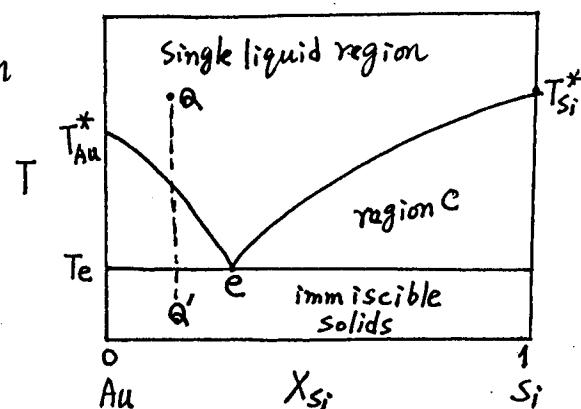


- Suppose 6 mol of an ideal gas at 25.0°C are allowed to expand isothermally and reversibly from an initial volume of 5 dm<sup>3</sup> to a final volume of 15 dm<sup>3</sup>.
  - How much work is done by the gas? (6%)
  - What are  $\Delta U$  and  $\Delta H$ ? (4%)
- A mole of hydrogen gas is heated from T=300 K to 1000 K at constant volume. Calculate the entropy change.  
 $(\bar{C}_v = 18.97 + 3.26 \times 10^{-3} T + 5.0 \times 10^4 T^{-2} \text{ J K}^{-1} \text{ mol}^{-1})$ . (8%)
- (a) Liquid water at 100°C is in equilibrium with water vapor at 1 atm.  
 $(\Delta H_{\text{vap}} = 40.60 \text{ kJ mol}^{-1})$ , what are  $\Delta G$  and  $\Delta S$ ? (6%)
  - Suppose that water at 100°C is in contact with water vapor at 0.9 atm. Calculate  $\Delta G$  and  $\Delta S$  for this process. (6%)
- The Gibbs energies of formation of NO<sub>2</sub>(g) and N<sub>2</sub>O<sub>4</sub>(g) are 51.30 and 102.0 kJ mol<sup>-1</sup>, respectively at 1 atm and 25°C.
  - Calculate  $K_p$  for the reaction  $\text{N}_2\text{O}_4(\text{g}) \rightleftharpoons 2\text{NO}_2(\text{g})$ . (5%)
  - At what pressure is N<sub>2</sub>O<sub>4</sub> 50% dissociated? (6%)
- Prove that for a gas obeying the van der Waals equation  $(P + \frac{a}{V_m^2})(V_m - b) = RT$ , the internal pressure is  $a/V_m^2$ . (6%)
- Calculate the activation energy for a reaction whose rate constant at 25°C is doubled by a 10°C increase in temperature. (6%)
- Given the phase diagram of the gold-silicon system

(a) Where is the eutectic point? (2%)

(b) At constant pressure, calculate the degree of freedom of the system at point Q, e, and Q'. (6%)

(c) What is the solid phase in region C? (2%)



$T_{\text{Au}}^*$ : m.p. of Au

$T_{\text{Si}}^*$ : m.p. of Si

$T_e$ : eutectic temperature

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8. Find the following expectation values of  $\hat{H}_{\text{atom}}$  using the wavefunction

$\psi_{1s}$  & :

- (a)  $\langle \hat{U}^2 \rangle$ , (b)  $\langle \hat{U}_z \rangle$ , (c)  $\langle \hat{S}^2 \rangle$ , (d)  $\langle \hat{S}_z \rangle$ , (e)  $\langle \hat{H} \rangle$  (10%)

9. (a) Write the energy expressions of (i) rigid rotor, (ii) harmonic oscillator

(b) Find the minimum values of these energies

(c) Write the selection rules between the energy levels of rigid rotor. (9%)

10. For a free particle moving in one dimensional space, write the operators of (a) momentum, (b) kinetic energy, (c) total energy. (9%)

11. (a) Write the expression of wavefunctions of (i) one particle in one dimensional space, (ii) two particles in three dimensional space

(b) Write the expressions of probability density and the expectation value of operator  $\hat{p}_x$ . (9%)