

# MSE 160 Lecture Notes

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MSE 160

*"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:

$$\sigma = \frac{F}{A_0} \quad (1)$$

**Engineering Strein** Also:

$$\epsilon = \frac{\Delta l}{l_0} \quad (2)$$

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

$$\sigma = E\epsilon \quad (3)$$

**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 engineeing 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. Schematically, we can represent the atomic configuration as a spring system:

1. **Initial - 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 proportional to the slope of the interatomic force-separation curve.

**Force-Separation Curve** The force-separation 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.

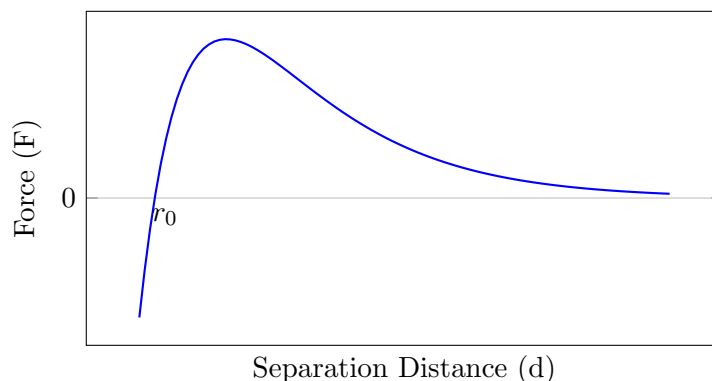


Figure 1: Force-Separation Curve (Lennard-Jones Force)

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

**Definition 1.1.1** (Equilibrium interatomic separation distance). The equilibrium interatomic separation 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.

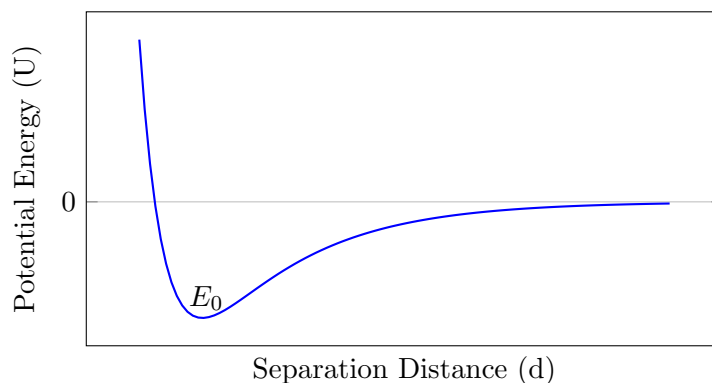


Figure 2: Potential Energy-Separation Curve

**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 symmetric 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-separation curve at  $r_0$ , the higher the elastic modulus.
3. **Lower Coefficient of Thermal Expansion** The more symmetric 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:

$$\tau = \frac{F}{A_0} \quad (5)$$

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

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

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

$$\tau = G\gamma \quad (7)$$

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

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

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:

$$\nu = -\frac{\epsilon_{\text{lat}}}{\epsilon_{\text{axial}}} \quad (9)$$

Constants and conversions

1 atm = 101.325 kPa = 1.013 25 bar = 14.696 psi  
N<sub>A</sub> = 6.022 × 10<sup>23</sup> mol<sup>-1</sup>  
e = 1.602 × 10<sup>-19</sup> C  
1 eV = 1.602 × 10<sup>-19</sup> J  
ε<sub>0</sub> = 8.854 × 10<sup>-12</sup> F m<sup>-1</sup>  
R = 8.314 J mol<sup>-1</sup> K<sup>-1</sup>  
0.082 067 L atm mol<sup>-1</sup> K<sup>-1</sup>  
0 °C = 273.15 K  
k = 8.62 × 10<sup>-5</sup> eV atom<sup>-1</sup> K<sup>-1</sup>  
1.38 × 10<sup>-23</sup> J atom<sup>-1</sup> K<sup>-1</sup>  
F = 96 486 C mol<sup>-1</sup>  
h = 6.626 × 10<sup>-34</sup> J s  
4.136 × 10<sup>-15</sup> eV s  
c = 2.99 × 10<sup>8</sup> m s<sup>-1</sup>  
g = 9.81 m s<sup>-2</sup>

Microstructure

$LD = \frac{\#}{\text{Length}}$   
 $PD = \frac{\#}{\text{Area}}$   
 $V = \frac{4}{3}\pi r^3$   
 $A_{\text{triangle}} = \frac{1}{2}bh$   
 $\rho = \frac{n_A A_A + n_C A_C}{V_{CNA}}$   
 $N = \frac{N_A \rho}{A}$   
 $a = 2\sqrt{2}R$   
 $d_{\text{hkl}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$   
 $n_n = \frac{M_w}{\overline{m}}$

Mechanical Behaviour

$\sigma = \frac{F}{A_0}$   
 $\sigma = E\epsilon$   
 $\sigma_T = \sigma(1 + \epsilon)$   
 $\sigma_T = \frac{F}{A_i}$   
 $E = 2G(1 + \nu)$   
 $\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$

Magnetic Behaviour

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

Electrical Behaviour

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

Electrochemistry

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

Thermodynamics

$PV = nRT$      $\Delta U = q + w$   
 $\Delta U = q - P_{\text{ext}}\Delta V$      $H \equiv U + PV$   
 $G \equiv H - TS$      $\Delta S = \frac{q_{\text{rev}}}{T}$   
constant T:  $\Delta G = \Delta H - T\Delta S$   
 $q = mc\Delta T$      $q = nC_P\Delta T$   
For  $aA + bB \rightarrow cC + dD$ ,  $Q = \frac{a^c c^d}{a^a a^b}$   
 $\Delta_r G = \Delta G^\circ + RT \ln Q$   
 $\Delta_r H^\circ = (\sum v_i \Delta_f H^\circ)_{\text{prod.}} - (\sum v_i \Delta_f H^\circ)_{\text{react.}}$   
 $\Delta_r S^\circ = (\sum v_i \Delta_f S^\circ)_{\text{prod.}} - (\sum v_i \Delta_f S^\circ)_{\text{react.}}$   
 $W_{\text{phase}} = \frac{\text{length of opp. side of lever}}{\text{total length of lever}}$   
 $E = h\nu = \frac{hc}{\lambda}$   
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 <sub>2</sub> (g)	0.843	37.1
H <sub>2</sub> (g)	14.304	28.836
H <sub>2</sub> O(g)	2.03	36.4
H <sub>2</sub> O(l)	4.184	75.3
H <sub>2</sub> O(s)	2.09	37.7
NaCl	0.853	50.5
O <sub>2</sub> (g)	0.918	29.378

Temperatures and enthalpies of phase changes

Substance	M.P. (°C)	$\Delta_{fus} H \left( \frac{kJ}{mol} \right)$	B.P. (°C)	$\Delta_{vap} H \left( \frac{kJ}{mol} \right)$
Al	658	10.6	2467	284
Ca	851	9.33	1487	162
CH <sub>4</sub>	-182	0.92	-164	8.18
H <sub>2</sub> O	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	$\Delta_f H^\circ \left( \frac{kJ}{mol} \right)$	$S^\circ \left( \frac{J}{mol \cdot K} \right)$	$\Delta_f G^\circ \left( \frac{kJ}{mol} \right)$
C	0	5.74	0
CH <sub>4</sub> (g)	-74.81	186.2	-50.75
C <sub>2</sub> H <sub>2</sub> (g)	-83.9	200.93	-
C <sub>3</sub> H <sub>8</sub> (g)	-103.8	269.9	-23.49
CaC <sub>2</sub> (s)	-59.8	70.3	-
CaO(s)	-635	38.1	-
CaF <sub>2</sub> (s)	-1225	68.87	-1162
CaF <sub>2</sub> (l)	-1186	92.6	-
Ca(OH) <sub>2</sub> (s)	-987.0	83.0	-
CO <sub>2</sub> (g)	-393.5	213.6	-394.4
Cu <sub>2</sub> O(s)	-168.6	93.1	-
Cu <sub>2</sub> O(l)	-154.79	-	-
Cu(s)	-	33.2	-
Fe(s)	0	27.3	0
Fe <sub>2</sub> O <sub>3</sub> (s)	-824.2	87.4	-
H <sub>2</sub> (g)	-	130.68	-
H <sub>2</sub> O(g)	-241.8	188.7	-228.6
H <sub>2</sub> O(l)	-285.8	69	-
O <sub>2</sub> (g)	0	205.0	0

Miscellaneous enthalpies

Substance	Reaction	$\Delta H \left( \frac{kJ}{mol} \right)$
F <sub>2</sub>	$F_2 \rightarrow F(g)$	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

# IUPAC Periodic Table of the Elements

1 <b>H</b> hydrogen 1.0080 ± 0.0002	2 <b>He</b> helium 4.0026 ± 0.0001	3 <b>Li</b> lithium 6.94 ± 0.001	4 <b>Be</b> beryllium 9.0122 ± 0.0001	5 <b>B</b> boron 10.81 ± 0.02	6 <b>C</b> carbon 12.011 ± 0.002	7 <b>N</b> nitrogen 14.007 ± 0.001	8 <b>O</b> oxygen 15.999 ± 0.001	9 <b>F</b> fluorine 18.998 ± 0.001	10 <b>Ne</b> neon 20.180 ± 0.001	11 <b>Na</b> sodium 22.990 ± 0.001	12 <b>Mg</b> magnesium 24.305 ± 0.002	13 <b>Al</b> aluminium 26.982 ± 0.001	14 <b>Si</b> silicon 28.085 ± 0.001	15 <b>P</b> phosphorus 30.974 ± 0.001	16 <b>S</b> sulfur 32.06 ± 0.02	17 <b>Cl</b> chlorine 35.45 ± 0.01	18 <b>Ar</b> argon 39.95 ± 0.16
19 <b>K</b> potassium 39.098 ± 0.001	20 <b>Ca</b> calcium 40.078 ± 0.004	21 <b>Sc</b> scandium 44.956 ± 0.001	22 <b>Ti</b> titanium 47.867 ± 0.001	23 <b>V</b> vanadium 50.942 ± 0.001	24 <b>Cr</b> chromium 51.996 ± 0.001	25 <b>Mn</b> manganese 54.938 ± 0.001	26 <b>Fe</b> iron 55.845 ± 0.002	27 <b>Co</b> cobalt 58.933 ± 0.001	28 <b>Ni</b> nickel 58.693 ± 0.001	29 <b>Cu</b> copper 63.546 ± 0.003	30 <b>Zn</b> zinc 65.38 ± 0.02	31 <b>Ga</b> gallium 69.723 ± 0.001	32 <b>Ge</b> germanium 72.630 ± 0.008	33 <b>As</b> arsenic 74.922 ± 0.001	34 <b>Se</b> selenium 78.971 ± 0.008	35 <b>Br</b> bromine 79.904 ± 0.003	36 <b>Kr</b> krypton 83.798 ± 0.002
37 <b>Rb</b> rubidium 85.468 ± 0.001	38 <b>Sr</b> strontium 87.62 ± 0.01	39 <b>Y</b> yttrium 88.906 ± 0.001	40 <b>Zr</b> zirconium 91.224 ± 0.002	41 <b>Nb</b> niobium 92.906 ± 0.001	42 <b>Mo</b> molybdenum 95.95 ± 0.01	43 <b>Tc</b> technetium [97]	44 <b>Ru</b> ruthenium 101.07 ± 0.02	45 <b>Rh</b> rhodium 102.91 ± 0.01	46 <b>Pd</b> palladium 106.42 ± 0.01	47 <b>Ag</b> silver 107.87 ± 0.01	48 <b>Cd</b> cadmium 112.41 ± 0.01	49 <b>In</b> indium 114.82 ± 0.01	50 <b>Sn</b> tin 118.71 ± 0.01	51 <b>Sb</b> antimony 121.76 ± 0.01	52 <b>Te</b> tellurium 127.60 ± 0.03	53 <b>I</b> iodine 126.90 ± 0.01	54 <b>Xe</b> xenon 131.29 ± 0.01
55 <b>Cs</b> caesium 132.91 ± 0.01	56 <b>Ba</b> barium 137.33 ± 0.01	57-71 lanthanoids	72 <b>Hf</b> hafnium 178.49 ± 0.01	73 <b>Ta</b> tantalum 180.95 ± 0.01	74 <b>W</b> tungsten 183.84 ± 0.01	75 <b>Re</b> rhenium 186.21 ± 0.01	76 <b>Os</b> osmium 190.23 ± 0.03	77 <b>Ir</b> iridium 192.22 ± 0.01	78 <b>Pt</b> platinum 195.08 ± 0.02	79 <b>Au</b> gold 196.97 ± 0.01	80 <b>Hg</b> mercury 200.59 ± 0.01	81 <b>Tl</b> thallium 204.38 ± 0.01	82 <b>Pb</b> lead 207.2 ± 1.1	83 <b>Bi</b> bismuth 208.98 ± 0.01	84 <b>Po</b> polonium [209]	85 <b>At</b> astatine [210]	86 <b>Rn</b> radon [222]
87 <b>Fr</b> francium [223]	88 <b>Ra</b> radium [226]	89-103 actinoids	104 <b>Rf</b> rutherfordium [261]	105 <b>Db</b> dubnium [268]	106 <b>Sg</b> seaborgium [269]	107 <b>Bh</b> bohrium [270]	108 <b>Hs</b> hassium [269]	109 <b>Mt</b> meitnerium [271]	110 <b>Ds</b> darmstadtium [281]	111 <b>Rg</b> roentgenium [282]	112 <b>Cn</b> copernicium [285]	113 <b>Nh</b> nihonium [286]	114 <b>Fl</b> flerovium [290]	115 <b>Mc</b> moscovium [290]	116 <b>Lv</b> livermorium [293]	117 <b>Ts</b> tennessine [294]	118 <b>Og</b> oganesson [294]

Key:
atomic number
Symbol
name
abridged standard
atomic weight



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