Exercise for the Lecture on Materials Science

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Exercise Sheet 6

Discussion on June 4, 2025

Exercise 1: Water

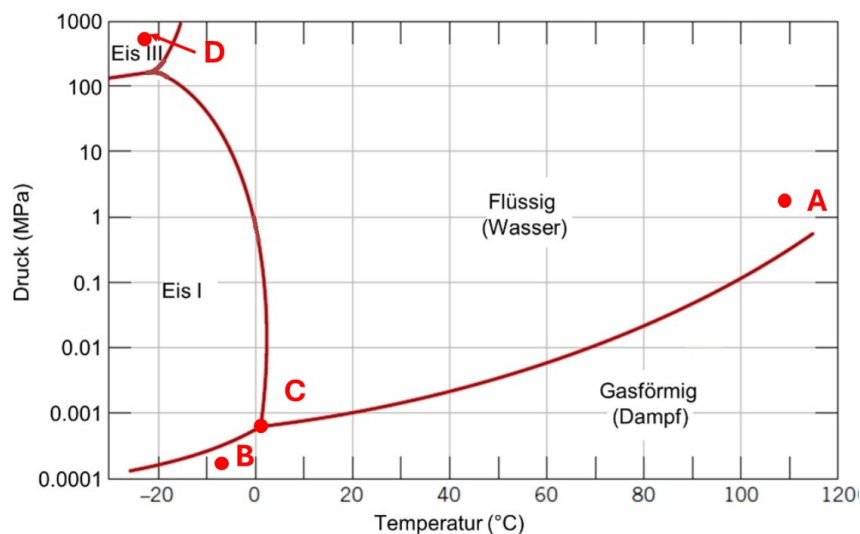Figure 1 shows the single-component phase diagram of H_2O.

Figure 1: Single-component phase diagram of H_2O

1. Use the Gibbs phase rule to determine the number of degrees of freedom F at points A to D.
   Also explain the physical meaning of the number of degrees of freedom.

2. Why can water remain liquid below $0\,°C$, even though this is below the freezing point? Explain the physical mechanism behind this phenomenon.

3. Calculate the critical radius of an ice nucleus for an undercooling of $10\,K$. Use the following values:
   $$\gamma = 0{,}033\,\text{J/m}^2, \quad \Delta H_f = 3{,}3 \cdot 10^8\,\text{J/m}^3, \quad T_m = 273{,}15\,\text{K}$$

4. Explain the difference between homogeneous and heterogeneous nucleation during the freezing of water. Give typical examples from nature or technology.

5. How do dust particles or impurities affect the probability of ice nucleation in clouds?

Exercise 2: Spinodal decomposition in a binary alloy

A binary alloy A–B is rapidly quenched from the single-phase region at high temperature into the two-phase region below the critical temperature. The free enthalpy of mixing is

given by:

$$G(c) = \Omega c(1 - c) + RT\left[c \ln c + (1 - c) \ln(1 - c)\right]$$

where c is the concentration of component B, $\Omega > 0$ is an interaction parameter, R is the gas constant, and T is the temperature.

1. Explain the physical difference between spinodal and binodal decomposition.

2. Derive the condition for spinodal instability from the given function $G(c)$.

3. For which concentration range within $c \in [0, 1]$ does spinodal decomposition occur at $T = 300\,\text{K}$, with $\Omega = 2{,}5\,\text{kJ/mol}$, and $R = 8{,}314\,\text{J/mol\,K}$?

4. What kind of microstructure (morphology) do you typically expect from spinodal decomposition? Give examples.

Exercise 3: Time-Temperature-Transformation Diagram

Below is the time-temperature-transformation (TTT) diagram for a steel with $0{,}45$ wt.-% C. The phases shown in the diagram are austenite (A), ferrite (F), pearlite (P), bainite (B), and martensite (M).
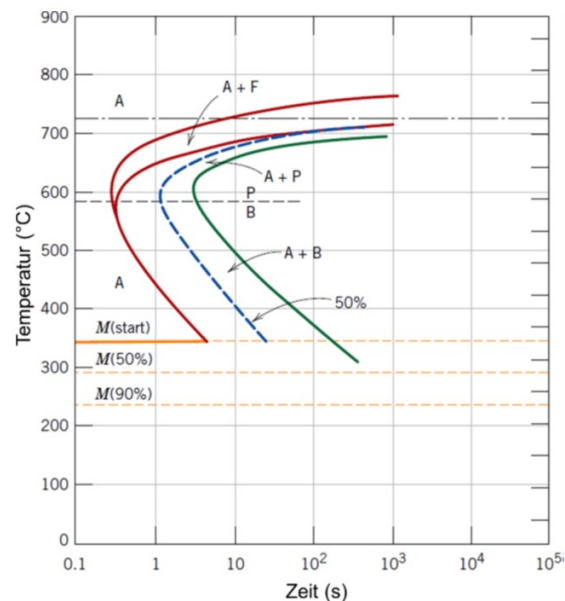

Figure 2: Time-temperature-transformation (TTT) diagram for a Fe–C alloy with $0{,}45$ wt.-% C.

1. Sketch suitable time-temperature paths in Figure 2 to produce the following microstructures:

   (a) $42\,\%$ proeutectoid ferrite and $58\,\%$ pearlite

   (b) $50\,\%$ pearlite and $50\,\%$ bainite

   (c) $100\,\%$ martensite

(d) 50 % martensite and 50 % retained austenite

2. Briefly explain for each case why your chosen path leads to the desired microstructure. In particular, refer to critical temperatures, cooling rates, and whether the transformation curves in the TTT diagram are crossed or not.

Exercise 4: MgO–Al$_2$O$_3$ System

In the MgO–Al$_2$O$_3$ system, the spinel phase (MgAl$_2$O$_4$) forms stably over a certain range of non-stoichiometric compositions. This phase tolerates both MgO and Al$_2$O$_3$ excess via point defects in the crystal lattice.

1. At 2000 °C, the spinel phase is stable up to 82 mol% (corresponding to 92 wt.-%) Al$_2$O$_3$.
   Assume a total of N stoichiometric units of MgAl$_2$O$_4$.
   What type of vacancy occurs with this Al$_2$O$_3$ excess, and what is the fraction of these vacancies (relative to the total number of cation sites)?

2. On the MgO-rich side, the maximum deviation from stoichiometry occurs at 39 mol% (corresponding to 62 wt.-%) Al$_2$O$_3$.
   Again, assume N stoichiometric units.
   What type of vacancy occurs in this case, and what is the fraction of these vacancies (relative to the number of oxygen sites)?