

### 3.020 – Thermodynamics of Materials Recitation 3

#### Problem 1

In this problem we will calculate and sketch a unary phase diagram of water using the equation of Clausius-Clapeyron and thermodynamic data given in the table below. We will integrate the equation of Clausius-Clapeyron using appropriate approximations to find the analytical expressions  $P(T)$  for three phase transformations in water.

$\Delta H_{fus}=6.01\text{kJ/mol}$	$V^s=1.958\cdot 10^{-5}\text{m}^3/\text{mol}$ ( $=1.09\text{cm}^3/\text{g}$ )	$T_{tri}=273.16\text{K}$
$\Delta H_{vap}=44.0\text{kJ/mol}$	$V^l=1.802\cdot 10^{-5}\text{m}^3/\text{mol}$ ( $=1.00\text{cm}^3/\text{g}$ )	$P_{tri}=611.73\text{Pa}$
$\Delta H_{sub}=51.1\text{kJ/mol}$	$V^v=RT/P$	

- a) Solid to liquid transformation:
  1. What are the required approximations for this transformation?
  2. Find the analytical expression  $P(T)$  that describes the two-phase equilibrium conditions after indefinite integration of the Clausius-Clapeyron equation for this transformation?
  3. Use the derived relation to verify the melting temperature of water at atmospheric pressure.
- b) Liquid to vapor transformation:
  1. What are the required approximations?
  2. Find analytically the  $P(T)$  two-phase equilibrium conditions for this transformation?
  3. Use the derived relation to verify the boiling temperature of water at atmospheric pressure.
- c) Solid to vapor transformation:
  1. Required approximations?
  2. Find the analytical  $P(T)$  equilibrium conditions?
  3. We do not know the sublimation temperature of water at atmospheric pressure, why?
- d) Sketch a  $\ln(P)$ - $T$  diagram of water around the triple point using the above derived analytical expressions for the three two-phase coexisting lines.

You have drawn your first (approximate) unary phase diagram!

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3.020 Thermodynamics of Materials  
Spring 2021

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