### MSE 160 Lecture Notes

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MSE 160

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 prootionally 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.

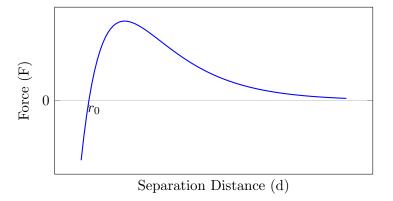


Figure 1: Force-Separation Curve (Lennard-Jones Force)

$$E \propto \frac{dF}{dr} \bigg|_{r_0}$$
 (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-separation curve is steeper at  $r_0$ .

### 1.2 Understanding Other Properties in terms of Atomic Configuration

**Potential Energy-Separation Curve** The potential energy-separation 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-separation 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.

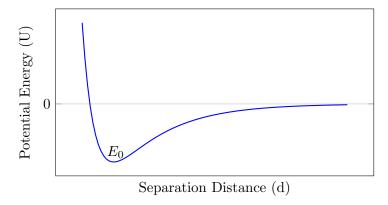


Figure 2: Potential Energy-Separation Curve

Coefficient of Thermal Expansion The coefficient of thermal expansion,  $\alpha$ , 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 following 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  $\nu$  is the Poisson's ratio.

**Poisson's Ratio** Poisson's ratio,  $\nu$ , 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

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

**Definition 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:

- $\bullet$  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 Selection 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:

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

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

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

**Definition 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:

$$APF = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}}$$
 (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: Al, Cu, Au, 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):

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

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:

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

$$= \frac{M}{4\sqrt{2}r^3 N_A}$$
(17)

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

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

$$\rho_{\rm HCP} = \frac{6M}{a^3 N_A} \tag{19}$$

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

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

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

**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:

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

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

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 position 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 = 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  $[\overline{2}01]$ .

**Family of Directions** A family of directions is a set of directions that are parallel to each other. It is denoted by  $\langle uvw \rangle$ .

**Example 4.1.2.** The family of directions < 100 > is the set of directions [100], [010], [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:

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$$
(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  $(h_1k_1l_1)$  and  $(h_2k_2l_2)$  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<sup>th</sup> order peak angle  $\theta_c$  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 Geometrically 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

**Definition 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:

$$\rho = \frac{4M_{\text{Na}} + 4M_{\text{Cl}}}{a^3 N_A} = \frac{4(22.99) + 4(35.45)}{a^3 N_A}$$

$$= \frac{4(22.99) + 4(35.45)}{(2\sqrt{2}r_{\text{Na}})^3 N_A} = \frac{4(22.99) + 4(35.45)}{(2\sqrt{2} \times 0.102)^3 N_A}$$

$$= \frac{4(22.99) + 4(35.45)}{(2\sqrt{2} \times 0.102)^3 N_A} = 2.16 \text{ g/cm}^3$$

**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  $r_{\rm Zn} = 0.074$  nm and the radius of Sulfur (Anion) is  $r_{\rm S} = 0.184$  nm. The ratio is:

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

**Example 4.3.4** (AX<sub>2</sub> Type: CaF<sub>2</sub>). The CaF<sub>2</sub> structure is an AX<sub>2</sub> 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:

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

1 atm = 101.325 kPa = 1.01325 bar = 14.696 psi $6.022 \times 10^{23} \, \mathrm{mol}^{-1}$ 

 $1.602 \times 10^{-19} \,\mathrm{C}$ 

 $1.602 \times 10^{-19} \,\mathrm{J}$ 1 eV

 $8.854 \times 10^{-12} \; \mathrm{F \, m^{-1}}$ 

 $8.314\,\mathrm{J}\,\mathrm{mol}^{-1}\,\mathrm{K}^{-1}$ 

 $0.082\,067\,\mathrm{L\,atm\,mol^{-1}\,K^{-1}}$ 

 $273.15\,\mathrm{K}$ 0°C  $8.62\times 10^{-5}\,{\rm eV\,atom^{-1}\,K^{-1}}$ 

 $1.38 \times 10^{-23} \, \mathrm{J} \, \mathrm{atom}^{-1} \, \mathrm{K}^{-1}$  $96486 \,\mathrm{C}\,\mathrm{mol}^{-1}$ 

 $6.626 \times 10^{-34} \,\mathrm{J\,s}$ 

 $4.136\times10^{-15}\,\mathrm{eV}\,\mathrm{s}$ 

 $2.99\times 10^8\,{\rm m\,s^{-1}}$ 

 $9.81\,\mathrm{m\,s^{-2}}$ 

### Microstructure

 $LPF = \frac{\text{length of atoms}}{\text{length of vector}}$   $PPF = \frac{\text{area of atoms}}{\text{area of plane}}$   $A = \pi r^2$  $n\lambda = 2d_{\rm hkl}\sin\theta$  $N_V = N \exp(-1)$  $\rho = \frac{nA}{V_C N_A}$  $APF = \frac{V_S}{V_C}$  $a = \frac{4}{\sqrt{3}}R$  $n_w = \overline{\frac{M_w}{\overline{m}}}$  $d_{\rm hkl} = \frac{1}{\sqrt{h^2 + k^2 + l^2}}$  $\rho = \frac{n_A A_A + n_C A_C}{V_C N_A}$  $A_{\text{triangle}} = \frac{1}{2}bh$  $LD = \frac{\#}{\text{Length}}$   $PD = \frac{\#}{\text{Area}}$   $V = \frac{4}{3}\pi r^3$  $a = 2\sqrt{2}R$  $N = \frac{N_A \rho}{M_A \rho}$  $n_n = \frac{\overline{N_n}}{\overline{m}}$ 

# Mechanical Behaviour

$\epsilon = rac{\Delta l}{l_0}$	$\sigma_{3\text{-point}} = \frac{3FL}{2wh^2}$	$\epsilon_T = \ln(1 + \epsilon)$	$\sigma_T = K \epsilon_T^n$	$ u = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z} $
$\sigma = rac{F}{A_0}$	$\sigma=E\epsilon$	$\sigma_T = \sigma(1+\epsilon)$	$\sigma_T = rac{F}{A_i}$	$E = 2G(1+\nu)$

## Magnetic Behaviour

$B_0=\mu_0 H$	$B=\mu_0 H + \mu_0 M$	$\mu_B = rac{e\hbar}{2m_e} = eta$	
$H = \frac{NI}{L}$	$M=\chi_m H$	$B = (1 + \chi_m)\mu_0 H$	$\beta = 9.27 \times 10^{-24} Am^2$

# Electrical Behaviour

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

### Electrochemistry

$$E = E^{\circ} - \frac{RT}{nF} \ln Q \qquad I = \frac{nC}{t}$$

$$E_{\text{at } 25 \circ \text{C}} = E^{\circ} - \frac{0.0592}{n} \ln Q$$

$$w = nFE^{\circ}$$

### Thermodynamics

$$PV = nRT \qquad \Delta U = q + w$$

$$\Delta U = q - P_{\text{ext}} \Delta V \qquad H \equiv U + PV$$

$$G \equiv H - TS \qquad \Delta S = \frac{q_{\text{rev}}}{T}$$

$$\text{constant T: } \Delta G = \Delta H - T\Delta S$$

$$q = mc\Delta T$$

For  $aA + bB \to cC + dD$ ,  $Q = \frac{a_C^c a_D^d}{a_A^d a_B^D}$ 

 $\Delta_{\rm r}G = \Delta G^\circ + RT \ln Q$ 

 $\Delta_{\rm r} H^{\circ} = (\Sigma v_i \Delta_{f,i} H^{\circ})_{\rm prod.} - (\Sigma v_i \Delta_{f,i} H^{\circ})_{\rm react.}$ 

 $\begin{array}{l} \Delta_{\rm r}S^{\circ} = (\Sigma v_{i}\Delta_{f,i}S^{\circ})_{\rm prod.} - (\Sigma v_{i}\Delta_{f,i}S^{\circ})_{\rm react.} \\ W_{\rm phase} = \frac{{\rm length\ of\ ope.\ side\ of\ lever}}{{\rm total\ length\ of\ lever}} \end{array}$ total length of lever

Specific heats and heat capacities

$C_P \left( \frac{J}{mol \cdot K} \right)$	
$c~(rac{J}{g\cdot K})$	7
${\bf Substance}$	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \

Air(g)	1.0	ı
$CO_2(g)$	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

omporance and compress of prime and see	MILE OTTO	arbice of bu	1100110	200
Substance	$M.P.$ $(^{\circ}C)$	$\Delta_{\substack{fus \ ootnotebox[k,t] \ mol}} H$	B.P. (°C)	$\Delta_{vap}H = rac{kJ}{mol}$
Al	829	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

$\frac{\Delta_f G^{\circ}}{(\frac{kJ}{mol})}$	0 50 75		-23.49	ı	ı	-1162	ı	ı	-394.4	ı	ı	ı	0	ı	ı	-228.6	1	0
$S^{\circ} \atop (\frac{J}{mol \cdot K})$	5.74	200.93	269.9	70.3	38.1	68.87	92.6	83.0	213.6	93.1	ı	33.2	27.3	87.4	130.68	188.7	69	205.0
$\frac{\Delta_f H^{\circ}}{(\frac{kJ}{mol})}$	0 7.7.81	-74.31	-103.8	-59.8	-635	-1225	-1186	-987.0	-393.5	-168.6	-154.79		0	-824.2		-241.8	-285.8	0
Species	C	$C_2H_2(g) \ C_2H_2(g)$	$C_3H_8(g)$	$CaC_2(s)$	CaO(s)	$CaF_2(s)$	$CaF_2(l)$	$Ca(OH)_2(s)$	$CO_2(g)$	$Cu_2O(s)$	$Cu_2O(l)$	Cu(s)	Fe(s)	$Fe_2O_3(s)$	$H_2(g)$	$H_2O(g)$	$H_2O(l)$	$O_2(g)$

### Miscellaneous enthalpies

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

Scott Ramsay, December 2024

# **IUPAC Periodic Table of the Elements**

18	2 Helium 4.0026 ± 0.0001	10 neon 20.180	<b>Ar</b> argon 39.95 ±0.16	36 <b>Kr</b> krypton 83.798 ± 0.002	54 Xe xenon 131.29 ± 0.01	86 <b>Rn</b> radon	0 <b>g</b> oganesson [294]
	17	9 fluorine 18.998	chlorine 35.45	35 <b>Br</b> bromine 79.904 ± 0.003	53 iodine 126.90 ± 0.01	At astatine	T17 TS tennessine
	9	0 0 0 0 0 15.999 0 0.001	16 sulfur 32.06 ± 0.02	34 <b>Se</b> selenium 78.971 ± 0.008	52 <b>Te</b> tellurium 127.60 ± 0.03	84 <b>Po</b> polonium [209]	116 <b>LV</b> livermorium [293]
	15	7 nitrogen 14.007 ± 0.001	15 Phosphorus 30.974 ± 0.001	33 <b>AS</b> arsenic 74.922 ± 0.001	51 <b>Sb</b> antimony 121.76 ± 0.01	83 <b>Bi</b> bismuth 208.98 ± 0.01	Mc moscovium
	4	6 Carbon 12:011	14 Silicon 28.085	32 <b>Ge</b> germanium 72.630 ± 0.008	50 <b>Sn</b> tin 118.71 ± 0.01	82 <b>Pb</b> lead 207.2 ± 1.1	114 <b>FI</b> flerovium [290]
	5	5 <b>D</b> boron 10.81	13 AI aluminium 26.982 ± 0.001	31 <b>Ga</b> gallium 69.723 ±0.001	49 Indium 114.82	81 thallium 204.38 ± 0.01	113 <b>Nh</b> nihonium [286]
			12	30 <b>Zn</b> zinc 65.38 ± 0.02	48 <b>Cd</b> cadmium 112.41 ± 0.01	80 <b>Hg</b> mercury 200.59 ± 0.01	8
			£	29 <b>Cu</b> copper 63.546 ±0.003	47 <b>Ag</b> silver 107.87 ± 0.01	79 <b>Au</b> gold 196.97 ± 0.01	Rg m roentgenium
			10	28 nickel 58.693 ± 0.001	46 <b>Pd</b> palladium 106.42 ± 0.01	78 Pt 195.08 ± 0.02	
			o	27 <b>Co</b> cobalt 58.933 ± 0.001	45 <b>Rh</b> rhodium 102.91 ± 0.01	77 	E
			ω	26 <b>Fe</b> iron 55.845 ±0.002	44 <b>RU</b> ruthenium 101.07 ± 0.02	76 <b>Os</b> osmium 190.23 ± 0.03	108 <b>HS</b> hassium [269]
			٢	25 <b>Mn</b> manganese 54.938 ± 0.001	Tc Tc technetium	75 <b>Re</b> rhenium 186.21	107 <b>Bh</b> bohrium [270]
			9	24 <b>Cr</b> chromium 51.996 ± 0.001	42 <b>Mo</b> molybdenum 95.95 ± 0.01	74 W tungsten 183.84 ± 0.01	Sg seaborgium
		ber and	ro	23 <b>V</b> vanadium 50.942 ± 0.001	41 <b>Nb</b> niobium 92.906 ± 0.001	73 <b>Ta</b> tantalum 180.95 ± 0.01	105 <b>Db</b> dubnium [268]
	Key:	atomic number Symbol name abridged standard atomic weight	4	22 <b>Ti</b> titanium 47.867 ± 0.001	40 <b>Z f</b> zirconium 91.224 ± 0.002	72 <b>Hf</b> hafnium 178.49 ± 0.01	104 <b>Pf</b> rutherfordium [267]
			ю	21 <b>Sc</b> scandium 44.956 ± 0.001	39 Yttrium 88.906 ± 0.001	57-71 lanthanoids	89-103 actinoids
	0	4 <b>Be</b> beryllium 9.0122 ± 0.0001	12 <b>Mg</b> magnesium 24.305 ± 0.002	20 <b>Ca</b> calcium 40.078 ± 0.004	38 <b>Sr</b> strontium 87.62 ± 0.01	56 <b>Ba</b> barium 137.33 ± 0.01	88 <b>Ra</b> radium [226]
-	hydrogen 1.0080 ± 0.0002	3 lithium 6.94 ± 0.06	22.990 ***********************************	19 K potassium 39.098 ± 0.001	37 <b>Rb</b> rubidium 85.468 ± 0.001	55 Csesium 132.91 ± 0.01	87 <b>Fr</b> francium [223]



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71 <b>Lu</b> lutetium 174.97 ± 0.01	103 <b>Lr</b> lawrencium [262]
70 <b>Yb</b> ytterbium 173.05 ± 0.02	102 <b>No</b> nobelium [259]
69 Tm thulium 168.93 ± 0.01	Md mendelevium [258]
68 <b>Er</b> erbium 167.26 ±0.01	100 <b>Fm</b> fermium [257]
67 <b>Ho</b> holmium 164.93 ± 0.01	99 <b>ES</b> einsteinium [252]
66 <b>Dy</b> dysprosium 162.50 ± 0.01	98 Cf californium [251]
65 <b>Tb</b> terbium 158.93 ± 0.01	97 <b>BK</b> berkelium [247]
64 <b>Gd</b> gadolinium 157.25 ± 0.03	96 <b>Cm</b> curium [247]
63 Europium 151.96 ± 0.01	95 <b>Am</b> ameridum [243]
62 Samarium 150.36 ± 0.02	94 <b>Pu</b> plutonium [244]
61 <b>Pm</b> promethium	ND neptunium [237]
60 Nd neodymium 144.24 ± 0.01	92 uranium 238.03 ± 0.01
59 <b>Pr</b> praseodymium 140.91 ± 0.01	91 <b>Pa</b> protactinium 231.04 ±0.01
58 Cerium 140.12 ± 0.01	90 Thorium 232.04 ± 0.01
57 <b>La</b> lanthanum 138.91 ± 0.01	89 <b>Ac</b> actinium

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