.133} = 0.74$$

5 Stress-Strain Behavior

Uniformly Distributed Elongation The elongation of a material is uniformly distributed within the gauge length. The initial values, referred to as the "elastic region," are characterized as uniformly elastic.

Non-Linear Elastic There is also a non-linear region where the material remains elastic but is not uniformly distributed.

Localized Plastic Deformation The material then enters the plastic region where the deformation is localized. The material is permanently deformed. This is characterized by the ultimate tensile strength (this is bad when it happens).

Necking The material then necks, where the cross-sectional area decreases. The material is then strained until it breaks.

True Stress The true stress is given by:

$$\sigma_T = \frac{F}{A_i} \tag{27}$$

, where A_i is the instantaneous cross-sectional area.

Ultimate Tensile Strength The ultimate tensile strength is the maximum stress on the stress-strain curve.

Strengthening Plastic deformation is made more difficult by the following mechanisms:

1. **Strain Hardening** Preloading beyond the elastic region - upon plastic deformation, the material will have a higher yield strength.

2. **For Metals and Alloys** The following mechanisms are used:

Strain Hardening Equation The true stress-strain curve can be emprically described by the following equation:

$$\sigma_T = K\epsilon_T^n \tag{28}$$

, where K is the Strain Hardening coefficient and n is the strain hardening exponent. Both of these values are material properties.

True Strain   Since $\epsilon_i = \frac{\Delta l_i}{l_0 + \Delta l_{i-1}}$ we can compute a Rieman sum to get the true strain:

$$\epsilon_T = \int_{l_0}^{l_f} \frac{dl}{l} = \ln\left(\frac{l_f}{l_0}\right) \tag{29}$$

Strain Rate   The strain rate is the rate at which the material is deformed. It is given by:

But, before necking, we can assume $V_0 = V_i$ and $A_i = \frac{A_0 l_0}{l_i}$. Thus, we have:

$$\sigma_T = \frac{F}{A_i} = \frac{F}{\frac{A_0 l_0}{l_i}} = \frac{F l_i}{A_0 l_0} = \frac{F}{A_0} \cdot \frac{l_i}{l_0} = \sigma \cdot \frac{l_i}{l_0}$$
$$= \sigma \cdot (1 + \epsilon) \tag{30}$$

and,

$$\epsilon_T = \ln(1 + \epsilon) \tag{31}$$

5.1 Imperfections

Dislocation   Recal that plastic deformation occurs by step-wise breaking of atomic bonds. This is done by the movement of dislocations. **Strengthening mechanisms in Metals** rely on inhibiting the movement of dislocations.

Definiton 5.1.1 (Dislocation). A dislocation is the breaking and reforming of bonds, one row at a time. It is a line defect in the crystal structure.

Crystalline Imperfections   We use crystalline imperfections to inhibit the movement of dislocations. These imperfections include:

- **Point Imperfections (Defects)** Vacancies, interstitials, and substitutional atoms. (Example) Solid solution strengthening.

- **Line Imperfections** Dislocations.

- **Area Imperfections** Grain boundaries of the interface between two grains and free surfaces.

- **Volume Imperfections** Second phase particles.

Solid Solution Strengthening   [Alloying] The addition of a solute to a solvent to inhibit the movement of dislocations. There is two types:

1. **Interstitial Impurities** The solute atoms are smaller than the solvent atoms. This the impurites to be in the interstitial sites.

2. **Substitutional Impurities** The solute atoms are larger than or as large as the solvent atoms ($< 10\%\Delta\varnothing$, similar electornegativity.). This causes the impurities substitute the lattice sites.

It slightly nudges nearby atoms, creating **lattice strain** that make it harder for dislocations to move.

Machaism - Diffusion of Impurities In positve edge dislcation, it has compession above disvlation line, and tension below. The impurities will 'pin' the dislocation, making it harder to move.

Plastic Deformation We can also strengthen the material by increasing the number of dislocations. This is done by plastic deformation methods:

1. Cold Work

2. Forging/Strain Hardening

Mechanisms of Strengthening Plastic deformation increases number of dislocations, which inhibits one another due to the strain fields.

Definiton 5.1.2 (Grain Boundaries)**.** Grain boundaries are the interface between two grains. Grains are regions of the same crystal structure but with different orientations.

Grain Size Reduction Dislcations tend to move in the direction of the grain boundry (GB). Thus, reducing the grain size reduces the distance the dislocation can move. In addition, there are atomic strain due to the difference of bond lenght between grains, contributing to the strain field. It is given by:

$$\sigma = \sigma_0 + \frac{K_y}{d} \tag{32}$$

Second Phase Particles Second phase particles are particles of a different phase in the material. They can be used to inhibit the movement of dislocations. They are often hard, brittke phases.

Constants and conversions

1 atm = 101.325 kPa = 1.01325 bar = 14.696 psi
N_A $6.022 \times 10^{23}\,\text{mol}^{-1}$
e $1.602 \times 10^{-19}\,\text{C}$
1 eV $1.602 \times 10^{-19}\,\text{J}$
ϵ_0 $8.854 \times 10^{-12}\,\text{F m}^{-1}$
R $8.314\,\text{J mol}^{-1}\,\text{K}^{-1}$
  $0.082067\,\text{L atm mol}^{-1}\,\text{K}^{-1}$
0°C $273.15\,\text{K}$
k $8.62 \times 10^{-5}\,\text{eV atom}^{-1}\,\text{K}^{-1}$
  $1.38 \times 10^{-23}\,\text{J atom}^{-1}\,\text{K}^{-1}$
F $96.486\,\text{C mol}^{-1}$
h $6.626 \times 10^{-34}\,\text{J s}$
  $4.136 \times 10^{-15}\,\text{eV s}$
c $2.99 \times 10^{8}\,\text{m s}^{-1}$
g $9.81\,\text{m s}^{-2}$

Microstructure

$LD = \frac{\#}{\text{Length}}$ $LPF = \frac{\text{length of atoms}}{\text{length of vector}}$

$PD = \frac{\#}{\text{Area}}$ $PPF = \frac{\text{area of atoms}}{\text{area of plane}}$

$V = \frac{4}{3}\pi r^3$ $A = \pi r^2$

$A_{\text{triangle}} = \frac{1}{2}bh$ $\rho = \frac{nA}{V_C N_A V_s}$

$\rho = \frac{n_A A + n_C A_C}{V_C N_A}$ $APF = \frac{V_s}{V_C}$

$N = \frac{N_A \rho}{A}$ $N_V = N\exp\left(-\frac{Q_V}{kT}\right)$

$a = 2\sqrt{2}R$ $a = \frac{4}{\sqrt{3}}R$

$d_{\text{hkl}} = \frac{a}{\sqrt{h^2+k^2+l^2}}$ $n\lambda = 2d_{\text{hkl}}\sin\theta$

$n_n = \frac{M_n}{m}$ $n_w = \frac{M_w}{m}$

Mechanical Behaviour

$\sigma = \frac{F}{A_0}$ $\epsilon = \frac{\Delta l}{l_0}$

$\sigma = E\epsilon$ $\sigma_{\text{3-point}} = \frac{3FL}{2wh^2}$

$\sigma_T = \sigma(1+\epsilon)$ $\epsilon_T = \ln(1+\epsilon)$

$\sigma_T = \frac{F}{A_i}$ $\sigma_T = K\epsilon_T^n$

$E = 2G(1+\nu)$ $\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$

Magnetic Behaviour

$H = \frac{NI}{L}$ $B_0 = \mu_0 H$

$M = \chi_m H$ $B = \mu_0 H + \mu_0 M$

$B = (1+\chi_m)\mu_0 H$ $\mu_B = \frac{e\hbar}{2m_e} = \beta$

$\beta = 9.27 \times 10^{-24}\,Am^2$

Electrical Behaviour

$$\sigma = n|e|\mu_e + p|e|\mu_h \qquad \sigma = n|e|\mu_e$$
$$\sigma = p|e|\mu_h$$

Electrochemistry

$$E = E° - \frac{RT}{nF}\ln Q \qquad I = \frac{nC}{t}$$
$$E_{\text{at 25°C}} = E° - \frac{0.0592}{n}\ln Q$$
$$w = nFE°$$

Thermodynamics

$$PV = nRT \qquad \Delta U = q + w$$
$$\Delta U = q - P_{\text{ext}}\Delta V \qquad H = U + PV$$
$$G \equiv H - TS \qquad \Delta S = \frac{q_{\text{rev}}}{T}$$
$$\text{constant T: } \Delta G = \Delta H - T\Delta S$$
$$q = mc\Delta T \qquad q = nC_P\Delta T$$
$$\text{For } aA + bB \rightarrow cC + dD, \quad Q = \frac{a_C^c a_D^d}{a_A^a a_B^b}$$
$$\Delta_r G = \Delta G° + RT\ln Q$$
$$\Delta_r H° = (\Sigma v_i \Delta_{f,i} H°)_{\text{prod.}} - (\Sigma v_i \Delta_{f,i} H°)_{\text{react.}}$$
$$\Delta_r S° = (\Sigma v_i \Delta_{f,i} S°)_{\text{prod.}} - (\Sigma v_i \Delta_{f,i} S°)_{\text{react.}}$$
$$W_{\text{phase}} = \frac{\text{length of opp. side of lever}}{\text{total length of lever}}$$
$$E = h\nu = \frac{hc}{\lambda}$$

Specific heats and heat capacities

Substance	$c\left(\frac{J}{g \cdot K}\right)$	$C_P\left(\frac{J}{mol \cdot K}\right)$
Air(g)	1.0	-
$CO_2(g)$	0.843	37.1
$H_2(g)$	14.304	28.836
$H_2O(g)$	2.03	36.4
$H_2O(l)$	4.184	75.3
$H_2O(s)$	2.09	37.7
$NaCl$	0.853	50.5
$O_2(g)$	0.918	29.378

Temperatures and enthalpies of phase changes

Substance	M.P. (°C)	$\Delta_{fus}H$ $\frac{kJ}{mol}$	B.P. (°C)	$\Delta_{vap}H$ $\frac{kJ}{mol}$
Al	658	10.6	2467	284
Ca	851	9.33	1487	162
CH_4	-182	0.92	-164	8.18
H_2O	0	6.01	100	40.7
Fe	1530	14.9	2735	354

Standard formation enthalpy, standard entropy and standard formation Gibbs energy at 298.15 K

Species	$\Delta_f H°$ $\left(\frac{kJ}{mol}\right)$	$S°$ $\left(\frac{J}{mol \cdot K}\right)$	$\Delta_f G°$ $\left(\frac{kJ}{mol}\right)$
C	0	5.74	0
$CH_4(g)$	-74.81	186.2	-50.75
$C_2H_2(g)$	-83.9	200.93	-
$C_3H_8(g)$	-103.8	269.9	-23.49
$CaC_2(s)$	-59.8	70.3	-
$CaO(s)$	-635	38.1	-
$CaF_2(s)$	-1225	68.87	-1162
$CaF_2(l)$	-1186	92.6	-
$Ca(OH)_2(s)$	-987.0	83.0	-
$CO_2(g)$	-393.5	213.6	-394.4
$Cu_2O(s)$	-168.6	93.1	-
$Cu_2O(l)$	-154.79	-	-
$Cu(s)$	-	33.2	-
$Fe(s)$	0	27.3	0
$Fe_2O_3(s)$	-824.2	87.4	-
$H_2(g)$	-	130.68	-
$H_2O(g)$	-241.8	188.7	-228.6
$H_2O(l)$	-285.8	69	-
$O_2(g)$	0	205.0	0

Miscellaneous enthalpies

Substance	Reaction	$\Delta H\left(\frac{kJ}{mol}\right)$
F_2	$F_2 \rightarrow F(g)$	157
F	$F(g) \rightarrow F^-(g)$	-328
Ca	$Ca(g) \rightarrow Ca^{2+}(g)$	1734
$NaCl$	$NaCl(s) \rightarrow$ $Na^+(aq) + Cl^-(aq)$	3.9

Scott Ramsay, December 2024

IUPAC Periodic Table of the Elements

Key:

atomic number
Symbol
name
abridged standard atomic weight

1	2												13	14	15	16	17	18
1 **H** hydrogen 1.0080 ± 0.0002																		2 **He** helium 4.0026 ± 0.0001
3 **Li** lithium 6.94 ± 0.06	4 **Be** beryllium 9.0122 ± 0.0001												5 **B** boron 10.81 ± 0.02	6 **C** carbon 12.011 ± 0.002	7 **N** nitrogen 14.007 ± 0.001	8 **O** oxygen 15.999 ± 0.001	9 **F** fluorine 18.998 ± 0.001	10 **Ne** neon 20.180 ± 0.001
11 **Na** sodium 22.990 ± 0.001	12 **Mg** magnesium 24.305 ± 0.002	3	4	5	6	7	8	9	10	11	12		13 **Al** aluminium 26.982 ± 0.001	14 **Si** silicon 28.085 ± 0.001	15 **P** phosphorus 30.974 ± 0.001	16 **S** sulfur 32.06 ± 0.02	17 **Cl** chlorine 35.45 ± 0.01	18 **Ar** argon 39.95 ± 0.16
19 **K** potassium 39.098 ± 0.001	20 **Ca** calcium 40.078 ± 0.004	21 **Sc** scandium 44.956 ± 0.001	22 **Ti** titanium 47.867 ± 0.001	23 **V** vanadium 50.942 ± 0.001	24 **Cr** chromium 51.996 ± 0.001	25 **Mn** manganese 54.938 ± 0.001	26 **Fe** iron 55.845 ± 0.002	27 **Co** cobalt 58.933 ± 0.001	28 **Ni** nickel 58.693 ± 0.001	29 **Cu** copper 63.546 ± 0.003	30 **Zn** zinc 65.38 ± 0.02		31 **Ga** gallium 69.723 ± 0.001	32 **Ge** germanium 72.630 ± 0.008	33 **As** arsenic 74.922 ± 0.001	34 **Se** selenium 78.971 ± 0.008	35 **Br** bromine 79.904 ± 0.003	36 **Kr** krypton 83.798 ± 0.002
37 **Rb** rubidium 85.468 ± 0.001	38 **Sr** strontium 87.62 ± 0.01	39 **Y** yttrium 88.906 ± 0.001	40 **Zr** zirconium 91.224 ± 0.002	41 **Nb** niobium 92.906 ± 0.001	42 **Mo** molybdenum 95.95 ± 0.01	43 **Tc** technetium [97]	44 **Ru** ruthenium 101.07 ± 0.02	45 **Rh** rhodium 102.91 ± 0.01	46 **Pd** palladium 106.42 ± 0.01	47 **Ag** silver 107.87 ± 0.01	48 **Cd** cadmium 112.41 ± 0.01		49 **In** indium 114.82 ± 0.01	50 **Sn** tin 118.71 ± 0.01	51 **Sb** antimony 121.76 ± 0.01	52 **Te** tellurium 127.60 ± 0.03	53 **I** iodine 126.90 ± 0.01	54 **Xe** xenon 131.29 ± 0.01
55 **Cs** caesium 132.91 ± 0.01	56 **Ba** barium 137.33 ± 0.01	57-71 lanthanoids	72 **Hf** hafnium 178.49 ± 0.01	73 **Ta** tantalum 180.95 ± 0.01	74 **W** tungsten 183.84 ± 0.01	75 **Re** rhenium 186.21 ± 0.01	76 **Os** osmium 190.23 ± 0.03	77 **Ir** iridium 192.22 ± 0.01	78 **Pt** platinum 195.08 ± 0.02	79 **Au** gold 196.97 ± 0.01	80 **Hg** mercury 200.59 ± 0.01		81 **Tl** thallium 204.38 ± 0.01	82 **Pb** lead 207.2 ± 1.1	83 **Bi** bismuth 208.98 ± 0.01	84 **Po** polonium [209]	85 **At** astatine [210]	86 **Rn** radon [222]
87 **Fr** francium [223]	88 **Ra** radium [226]	89-103 actinoids	104 **Rf** rutherfordium [267]	105 **Db** dubnium [268]	106 **Sg** seaborgium [269]	107 **Bh** bohrium [270]	108 **Hs** hassium [269]	109 **Mt** meitnerium [277]	110 **Ds** darmstadtium [281]	111 **Rg** roentgenium [282]	112 **Cn** copernicium [285]		113 **Nh** nihonium [286]	114 **Fl** flerovium [290]	115 **Mc** moscovium [290]	116 **Lv** livermorium [293]	117 **Ts** tennessine [294]	118 **Og** oganesson [294]

57 **La** lanthanum 138.91 ± 0.01	58 **Ce** cerium 140.12 ± 0.01	59 **Pr** praseodymium 140.91 ± 0.01	60 **Nd** neodymium 144.24 ± 0.01	61 **Pm** promethium [145]	62 **Sm** samarium 150.36 ± 0.02	63 **Eu** europium 151.96 ± 0.01	64 **Gd** gadolinium 157.25 ± 0.03	65 **Tb** terbium 158.93 ± 0.01	66 **Dy** dysprosium 162.50 ± 0.01	67 **Ho** holmium 164.93 ± 0.01	68 **Er** erbium 167.26 ± 0.01	69 **Tm** thulium 168.93 ± 0.01	70 **Yb** ytterbium 173.05 ± 0.02	71 **Lu** lutetium 174.97 ± 0.01
89 **Ac** actinium [227]	90 **Th** thorium 232.04 ± 0.01	91 **Pa** protactinium 231.04 ± 0.01	92 **U** uranium 238.03 ± 0.01	93 **Np** neptunium [237]	94 **Pu** plutonium [244]	95 **Am** americium [243]	96 **Cm** curium [247]	97 **Bk** berkelium [247]	98 **Cf** californium [251]	99 **Es** einsteinium [252]	100 **Fm** fermium [257]	101 **Md** mendelevium [258]	102 **No** nobelium [259]	103 **Lr** lawrencium [262]

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PURE AND APPLIED CHEMISTRY

Dislcations (Slips)   Occurs on the plane with the highest planar density. The slip direction is the direction with the highest linear density. The slip system is the combination of the slip plane and slip direction.

FCC has 4 unique planes, each with 3 unique directions. Thus, there are 12 unique slip systems. Compare this to HCP, which has only base plane.

Resolved Stear Stress   Consider single crystal with a certain plane. Let ϕ be the angle between the normal of the plane and the direction of the applied stress, and λ be the angle between the plane and the orthonal of the applied stress. The resolved shear stress is given by:

$$\tau = \sigma \cos\phi \cos\lambda \tag{33}$$

Critcal Resolved Shear Stress   The critical resolved shear stress is the minimum shear stress required to move a dislocation. When the resolved shear stress equal the critical resolved shear stress, the dislocation will move, and:

$$\sigma = \sigma_y \tag{34}$$

So,

$$\tau_{\text{CRSS}} = \sigma_y \cos\phi \cos\lambda \tag{35}$$

Note   Most crystals are polycrystalline, so dislocation must be able to move to the neibouring crystal.

Burgers Vector   The Burgers vector is the vector that describes the dislocation. It is the vector that closes the loop of the dislocation. It is given by: