EXAM #1 – PRACTICE QUESTIONS - SOLUTIONS

Note: We will go over the answers of the following questions during the recitation session on Thursday, Feb 24th. In the exam, you are expected to remember basic formulas such as atomic packing factor calculations, theoretical density calculations, Miller indices or the formula for the lever rule. Information related to the periodic table (e.g. atomic number, electronegativities) will be given in the questions.

Q1: Please indicate whether the following statements are TRUE or FALSE

1. HCP crystal structures are generated by stacking of hexagonal close-packed planes of atoms in ABCABC sequence. **FALSE**
2. Strongly bonded materials have a lower thermal expansion and higher melting temperature. **TRUE**
3. The equilibrium separation between atoms can easily be found by finding the distance at which the net bonding energy between the two atoms has minimum value. **TRUE**
4. Valence electron occupy the last orbital in each atom and some of them are shared in ionic bonds between two or more atoms. **FALSE**
5. The tendency of a polymer to crystallize increases with increasing molecular weight. **FALSE**

Q2a: Give the electron configurations for the following atoms or ions. (Atomic numbers for Si, Co and Fe are 14, 27 and 26, respectively.)

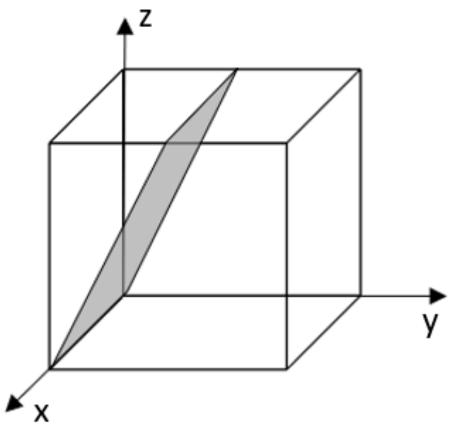
1. Si^{4-} $1s^2 2s^2 2p^6 3s^2 3p^6$
2. Co $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
3. Fe^{3+} $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$

Q2b: Match the electron structure below with the element type it represents.

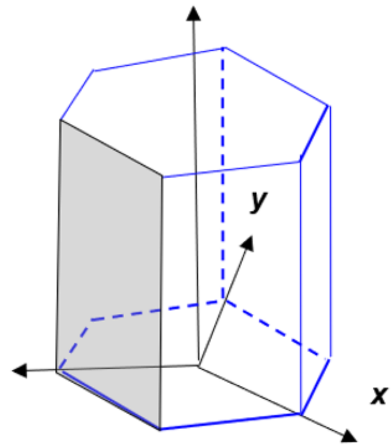
$1s^2 2s^2 2p^6 3s^2 3p^5$

a. Halogen
b. Alkaline earth metal
c. Transition metal
d. Inert gas
e. Alkali metal

Q3: Determine the indices for the planes shown in the following unit cells.

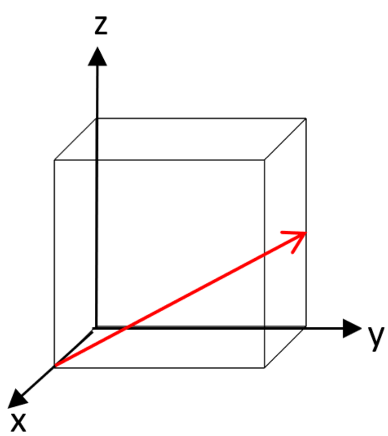


(a) $(02\bar{1})$

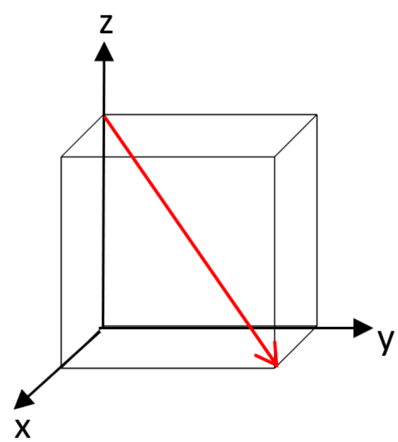


(b) $(0\bar{1}10)$

Q4: Determine the indices for the directions shown in the following unit cells.



(a) $[\bar{2}21]$



(b) $[11\bar{1}]$

Q5: The Pauli Exclusion Principle states that each electron state can hold no more than ___**2**______ electrons which must have opposite/same (circle correct answer) spins.

Q6: a) Calculate the radius of a gold atom. Given that Au has an FCC crystal structure, a density of 22.4 g/cm^3, and an atomic weight of 196.97 g/mol. **b)** Using the radius calculated in part a, calculate the planar density of the (100) face.

$$\rho = \frac{nA}{V_c N_A}$$

When n = number of atoms/unit cell

A = atomic weight

V_C = volume of unit cell = a^3 for cubic

N_A = Avogadro's number = 6.022×10^{23} atoms/mol

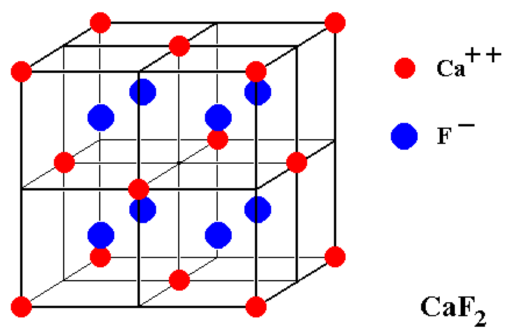
$a = 2\sqrt{2}\, r$ (For an FCC crystal structure)

n=4 atoms/unit cell (For an FCC crystal structure)

$$22.4 = \frac{(4)(196.97)}{(2\sqrt{2}\, r)^3\, (6.022 \times 10^{23})} \rightarrow r = 0.137\ nm$$

$$Planar\ density = \frac{\#\ of\ atoms\ in\ the\ plane}{area\ of\ the\ plane} = \frac{2}{(2\sqrt{2} \times 0.137)^2} = 13.3(1/nm^2)$$

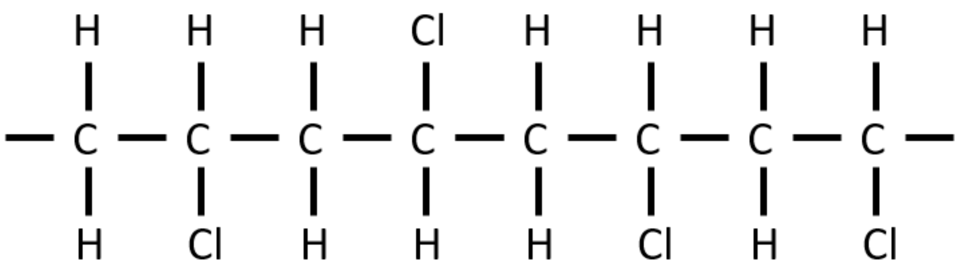
Q7: For the CaF_2 with the rock salt structure (see figure below), what are the coordination numbers of Ca^{2+} (8) and F^- ions (4) ? How many Ca^{2+} (4) and F^- (8) ions are there in the unit cell?



Q8: Describe the type of bonding for each of the following materials

1. Solder: METALLIC
2. Rubber: COVALENT AND VAN DER WAALS
3. Diamond: COVALENT

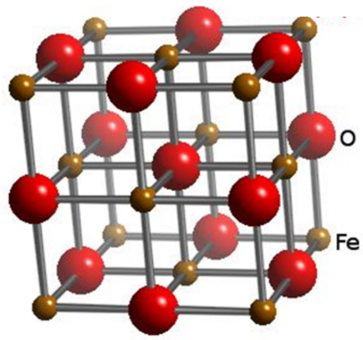
Q9a: Write the repeating unit for the following polymer. **-(CH_2-CHCl)-**



Q9b: Is this polymer

a. Isotactic
b. Atactic
c. Syndiotactic
d. Random copolymer

Q10: a) Compute the theoretical density of MgO, the lattice structure of which is shown in the figure below. **b)** Compute the atomic packing factor of MgO (in decimal form, not percentage) using the data: Radius of Mg^{2+} is 0.072 nm, radius of O^{2-} is 0.140 nm, atomic weight of Mg is 24.31 g/mol, atomic weight of O is 16.00 g/mol



(a) Calculate the density

Lattice parameter is:

$$a = 2r_{Fe^{2+}} + 2r_{O^{2-}} = 2(0.072nm) + 2(0.140nm) = 0.424nm$$

Density equation:

$$\rho = \frac{n'(A_{Fe} + A_O)}{V_C N_A} = \frac{n'(A_{Fe} + A_O)}{a^3 N_A}$$

For FeO, n'=4 formula units/unit cell

$$\rho = \frac{(4 \text{ formula units/unit cell})(24.31 \text{ g/mol} + 16.00 \text{ g/mol})}{(4.24 \times 10^{-8} \text{cm})^3 (6.022 \times 10^{23} \text{ formula units/mol})} = 3.51 g/cm^3$$

(b) Calculate the Atomic Packing Factor

From above, there are 4 Mg ions and 4 O ions per unit cell, sphere volume is:

$$V_S = 4 \times \frac{4}{3}\pi \left[(0.072nm)^3 + (0.140nm)^3 \right] = 0.0522nm^3$$

a value found in part (a), $V_C = a^3 = 0.0762nm^3$

$$APF = \frac{V_S}{V_C} = \frac{0.0522nm^3}{0.0762nm^3} = 0.685$$

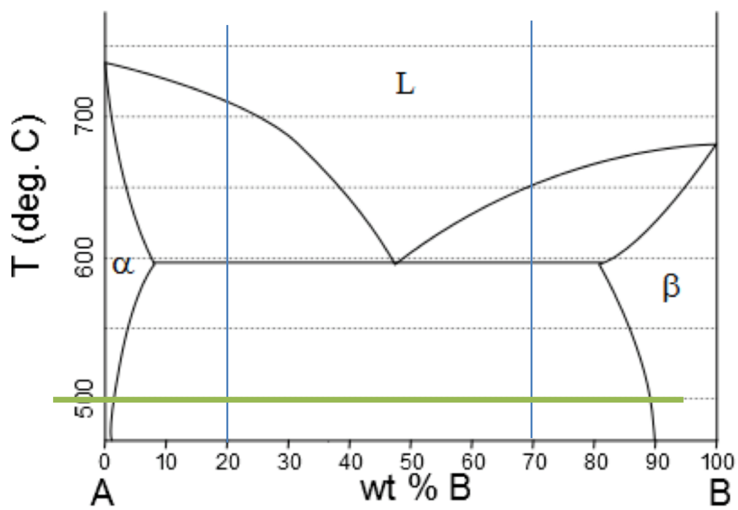
Q11: For the phase diagram below:

a) Given a starting composition of 30 wt% A, and starting from pure Liquid (L)
   a. At what temperature would the material first begin to solidify? Around 650 °C
   b. At what temperature would the material be completely solid? Around 600 °C, just below the eutectic temperature

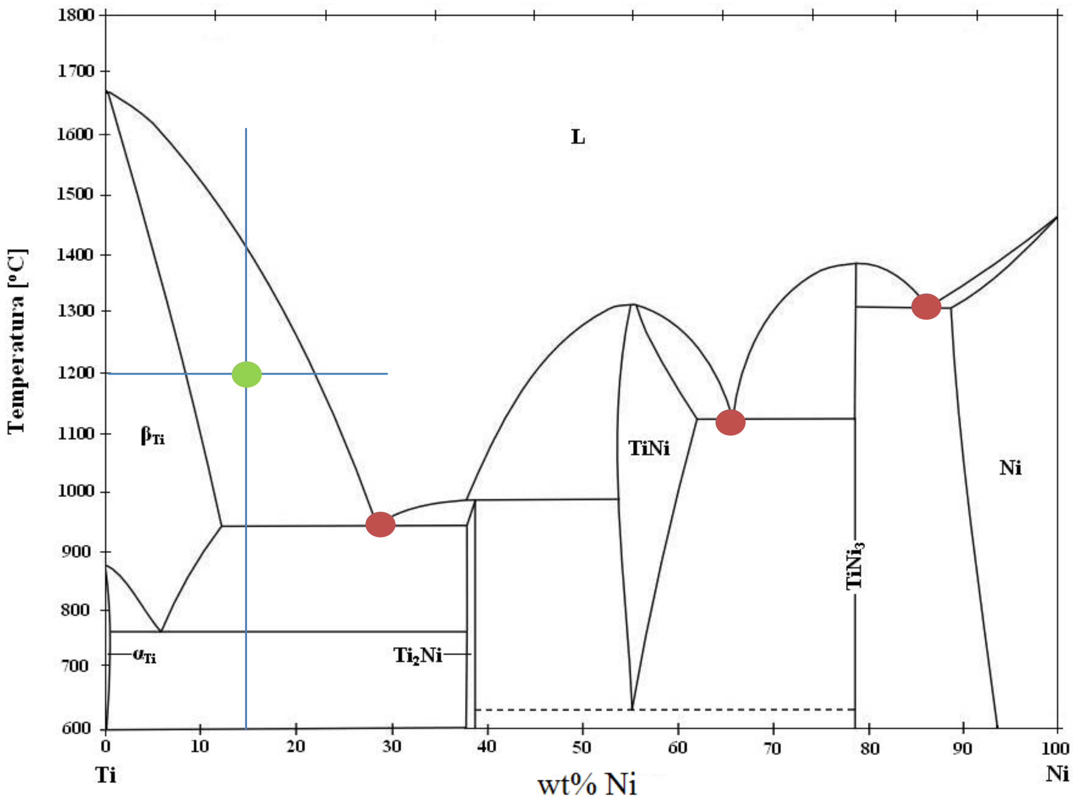
b) Given a starting composition of 80 wt% A,
   a. What phases are present at 500 °C? Alpha and Beta
   b. Estimate the composition of all phases present at 500 °C. Alpha has around 2-3 wt% B, whereas Beta has 90 wt% B. (Check the green horizontal line)
   c. What is the relative concentration of the phases present at 500 °C (in wt%)? Use the tie line to calculate the concentrations.

$$Alpha: \frac{90-20}{90-3} = 0.8$$

$$Beta: 1 - 0.8 = 0.2$$



Q12: The Ti-Ni binary system has the following phase diagram



a. Find and show eutectic points in the diagram. Shown with red dots

b. <u>For a system with 15 wt.% Ni at 1200 ˚C</u>

   i. What phases are present? BetaTi + Liquid

   ii. What is/are the compositions of that/those phase(s)? BetaTI has around 10 wt% Ni, whereas Liquid has around 22 wt% Ni.

   iii. What is the weight fraction of each phase present? Use the tie line, lever method to find the weight fractions.

$$BetaTi: \frac{22-15}{22-10} = 0.58$$

$$Liquid: 1 - 0.58 = 0.42$$

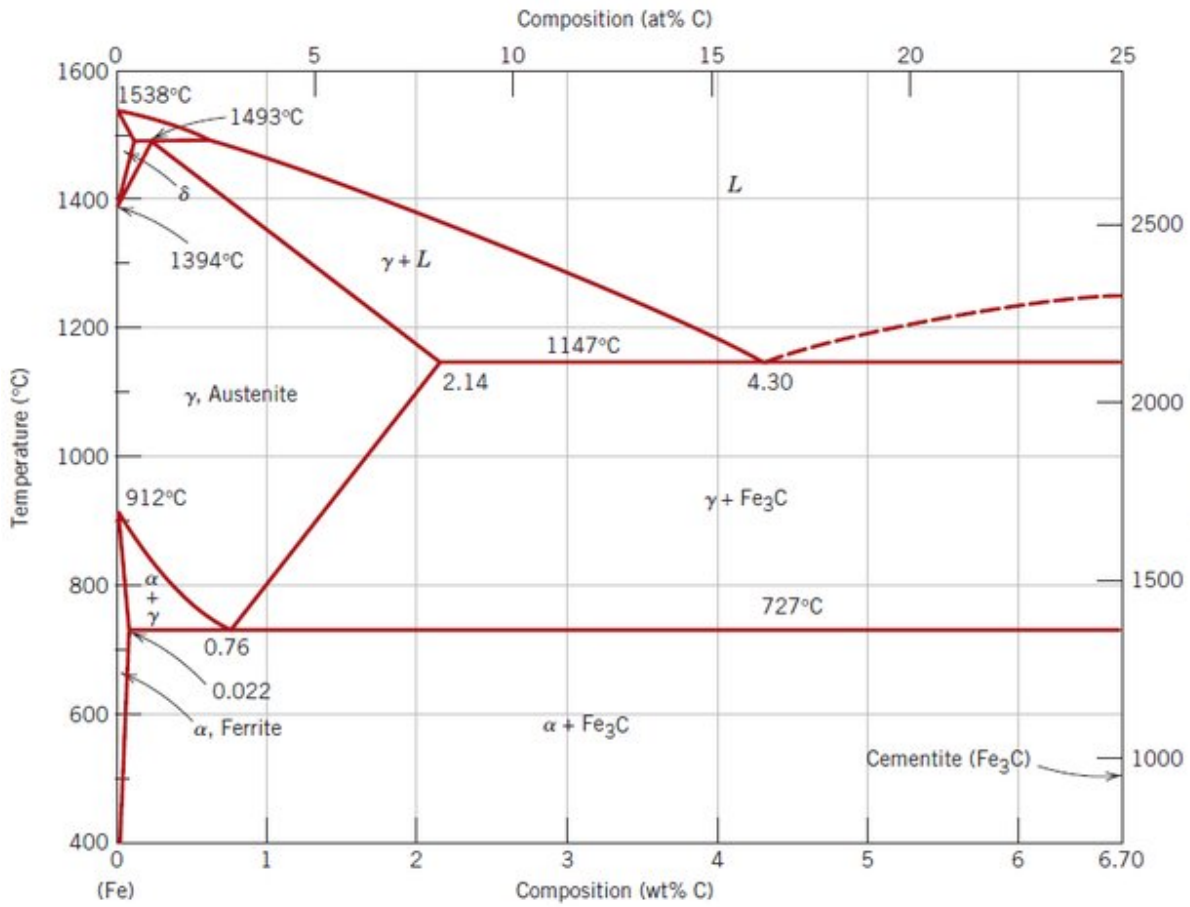
c. <u>For a system with 58 wt.% Ni at 1000 ˚C</u>

   i. What phase(s) is/are present? TiNi

   ii. What is/are the compositions of that/those phase(s)? Single phase, <u>58 wt.% Ni</u>

   iii. What is the weight fraction of each phase present? 100% since single phase.

Q13: For the iron-carbon phase diagram shown below, answer the following questions



a. What is the composition at the eutectic point? What is the temperature of the eutectic reaction? Fe-4.3 wt%C, 1147 °C
b. What is the composition at the eutectoid point? What is the temperature of the eutectic reaction? Fe-0.76 wt%C, 727 °C
c. What is the lowest melting temperature an iron-carbon alloy can have? 1147 °C
d. What is special about the value 2.14 wt% C? If the composition of carbon is less than 2.14 wt%, then the alloy is a steel—if greater that 2.14 wt% it is a cast iron.

Q14: a) For a steel with 2 wt% C, what is the concentration of carbon inside the γ(austenite) phase at 800 °C and 1200 °C? b) For a steel with 3 wt% C, How does the concentration of carbon inside the γ(austenite) change compared to the steel with 2 wt% C at the same temperatures?

a) Draw horizontal line at 800C and 1200 C and see where it touches the phase boundary of austenite – it should occur at somewhere around 1% carbon at 800C and 1.7% carbon at 1200C. Note that the question is not asking for the volume fraction of austenite at these temperatures!
(Note, if you are off by a few %, it's fine – as long as you indicate how you got your answer)

b) No change in austenite composition: compositions of the phases are not changed within the two-phase mixture region at a constant temperature – the only thing that changes is the amount of each phase in the mixture.

Q15: For some iron-carbon alloy, the mass fractions of total ferrite and total cementite are 0.55 and 0.45, respectively. (a) On the basis of carbon content is this alloy classified as a steel or a cast iron? Why? (b) If the alloy is a steel, is it hypoeutectoid or hypereutectoid? If a cast iron, is it hypoeutectic or hypereutectic? Why?

(a) To solve this part of the problem, it is necessary to determine the composition of the alloy in terms of weight percent carbon. If the composition of carbon is less than 2.14 wt%, then the alloy is a steel—if greater that 2.14 wt% it is a cast iron. The lever-rule expression for mass fraction of total ferrite is as follows:

$$W_\alpha = \frac{6.70 - C_0}{6.70 - 0.022}$$

where compositions are in weight percent carbon and C0 is the alloy composition. (Alternatively, a lever rule expression for total cementite is possible, which will yield the same value for C0.) Solving for C0 in the above equation, when Wα = 0.55 leads to C0 = 3.03 wt% C. Therefore, this alloy is a cast iron since the composition of carbon is greater than 2.14 wt%.

(b) From the Fe-Fe3C phase diagram, Figure 10.28, the eutectic composition is 4.30 wt% C. Because this composition (3.03 wt% C) is less than the eutectic, the alloy is a hypoeutectic one