UNIVERSITI SAINS MALAYSIA

First Semester Examination
Academic Session 2009/2010

November 2009

EBB 236/3 - Materials Thermodynamics
[Termodinamik Bahan]

Duration : 3 hours
[Masa : 3 jam]

Please ensure that this examination paper contains EIGHT printed pages before you begin the examination.
[Sila pastikan bahawa kertas peperiksaan ini mengandungi LAPAN muka surat yang bercetak sebelum anda memulakan peperiksaan ini.]

This paper consists of SEVEN questions. ONE question in PART A, THREE questions in PART B and THREE questions in PART C.
[Kertas soalan ini mengandungi TUJUH soalan. SATU soalan di BAHAGIAN A, TIGA soalan di BAHAGIAN B dan TIGA soalan di BAHAGIAN C.]

Instruction: Answer **FIVE** questions. Answer **ALL** questions from PART A, **TWO** questions from PART B and **TWO** questions from PART C. If candidate answers more than five questions only the first five questions answered in the answer script would be examined.
*[**Arahan**: Jawab **LIMA** soalan. Jawab **SEMUA** soalan dari BAHAGIAN A, **DUA** soalan dari BAHAGIAN B dan **DUA** soalan dari BAHAGIAN C. Jika calon menjawab lebih daripada lima soalan hanya lima soalan pertama mengikut susunan dalam skrip jawapan akan diberi markah.]*

The answers to all questions must start on a new page.
[Mulakan jawapan anda untuk semua soalan pada muka surat yang baru.]

You may answer a question either in Bahasa Malaysia or in English.
[Anda dibenarkan menjawab soalan sama ada dalam Bahasa Malaysia atau Bahasa Inggeris.]

In the event of any discrepancies, the English version shall be used.
[Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah diguna pakai.]

PART A

BAHAGIAN A

1. [a] Assuming that the pressure dependence of the transformation temperatures can be neglected below one atmosphere, calculate the pressure at the triple point (α, γ, G), (γ, δ, G) and (δ, L, G) for pure iron. Assume also that all heats of transformation are temperature independent. For iron T_v = 3008 K, T_m = 1808 K, $T^{\alpha\gamma}$ = 1180 K, $T^{\gamma\delta}$ = 1673 K. Corresponding heats of transformation are respectively 354.1, 16.15, 0.91 and 0.63 (KJ/gm atom).

Andaikan kesandaran suhu transformasi terhadap tekanan diabaikan di bawah satu atmosfera, kirakan tekanan pada titik triple (α, γ, G), (γ, δ, G) dan (δ, L, G) untuk ferum tulen. Juga andaikan semua haba transformasi adalah tak bersandar kepada suhu. Untuk Ferum T_v = 3008 K, T_m = 1808 K, $T^{\alpha\gamma}$ = 1180 K, $T^{\gamma\delta}$ = 1673 K. Haba transformasi yang bersepadanan masing-masing adalah 354.1, 16.51, 0.91 dan 0.63 (KJ/gm atom).

(50 marks/*markah*)

[b] Prove that the change in entropy of a system undergoing a thermodynamic change is always positive.

Buktikan perubahan entropi sesuatu sistem yang mengalami perubahan termodinamik adalah sentiasa positif.

(20 marks/*markah*)

[c] Consider the nucleation of bubbles of CO gas in a liquid steel melt. Mathematically show why the nucleation starts at the interface between the steel and the container rather than in the melt itself.

Anggap penukleusan gelombang gas CO di dalam cecair leburan keluli. Secara matematik tunjukkan mengapa penukleusan bermula pada antaramuka keluli dan bekas berbanding dengan leburan tersebut.

(30 marks/*markah*)

…3/-

PART B

BAHAGIAN B

2. [a] Derive the expression for a spherical nucleus of critical size and the free energy of formation of such a nucleus in a vapour-liquid transformation.

Terbitkan ungkapan bagi nukleus sfera yang bersaiz kritikal dan tenaga bebas pembentukan sesuatu nukleus dalam perubahan gas-cecair.

(40 marks/*markah*)

[b] In the solidification of aluminium by homogeneous nucleation, the undercooling required is 60K in a specific case. Assume γ_{SL} to be 0.034J/m^2, v = 10^{12}/s, the factor (s*pd) is estimated at 10^{28}/m^3 and neglect activation energy for the activated complex. ΔH for solidification of aluminium = 4 x 10^5 J/kg. Specific gravity of liquid aluminium is 2.4. The melting point T_m = 931.7 K and k = 1.38x10^{-23} J/K.

(i) Find the bulk energy change and the free energy change for the critical nucleus, in joules per m^3.

(ii) Find the rate of nucleation in nuclei/s/m^3.

Dalam pemejalan aluminium melalui nukleasi seragam, penyejukan yang diperlukan dalam kes tertentu adalah 60K. Andaikan γ_{SL} adalah 0.034 J/m^2, v = 10^{12}/s, faktor (s*pd) ditaksirkan pada 10^{28}/m^3 dan tenaga pengaktifan bagi kompleks-teraktif diabaikan. ΔH bagi pemejalan aluminium = 4 x 10^5 J/kg. Spesifik graviti bagi cecair aluminium adalah 2.4. Takat lebur T_m = 931.7 K dan k = 1.38x10^{-23} J/K.

(i) Kirakan perubahan tenaga pukal dan perubahan tenaga bebas bagi nukleus kritikal, dalam joule per m^3.

(ii) Kirakan kadar penukleusan dalam nuklei/s/m^3.

(60 marks/*markah*)

3. [a] What is divacancy? How can the number of divacancies in a crystal be approximately estimated?

Apakah maksud dwikekosongan? Bagaimana bilangan dwikekosongan di dalam sesuatu hablur dianggarkan?

(30 marks/*markah*)

[b] Beryllium Oxide (BeO) is known to have Schottky defect,

(i) Write an equation to express the formation of Schottky defect in BeO using Kronger-Vink notation.

(ii) Calculate cation vacancy concentration in vacancy/cm^3.

(iii) A sample of BeO is consisting of 0.01 mol% soluble Li_2O. Calculate the vacancy fraction of anion sites with assumption the beryllium lattice sites are replaced by litium ion.

(iv) Calculate cation vacancy concentration in vacancy/cm^3.

Given

$\rho_{BeO} = 3.02$

$\Delta H_{s(BeO)} = 6$ eV

Exp $(\Delta S_{s(BeO)} K^{-1}) = 100$

Beryllium Oksida diketahui membentuk kecacatan Schottky.

(i) Tuliskan persamaan untuk pembentukan cacat Schottky dalam BeO menggunakan tatatanda Kronger-Vink.

(ii) Kirakan kepekatan kekosongan kation dalam sebutan kekososngan/cm^3.

(iii) Sampel BeO mangandungi 0.01 mol% Li_2O terlarut. Kirakan pecahan tapak anion yang kosong dengan andaian tapak kekisi beryllium digantikan oleh ion litium.

(iv) Kirakan kepekatan kekosongan kation dalam sebutan kekosongan/cm^3.

Diberi

$\rho_{BeO} = 3.02$

$\Delta H_{s(BeO)} = 6$ *eV*

Exp $(\Delta S_{s(BeO)} K^{-1}) = 100$

(70 marks/*markah*)

…5/-

4. [a] Below the triple point (-56.2^{o}C) the vapour pressure of solid CO_2 is given by

$$\ln P\ (atm) = -3116/T + 16.01$$

The heat of fusion is 8330J/mole. What is the heat of sublimation and the heat of evaporation?

Di bawah takat triple (-56.2^{o}C) tekanan wap bagi CO_2 pepejal diberi sebagai

$$\ln P\ (atm) = -3116/T + 16.01$$

Haba lakuran ialah 8330J/mole. Apakah haba pemejalwapan dan haba penyejatan?

(25 marks/*markah*)

[b] What is the pressure at the triple point?

Apakah tekanan pada takat triple?

(25 marks/*markah*)

[c] What would be the vapour pressure of liquid CO_2 at 298K?

Apakah tekanan wap CO_2 pada 298K?

(25 marks/*markah*)

[d] Draw a sketch of the system and state why solid CO_2 on a laboratory bench evaporates rather than melts.

Lakarkan gambarajah fasa sistem ini dan nyatakan sebab mengapa CO_2 pepejal, di meja makmal mengalami pemejalwapan bukan peleburan.

(25 marks/*markah*)

PART C

BAHAGIAN C

5. [a] What is Ellingham's diagram and its principle of construction? How can such a diagram be used to compare the relative possibility of occurrence between two chemical reactions in a particular system? Point out the major limitations of this diagram.

Apakah gambarajah Ellingham dan prinsip-prinsip pembinaannya? Bagaimana gambarajah sebegini dapat digunakan untuk membandingkan kemungkinan relatif kejadian antara dua tindakbalas kimia dalam sesebuah sistem? Senaraikan had-had major gambarajah ini.

(50 marks/*markah*)

[b] Consider the following chemical reaction indicating the oxidation of pure nickel:

$$<Ni> + (H_2O) = <NiO> + H_2$$

Is it possible to anneal pure Ni sheet at 750^oC in an atmosphere containing a mixture of 90%H_2O and 10%H_2 by volume without oxidation? Given that:

$$<Ni> + \frac{1}{2}(O_2) = <NiO>, \qquad \Delta G^o = -58{,}450 + 23.55T \text{ cal}$$

$$(H_2) + \frac{1}{2}(O_2) = (H_2O), \qquad \Delta G^o = -58{,}900 + 13.1T \text{ cal}$$

Pertimbangkan tindakbalas kimia berikut menunjukkan proses pengoksidaan nikel asli:

$$<Ni> + (H_2O) = <NiO> + H_2$$

Adakah mustahil bagi menyepuhlindap kepingan asli Ni pada suhu 750^oC dalam atmosfera yang mengandungi campuran isipadu 90% H_2O dan 10% H_2 tanpa pengoksidaan. Diberikan:

$$<Ni> + \frac{1}{2}(O_2) = <NiO>, \qquad \Delta G^o = -58{,}450 + 23.55T \text{ cal}$$

$$(H_2) + \frac{1}{2}(O_2) = (H_2O), \qquad \Delta G^o = -58{,}900 + 13.1T \text{ cal}$$

(50 marks/*markah*)

6. [a] What is a regular solution? How do you check the regularity of a solution?

Apakah persamaan biasa? Bagaimana anda memastikan kebiasaan persamaan?

(40 marks/*markah*)

[b] Derive Sievert's Law and briefly discuss its major applications.

Terbitkan Hukum Sievert dan terangkan dengan ringkas tentang aplikasi utamanya.

(30 marks/*markah*)

[c] While making liquid steel in a steel plant, the steel at 1600^{o}C comes in contact with open atmosphere leading to oxygen absorption of 0.001%. How can this steel be degassed by controlling the atmosphere in contact with its top surface to bring down the oxygen content to 0.0005%?

Apabila menghasilkan cecair keluli dalam sesebuah loji keluli tersebut pada 1600^{o}C akan terdedah pada atmosfera terbuka dan menyebabkan berlakunya penyerapan oksigen pada 0.001%. Bagaimana keluli ini boleh dinyahgas melalui pengawalan atmosfera yang bersentuhan dengan permukaan atas dengan menurunkan kandungan oksigen kepada 0.0005%.

(30 marks/*markah*)

7. [a] Discuss the criteria of spontaneity based on entropy and free energy of a thermodynamic system.

Bincangkan kriteria kespontanan berdasarkan entropi dan tenaga bebas sistem termodinamik.

(40 marks/*markah*)

[b] Droplets of gold are observed to supercool by a maximum amount of 230°C. What is the entropy change associated with the isothermal solidification of 1 g-atom of supercooled gold? Given that, $C_{P,<Au>}$ = 5.0 cal/deg/mole, $C_{P,\{Au\}}$ = 7.0 cal/deg/mole, Melting point of Au = 1063°C, Heat of fusion of Au, ΔH_f = 3050 cal/mole.

Titisan emas diperhatikan menyejuk dengan jumlah maksimum pada suhu 230°C. Apakah perubahan entropi dihubungkait dengan pemejalan isotermal 1 g atom emas yang disejuklampau? Diberikan $C_{P,<Au>}$ *= 5.0 cal/deg/mol,* $C_{P,\{Au\}}$ *= 7.0 cal/deg/mol, Takat lebur Au = 1063°C, Haba Au,* ΔH_f *= 3050 cal/mol.*

(60 marks/*markah*)

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