MSE 160 Lecture Notes

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Molecules and Materials, Winter 2024 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 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.

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	$8.854 \times 10^{-12}\,\text{F m}^{-1}$
R	$8.314\,\text{J mol}^{-1}\,\text{K}^{-1}$
	$0.082\,067\,\text{L atm mol}^{-1}\,\text{K}^{-1}$
0 °C	273.15 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

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

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

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

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

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

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

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

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

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

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

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

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

$w = nFE^\circ$

Thermodynamics

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

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

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

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

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

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

$\Delta_r G = \Delta G^\circ + RT\ln Q$

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

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

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

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

Specific heats and heat capacities

Substance	c $(\frac{J}{g\cdot K})$	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	$\Delta_f H^\circ$ $(\frac{kJ}{mol})$	S° $(\frac{J}{mol\cdot K})$	$\Delta_f G^\circ$ $(\frac{kJ}{mol})$
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	$F_2 \rightarrow F(g)$	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

1																	18
1 **H** hydrogen 1.0080 ± 0.0002	2		Key:									13	14	15	16	17	2 **He** helium 4.0026 ± 0.0001
3 **Li** lithium 6.94 ± 0.06	4 **Be** beryllium 9.0122 ± 0.0001		atomic number **Symbol** name abridged standard atomic weight									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]

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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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