MSE104 Fall 2017 Midterm Review

Problem 1: Short Answer

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

Melting temperature

Hardness

Elastic modulus

Fracture toughness

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

c) 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.

d) FeO has a molecular weight of 71.844 g/mole and a density of 5.74 g/cm^3. In one mole of $Fe_{0.988}O$, there is 0.988 mole of Fe per 1 mole of O. In one mole of $Fe_{0.988}O$, what is the number density of Fe^{+3} (ions/m^3)? Assume there are no impurities in this material and no oxygen defects.

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, and atomic weight of 14.0 g/mole for N and 27.0 g/mole for Al, determine the following:

a) Calculate the density of AlN

b) Calculate the atomic packing factor (APF) of AlN

c) What would the number density (number per volume) of *Al vacancies* be at 1000K 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 density does not change with temperature.

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?

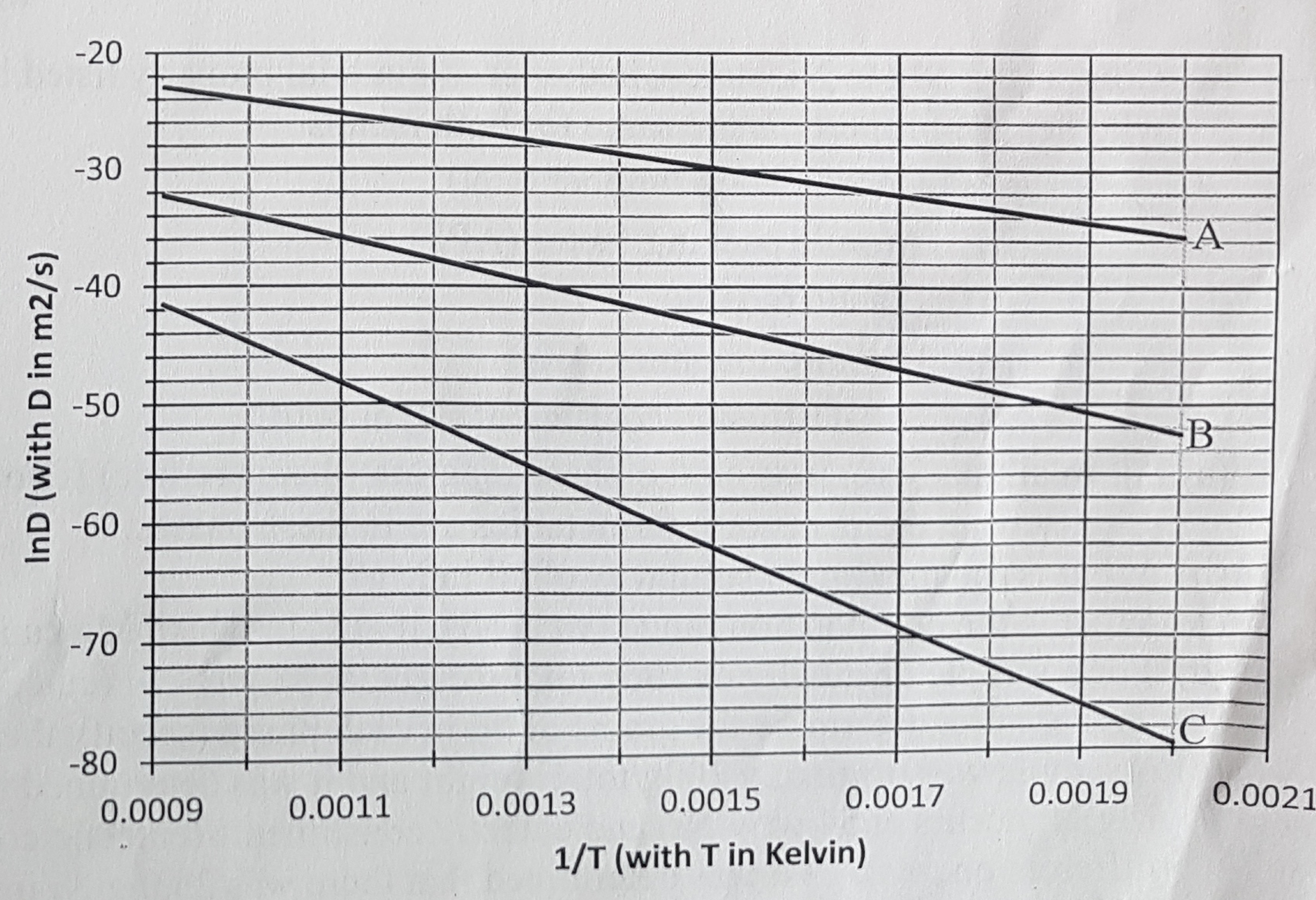
Problem 3: Diffusion

The diffusion data for three different atoms (A, B, C) in the same host material are plotted on the same graph. On the y-axis is lnD (D is in m^2/s), and on the x-axis is 1/T (T is in Kelvin).

(a) Determine the activation energy and D_o for diffusion of A in the host. Remember to include units.

(b) At 1000K, if atom A is diffused into the host for 100 min, calculate the diffusion time required at 1000K for atom B to achieve the same concentration at the same position. Assume that surface concentration remains the same.

(c) Do you expect atom A or atom B to have larger size (larger radius)?



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MSE 104, Midterm (2hrs)
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1 (12 pts)	8
2 (20 pts)	20
3 (20 pts)	20
4 (20 pts)	20
5 (15 pts)	15
6 (13 pts)	13.
Total	96

All work must be clearly shown with proper units in the final answer to receive full credit.

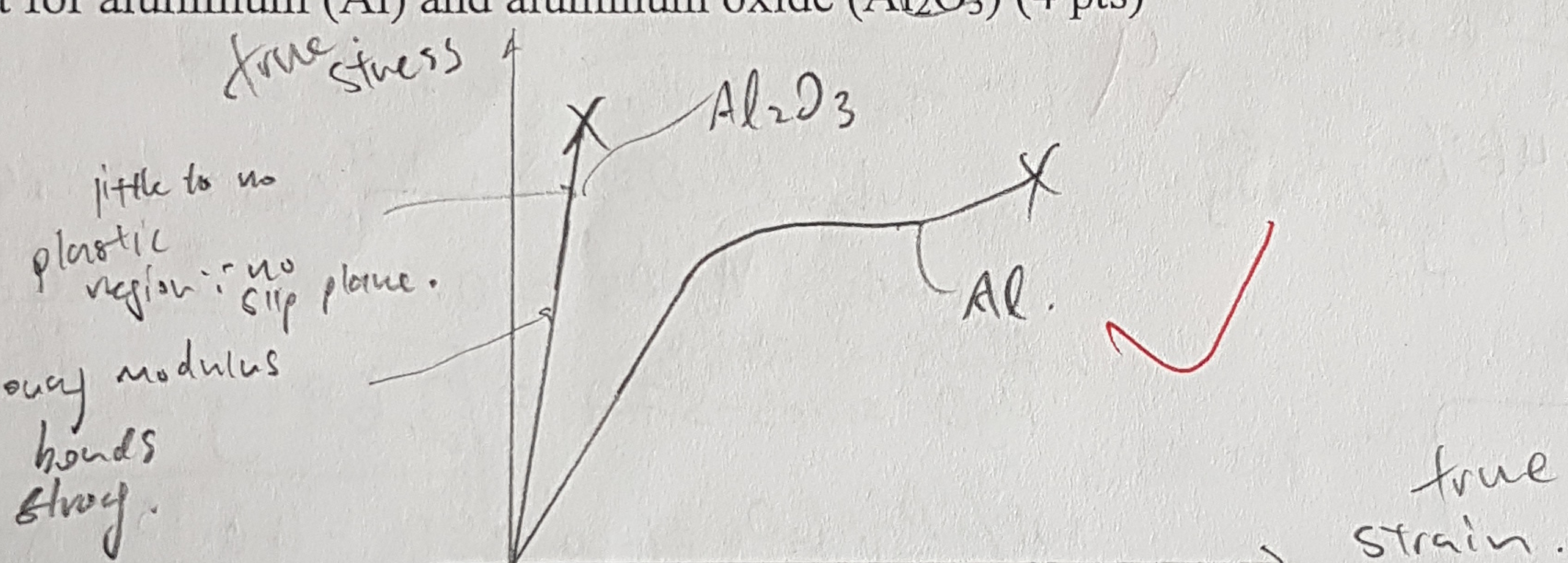
Please check that ALL parts are answered.

If there is conflicting work shown, you must CIRCLE your final answer to receive proper credit.

Problem 1 (10pt)

a) Superimpose on the same stress-strain graph (plot stress on y-axis and strain on x-axis) the curves you expect for aluminum (Al) and aluminum oxide (Al_2O_3) (4 pts)

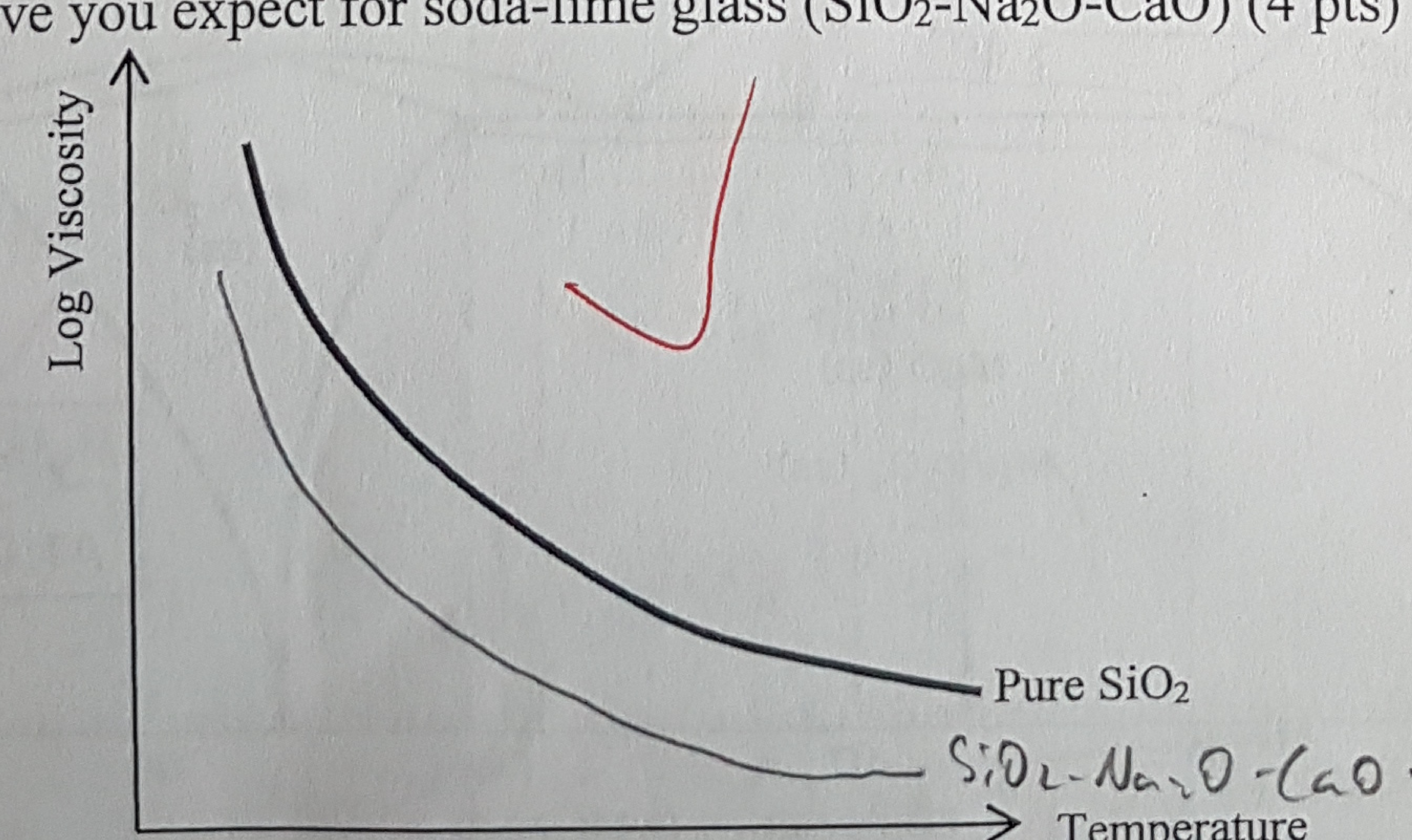
ionic . ceramic .



b) It is known that silica glasses expand when the temperature is raised (although the expansion is significantly less than that of metals). Which material would you expect to have greater expansion with the same increase in temperature – pure SiO_2 glass or soda-lime glass (SiO_2-Na_2O-CaO)? No explanation necessary (4 pts).

SiO_2

c) A plot of log viscosity (y-axis) vs. temperature (x-axis) is shown below, with the curve for pure SiO_2 drawn. On this plot, draw the curve you expect for soda-lime glass (SiO_2-Na_2O-CaO) (4 pts)



Excellent

Problem 2 (20pt)

The MgO-Al_2O_3 phase diagram is shown below (ss denotes a solid solution). Show all work and as long as reasoning is correct, you will receive full credit.

a) Fill in for each box the phase(s) that are present (5 pts) +5

b) At a temperature slightly below 2000°C, list two different compositions at which the mass fraction of the "primary phase" is 0.60 and the "eutectic phase" is 0.40. (6 pts)

60% of 4.1 cm (see figure below) = 2.46 cm
∴ 60% primary phase = 2.46 cm from right edge.

answer: 34% wt Al_2O_3 ⇕ 66% wt MgO

60% of 1.1 cm (see figure below) = 0.44 cm.
60% primary phase = 0.44 cm from left edge.

answer. 58% wt Al_2O_3 ⇕ 42% wt MgO.

+6

c) For a system containing originally 40g pure Al_2O_3 and 60g pure MgO that was hypothetically melted and slowly cooled to a temperature right below 2000°C, what is the mass (in grams) of Al_2O_3 in the primary phase, in the eutectic MgO (ss) and in the eutectic $MgAl_2O_4$ (ss)? (9 pts)

Primary Phase: MgO

40 wt% 60 wt%

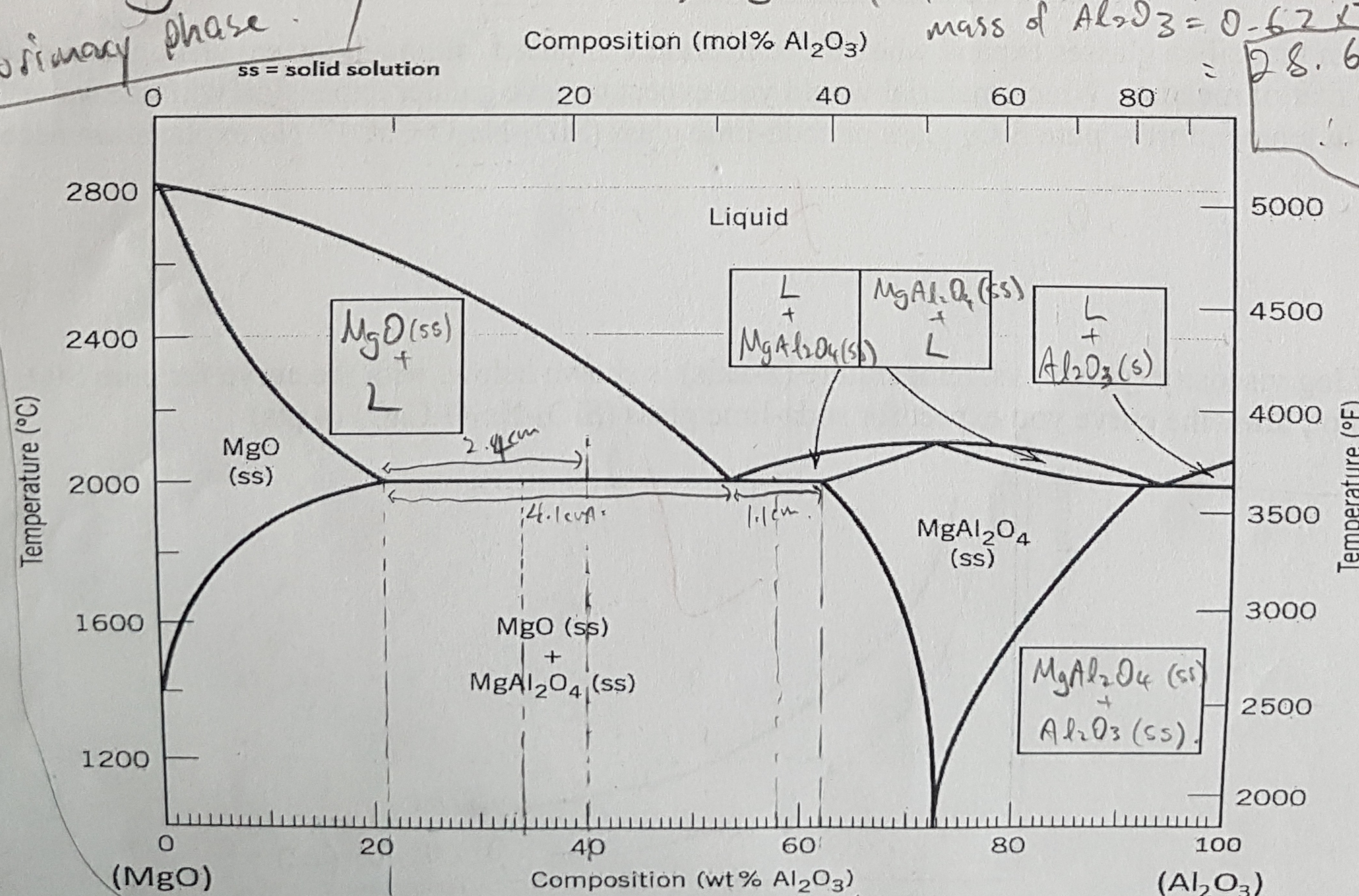
+9

wt% of primary MgO (ss) = $\frac{4.1-2.4}{4.1} \times 100$
= 41.46 % ∵ total 100g
= 41.46 g

∴ mass of Al_2O_3
= 0.21 × 41.46
= 8.707 g in primary phase.

Eutectic:
Total tie line length = 5.2 cm.
wt% MgO: $\frac{5.2-2.4}{5.2} \times 100$ = 53.846 %wt
mass of Al_2O_3 = 0.21 × 53.846 = 11.3 g.
∴ Al_2O_3 in eutectic MgO = 11.3 − 8.707 = 2.600 g = Al_2O_3 in eutectic MgO

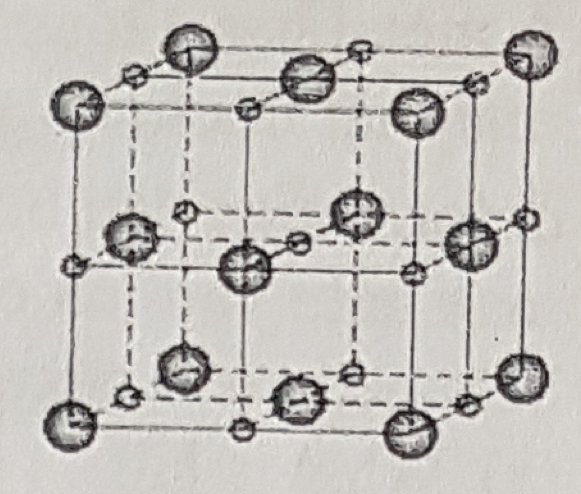
wt% $MgAl_2O_4$ = 1 − 0.53846 = 46.153
mass of Al_2O_3 = 0.62 × 46.153 g
= 28.6 g = Al_2O_3 in eutectic $MgAl_2O_4$



21% 62%

Problem 3. (20pt) 20

MgO has rock salt (NaCl) structure. The ionic radius of Mg^{+2} is 0.072 nm, the ionic radius of O^{-2} is 0.140 nm. The atomic weight of Mg is 24.31 g/mol and the atomic weight of O is 16.00 g/mol. Avogadro's number: 6.02×10^{23} atoms/mol. Boltzman constant: 8.62×10^{-5} eV/atom-K. $\rho = nA/V_cN_A$ APF = V_s/V_c



(a) State the coordination number for the anions (2 pts)

(b) Calculate the density of MgO in g/cm³ (6 pts)

(c) Calculate the atomic packing factor of MgO (6 pts)

(d) The activation energy for formation of Schottky defects (cation vacancy – anion vacancy pair) in MgO has been estimated to be 6.5 eV. What is the number density (number/nm³) of O^{2-} vacancies at 1500K? (6 pts)

$$N_S = N \exp\left(-\frac{Q_S}{2kT}\right)$$ N is for a perfect crystal

1 cm = 10^7 nm. 1 cm³ = $(10^7)^3 = 1 \times 10^{21}$.

a) Coordination Number = 6 ✓ 2

b) $\rho = \frac{n'(\Sigma A_A + \Sigma A_C)}{V_c N_A}$

$n' = \frac{\frac{1}{8}(8)+\frac{1}{2}(6)+\frac{1}{4}(12)+1}{2} = 4$

if digonals touch, $\sqrt{2}a = 4(0.140)$, $a = 0.3959$ nm $< 2(0.072)+2(0.140) = 0.424$ nm

∴ NOT digonal touch [see figure 1 for elaboration]

∴ $a = 2(0.072)+2(0.140) = 0.424$ nm

$\therefore \rho = \frac{4(24.31+16.00)}{(0.424\times10^{-7})^3(6.02\times10^{23})}$

$= 3.51$ g/cm³ ✓

c) APF

Volume of atoms

vol O^{2-} $= \left[\frac{1}{8}(8)+\frac{1}{2}(6)\right]\times\frac{4}{3}\pi(0.072)^3 = 0.0062538$ nm³

vol Mg^{2+} $= \left[\left[\frac{1}{4}\right]12+1\right]\frac{4}{3}\pi(0.140)^3 = 0.045976$ nm³

vol. unit cell $= a^3 = 0.424^3 = 0.076225$ nm³

∴ APF $= \frac{0.0062538+0.045976}{0.076225}\times100$

$= 68.5\%$ = APF ✓

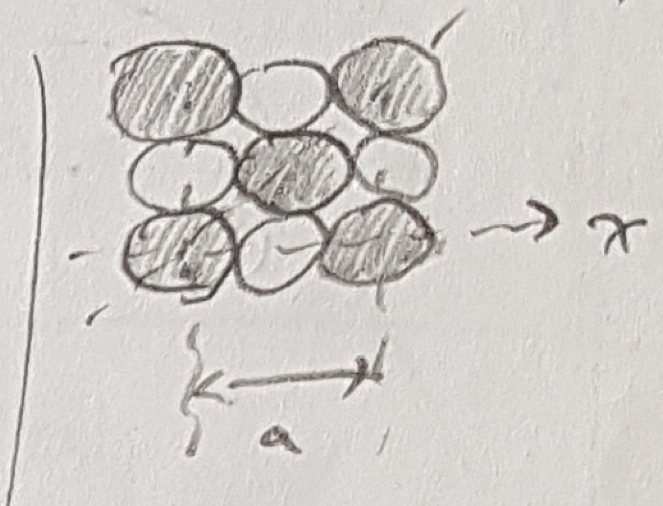


figure 1.

d) $N = \frac{n'}{V_c} = \frac{\rho N_A}{\Sigma A_A + \Sigma A_C}$

$= \frac{3.51\times6.02\times10^{23}}{24.31+16} = 5.247\times10^{22}$

∴ $N_s = N\exp\left(-\frac{Q_s}{2kT}\right)$

$= (5.2419\times10^{22})\exp\left(-\frac{6.5}{2\times8.62\times10^{-5}\times1500}\right)$

$= 6.3653\times10^{11}$/cm³

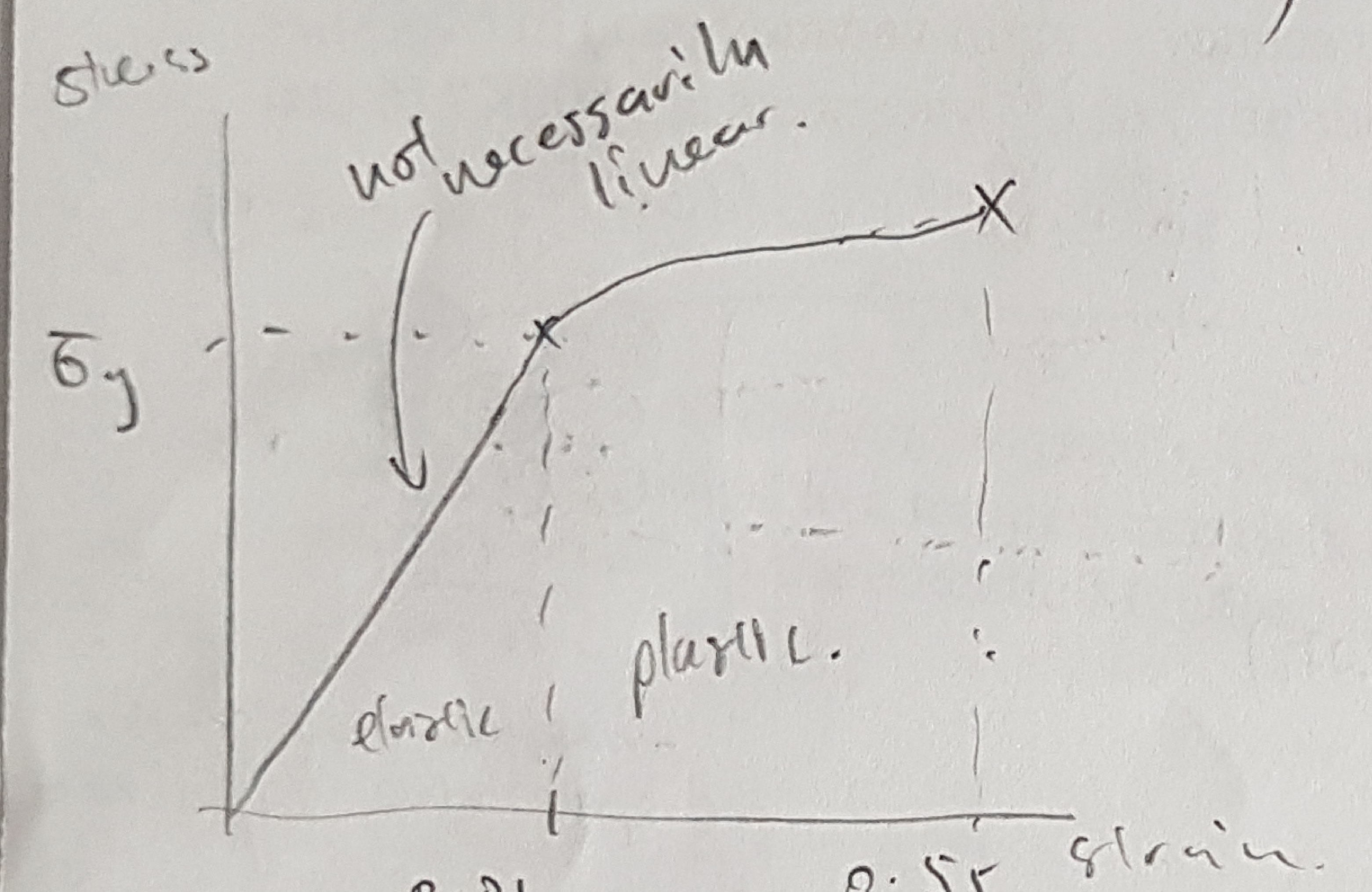
$= 6.370\times10^{-10}$/nm³ ✓

Problem 4. (20pt)

A metal has a toughness of 748 MJ/m^3 (or 748 MPa). Elastic deformation terminates at a strain of 0.010, and the material fractures at a total strain of 0.55. The modulus of resilience is 2.50 MJ/m^3 (2.50 MPa). Plastic deformation can be described the equation $\sigma = K\varepsilon^n$, where n is 0.18. A stress-strain diagram is *not required* but may help you in determining the answer. (With information given, student is expected to know relationship between yield stress and modulus of resilience from stress-strain diagram without equations).

(a) What is K?

(b) What is the yield stress?



b) Modulus of resilience = energy for yield = area under elastic region of stress-strain

$2.5\times10^6 = \frac{1}{2}(0.01)\times\sigma_y$ ← assume linear

→ $\sigma_y = 5\times10^8$ N/m²

a) $\int \sigma \, d\varepsilon$ = toughness − resilience (for plastic region)

$= K\int_{0.01}^{0.55} \varepsilon^{0.18} d\varepsilon = (748 - 2.5)\times10^6$

$= K \frac{1}{1.18} \varepsilon^{1.18} \Big|_{0.01}^{0.55} = 745.5\times10^6$

$K = \frac{745.5\times10^6\times1.18}{0.55^{1.18} - 0.01^{1.18}}$

$K = 1797037744$ N/m²

1797 MPa.

c) $\sigma = K\varepsilon^{0.18}$

sub $\sigma_y = 500\,000 = K(0.01)^{0.18}$ boundary condition.

$K = \frac{500\,000}{(0.01)^{0.18}}$

$K = 1145433.826$ N/m²

b) at boundary condition,

$\sigma_y = K\varepsilon_y^{0.18}$

$= 1797037744(0.01)^{0.18}$

$\sigma_y = 784435426.4$ N/m²

784.4 MPa.

oblem 5. (15pt)

The diffusion coefficients for nickel (Ni) in iron (Fe) at two different temperatures are given below.
$D = D_o \exp(-Q_D/RT)$. R = 8.314 J/mol-K

(a) Determine the activation energy for diffusion of Ni in Fe (12 pts)
(b) Which would have the higher activation energy for diffusion: Ni in FCC Fe or Ni in BCC Fe? No explanation necessary (3 pts)

Temperature (K)	D (m^2/s)
1473	2.2×10^{-15}
1673	4.8×10^{-14}

a)

$D = D_o \exp\left(-\frac{Q_o}{RT}\right)$

①: $2.2 \times 10^{-15} = D_o \exp\left(-\frac{Q_o}{8.314 \times 1473}\right)$

②: $4.8 \times 10^{-14} = D_o \exp\left(\frac{-Q_o}{8.314 \times 1673}\right)$

① / ②:

$0.04583 = \exp\left(\frac{-Q_D}{8.314 \times 1473} + \frac{Q_o}{8.314 \times 1673}\right)$

$\frac{Q_D}{1673} - \frac{Q_D}{1473} = -25.6299$

$1473\,Q_D - 1673\,Q_D = -63160581.53$

$Q_D = 315802.9$ J/mol

b) FCC higher activation energy

Problem 6. (15pt)

ceramic. → no slip just fracture.

(a) Can the strength/hardness of Al_2O_3 be increased by cold-working or cold-rolling? No explanation necessary. (3 pts)

No

(b) A Schottky defect is a cation vacancy and anion vacancy, and a Frenkel defect is a cation vacancy and cation interstitial. Which defect would be more common in CaF_2? No explanation necessary. (3 pts)

Frenkel more common

more sites.

(c) A structural part for an airplane requires a fracture toughness or impact energy that can match that of metals. You wish not to use metals as they are too heavy (i.e. their density is too high). What is an alternative material? Hint: think of your homework CES problem. (3 pts)

carbon fibre composite

(d) FeO has a molecular weight of 71.844 g/mole and a density of 5.74 g/cm³. In one mole of $Fe_{0.975}O$, there is 0.975 mole of Fe per 1 mole of O. In one mole of $Fe_{0.975}O$, what is the number density of Fe^{+3} (ions/cm³)? Avogadro's number: 6.02 x 10^{23} atoms/mol. Assume there are no impurities in this material and no oxygen defects. (4 pts)

In 1 mole of O^{2-},
negative charges = 2x1 = 2 mole.
In 0.975 mole of Fe^{2+},
positive charges: 0.975x2 = 1.95 mole.
∴ need: 2 − 1.95 = 0.05 mole
more "+" charge for
charge neutrality condition.
$Fe^{3+} = Fe^{2+} + e^{+}$
∴ $Fe_{0.975}O$ (1 mole) contains 0.05 mole of Fe^{3+}

∴ $\frac{mole}{cm^3} = \frac{5.74 g/cm^3}{71.844 g/mole}$
= 0.0798953
∴ ions/mole of
Fe^{+3} = 0.0798953 x 0.05
= 0.00399 mol/cm³
x6.02x10²³
= 2.405x10²¹ ions/cm³