Uva Wellassa University, Sri Lanka
End Semester Examination – January 2010
SCT 331-3 Material Chemistry 1

Time: Three (03) hours

Total 09 Questions
Answer **02** questions from **Part-A** and **04** from **Part-B**

Universal gas constant $R = 8.314\ J\ K^{-1}mol^{-1}$
Boltzmann gas constant $k = 1.38 \times 10^{-23} J\ K^{-1}$
Velocity of light, $c = 2.99 \times 10^{10} cm\ s^{-1}$
Planck constant, $h = 6.626 \times 10^{-34} J\ s$ *and* $h/2\pi = 1.054 \times 10^{-34} Js$

PART - A

1) Construct and label the hypothetical phase diagram for metals A and B between room temperature (20 °C) and 700 °C given the following information:
   - The melting temperature of metal A is 480 °C.
   - The maximum solubility of B in A is 4 wt% B, which occurs at 420 °C.
   - The solubility of B in A at room temperature is 0 wt% B.
   - One eutectic occurs at 420 °C and 18 wt% B–82 wt% A.
   - A second eutectic occurs at 475 °C and 42 wt% B–58 wt% A.
   - The intermetallic compound A-B exists at a composition of 30 wt% B–70 wt% A, and melts congruently at 525 °C.
   - The melting temperature of metal B is 600 °C
   - The maximum solubility of A in B is 13 wt% A, which occurs at 475 °C.
   - The solubility of A in B at room temperature is 3 wt% A.

   i. What is the compound of A-B exists at 30 wt% B–70 wt% A?

   (20 marks)

   ii. If a A - B alloy of composition 30 wt% A –70 wt% B is slowly heated from a temperature of 20 °C,
      a. At what temperature does the first liquid phase form?
      b. What is the composition of this liquid phase?
      c. At what temperature does complete melting of the alloy occur?
      d. What is the composition of the last solid remaining prior to complete melting?

   (40 marks)

iii. Draw microstructures form for the alloy stated in (ii) above when it slowly heated from room temperature to 650°C.

(40 marks)

2) After austenizing eutectoid steel (shown in Fig Q2) at 800°C, is subjected to heat-treatments as listed below.

   i. Using the isothermal transformation diagram determine the microstructure of the sample after each heat-treatment.
      a. Quenched to 150°C.
      b. Quenched to 690°C and held there for 2 hr.
      c. Quenched to 610°C and held for 3 min.
      d. Quenched to 300°C and held there for 30 min.
      e. Quenched to 300°C and held there for 5 hr.

(50 marks)

   ii. It is necessary to create following microstructures using the eutectoid steel in (i). Give the required cooling rates and temperature data necessary for these processes.
      a. 100% martensite.
      b. 30% fine pearlite and 70% martensite.
      c. 100% fine pearlite.
      d. 50% fine pearlite and 50% bainite.
      e. 50% bainite and 50% martensite.

(50 marks)

3) Consider the continuous cooling transformation of eutectoid steel, Fig Q3.

   i. State the product(s) that would be obtained at the end of each of the following process carried out on fully annealed steel at 760°C cooled at the rate of
      a. 1°C/min for 1 hr, and then quenched to 20°C.
      b. 2.5°C/min for 1 hr, and then quenched to 20°C.
      c. 20°C/s up to a temperature of 600°C and then quenched to 0°C.
      d. 150°C/s for 5 s, then maintained at a constant temperature for 1 min; then reheated to 300°C for very long time.

(40 marks)

   ii. Discuss the effect of the microstructure on the hardness of the material.

(30 marks)

   iii. Explain how you can determine the hardness of a 1060 steel specimen considering its history of heat-treatment and the industrial isothermal transformation diagram.

(30 marks)

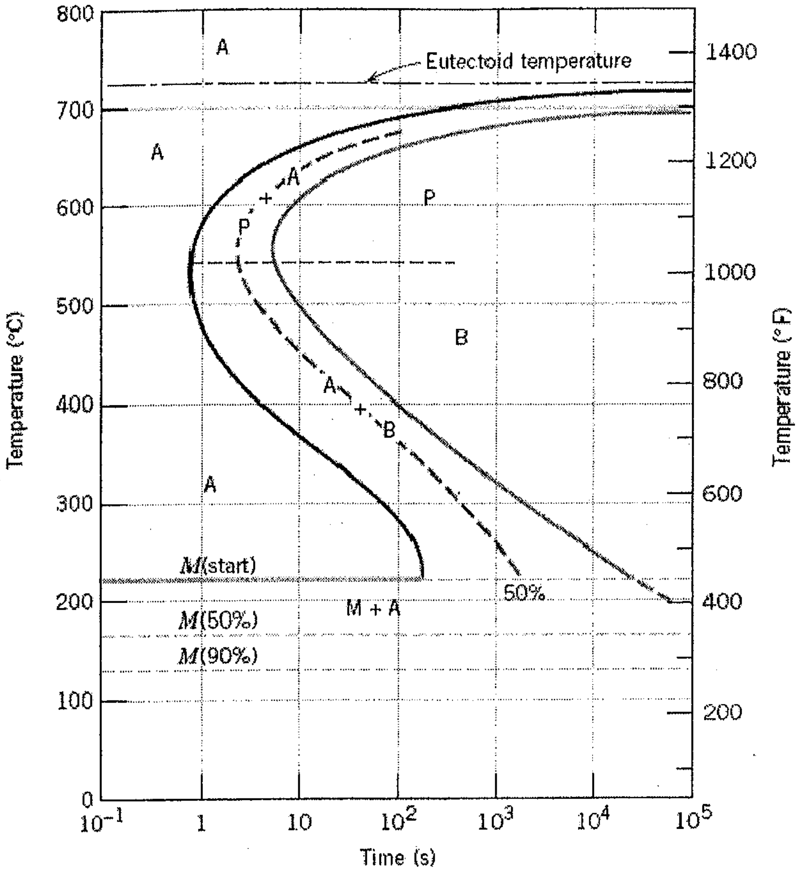
800
700
600
500
400
300
200
100
0
Temperature (°C)
1400
1200
1000
800
600
400
200
Temperature (°F)
A
Eutectoid temperature
A
P
A + P
P
B
A + B
A
M(start)
M(50%)
M(90%)
M + A
50%
10^{-1}
1
10
10^2
10^3
10^4
10^5
Time (s)

Fig Q2

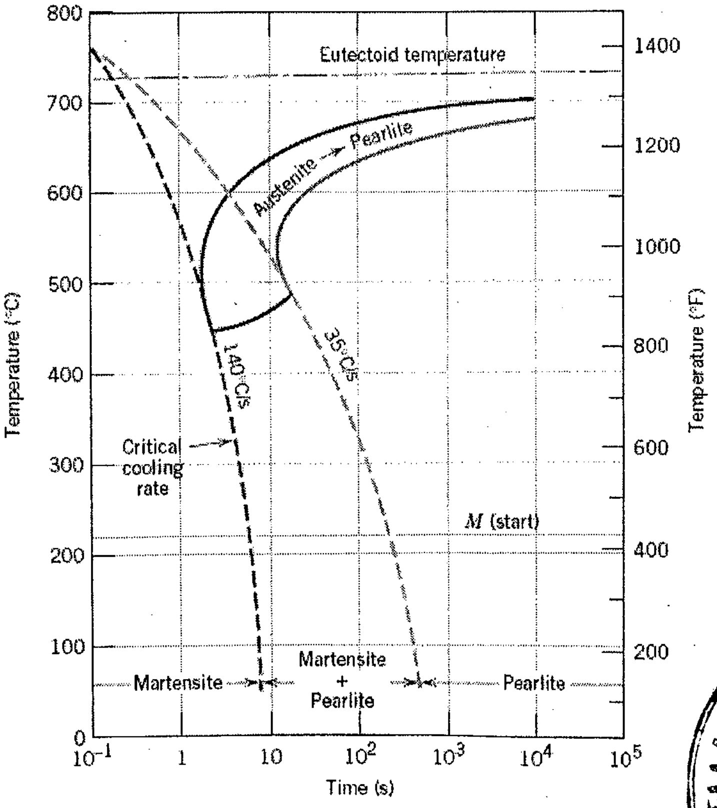
800
700
600
500
400
300
200
100
0
Temperature (°C)
1400
1200
1000
800
600
400
200
Temperature (°F)
Eutectoid temperature
Austenite → Pearlite
140°C/s
35°C/s
Critical cooling rate
M (start)
Martensite
Martensite + Pearlite
Pearlite
10^{-1}
1
10
10^2
10^3
10^4
10^5
Time (s)

Fig Q3

PART - B

4)

i. Define reduced variables of a given gas.

(15 marks)

ii. State the principle of corresponding states of a real gas.

(20 marks)

iii. The van der Waals equation of a gas is given as,

$$p = \frac{RT}{V_m - b} - \frac{a}{V_m^2}.$$

Define the meaning of symbols stated therein. Relate the V, P and T at the critical state to van der Waals parameters.

(50 marks)

iv. The critical constants of ethane are $p_c = 48.20$ atm, $V_c = 148$ cm^3 mol^{-1}, and $T_c = 305.4$ K. Calculate the van der Waals parameters of the gas and estimate the radius of the molecules (assume gas molecules are spherical in shape).

(15 marks)

5)

i. According to Maxwell's theory, the speed distribution of gas molecules is given as

$$f(v) = 4\pi\left(\frac{M}{2\pi RT}\right)v^2 e^{-\frac{Mv^2}{2RT}}$$

Identify all symbols given in. State the physical meaning of following terms. Whenever possible evaluate them:

(*i*). $\int_0^{\infty} v f(v)dv$ (ii). $vf(v)dv$ (iii). $\int_0^{\infty} f(v)dv$

(20 marks)

ii. According to transition state theory, the rate constant, *k* of the reaction

$$A_g + B_g \rightarrow C_g$$

is expressed a;

$$k = \frac{k_b T}{h}\frac{Q^{\#}}{Q_A Q_B}e^{\frac{-E_a}{RT}}$$

Define all terms therein. The value of $\Delta S^{\#}$ for a reaction has been obtained as -80.5 J K^{-1} mol^{-1} at 400°C. Find the value of exponential factor (A).

(30 marks)

iii. Define following terms:

a. Number density (N)
b. Collision frequency (z)

c. Mean free path (λ)

d. Prove that the collision density of identical particles in gaseous state is $z = \sqrt{2}N\sigma_0\bar{c}$. All symbols carry standard meanings.

(20 marks)

iv. Based on collision theory, for unlike molecules the rate of a reaction (in gas state) is given as,

$$\text{the rate} = p\left(\frac{8\,(k_bT}{\mu}\right)^{\frac{1}{2}} d_{AB}^2 n_A n_B e^{\frac{-Ea}{RT}}$$

Deduce an expression for reaction rate when molecules are similar. State the units of the rate expression clearly.

(30 marks)

6)

i. Which of the following molecules show infrared activity?

a. H_2O

b. CO_2

c. O_2

(10 marks)

ii. What are the gross and specific selections rules of harmonic and anharmonic oscillators. In vibrational spectroscopy define fundamental and overtone frequencies.

(10 marks)

iii. The form of the anharmonic Morse potential is $V(x) = D(1 - \exp(-\beta x^{\dagger}2)$. The Morse energy eigen values are given by

$$E_v = \breve{\upsilon}\left(1+\frac{1}{2}\right) - \breve{\upsilon}\breve{x}\left(1+\frac{1}{2}\right)^2 \qquad (\breve{x} \geq 0).$$

Draw the harmonic potential on the left and a Morse potential on the right. Draw and label horizontal lines for the energy levels of both harmonic oscillator and Morse potential for the quantum numbers $v = 0, 1, 2,$ and 3 comparing relative energies for a given quantum number.

(20 marks)

iv. Consider the IR spectrum of CO given below (Fig Q6). From the wave number measurements on the spectrum assign the spectrum, hence determine harmonic frequency and anharmonicity constant (in cm⁻¹). Estimate the bond dissociation for this molecule (hint: identify the fundamental and first overtone from the spectrum).

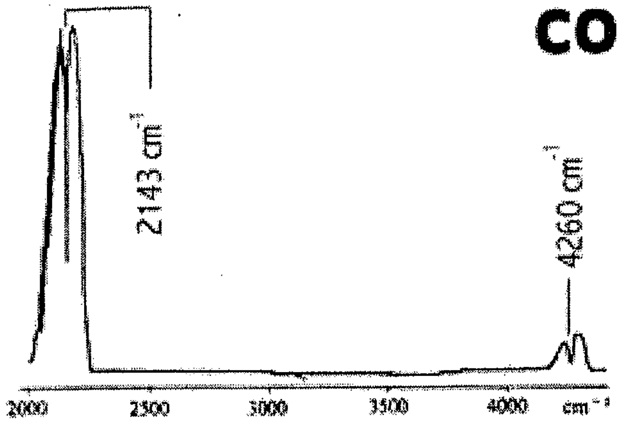

Fig Q6

(60 marks)

7)

i. What is diffusion? Explain briefly the vacancy diffusion. How it differs from self diffusion.

(25 marks)

ii. What is Debye frequency of diffusion? Generally, the activation energy of diffusion (Q) is divided into two parts, i.e. the enthalpy of vacancy formation (ΔH_v) and the enthalpy of atoms migration (ΔH_m) $Q = \Delta H_v + \Delta H_m$. Why the ΔH_v term is zero in interstitial diffusion?

(25 marks)

iii. Write Fick's first law of diffusion of mass transfer and identify all terms therein. Define the heat and current fluxes and relate them in analogous manner to Fick's first law.

(25 marks)

iv. Determine the rate at which helium (He) held at 5 atm. and 200°C in a Pyrex glass bulb of 50 cm diameter and a wall thickness of 0.1 cm, diffuse through the Pyrex to outside ($D = 1 \times 10^{-9}$ cm^2 s/atm.).

(25 marks)

8)

i. Explain briefly steady state and non-steady state diffusion.

(10 marks)

ii. State Fick's 2nd law of diffusion. Identify all terms therein.

(20 marks)

iii. A solution to the Fick's 2nd law is given as

$$\frac{C}{C_s} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right).$$

State the initial and boundary conditions assumed to validate this solution.

(30 marks)

iv. Ga is diffused into a thick slice of silicon at a temperature of 1100°C for three (3) hours. What is, after that time, the Ga concentration (Ga/cm^3) at a depth of:

(a) 1×10^{-4} cm and
(b) 3×10^{-4} cm?
(A constant Ga source is used at the surface,
$C_o = 1018/\text{cm}^3$; $D_{1100°C} = 7 \times 10^{-13}$ cm^2/s.)

(40 marks)

9)

i. Provide a typical energy corresponding to the lowest energy quantum transitions from the ground state to the first excited state for the following molecular processes. Clearly state units, using the same units for all four processes.

a. electronic transition
b. rotational transition
c. vibrational transition

(25 marks)

ii. Which molecules below can absorb or emit microwave radiation?
a. C_6H_6
b. H_2O
c. HCN
d. SF_6
e. CH_3Cl

(25 marks)

iii. Categorize each of the molecules above as belonging to one of the rotor types in the list below.
a. Linear
b. Symmetric (prolate and oblate)
c. Spherical
d. Asymmetric

(25 marks)

iv. The rotational constant of $^{12}C^{16}O_2$ is 0.39021 cm^{-1}. Calculate the bond length of the molecule ($m(^{12}C)$ = 12 u exactly, $m(^{16}O)$ = 15.9949 u).

(25 marks)

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The Error Function

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