### 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:

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

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.

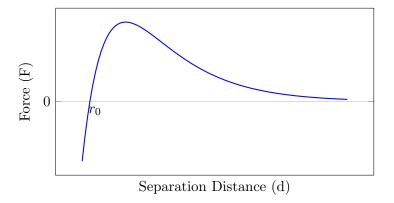


Figure 1: Force-Separation Curve (Lennard-Jones Force)

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

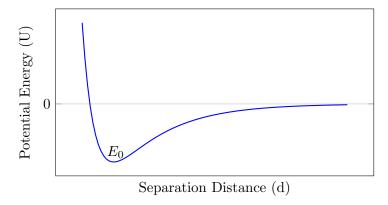


Figure 2: Potential Energy-Separation Curve

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.
- $\bullet$  b is the width of the sample
- d is the thickness/depth of the sample

### 2 Selection of Materials

**Example 2.0.1** (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:

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

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) = 
$$\frac{E^{\frac{1}{2}}}{\rho}$$
 (11)

**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.

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

 $8.62\times 10^{-5}\,{\rm eV\,atom^{-1}\,K^{-1}}$  $1.38 \times 10^{-23} \, \mathrm{J} \, \mathrm{atom}^{-1} \, \mathrm{K}^{-1}$ 

 $96486 \,\mathrm{C}\,\mathrm{mol}^{-1}$ 

 $4.136 \times 10^{-15} \, \mathrm{eV} \, \mathrm{s}$  $6.626 \times 10^{-34} \,\mathrm{J\,s}$ 

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

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

### 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

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

## 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

 $E_{\rm at\ 25\,\circ C} = E^{\circ} - \frac{0.0592}{n} \ln Q$  $E = E^{\circ} - \frac{RT}{nF} \ln Q$  $w = nFE^{\circ}$ 

### Thermodynamics

 $H \equiv U + PV$  $\Delta U = q + w$  $q=nC_P\Delta T$  $\Delta S = \frac{q_{\rm rev}}{T}$ constant T:  $\Delta G = \Delta H - T\Delta S$  $\Delta U = q - P_{\rm ext} \Delta V$  $G \equiv H - TS$  $q = mc\Delta T$ PV = nRT

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

Substance	$c\;(\frac{J}{g\cdot K})$	$C_P \left( \frac{J}{mol \cdot K} \right)$
$\operatorname{Air}(g)$	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

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ubstance	M.P.	$\Delta_{fus}H$	B.P.	$\Delta_{vap}H$
	$(_{\mathcal{O}}_{\circ})$	$\frac{kJ}{mol}$	$(_{\mathcal{O}}_{\mathcal{O}})$	$\frac{k\bar{J}}{mol}$
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	ı	-23.49	ı <b>ı</b>	-1162	ı	ı	-394.4	ı	ı	ı	0	ı	ı	-228.6	ı	0
$S^{\circ} \choose \frac{J}{mol \cdot K}$	5.74	200.93	269.9	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 -74.81	-83.9	-103.8	-635	-1225	-1186	-987.0	-393.5	-168.6	-154.79	1	0	-824.2	1	-241.8	-285.8	0
Species	$C$ $CH_{A}(a)$	$C_2H_2(g)$	$C_3H_8(g)$	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	$F_2$	ĽΉ	Ca	NaCl	

Scott Ramsay, December 2024

# **IUPAC Periodic Table of the Elements**

18 2 P Helium Helium 4.0026	10 10 10 10 10 10 10 10 10 10 10 10 10 1	18 argon 39.95 ±0.16	36 <b>Kr</b> krypton 83.798 ±0.002	54 Xenon xenon 131.29 ± 0.01	86 radon	118 <b>Og</b> oganesson [294]
7	9 fluorine 18.998 ± 0.001	17 Chlorine 35.45 ± 0.01	35 <b>Br</b> bromine 79.904 ± 0.003	53 lodine 126.90 ± 0.01	At At astatine	TS TS tennessine [294]
4	8 0xygen 15.999 ± 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> Iivermorium [293]
<u>ر</u> بر	7 nitrogen 14.007	15 phosphorus 30.974 ± 0.001	33 <b>AS</b> arsenic 74.922 ± 0.001	Sb antimony 121.76 ± 0.01	83 <b>Dismuth</b> 208.98 ± 0.01	Mc moscovium [290]
-	6 Carbon 12.011	28.085 ± 0.001	32 <b>Ge</b> germanium 72.630 ± 0.008	50 Sn tin 118.71 ± 0.01	82 <b>Pb</b> lead 207.2 ± 1.1	114 <b>FI</b> flerovium [290]
ç	5 Doron boron ± 0.02	13 AI aluminium 26.982 ± 0.001	31 <b>Ga</b> gallium 69.723 ± 0.001	49	### ##################################	Nh nihonium [286]
		25	30 <b>Zn</b> zinc 65.38 ± 0.02	48 Cadmium 112.41 ± 0.01	## 80 mercury 200.59 # 0.01	112 <b>Cn</b> copernicium [285]
		E	29 <b>Cu</b> copper 63.546 ± 0.003	47 Silver 107.87	79 <b>Au</b> gold 196.97 ± 0.01	Rg roentgenium
		10	28 <b>Ni</b> nickel 58.693	46 <b>Pd</b> palladium 106.42 ± 0.01	78 platinum 195.08 ± 0.02	DS darmstadfium
		0	27 <b>Co</b> cobalt 58.933 ± 0.001	45 <b>Rh</b> rhodium 102.91 ± 0.01	77 	109 Mt meitnerium
		∞	26 Fe iron 55.845 ± 0.002	<b>Ru</b> ruthenium 101.07 ± 0.02	76 Osmium 190.23 ± 0.03	108 <b>HS</b> hassium [269]
		<b>~</b>	25 <b>Wn</b> manganese 54.938 ± 0.001	Tc Tc technetium	75 <b>Re</b> rhenium 186.21 ± 0.01	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 tungsten 183.84 ± 0.01	Sg seaborgium
	oer I	ω	23 V vanadium 50.942 ± 0.001	Nb niobium 92.906 ± 0.001	73 Ta tantalum 180.95 ± 0.01	105 <b>Db</b> dubnium [268]
	atomic number Symbol name abridged standard atomic weight	4	22 <b>Ti</b> titanium 47.867 ± 0.001	40 <b>Zr</b> zirconium 91.224 ± 0.002	72 <b>Hf</b> hafnium 178.49 ± 0.01	104 <b>Rf</b> rutherfordium
		ო	21 Scandium 44.956 ± 0.001	39 Yttrium 88.906 ± 0.001	57-71 lanthanoids	89-103 actinoids
c	4 <b>Be</b> beryllium 9.0122 ± 0.0001	12 Mg 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]
1 <b>T</b> hydrogen 1,0080	3 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	22.990 ± 0.001	19 K potassium 39.098 ± 0.001	37 <b>Rb</b> rubidium 85.468 ± 0.001	55 <b>CS</b> caesium 132.91 ± 0.01	87 <b>Fr</b> francium [223]



103 <b>Lr</b> lawrencium [262]
102 <b>No</b> nobelium [259]
Md mendelevium [258]
100 <b>Fm</b> fermium [257]
99 <b>ES</b> einsteinium [252]
98 Cf californium [251]
97 <b>BK</b> berkelium [247]
96 <b>Cm</b> curium
95 Am ameridum [243]
94 Pu plutonium [244]
Np neptunium
92 uranium 238.03 ± 0.01
91 <b>Pa</b> protactinium 231.04 ± 0.01
90 Th thorium 232.04 ± 0.01
89 Ac actinium

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