Department of Materials Science and Engineering
Henry Samueli School of Engineering and Applied Science
University of California, Los Angeles

MSE 104, Midterm version 2
Winter 2017, February 15, 2017

Name: Seulki Koo

UCLA ID: [redacted]

All work must be clearly shown with proper units in the final answer to receive full credit. Check that all parts are answered.

1 (12 pts)	7
2 (20 pts)	20
3 (20 pts)	15.5
4 (20 pts)	20
5 (28 pts)	17.5
Total	80

Problem 1: Short Answer

a) For aluminum (Al), would its density increase or decrease if the temperature is increased (no explanation necessary). (2 pts)

Decrease ✓

b) FeO has rock salt (NaCl) structure, would you expect the activation energy for Schottky defects to be higher or the activation energy for Frenkel defects to be higher (no explanation necessary). A Schottky defect is a cation vacancy and anion vacancy, and a Frenkel defect is a cation vacancy and cation interstitial. (2 pts)

Schottky defect activation energy is higher. ✗ −2

c) When comparing aluminum (Al) with aluminum nitride (AlN), state for each material property below which material (Al or AlN) will have the higher value (4 pts)

Elastic modulus AlN ✓
Hardness AlN ✓
Fracture toughness AlN ✗
Melting temperature AlN ✓

−1

d) FeO has a molecular weight of 71.844 g/mole and a density of 5.74 g/cm³. In one mole of $Fe_{0.992}O$, there is 0.992 mole of Fe per 1 mole of O. In one mole of $Fe_{0.992}O$, what is the number density of Fe^{+3} (ions/m³)? Assume there are no impurities in this material and no oxygen defects. (4 pts)

$1-x$

$\frac{n \times N_v}{V_c}$

$1 - x = 0.992$ ✓

$x = 0.008$ mole

3 mol ↓ 1 mol → Total 2 mol ↓

$\Rightarrow 0.004$ mol Fe^{+3} formed.

0.016 Fe^{+3}

$3\ Fe^{2+} \downarrow \quad 1\ Fe^{3+} \uparrow$

$\frac{n}{V_c} = \frac{\rho N_A}{A} = \frac{(5.74)(6.022\times10^{23})}{(71.844)} = 4.811\times10^{22}$ ions/m³ for FeO

$4.811\times10^{22}\ \frac{\text{ions}}{\text{m}^3} \times \frac{1}{2} = 2.406\times10^{22}$ Fe ions/m³

$2.406\times10^{22} \times 0.004 = 9.622\times10^{19}$ ions/m³ Fe^{+3} ✗

−2

(20)

Problem 2: Crystal Structure

Assume AlN has zinc blende (ZnS) structure. Using an effective radius of 0.070 nm for N and 0.120 nm for Al atomic weight of 14.0 g/mole for N and 27.0 g/mole for Al, determine the following:

a) Calculate the atomic packing factor (APF) of AlN (5 pts)

b) Calculate the density of AlN (5 pts)

c) What would the number density (number per volume) of *Al vacancies* be at 1200K if it forms Frenkel defects (a Frenkel defect is a cation vacancy and cation interstitial pair). Assume activation energy for Frenkel defects is 6.6 eV and does not vary with temperature. (5 pts)

d) The packing of atoms of different sizes (a larger one and a smaller one) usually results in higher APF, so why is the APF of AlN lower than that of pure Al which has FCC structure? (5 pts)

a) $APF = \frac{V_S}{V_C} = \frac{4 \times \frac{4}{3}\pi (r_N^3 + r_{Al}^3)}{a^3} = \frac{\frac{16}{3}\pi (0.07^3 + 0.12^3)}{0.439^3}$

$\frac{\sqrt{3}}{4} a = r_N + r_{Al} = 0.19$

$a = 0.439$ nm ✓

$= \underline{0.410}$ ✓

b) $\rho = \frac{nA}{N_A V_C} = \frac{4(14 g/mol + 27.0 g/mol)}{(6.022 \times 10^{23})(0.439 \times 10^{-9})^3} = 3.22 \times 10^6 g/m^3 = \underline{3.22 g/cm^3}$ ✓

c) $N_{fr} = N \exp\left(-\frac{Q_{fr}}{2kT}\right)$ $N = \frac{4}{V_c} = \frac{4}{(0.439 \times 10^{-9})^3}$

$= \frac{4}{(0.439 \times 10^{-9})^3} \exp\left(-\frac{6.6}{2(8.62 \times 10^{-5})(1200)}\right) = \underline{6.60 \times 10^{-4} /m^3}$ ✓

d) Since zinc blend structure has covalent bonds, the bonding is directional. Also, atoms are needed to form specific angles. AlN has less closed packed than Al, which cause less APF.

30

Mechanical Properties

A metal alloy has a modulus of resilience of 11.5 MJ/m^3 (recall that 1 MJ/m3 is equal to 1 MPa). The yield strength of this alloy is the same as its tensile strength. The toughness of this metal alloy is 325 MJ/m^3. If a sample of this alloy originally 10.0 cm was elongated 6% (or strain of 0.06), *which is greater than the yield strain and the load is then released*, the final length of the sample was 10.32 cm. Assume yield strength and tensile strength do not change. Based on this information, determine the following (a stress-strain diagram is not required but you may find drawing one to be helpful)

(1) The yield strength and tensile strength of the alloy (same value) $\sigma_y = T.S$

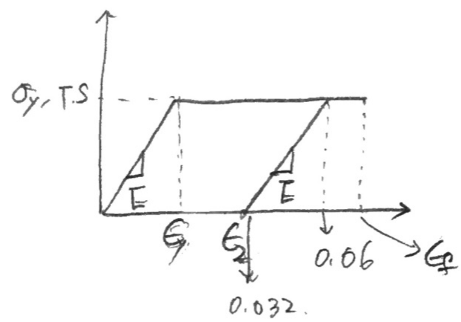
(2) The total strain at which fracture occurred.

$E\epsilon = \sigma$

(1)

$U_r = 11.5 MJ/m^3$

Toughness $= 325 MJ/m^3$



$\epsilon_2 = \frac{10.32 - 10}{10} = 0.032$

$E = \frac{\sigma}{\epsilon} = \frac{\sigma_y}{0.06 - 0.032} = \frac{\sigma_y}{0.028}$

$U_r = \frac{1}{2}\epsilon_y \sigma_y = \frac{\sigma_y^2}{2E} = \frac{\sigma_y^2}{2\left(\frac{\sigma_y}{0.028}\right)} = \frac{\sigma_y}{\frac{2}{0.028}} = \frac{\sigma_y}{71.4} = 11.5 MPa$

$\sigma_y = 71.4 \times 11.5 = 821.1 MPa \Rightarrow \underline{\sigma_y = T.S = 821.1 MPa}$

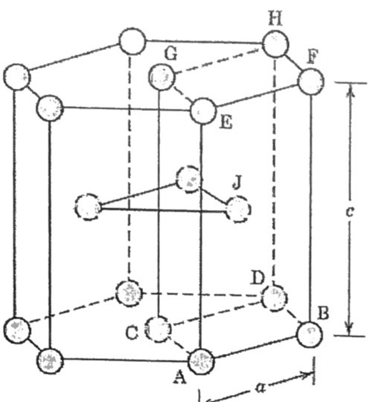
(2) Toughness $= U_r + \sigma_y(\epsilon_f - \epsilon_y) = U_r + \sigma_y \epsilon_f - \sigma_y \epsilon_y$ ($\sigma_y \epsilon_y \to 2U_r$)

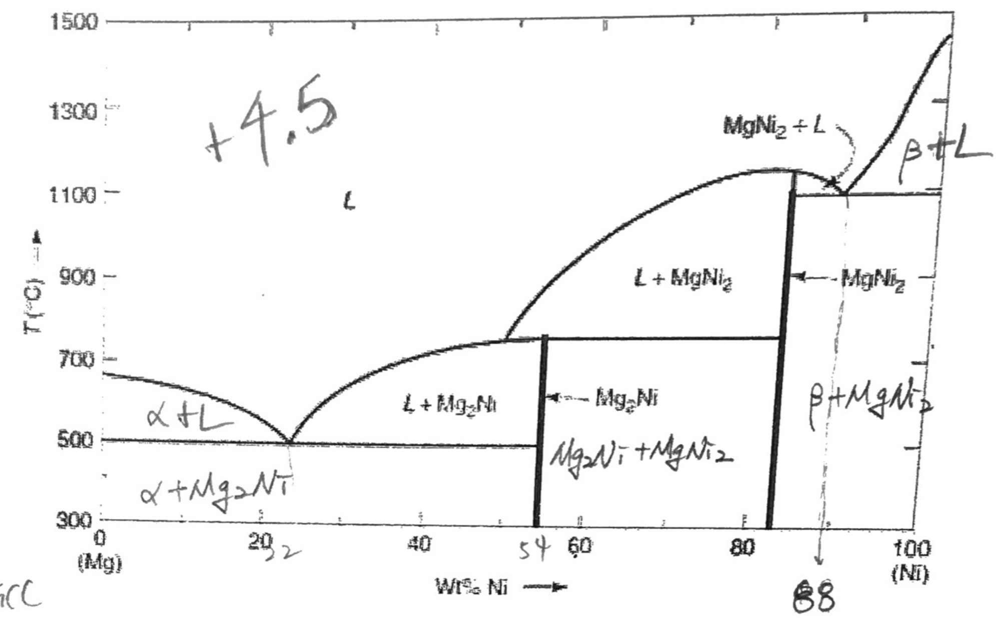
$= \sigma_y \epsilon_f - U_r = 325 MPa$

$\epsilon_f = \frac{325 + U_r}{\sigma_y} = \frac{325 + 11.5}{821.1} = \underline{0.410}$

17.5

5. **Mg-Ni Phase Diagram**
The magnesium-nickel (Mg-Ni) phase diagram is shown below. Ni is FCC and Mg is HCP, and the HCP unit cell is shown below. There are two intermetallic phases, one is Mg_2Ni which occurs only at a composition of 54 wt% Ni, and the other is $MgNi_2$ which occurs only at a composition of 83 wt% Ni. Answer the following:





Comparing pure Mg to pure Ni, state whether each material property listed below is higher for Mg, higher for Ni, or whether the property is the same for both metals (5 pts)

(i) Elastic modulus (E) ~~Mg~~

+2 (ii) Fracture toughness (K_{IC}) ~~Mg~~

(iii) Self-Diffusion coefficient (D) at 400C ~~Ni~~

(iv) Coordination number (CN) Same

(v) Atomic packing factor (APF) Same

(a) Fill in all blank regions on the phase diagram (there are five) If you use symbols such as α, β, etc. you must specify what elements or intermetallics are in these phases. (5 pts) (α → ~~rich in~~ Mg (~~both Mg, Ni exist~~) β → ~~rich in~~ Ni (~~both Mg, Ni exist~~) pure.

(b) What is the maximum solubility of Mg in Ni? (2 pts) 12wt % Mg 0

(c) What is the composition range (wt% Mg), if any, in which Ni can be precipitation hardened with Mg? (2 pts)
0 wt % Mg < wt% Mg < 12 wt % Mg 0

(d) For a sample originally of 100g total weight, at 88 wt% Ni (eutectic composition), right below the eutectic temperature, determine the grams of Ni in each phase (specify the phase). (6 pts)

Eutectic Ni & $MgNi_2$

wt Eutectic Ni = $\frac{88-80}{100-80} \times 100 = 40\%$

+3 Wt eutectic $MgNi_2$ = 100 − 40 = 60 %

88g Ni total.

Should be 83

(M eutectic Ni) = (M_{TOT})(0.4)(1) = 40g

(M eutectic $MgNi_2$) = (100)(0.88) − 40 = 48g ??

Not correct.

(e) A sample was originally 100g total weight and it was determined that the sample had primary Mg_2Ni (recall that Mg_2Ni occurs at 54 wt% Ni) and eutectic constituents (eutectic constituents are alternating layers of two different phases). If it was determined that there was 30.0 g Ni in only the *primary* Mg_2Ni, determine the original composition. (8 pts)

(M_{TOTAL})(wt_{Mg_2Ni})($wt_{primary}$) = 30

$Wt_{primary} = \frac{30}{100 \cdot 0.54} = 0.556 = \frac{C_0 - 22}{54 - 22} \Rightarrow 39.8 = C_0$ +8

39.8 wt% Ni − 60.2 wt % Mg good

$N_A = 6.023 \times 10^{23}$ molecules/mol
$k = 1.38 \times 10^{-23}$ J/atom-K $= 8.62 \times 10^{-5}$ eV/atom-K
$R = 8.31$ J/mol-K

Factor by Which Multiplied	Prefix
10^{9}	giga
10^{6}	mega
10^{3}	kilo
10^{-2}	centi[a]
10^{-3}	milli
10^{-6}	micro
10^{-9}	nano
10^{-12}	pico

$$a = 2R\sqrt{2} \qquad a = \frac{4R}{\sqrt{3}} \qquad APF = \frac{V_S}{V_C}$$

$$\rho = \frac{nA}{V_C N_A} \qquad N_v = N_o \exp\left(-\frac{Q_v}{kT}\right) \qquad N_{fr} = N \exp\left(-\frac{Q_{fr}}{2kT}\right)$$

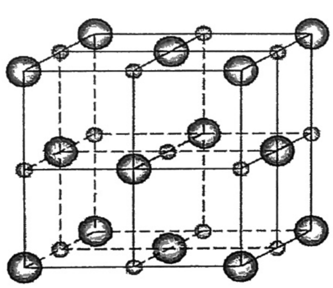
N_o is for perfect lattice — N total number of lattice sites

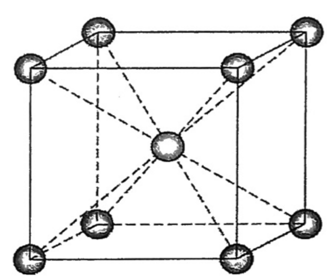
$$\sigma = \frac{F}{A_o} \qquad \varepsilon = \frac{l - l_o}{l_o} = \frac{\Delta l}{l_o} \qquad \sigma = E\varepsilon \qquad \tau = G\gamma$$

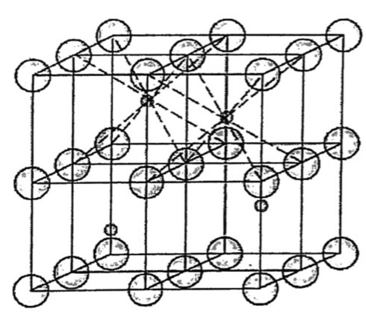
$$\nu = -\frac{\varepsilon_x}{\varepsilon_z} = -\frac{\varepsilon_y}{\varepsilon_z} \qquad E = 2G(1+\nu) \qquad \sigma_m = 2\sigma_o\left(\frac{a}{\rho_t}\right)^{1/2} \qquad \sigma_c = \left(\frac{2E\gamma_s}{\pi a}\right)^{1/2}$$

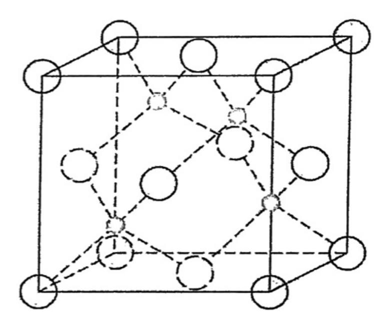
$$\%EL = \left(\frac{l_f - l_o}{l_o}\right) \times 100 \qquad U_r = \frac{1}{2}\sigma_y \varepsilon_y = \frac{\sigma_y^2}{2E} \qquad K_c = Y\sigma\sqrt{\pi a} \qquad K_{Ic} = Y\sigma\sqrt{\pi a}$$

$$\dot{\varepsilon}_s = K\sigma^n \exp\left(-\frac{Q_c}{RT}\right) \qquad \frac{C_x - C_o}{C_s - C_o} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right) \qquad D = D_o \exp\left(-\frac{Q_d}{RT}\right)$$









Metal
Nonmetal
Intermediate

Key: 29 (Atomic number), Cu (Symbol), 63.54 (Atomic weight)

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 1.0080																	2 He 4.0026
3 Li 6.939	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.183
11 Na 22.990	12 Mg 24.312											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
19 K 39.102	20 Ca 40.08	21 Sc 44.956	22 Ti 47.90	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.71	29 Cu 63.54	30 Zn 55.37	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.91	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.40	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.34	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.98	84 Po (210)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	Acti-nide series															