



WELDING LMECA2860

PHASE TRANSFORMATIONS IN METALS AND ALLOYS

HOMEWORK 1 REPORT

Work performed by:

Vansnick François

1 Summarize Chapter 1 of the book

1.1 Equilibrium

For transformations that occur at constant temperature and pressure the relative stability of a system is determined by its Gibbs free energy (G).

$$G = H - TS$$

$$H = E + PV$$

A system is at equilibrium when it is in the most stable state, i.e. shows no desire to change ad infinitum. Will be in stable equilibrium if it has the lowest possible value of the Gibbs free energy.

$$dG = 0$$

Configurations that are a local minimum are called **metastable**. Any transformation that results in a decrease in Gibbs free energy is possible:

$$\Delta G = G_2 - G_1 < 0$$

 G_1 is initial state and G_2 final state.

Intensive properties: T,P (independent of the size)

extensive properties: V, E, H, S and G (proportional to the quantity of material in the system)

1.2 Single Component Systems

Specific heat at constant pressure:

$$C_p = (\frac{\partial H}{\partial T})_p$$

H can be defined as:

$$H = \int_{298}^{T} C_p \, dT$$

We can also derived entropy from C_p :

$$\frac{C_p}{T} = (\frac{\partial S}{\partial T})_p$$

$$S = \int_0^T \frac{C_p}{T} \, dT$$

By combining those equations we found :

$$dG = -SdT + VdP$$

At all temperatures the liquid has a higher enthalpy (internal energy) than the solid. At constant temperature the free energy of a phase increases with pressure such that:

$$(\frac{\partial G}{\partial P})_T = V$$

Free energy of each phase will not increase by the same amount so:

$$dG^{\alpha} = V_m^{\alpha} dP - S^{\alpha} dT$$

$$dG^{\beta} = V_m^{\beta} dP - S^{\beta} dT$$

At equilibrium, Clausius-Claypeyron equatiopn:

$$(\frac{dP}{dT_{eq}}) = \frac{\Delta H}{T_{eq}\Delta V}$$

The difference in free energy between two phases at temperatures away from the equilibrium temperature. Solidification will be accompanied by a decrease in free energy.

$$G^L = H^L - TS^L$$

$$G^S = H^S - TS^S$$

1.3 Binary Solutions

$$X_A + X_B = 1$$

With X_x mole fraction of the element x. And so the free energy of the whole system is:

$$G_1 = X_A G_A + X_B G_B$$

Boltzman's formula is based on the number of possible atoms arranged randomly. Finally we end up with :

$$\Delta G_{mix} = RT(X_A ln X_A + X_B ln X_B)$$

We can also rewrite the equation via the chemical potential:

$$G = \mu_A X_A + \mu_B X_B$$

The internal energy of the solution depends on the number of bonds P_{xx}

$$E = P_{AA}\epsilon_{AA} + P_{BB}\epsilon_{BB} + P_{CC}\epsilon_{CC}$$

At the end for a regular solution we get:

$$G = X_A G_A + X_B G_B + \Omega X_A X_B + RT(lnX_A + X_B lnX_B)$$

a is the activity of element A, and $\gamma_a = a_a/X_a$ (cfr Raoult's and Henry's law)

1.4 Equilibrium in Heterogeneous Systems

In alloy systems with two phases (e.g., fcc and bcc), each phase has a unique free energy curve. The system minimizes free energy by separating into two phases with compositions determined by the lever rule. Equilibrium is reached when the chemical potentials of each component are equal in both phases.

1.5 Binary Phase Diagrams

Equilibrium melting T° when $G^S = G^L$ at $T_m(A) = T_m(B)$. The Gibbs Phase rule (for the component X):

$$\mu_X^{\alpha} = \mu_X^{\beta} = \mu_X^{\gamma}$$

Equilibrium the number of degrees of freedom F is given by:

$$P + F = C + 1$$

A degree of freedom is an intensive variable that can be varied independently while still maintaining equilibrium.

Let us now consider the possibility that some sites remain without atoms, that is, there are vacancies in the lattice.

$$\Delta H = \Delta H_v X_v$$

2 TP1

Exercice 1

Données : Alloy of 20% Sn and 80% Pb

1. Temperature of 260°C

- The alloy is located in the two-phase region liquid $+ \beta$.

Phase compositions:

- Liquid: approximately 28% Sn, 72% Pb.
- β : approximately 8% Sn, 92% Pb.

Calculation of fractions by weight (Lever rule):

Liquid fraction =
$$\frac{X_{\beta}^S - X_0}{X_{\beta}^S - X_{\beta}^L} = \frac{92 - 80}{92 - 72} = \frac{12}{20} = 0.6$$

Fraction of
$$\beta = \frac{X_0 - X_{\beta}^L}{X_{\beta}^S - X_{\beta}^L} = \frac{80 - 72}{92 - 72} = \frac{8}{20} = 0.4$$

1. Temperature of 200°C

- The alloy is located in the two-phase region liquid $+ \beta$.

Phase compositions:

- Liquid : approximately 55% Sn, 45% Pb.
- β : approximately 15% Sn, 85% Pb.

Calculation of fractions by weight (Lever rule):

Liquid fraction =
$$\frac{X_{\beta}^S - X_0}{X_{\beta}^S - X_{\beta}^L} = \frac{85 - 80}{85 - 45} = \frac{5}{40} = 0.125$$

Fraction of
$$\beta = \frac{X_0 - X_{\beta}^L}{X_{\beta}^S - X_{\beta}^L} = \frac{80 - 45}{85 - 45} = \frac{8}{20} = 0.875$$

1. Temperature of 150°C

- The alloy is located in the two-phase region $\alpha + \beta$.

Phase compositions:

- α : approximately 99% Sn, 1% Pb.
- β : approximately 5% Sn, 95% Pb.

Calculation of fractions by weight (Lever rule):

Fraction of
$$\alpha = \frac{X_{\beta}^S - X_0}{X_{\beta}^S - X_{\beta}^L} = \frac{95 - 80}{95 - 1} = \frac{15}{94} = 0.16$$

Fraction of
$$\beta = \frac{X_0 - X_{\beta}^L}{X_{\beta}^S - X_{\beta}^L} = \frac{80 - 1}{95 - 1} = \frac{79}{94} = 0.84$$

- Complete liquefaction temperature: the liquidus point for that specific composition is 220°C.
- Complete solidification temperature: the solidus point for this composition is 100°C.

2. Temperature of 250°C

- The alloy is in the **liquid** region.
- Phases present: Liquid.
- Molar fraction: 100% liquid.

3. Temperature of 200°C

- The alloy is in the two-phase region liquid + solid.
- Phases present: Liquid and solid.
- Molar fraction of phases:
- Solid = $\frac{3}{4} = 0.75$
- Liquid = $\frac{1}{4}=0.25$

4. Temperature of 140°C

- This is the eutetic temperature, the alloy is in a one-phase region solid α .
- Phases present: α (rich in Sn).
- Calculation of mole fractions: 100 % α

5. Temperature of 50°C

- At 50°C, the alloy is entirely in the solid phase $\alpha + \beta$.
- Phases present: α and β (constitute solid phases at this temperature).
- Molar fraction:
- $\beta = \frac{6.9-2}{100-2} = 0.05$
- $-\alpha = 1 0.05 = 0.95$

At room temperature (around 25°C), with a composition of 85% Al and 15% Cu, the alloy is in the two-phase region $\alpha + \beta$.

- Phase α : a solid solution of Al with a small percentage of Cu.
- Phase β : an intermetallic compound rich in Cu.

Calculation of mass fractions:

- 1. Phase composition α : Approximately 97% Al, 3% Cu.
- 2. Phase composition β : Approximately 47% Al, 53% Cu.

Fraction of
$$\alpha = \frac{X_0 - X_\beta}{X_\alpha - X_\beta} = \frac{85 - 47}{97 - 47} = \frac{35}{50} = 0.76$$

Fraction of $\beta = 1 - \alpha = 0.24$

Results: At room temperature, the alloy is composed of:

- 76% of the phase α (97% Al, 3% Cu)
- 24% of the phase β (53% Al, 47% Cu)

2. Melting temperature

The melting temperature is 820°C.

At 650°C, for an alloy containing 75% Al and 25% Si, we must refer to the Al-Si phase diagram. At this temperature, and for this composition, the alloy is in a two-phase region liquid + solid (Si).

- Liquid phase: rich in aluminum.
- Solid phase (Si): mainly silicon.
- 1. Composition of the liquid phase: Approximately 83% Al, 17% Si. 2. Composition of the solid phase (Si): 100% Si.

The mass fraction of each phase is given by:

Liquid fraction =
$$\frac{X_0 - X_{\beta}}{X_{\alpha} - X_{\beta}} = \frac{25 - 100}{17 - 100} = \frac{-75}{-83} = 0.9$$

Si fraction =
$$1 - \alpha = 0.1$$

Al-Cu phase diagram

In the Aluminum-Copper phase diagram, we identify the following triple points:

1. Eutectic point (Pb-Sn):

- Composition : Approximately 72% Sn, 38% Pb.
- Temperature : Approximately 185°C.
- Reaction : $L \to \alpha + \beta$
- **Description**: the liquid phase transforms into two solid phases, α and θ .

2. Peritectic point:

- Composition : Approximately 3% Pb, 97% Sn.
- Temperature : Approximately 185°C.
- Reaction : $L + \alpha \rightarrow \beta$
- **Description**: a liquid phase and the solid phase α transform into the phase β .

3. Peritectic point:

- Composition: Approximately 84% Pb, 16% Sn.
- **Temperature** : Approximately 185°C.
- Reaction : $L + \beta \rightarrow \alpha$
- **Description**: a liquid phase and the solid phase α transform into the phase α .

Sn-Bi phase diagram

1. Eutectic point:

- Composition : Approximately 43% Bi, 57% Sn.
- Temperature : 139°C.
- Reaction : $L \to \alpha + \beta$

• **Description**: the liquid phase transforms into two solid phases, α and θ .

2. Peritectic point:

- \bullet Composition : Approximately 13.1% Bi, 86.9% Sn.
- **Temperature** : Approximately 139°C.
- Reaction : $L + \alpha \rightarrow \beta$
- **Description**: a liquid phase and the solid phase α transform into the phase β .

Al-Cu phase diagram

1. Eutectic point:

- Composition: Approximately 33% Cu, 67% Al.
- Temperature : 820°K.
- Reaction : $L \to \alpha + \beta$
- **Description**: the liquid phase transforms into two solid phases, α and θ .

2. Peritectic point:

- \bullet Composition : Approximately 5.7% Cu, 94.3% Al.
- Temperature : 820°K.
- Reaction : $L + \alpha \rightarrow \beta$
- **Description**: a liquid phase and the solid phase α transform into the phase β .

3. Peritectic point:

- Composition : Approximately 53.5% Cu, 46.5% Al.
- Temperature : 820°K.
- Reaction : $L + \beta \rightarrow \alpha$
- **Description**: a liquid phase and the solid phase α transform into the phase α .

Al-Si phase diagram

1. Eutectic point:

- Temperature : 577°C.
- Reaction : $L \to \alpha + \beta$
- **Description**: the liquid phase transforms into two solid phases, α and θ .

2. Peritectic point :

- Composition : Approximately 2% Si, 98% Al.
- Temperature : 577°C.
- Reaction : $L + \alpha \rightarrow \beta$
- **Description** : a liquid phase and the solid phase α transform into the phase β .

Fe-C phase diagram (steel)

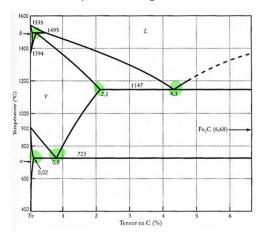


Figure 1: Fe-C

T	900°C		$723 + \epsilon$ °C		723 − ε °C	
Phases	%C	fraction	%C	fraction	%C	fraction
Austenite (γ)	0.4	1	0	0	0	0
Ferrite pro (α)	0	0	0	0.51	0	0
Cementite pro (Fe_3C)	0	0	0.4	0.49	0	0
Pearlite	0	0	0	0	0.4	1

Table 1 – Steel with 0.4 wt.%C

T	900°C		$723 + \epsilon$ °C		$723 - \epsilon$ °C	
Phases	%C	fraction	%C	fraction	%C	fraction
Austenite (γ)	0.8	1	0.8	1	0	0
Ferrite pro (α)	0	0	0	0	0	0
Cementite pro (Fe_3C)	0	0	0	0	0	0
Pearlite	0	0	0	0	0.8	1

Table 2 – Steel with 0.8 wt.%C

T	900°C		$723 + \epsilon$ °C		$723 - \epsilon$ °C	
Phases	%C	fraction	%C	fraction	%C	fraction
Austenite (γ)	0.4	1	0	0	0	0
Ferrite pro (α)	0	0	0	0.99	0	0
Cementite pro (Fe_3C)	0	0	1.2	0.1	0	0
Pearlite	0	0	0	0	0.4	1

Table 3 – Steel with 1.2 wt.% C

Figure 2: Table of composants