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Task 1. Diffusion (10 points, Lecture 7)

1.1 For a steel alloy it has been determined that a carburizing heat treatment of 17 h duration at 763 °C will raise the carbon concentration to 0.56 wt% at a point 2.2 mm from the surface. Estimate the time necessary to achieve the same concentration at a 5.3 mm position for an identical steel and at a carburizing temperature of 1000 °C. Assume that D_0 is $1.5 \times 10^{-5} \text{ m}^2/\text{s}$ and Q_d is 104 kJ/mol. Gas constant is 8.31 J/mol·K and Planck's constant is $6.63 \times 10^{-34} \text{ J} \cdot \text{s}$. (Please give the detailed calculation process)

Task 1.1

$$D_0 = 1.5 \times 10^{-5} \text{ m}^2/\text{s} \quad Q_d = 104 \text{ kJ/mol} \quad R = 8.31 \text{ J/mol} \cdot \text{K}$$

$$\text{First phase: } t_1 = 17 \text{ h}, \quad x_1 = 2.2 \text{ mm}, \quad T_1 = 763^\circ\text{C} = 1036.15^\circ\text{K}$$

$$\text{Second phase: } t_2 = ?, \quad x_2 = 5.3 \text{ mm}, \quad T_2 = 1000^\circ\text{C} = 1273.15^\circ\text{K}$$

We will find the diffusion coefficient of the two phases:

$$D_1 = D_0 \cdot e^{(-Q_d/RT_1)} = 1.5 \times 10^{-5} \cdot e^{(-104 \times 10^3 / (8.31 \times 1036.15))} = 8.5213 \times 10^{-11}$$

$$D_2 = D_0 \cdot e^{(-Q_d/RT_2)} = 1.5 \times 10^{-5} \cdot e^{(-104 \times 10^3 / (8.31 \times 1273.15))} = 8.072 \times 10^{-10}$$

Since the process is non-steady state diffusion $\Rightarrow \frac{x^2}{Dt} = \text{constant}$

$$\Rightarrow \frac{x_1^2}{D_1 t_1} = \frac{x_2^2}{D_2 t_2} = \text{constant}$$

$$\Rightarrow t_2 = \frac{x_2^2 D_1 t_1}{x_1^2 D_2} = \frac{(5.3)^2 \times 8.5213 \times 10^{-11} \cdot 17}{(2.2)^2 \times 8.072 \times 10^{-10}} = 10.415 \text{ h (answer)}$$

1.2 Answer these questions

(a) If [m] atoms of helium pass through a [a] square meter plate area every [t] hours, and if this flux is constant with time, compute the flux of helium in units of atoms per square meter per second.

(b) If water molecules pass through a membrane with a steady-state flux of [j] mole/(m² day), how long will it take, in hours, for [m] kg of water to pass through a [a] square centimeter of the membrane? (Please give the detailed calculation process.)

Task 1.2

a) Since flux J is constant, it only depends on unit of time

$$\text{We have: } t \text{ (hour)} = 3600 \cdot t \text{ (second)}$$

$$\Rightarrow \text{Flux of helium passing through the plate: } J = \frac{m}{3600 a t} \left(\frac{\text{atom}}{\text{m}^2 \text{s}} \right) \text{ (answer)}$$

$$\text{b) We have unit of flux: } J = \frac{\text{mole}}{\text{m}^2 \text{day}} \Rightarrow \text{flux in hours} = \frac{J}{24} \left(\frac{\text{mole}}{\text{m}^2 \text{hour}} \right)$$

Water is H₂O \Rightarrow water molar mass is $(1 \times 2) + 16 = 18 \text{ kg/mole}$

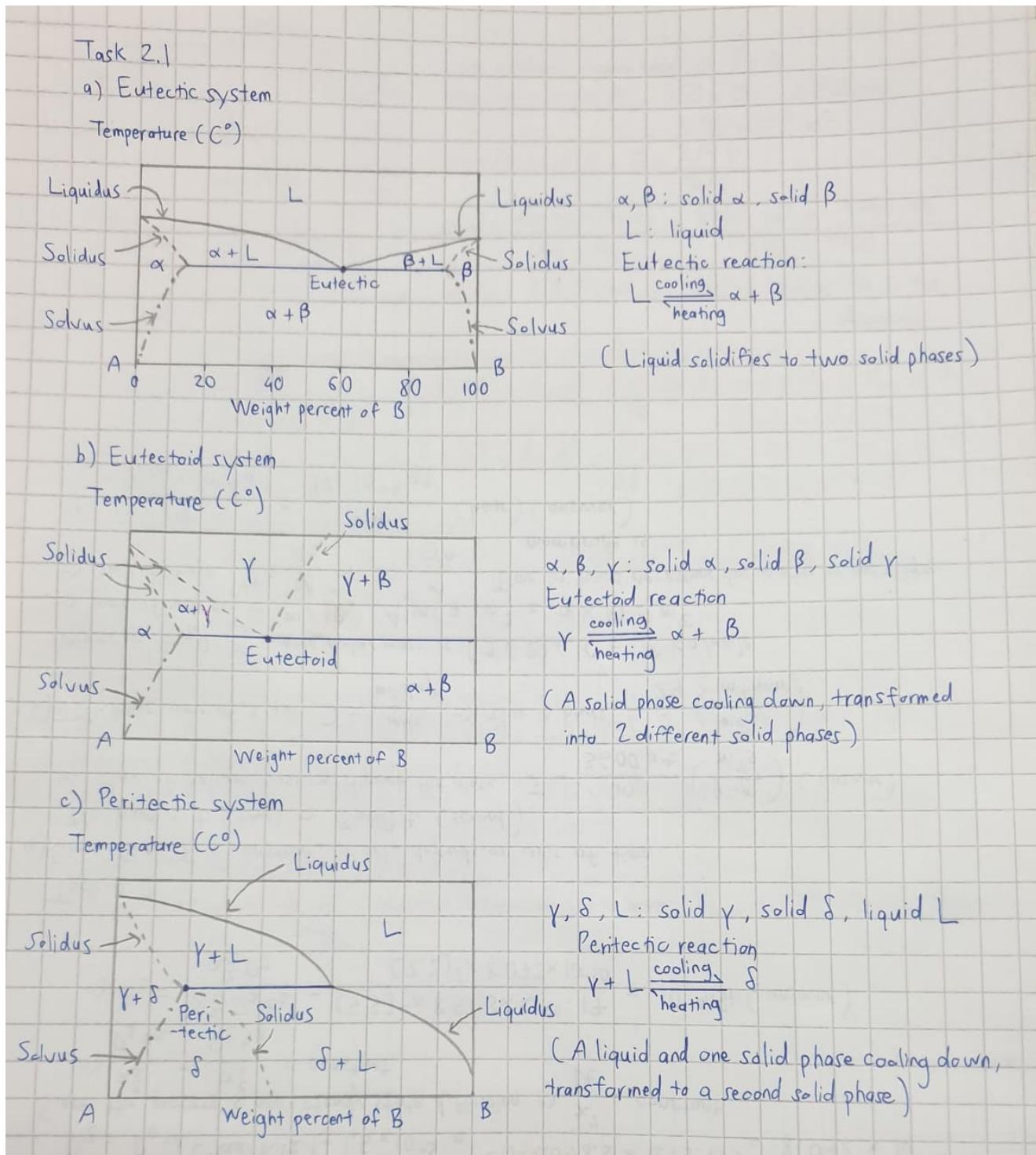
$$\Rightarrow \text{mole of water} = \frac{m}{18}. \text{ Also } \text{a cm}^2 = a \times 10^{-4} \text{ m}^2$$

$$\Rightarrow \text{Flux formula: } J = \frac{M}{At} \Rightarrow t = \frac{m}{JA} \quad \text{Time in hours necessary for water to pass the membrane is}$$

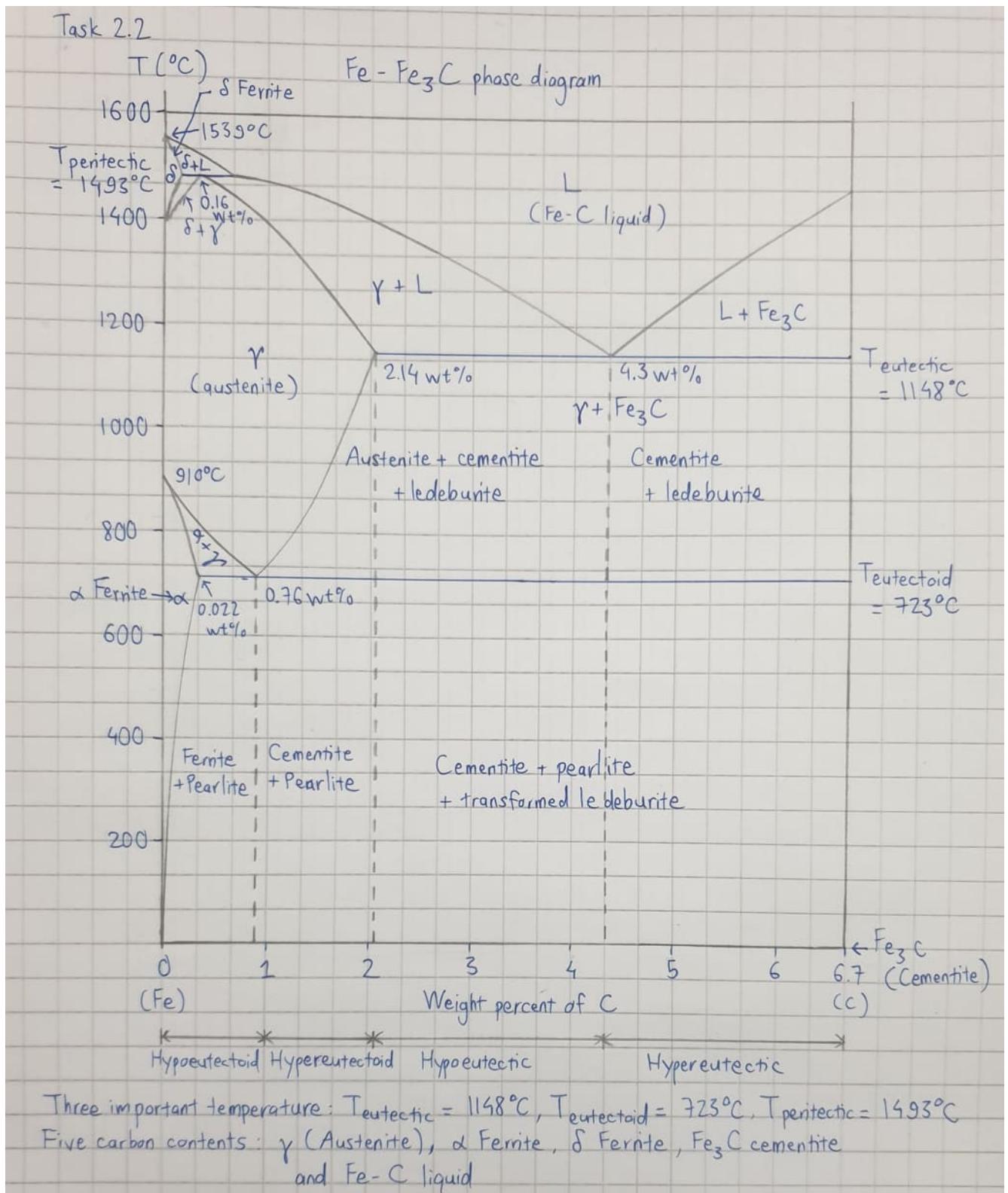
$$t = \frac{m/18}{J/24 \cdot 10^{-4} a} = \frac{24m}{18 \times 10^{-4} a J} \text{ (hour) (answer)}$$

Task 2. Phase diagram (45 points, Lecture 8)

2.1 Give the schematic sketch of binary phase diagrams of (a) eutectic system, (b) eutectoid system, and (c) peritectic system. On your schematic drawings, label the various phase regions, liquidus, solidus, and solvus lines, and give the reaction equations for these three systems. (Please create it on your own, copy/paste from textbook/slides is not accepted!)



2.2 Draw the Fe–Fe₃C phase diagram with the carbon content in the range of 0-6.7 wt%, indicate the phases, mark three important temperatures and five carbon contents. (Please create it on your own, copy/paste from textbook/slides is not accepted!)



2.3 For a 99.6 wt% Fe-0.40 wt% C steel at a temperature just below the eutectoid, determine the following:

- The compositions of Fe_3C and ferrite (α).
- The amount of cementite (in grams) that forms in 100 g of steel.
- The amounts of pearlite and proeutectoid ferrite (α) in the 100 g.

Task 2.3

Given 99.6 wt% Fe - 0.4 wt% C steel at temperature below eutectoid

- Compositions of Fe_3C and ferrite (α)

We have $C_0 = 0.4$ wt% carbon

According to the graph in task 2.2 \Rightarrow At temperature right below the eutectoid

$$\Rightarrow C_{\text{Fe}_3\text{C}} = 6.7 \text{ wt% carbon}, C_\alpha = 0.022 \text{ wt% carbon} \text{ (answer)}$$

- Amount of cementite in 100 g of steel

$$\begin{aligned} \text{We have: } m_{\text{Fe}_3\text{C}} &= \frac{m_{\text{Fe}_3\text{C}}}{m_{\text{Fe}_3\text{C}} + m_\alpha} m_{\text{steel}} = \frac{C_0 - C_\alpha}{C_{\text{Fe}_3\text{C}} - C_\alpha} \cdot 100\text{g} \\ &= \frac{0.4 - 0.022}{6.7 - 0.022} \times 100\text{g} = 0.0566 \times 100\text{g} = 5.66\text{ g (answer)} \end{aligned}$$

- Amount of pearlite and proeutectoid ferrite (α) in the 100g

According to the graph, pearlite and proeutectoid ferrite (α) are from 0.022 wt% C to 0.76 wt% C = C_y

$$\begin{aligned} \text{We have: } m_{\text{pearlite}} &= \frac{m_{\text{pearlite}}}{m_{\text{pearlite}} + m_\alpha} m_{\text{steel}} = \frac{C_0 - C_\alpha}{C_y - C_\alpha} \cdot 100\text{g} \\ &= \frac{0.4 - 0.022}{0.76 - 0.022} \times 100\text{g} = 51.22\text{ g (answer)} \end{aligned}$$

$$\Rightarrow m_{\text{proeutectoid ferrite } \alpha} = m_\alpha = 100 - m_{\text{pearlite}} = 48.78\text{ g (answer)}$$

Task 3. Phase transformation (45 points, Lecture 8)

3.1 Answer these questions

- List at least six important phases that are found in steel alloys.

Six important phases found in steel alloys are: cementite, α - ferrite, γ - austenite, pearlite, bainite and martensite

- Give the crystal structure and describe the microstructure for each.

+ Cementite: having orthorhombic crystal structure. Its microstructure is a single phase of intermetallic compound iron carbide Fe_3C .

+ α - ferrite: Solid solution of carbon in α -iron, having BCC crystal structure in pure iron

+ γ - Austenite: interstitial solid solution of carbon in γ -iron, having FCC crystal structure

+ Pearlite: slow cooling from austenite. It is a fine mixture of ferrite and cementite arranged in lamellar structure

- + Bainite: moderating cooling from austenite, made of elongated, feather-like Fe_3C particles mixed in α - ferrite matrix. It has fine non-lamellar structure
- + Martensite: rapid quenching from austenite. It is a single phase with body centered tetragonal (BCT) structure. Martensite has a fine needle-shaped microstructure

(c) Discuss and compare their mechanical properties.

- + Cementite: hard, brittle and insulating phase. It can be categorized as a ceramic
- + α - ferrite: very soft, ductile phase. It may lose its toughness below some critical temperature
- + γ - Austenite: not stable at room temperature. It is a soft, ductile and non-magnetic phase that can be hardened to high strength levels. It can be cooled in different ways to produce pearlite, bainite and martensite.
- + Pearlite: it has properties medium to soft, ductile α -ferrite and hard, brittle cementite. Coarse pearlite formed at higher temperatures is quite soft while fine pearlite formed at lower temperatures is relatively hard
- + Bainite: Hard, high yield strength but with low ductility. It is not as hard as martensite but not completely brittle
- + Martensite: is brittle and has very high strength. Tempered martensite gains more ductility without losing much strength

3.2 Give the definition of martensite phase transformation. Explain the reasons for the high strength of martensite.

+ Martensite phase transformation definition: Martensite is formed in carbon steel alloy by rapid cooling or quenching process of γ - austenite iron such as Fe_3C . Tempered martensite is produced by reheating martensite, resulting in α - ferrite and fine Fe_3C particles

+ Reasons for the high strength of martensite:

- Rapid cooling from austenite disallow carbon diffusion. In other words, martensite is diffusionless. Thus, the martensite phase consists of a metastable iron phase oversaturated in carbon. High amount of carbon makes martensite very hard and brittle
- Dispersion work-hardening precipitation of carbon increases martensite's hardness.
- Martensite's BCT structure with carbon located between the edges makes martensite have high yield strength, as BCT structure has low number of slip planes
- Martensite has high dislocation density due to shear transformation. These dislocations restrict each other's displacement, which increases residual stresses and hardens martensite.
- High density of block (group of parallel laths) boundaries is also another factor

3.3 Calculate the average phase transformation rate based on the following JMAK function:

$y = 1 - \exp(-kt^n)$ where y is the fraction of the transformed phase, t is the time in second, and the parameters $k = 0.02 \text{ s}^{-n}$, $n=2$

Task 3.3

Average phase transformation rate is $\frac{1}{t_{0.5}}$

$$\text{JMF function: } y = 1 - e^{(-0.02t^2)} = 0.5$$

$$\Rightarrow e^{(-0.02t^2)} = 0.5 \Rightarrow -0.02t^2 = \ln(0.5) \Rightarrow t = \sqrt{-\frac{\ln(0.5)}{0.02}}$$

$$\Rightarrow t = t_{0.5} = 5.887 \text{ (s)}$$

$$\text{Average rate: } \frac{1}{t_{0.5}} = \frac{1}{5.887} = 0.1698 \text{ (answer)}$$