

**COE-C2004 - Materials Science and Engineering**  
**2021-2022 Autumn II**

**Assignment 4, 22.11.2021**

**Task 1. Diffusion (10 points, Lecture7)**

**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.)

**Solution:**

According to Fick's second law:

$$\frac{x^2}{Dt} = \text{constant} \quad \text{Eq. 1 (1 point)}$$

For two given temperatures, we may write the following expression:

$$\frac{x_1^2}{D_1 t_1} = \frac{x_2^2}{D_2 t_2} \quad \text{Eq. 2 (1 point)}$$

According to the diffusion coefficient's relationship with temperature:

$$D = D_0 \cdot \exp\left(-\frac{Q_d}{RT}\right) \quad \text{Eq. 3 (1 point)}$$

We can derive the diffusion coefficients under different temperature:

$$D_1 = D_0 \cdot \exp\left(-\frac{Q_d}{RT_1}\right)$$

$$D_2 = D_0 \cdot \exp\left(-\frac{Q_d}{RT_2}\right)$$

Substituting the specific diffusion coefficients into Eq. 2:

$$\frac{x_1^2}{D_0 \cdot \exp\left(-\frac{Q_d}{RT_1}\right) \cdot t_1} = \frac{x_2^2}{D_0 \cdot \exp\left(-\frac{Q_d}{RT_2}\right) \cdot t_2} \quad \text{Eq. 4}$$

Then we can calculate the unknown time by:

$$t_2 = \frac{t_1 \cdot x_2^2 \cdot D_0 \cdot \exp\left(-\frac{Q_d}{RT_1}\right)}{x_1^2 \cdot D_0 \cdot \exp\left(-\frac{Q_d}{RT_2}\right)} = \left(\frac{t_1 \cdot x_2^2}{x_1^2}\right) \cdot \exp\left[-\frac{Q_d}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right] \quad \text{Eq. 5 (1 point)}$$

According to the problem statement:

$t_1 = 17 \text{ h}$ ,  $T_1 = 763 \text{ °C} = 1036 \text{ K}$ ,  $x_1 = 2.2 \text{ mm}$ ,  $T_2 = 1000 \text{ °C} = 1273 \text{ K}$ ,  $x_2 = 5.3 \text{ mm}$ ,  $Q_d = 104000 \text{ J/mol}$ , the universal gas constant  $R = 8.31 \text{ J/(mol} \cdot \text{K)}$ , so substituting those values to derive  $t_2$ :

$$t_2 = \left[\frac{(17 \text{ h}) \times (5.3 \text{ mm})^2}{(2.2 \text{ mm})^2}\right] \cdot \exp\left[-\frac{(104000 \frac{\text{J}}{\text{mol}})}{8.31 \frac{\text{J}}{\text{mol} \cdot \text{K}}} \times \left(\frac{1}{1036 \text{ K}} - \frac{1}{1273 \text{ K}}\right)\right] = 10.4093 \text{ h (2 points)}$$

- 1.2** (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/(m<sup>2</sup> 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.)

**Solution:**

**(a)**

The definition of flux is the quantity of something (which could be in terms of particle count, mass etc.) that passes through a specific unit of area in a specified unit of time.

In this case, we provided an atom count that pass through the known area each hour. Therefore, accounting for the seconds in each hour:

$$J = \frac{M}{A \cdot t} = \frac{[m]}{([a] \text{ m}^2) \cdot ([t] \text{ h} \cdot (3600 \text{ s/h}))} = 2.778 \times 10^{-4} \frac{[m]}{[a] \cdot [t] \text{ m}^2 \cdot \text{s}} \quad (2 \text{ points})$$

**(b)**

The molar mass of water is 18 g/mole, according to the definition of the flux, we can derive the time as follows:

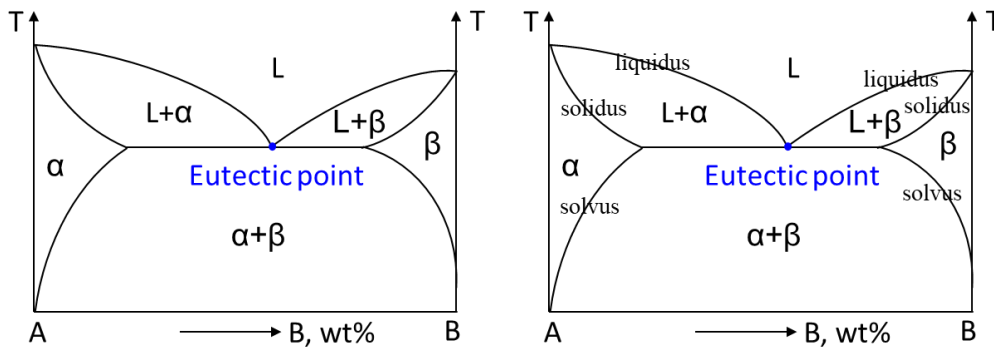
$$t = \frac{M}{A \cdot J} = \frac{[m] \text{ kg} \left( \frac{1000 \text{ g}}{1 \text{ kg}} \right) \left( \frac{1 \text{ mole}}{18 \text{ g}} \right)}{([a] \text{ cm}^2) \left( \frac{1 \text{ m}^2}{100^2 \text{ cm}^2} \right) \cdot ([j] \frac{\text{mole}}{\text{m}^2 \text{ day}})} \left( \frac{24 \text{ hr}}{1 \text{ day}} \right) = 1.333 \times 10^7 \frac{[m]}{[a] \cdot [j]} \text{ hours} \quad (2 \text{ points})$$

## Task 2. Phase diagram (45 points, Lecture7)

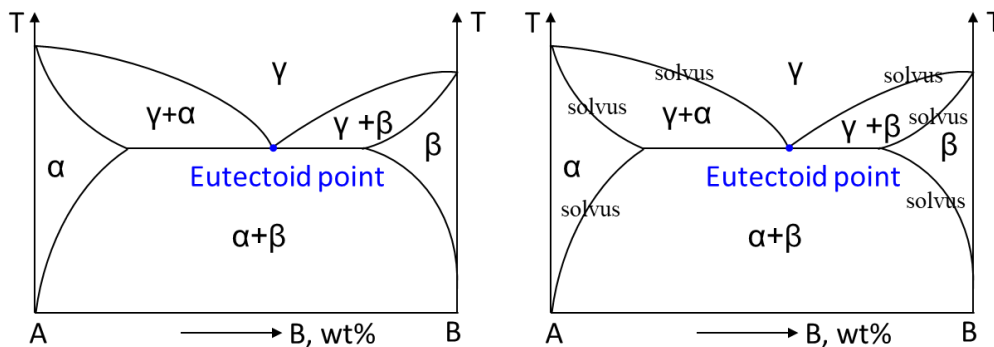
**2.1** Give the schematic sketch of binary phase diagrams of (a) eutectic system, (b) eutectoid system and (c) peritectic system. On your schematic drawings, label the various phase regions, liquidus, solidus, and solvus lines, and give the reaction equations for these three systems. (Please create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

### Solution:

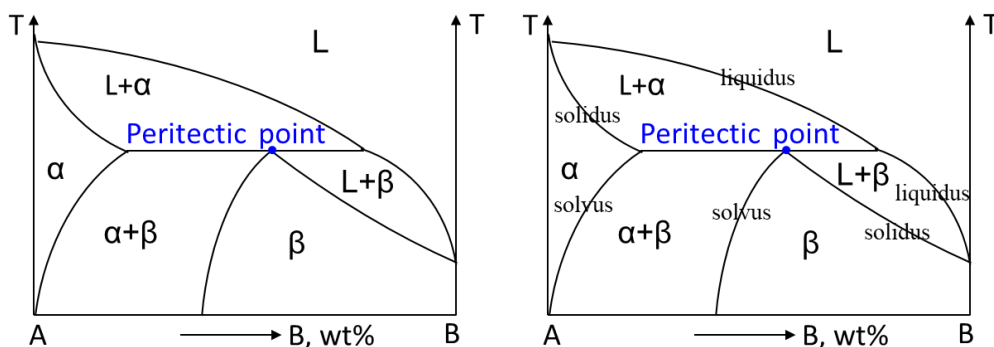
**(a)** Eutectic reaction:  $L \Leftrightarrow \alpha + \beta$



**(b)** Eutectoid reaction:  $\gamma \Leftrightarrow \alpha + \beta$



**(c)** Peritectic reaction:  $L + \alpha \Leftrightarrow \beta$



solvus line: the solid solubility limit line separating a homogeneous solid solution and the two-solid-phase region

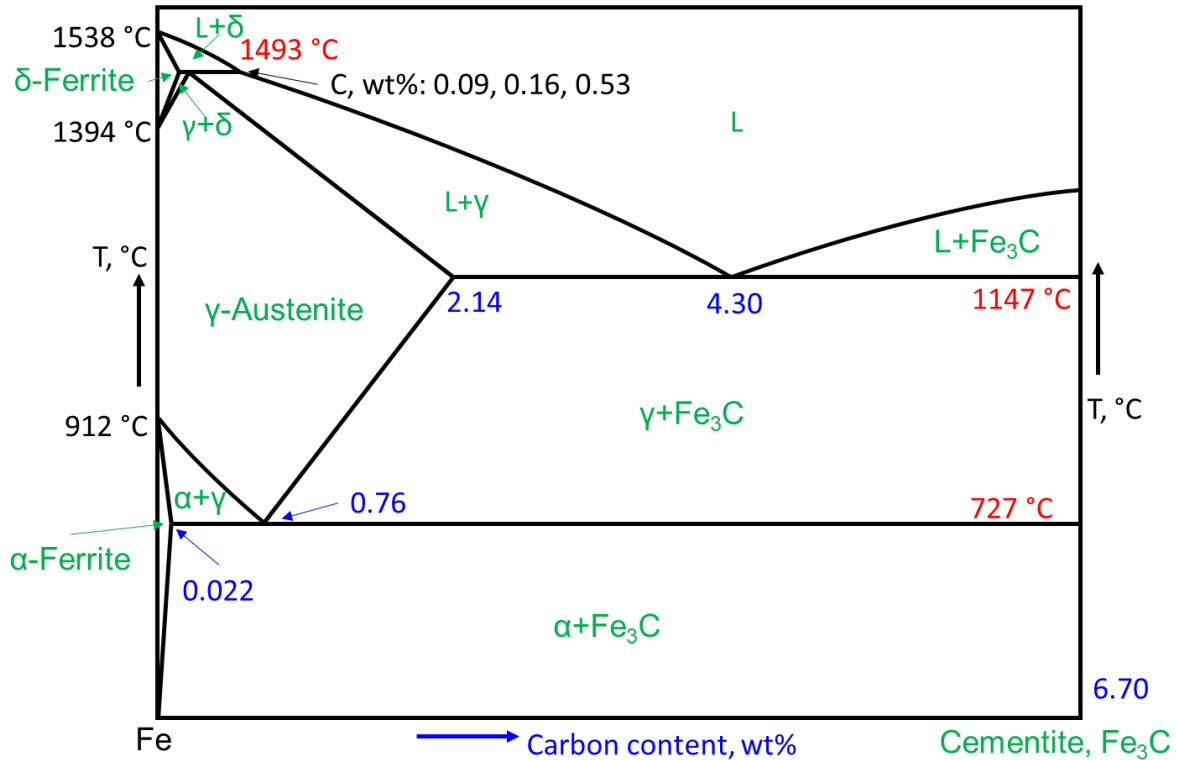
solidus line: the boundary between the single-solid-phase region and liquid-solid two-phase region

liquidus line: the boundary between the liquid-phase region and liquid-solid two-phase region

**(Reaction equations 2 points + Figure 2 points + Marks 2 point) \* 3 systems = 18 points**

**2.2** Draw the Fe–Fe<sub>3</sub>C phase diagram with 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!)

**Solution:**



Phase diagram 2 points

Marks of five phases 5 points

Key temperature 3 points

Key carbon content 5 points

**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<sub>3</sub>C 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.

**Solution:**

**(a)**

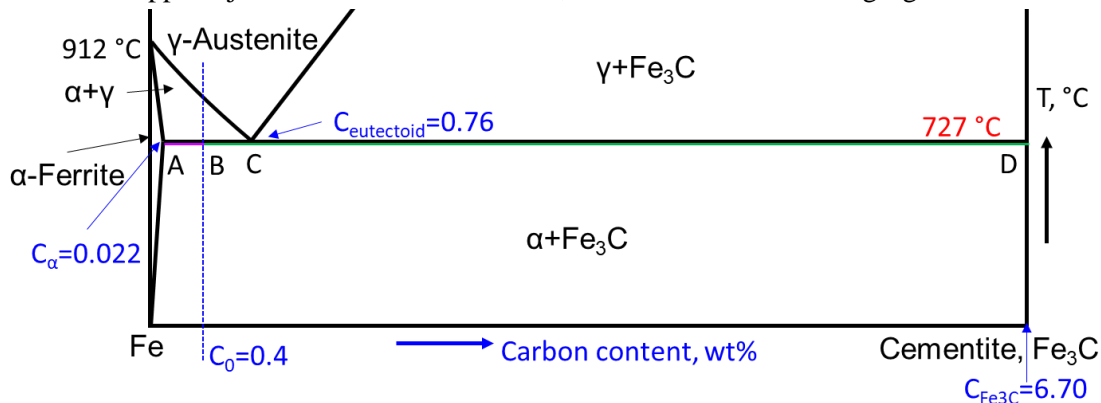
According to the Fe–Fe<sub>3</sub>C phase diagram, at a temperature just below the eutectoid, the carbon content is 0.022 wt% in α-ferrite and 6.7 wt% in cementite. The rest is iron. Therefore, the chemical composition is shown in the following table:

	Fe, wt%	C, wt%
α-ferrite	99.978	0.022
cementite	93.30	6.70

2 points

**(b)**

As 0.40 wt% is lower than the carbon content at eutectoid point, 0.76 wt%, the cementite is generated as a component in the pearlite when temperature is lower than the eutectoid temperature. Therefore, the level rule is applied just below the eutectoid line, as shown in the following figure:



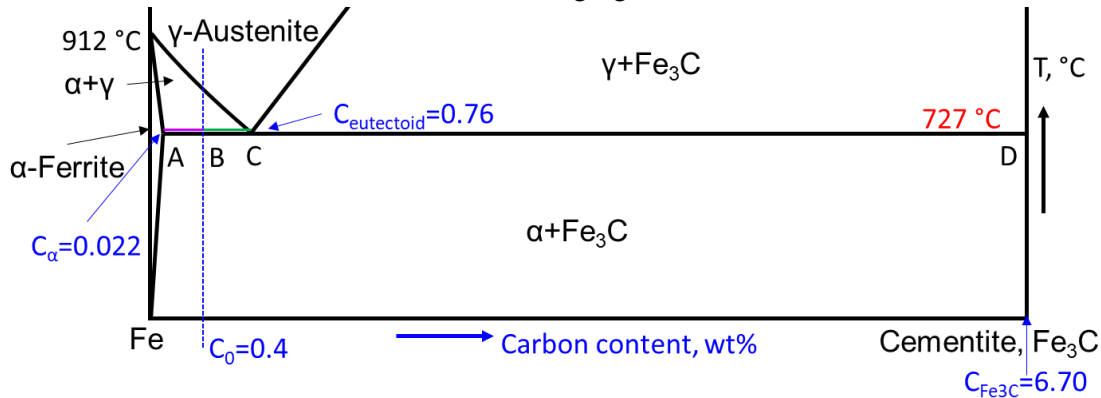
The weight percent of  $\text{Fe}_3\text{C}$  is:

$$W_{\text{Fe}_3\text{C}} = \frac{BC}{AC+CD} = \frac{AB}{AD} = \frac{C_0 - C_\alpha}{C_{\text{Fe}_3\text{C}} - C_\alpha} = \frac{0.40 - 0.022}{6.70 - 0.022} = 0.0566 \text{ (2+1+1 points)}$$

In 100 g steel, there are  $100 \text{ g} \times W_{\text{Fe}_3\text{C}} = 5.66 \text{ g}$  cementite. (1 point)

**(c)**

The proeutectoid  $\alpha$ -ferrite is generated after the temperature lower than boundary between  $\gamma$ -phase region and  $\alpha$ - $\gamma$ -two-phase region until the eutectoid temperature. Therefore, the level rule is applied just above the eutectoid line, as shown in the following figure:



The weight percent of proeutectoid  $\alpha$ -ferrite is:

$$W_\alpha = \frac{BC}{AB+BC} = \frac{BC}{AC} = \frac{C_{\text{eutectoid}} - C_0}{C_{\text{eutectoid}} - C_\alpha} = \frac{0.76 - 0.40}{0.76 - 0.022} = 0.4878 \text{ (2+1+1 points)}$$

In 100 g steel, there are  $100 \text{ g} \times W_\alpha = 48.78 \text{ g}$  proeutectoid ferrite.

After temperature is lower than the eutectoid temperature, all the left austenite is transformed into pearlite, therefore, the weight of pearlite in 100 g steel is:

$100 \text{ g} - 48.78 \text{ g} = 51.22 \text{ g}$ . (1 point)

### Task 3. Phase transformation (45 points, Lecture8)

3.1 (a) List at least six important phases that are found in steel alloys. (b) Give the crystal structure and describe the microstructure for each. (c) Discuss and compare their mechanical properties.

#### Solution:

Phase	Crystal structure / Microstructure	Mechanical property
Austenite	homogeneous face-center cubic (fcc) structure with carbon solute solution	Austenite is not a stable phase at room temperature. Alloying elements need to be added for austenite stabilization. end-user strength and ductility in a wide range depending on the alloying system
Ferrite	homogeneous body-center cubic (bcc) structure with limited carbon solute solution	low strength but high ductility
Cementite	a kind of carbides, chemical composition of $\text{Fe}_3\text{C}$ , orthorhombic crystal structure	highest hardness but very brittle
Pearlite	lamellar structure composes of alternating ferrite and cementite layers	in between the ferrite and cementite, i.e. higher strength and lower ductility than ferrite; lower hardness but higher ductility than cementite
Bainite	bcc ferritic matrix (plate-like shape named bainitic ferrite, BF) plus carbides (e.g. $\text{Fe}_3\text{C}$ ), the carbides could be dispersing in BF plates or precipitating among BF plates	generally higher carbon content than ferrite, results in higher strength and hardness but lower ductility compared to ferrite.
Martensite	body-center tetragonal (bct) structure, hierarchical microstructure with the basic unit of lath or plates-shaped crystals	high strength, hardness, but very brittle
Tempered martensite	very small $\text{Fe}_3\text{C}$ sphere particles in a ferrite matrix	strong, not as hard as martensite, but much more ductile than martensite

(Phase name 1 point + Crystal structure/Microstructure 2 points + Property 2 points) \* 6 = 30 points

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

#### Solution:

Martensitic transformation is a transformation without changes in concentration. It happens in many metal systems; the most important example is in steel. The entire area of austenitic crystals suddenly shears into a state, named martensite, without changes in local alloy composition occurring due to diffusion processes. It is not diffusion-controlled, i.e. a kind of diffusionless transformation. The direct change of the crystal structure from fcc to bct happens.

The change in volume and in configuration associated with this transformation causes **strong elastic lattice distortions**. The single atoms do not exchange places, instead only a cluster of atoms exchange place in a coordinated, coupled movement (cooperative shear movement of atoms). These complex lattice deformations are achieved through shear and tensile forces and resulting in **high dislocation density** and **increased residual stresses**. These microstructural features bring enhanced strength.

Besides, the **local carbon atoms** contribute to the **solid solution hardening**. In addition, metallographically, martensite forms very fine microstructure that has a similar effect as the grain refinement mechanism, the **fine-structure boundaries** enormously reduce dislocation mobility and contribute to the high strength and hardness of martensite. Furthermore, the high quenching speed also brings some **formation of Fe<sub>3</sub>C**, which increases the strength by **precipitation hardening** but also leads to the reduced ductility.

Definition 2 points

4 reasons \* 2 points

**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  $k=0.02 \text{ s}^{-n}$ ,  $n=2$ .

#### Solution 1:

According to the JMAK function, the transformed phase fraction y is

$$y = 1 - \exp(-kt^n) \quad \text{Eq. 6}$$

the average phase transformation rate v is defined as

$$v = \frac{1}{t_{0.5}} \quad \text{Eq. 7 (1 point)}$$

Therefore, solve Eq. 6 at  $y=0.5$  with parameters  $k=0.02 \text{ s}^{-n}$  and  $n=2$ ,

$$0.5 = 1 - \exp(-0.02 \text{ s}^{-n} \cdot t_{0.5}^2) \quad (1 \text{ point})$$

The time for 50% phase transformation is  $t_{0.5} = 5.8871 \text{ s}$  (2 points)

The average phase transformation rate is  $v = \frac{1}{t_{0.5}} = 0.1699 \text{ s}^{-1}$  (1 point)

#### Solution 2:

If you calculate  $t_{0.5}$  as the maximum rate point: the second derivative of JMAK function shall be zero.

$$y = 1 - \exp(-kt^n) \quad \text{Eq. 8}$$

The average phase transformation rate v is defined as

$$v = \frac{1}{t_{0.5}} \quad \text{Eq. 7 (1 point)}$$

The first and second derivative of JMAK function:

$$dy = kn \exp(-kt^n) t^{n-1} dt \quad \text{Eq. 9}$$

$$d^2y = [k^2 n^2 \exp(-kt^n) t^{2n-2} + kn(n-1) \exp(-kt^n) t^{n-2}] dt^2 \quad \text{Eq. 10 (1 point)}$$

When  $t = t_{0.5}$ ,  $\frac{d^2y}{dt^2} = 0$

Therefore, the time for 50% phase transformation is  $t_{0.5} = \sqrt[n]{\frac{(n-1)}{kn}} \quad (1 \text{ point})$

with parameters  $k=0.01 \text{ s}^{-n}$  and  $n=2$

$$t_{0.5} = \sqrt[n]{\frac{(n-1)}{kn}} = \sqrt[2]{\frac{(2-1)}{0.02 \times 2}} = \sqrt[2]{\frac{1}{0.04}} = 5 \text{ s} \quad (1 \text{ point})$$

The average phase transformation rate is  $v = \frac{1}{t_{0.5}} = 0.2 \text{ s}^{-1}$  (1 point)

**Due date: 18:00, 28.11.2021.**

**Contact: MyCourses 'General discussion' channel**