Uva Wellassa University, Sri Lanka

End Semester Examination – February 2011

SCT 331-3 Material Chemistry 1

Time: Three (03) Hours

Total 08 Questions

Answer two (02) questions from Part A and four (04) questions from Part B. Answer Part A and Part B in separate booklets.

All symbols carry standard meanings.

PART A

1. Given here are the solidus and liquidus temperatures for the copper–gold system.

Composition (wt% Au)	*Solidus Temperature (°C)*	*Liquidus Temperature (°C)*
0	1085	1085
20	1019	1042
40	972	996
60	934	946
80	911	911
90	928	942
95	974	984
100	1064	1064

   a. Construct the phase diagram for this system and label each region.

   b. A copper–gold alloy of composition 30 wt% Cu – 70 wt% Au is slowly heated from a temperature of 200°C.

      i. At what temperature does the first liquid phase form?

      ii. What is the composition of this liquid phase?

      iii. At what temperature does complete melting of the alloy occur?

      iv. What is the composition of the last solid remaining prior to complete melting?

   c. If a copper–gold alloy of composition 50 wt% Cu – 50 wt% Au is heated to 1100°C and slowly cooled to the room temperature draw the possible structures formed.

(100 marks)

31 | (08)

2. Fig. Q02 shows an IT Diagram for a sample of 1566 Steel. (Attach Fig Q02 with your answer script)
    a. Give the final structure with percentages of components and determine the range of hardness values for this specimen.
    b. Draw a cooling curve that can produce 25% fine pearlite, 25% bainite and 50% martensite. Determine the range of hardness values.
    c. Draw a cooling curve that can produce 50% fine pearlite and 50% bainite. Determine the range of hardness values.
    d. What is the effect of adding alloys to the material? Discuss with the help of sketches of IT diagrams.

(100 marks)

PART B

3.

a. State the Van der Waals equation of state for a real gas. Identify all terms therein.

(20 marks)

b. Plot the P – V isotherms of carbon dioxide at different temperatures. Your answer should show the variation of isotherms
(i). Above the critical temperature,
(ii). At the critical temperature,
(iii). Below the critical temperature of CO_2.

(20 marks)

c. Plot the same family of P-V curves of CO_2 accordance to Van der Waals equation. Identify the Van der Waals loop and show a method of correcting this effect (no mathematical derivations are required).

(20 marks)

d. The critical constants of CO_2 is given as P_c = 73.843 bar, V_c = 0.094 ($L.mol^{-1}$), and T_c = 304.14 K. Calculate the compressibility factor and the Van der Waals parameters of CO_2. Briefly explain the answer you received for compressibility factor.

(20 marks)

e. State the law of corresponding state of gases.

(20 marks)

4.

a. Maxwell Boltzmann distribution of speeds of gas molecules is given by the following equation: $F(u)du = \left(\frac{m}{2\pi k_b T}\right)^{3/2} u^2 e^{-mu^2/2k_bT} du$. Identify all terms therein. Plot the distribution of the velocity of a given gas according the Maxwell Boltzmann distribution. How the shape of the curve varies with the temperature.

(25 marks)

b. State the physical meaning of following expressions:

(i). $\int_{v1}^{v2} uF(u).du$ (ii). $\int_0^{\infty} F(u).du$ (iii). $\int_0^{\infty} uF(u).du$ (iv). $\int_0^{\infty} u^2F(u).du$

Write simplified expressions of the integrals (ii), (iii) and (iv) (no mathematical derivations are needed).

(25 marks)

c. Define following terms: (i). collision frequency, (ii). collision cross section, ~~(iii). mean~~ free path. Write mathematical expressions for each of these parameters.

31

II

(25 marks)

d. Calculate the frequency of nitrogen-nitrogen collisions in one cubic centimeter of air at one bar and 20^0C. Assume that 80% of the molecules in air are nitrogen molecules ($\sigma_{N2} = 4.50 \times 10^{-19}$ m^2). State clearly the calculation steps.

(25 marks)

5.

a. State the two assumptions made in the collision theory in deriving an expression for the rate of a reaction. Differentiate the meaning of collision cross section and reactive collision cross section.

(25 marks)

b. Prove that the reactive collision cross section of two dissimilar molecules in gaseous state is given by $\sigma(\epsilon) = \sigma_0\left(1 - \frac{\epsilon_a}{\epsilon}\right)$ for $\epsilon \geq \epsilon_a$. Deduce the value of $\sigma(\epsilon)$ when $\epsilon \leq \epsilon_a$. Rationalize your answer.

(25 marks)

c. According to the collision theory the rate of a reaction $A_g + B_g \rightarrow$ products is given as rate = $\sigma_0\left(\frac{8k_bT}{\pi\mu}\right)^{1/2} exp\left(-\frac{\epsilon_a}{k_bT}\right)N_AN_B$. Based on this expression write an expression for rate constant of the reaction. Write an expression for the pre-exponential factor of the Arrhenius model. How the Arrhenius pre-exponential factor depends on temperature.

(25 marks)

d. Calculate the rate constant for decomposition of HI at 500 K, if the energy of activation is 130 kJ.mol^{-1} and collision diameter of HI is 3.5 Å. Assume that every collision of two HI molecules yields decomposition.

(25 marks)

6.

a. What is the major assumption made in transition state theory? Prove that for a reaction, $A_g + B_g \rightarrow$ products, the rate constant is given by $k = \frac{k_bT}{h} K^{\#}$.

(30 marks)

b. Use the thermodynamics approach to prove that $k = \frac{k_bT}{h} e^{\Delta S^{\#}/R} e^{-E_a/RT}$. Following general thermodynamic relationships were given: $RTlnK = -\Delta G^o$; $\frac{dlnK}{dT} = \frac{\Delta U}{RT^2}$.

(40 marks)

c. The Arrhenius pre-exponential factor of a bimolecular reaction occurring at 350 ^{0}C is 8.0×10^{10} dm^{3}mol^{-1}s^{-1}. Calculate the entropy of activation.

(30 marks)

7.

a. State Fick's second law of diffusion. Define all terms therein. State all assumptions made.

(10 marks)

b. You are given two specimens of Pd, each of identical purity. Specimen A has a grain size of 3.091 μm; specimen B has a grain size of 441 μm. Which specimen will exhibit higher rate of diffusion of hydrogen through it? Explain the reason for your choice.

(20 marks)

c. The diffusion coefficient of O_2 in Si, D_0 has been measured to have following values:

D_0/ cm^2.s^{-1}	T /(^{0}C)
9.2×10^{-11}	1100
1.4×10^{-9}	1300

Show that in order to increase the value of D_0 by a factor x 10 greater than it is at 1300^{0}C would require raising the temperature above the melting point of Si (m.p. Si 1410^{0}C).

Make a crude estimate showing that it is feasible to remove oxygen from a silicon ribbon of thickness 0.1 μm by exposing the ribbon to vacuum for 10 minutes at a temperature of 1100°C.

(40 marks)

d. To increase its corrosion resistance, chromium (Cr) is diffused into steel at 980°C. If during diffusion the surface concentration of chromium remains constant at 100%, how long will it take (in days) to achieve a Cr concentration of 1.8% at a depth of 0.002 cm below the steel surface? ($D_o = 0.54\ \text{cm}^2/\text{s}$; $E_A = 286$ kJ/mol).

(30 marks)

8.

a. Briefly define following terms:

(i) Self diffusion (ii) Steady state diffusion (iii) Mass flux

b. State Fick's first law of diffusion. Define all terms therein.

c. There is a differential nitrogen pressure across a furnace wall made of steel measuring 2.22 mm in thickness. The concentration of nitrogen at the inner surface of the wall is held constant at 9.99 kg m^{-3}, while the concentration at the outer surface of the wall is held constant at 1.11 kg m^{-3}. The area of the wall is 3.33 m^2, and the diffusivity of nitrogen in steel at the furnace operating temperature is $D_N = 3.091 \times 10^{-10}\ m^2\ s^{-1}$. What is the total rate loss of nitrogen from the furnace at steady state? Express your answer in units of kg s^{-1}.

d. If the steel of the wall were replaced with another steel of the identical composition but with a grain size 10 x larger than that of the steel in part (c.), how would the loss of nitrogen from the furnace change? Explain.

(100 marks)

TABLE 2

The Error Function

z	erf(z)	z	erf(z)
0	0	0.85	0.7707
0.025	0.0282	0.90.	0.7970
0.05	0.0564	0.95	0.8209
0.10	0.1125	1.0	0.8427
0.15	0.1680	1.1	0.8802
0.20	0.2227	1.2	0.9103
0.25	0.2763	1.3	0.9340
0.30	0.3286	1.4	0.9523
0.35	0.3794	1.5	0.9661
0.40	0.4234	1.6	0.9763
0.45	0.4755	1.7	0.9838
0.50	0.5205	1.8	0.9891
0.55	0.5633	1.9	0.9928
0.60	0.6039	2.0	0.9953
0.65	0.6420	2.2	0.9981
0.70	0.6778	2.4	0.9993
0.75	0.7112	2.6	0.9998
0.80	0.7421	2.8	0.9999

SOURCE: The values of erf(z) to 15 places, in increments of z of 0.0001, can be found in the Mathematical Tables Project, "Table of Probability Functions . . .", vol. 1, Federal Works Agency, Works Projects Administration, New York, 1941. A discussion of the evaluation of erf(z), its derivatives and integrals, with a brief table is given by H. Carslaw and J. Jaeger, in Appendix 2 of "Conduction of Heat in Solids", Oxford University Press, Fair Lawn, NJ, 1959.

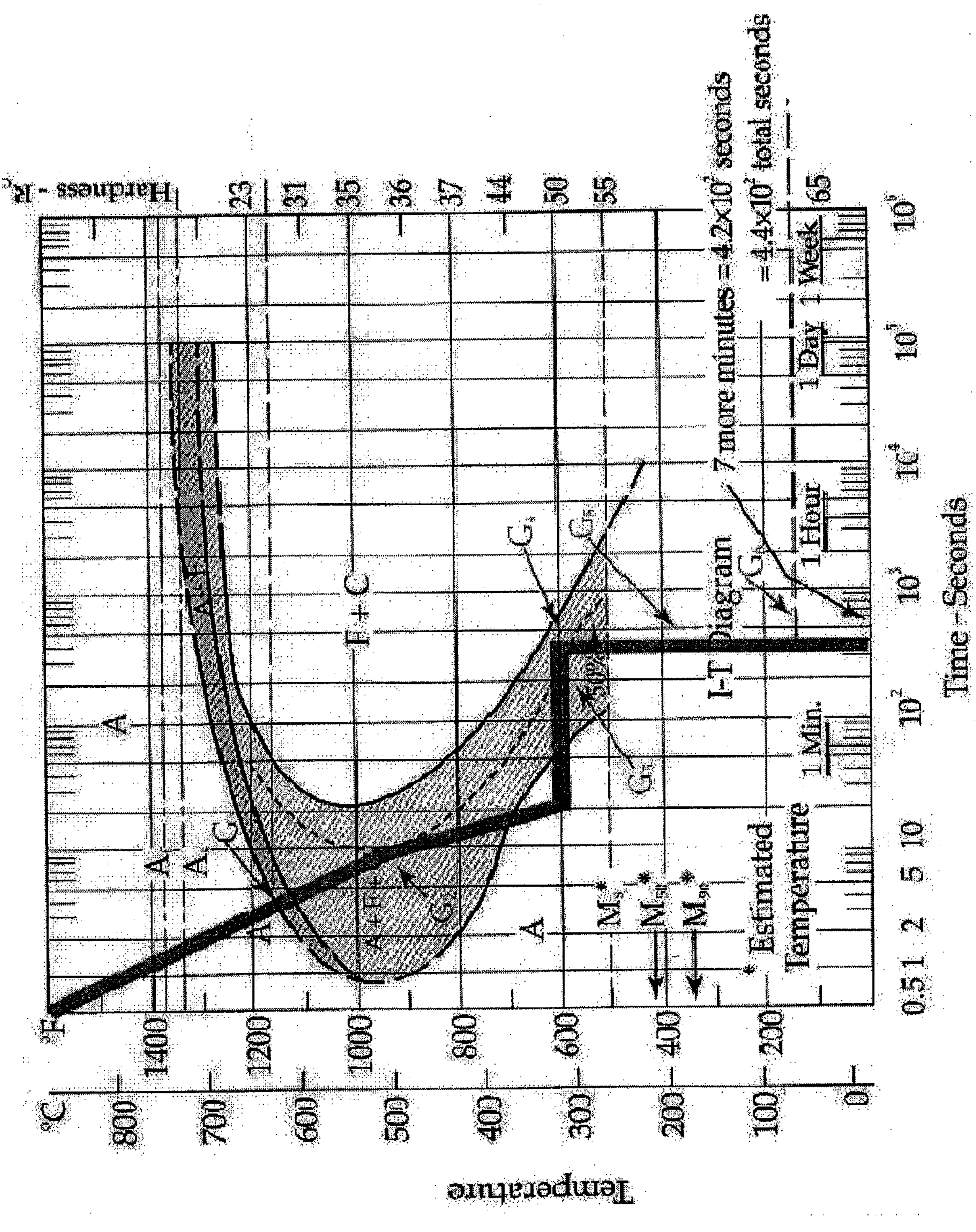
Temperature
°C
800
700
600
500
400
300
200
100
0
°F
1400
1200
1000
800
600
400
200
Hardness - R_c
23
31
35
36
37
44
50
55
65
A
A_1
A_3
A + F
A + F + C
F + C
A
C_s
C_f
50%
M_s*
M_50*
M_90*
* Estimated Temperature
I-T Diagram
7 more minutes = 4.2×10^2 seconds
= 4.4×10^2 total seconds
0.5 1 2 5 10
10^2
10^3
10^4
10^5
10^6
1 Min.
1 Hour
1 Day
1 Week
Time - Seconds

Fig. Q02