MSE 160 Lecture Notes

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Molecules and Materials, Winter 2024 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 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.

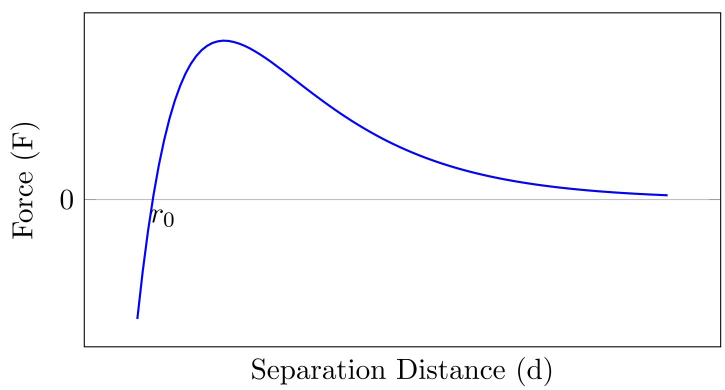

Figure 1: Force-Separation Curve (Lennard-Jones Force)

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

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.

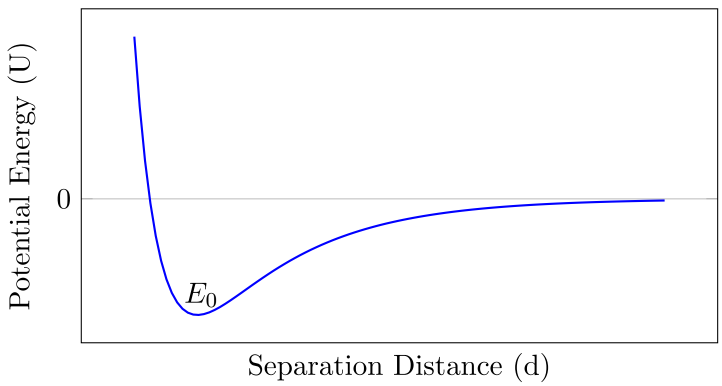

Figure 2: Potential Energy-Separation Curve

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

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:

$$\text{Material Performance Index (MSI)} = \frac{E^{\frac{1}{2}}}{\rho} \tag{11}$$

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.

Constants and conversions

$1\,\text{atm} = 101.325\,\text{kPa} = 1.013\,25\,\text{bar} = 14.696\,\text{psi}$

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	$8.854 \times 10^{-12}\,\text{F}\,\text{m}^{-1}$
R	$8.314\,\text{J}\,\text{mol}^{-1}\,\text{K}^{-1}$
	$0.082\,067\,\text{L}\,\text{atm}\,\text{mol}^{-1}\,\text{K}^{-1}$
$0\,°\text{C}$	$273.15\,\text{K}$
k	$8.62 \times 10^{-5}\,\text{eV}\,\text{atom}^{-1}\,\text{K}^{-1}$
	$1.38 \times 10^{-23}\,\text{J}\,\text{atom}^{-1}\,\text{K}^{-1}$
F	$96\,486\,\text{C}\,\text{mol}^{-1}$
h	$6.626 \times 10^{-34}\,\text{J}\,\text{s}$
	$4.136 \times 10^{-15}\,\text{eV}\,\text{s}$
c	$2.99 \times 10^{8}\,\text{m}\,\text{s}^{-1}$
g	$9.81\,\text{m}\,\text{s}^{-2}$

Microstructure

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

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

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

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

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

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

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

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

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

Mechanical Behaviour

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

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

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

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

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

Magnetic Behaviour

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

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

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

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

Electrical Behaviour

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

$\sigma = p|e|\mu_h$

Electrochemistry

$E = E° - \frac{RT}{nF}\ln Q$ $\quad I = \frac{nC}{t}$

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

$w = nFE°$

Thermodynamics

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

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

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

constant T: $\Delta G = \Delta H - T\Delta S$

$q = mc\Delta T$ $\quad q = nC_P\Delta T$

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

$\Delta_{\text{r}}G = \Delta G° + RT\ln Q$

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

$\Delta_{\text{r}}S° = (\Sigma v_i \Delta_{f,i}S°)_{\text{prod.}} - (\Sigma v_i \Delta_{f,i}S°)_{\text{react.}}$

$W_{\text{phase}} = \frac{\text{length of opp. side of lever}}{\text{total length of lever}}$

$E = h\nu = \frac{hc}{\lambda}$

Specific heats and heat capacities

Substance	c ($\frac{J}{g \cdot K}$)	C_P ($\frac{J}{mol \cdot K}$)
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	$\Delta_f H°$ ($\frac{kJ}{mol}$)	$S°$ ($\frac{J}{mol \cdot K}$)	$\Delta_f G°$ ($\frac{kJ}{mol}$)
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	$\Delta H(\frac{kJ}{mol})$
F_2	$F_2 \to F(g)$	157
F	$F(g) \to F^-(g)$	-328
Ca	$Ca(g) \to Ca^{2+}(g)$	1734
NaCl	$NaCl(s) \to Na^+(aq) + Cl^-(aq)$	3.9

Scott Ramsay, December 2024

IUPAC Periodic Table of the Elements

Key:

atomic number **Symbol** name abridged standard atomic weight

1	2	3	4	5	6	7	8	9	10	11	12	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											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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