Uva Wellassa University, Sri Lanka
Faculty of Science and Technology
Science and Technology Degree Programme
1st Semester Examination – March / April 2013

Uva Wellassa University

SCT 351-3 Materials Physics

Instructions to candidates

Number of questions: Six (06)
Time: Three (03) hours
Answer four (04) questions only
Total marks allocated: 400

Planck's constant = 6.626×10^{-34} J s^{-1}

Speed of light = 2.998×10^{8} m s^{-1}

Charge of an electron = 1.602×10^{-19} C

Mass of an electron = 9.109×10^{-34} kg

Faraday Constant = 96487 C mol^{-1}

1 amu = 1.66×10^{-27} kg

Universal gas constant = 8.314 J K^{-1} mol^{-1}

1. a.

   i. The volume of n moles of a perfect gas changes from V_1 to V_2 when it undergoes a reversible, isothermal expansion at temperature T. Derive an expression for the entropy change. (15 mark)

   ii. Derive an expression for the change in entropy for isothermal mixing of two inert perfect gases, A and B respectively, at the same temperature (T) and pressure (P) in terms of the number of moles (n_A and n_B) and mole fractions (X_A and X_B) of the gases. (20 mark)

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iii. A container of volume 5.0 ℓ is divided into two compartments of equal size. In the left compartment there is nitrogen at 1.0×10^5 N m^{-2} and 25 ºC, and in the right compartment there is hydrogen at the same temperature and pressure. Calculate the change in entropy when the partition is removed. State any assumptions you made in the calculation. (15 mark)

b.

i. Starting from the first law of thermodynamics, derive the Maxwell's relations,

$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$ and $\left(\frac{\partial V}{\partial T}\right)_P = -\left(\frac{\partial S}{\partial P}\right)_T$ for a closed system with PV work only. (15 mark)

ii. Using Maxwell relations, obtain an expression for volume dependence of entropy for a perfect gas. (20 mark)

iii. Give definitions for C_v and C_p. Using the definitions, show that the difference of C_p and C_v equals to nR. (15 mark)

2. a.

i. Briefly explain the following.

(I). Phase equilibrium

(II). Reaction equilibrium (20 mark)

ii. Starting from the thermodynamic definition of chemical potential, show that the flow of matter takes place from a place with a higher chemical potential to a place with a lower chemical potential. (30 mark)

b.

i. Two moles of an ideal mono atomic gas ($C_{v,m} = 3R/2$, $C_{p,m} = 5R/2$), at 300 K and 6 atm initially, undergo a reversible adiabatic expansion to half of its initial pressure. Calculate q, ΔT, ΔU, ΔH and work done for this process. (35 mark)

ii. What would be the entropy change you expect for a spontaneous natural process? Why? (15 mark)

3. a. The wave function of an electron in the ground state of a hydrogen atom is given by

$$\Psi = \left(\frac{1}{\pi\, a_o{}^3}\right)^{1/2} e^{-r/a_o}$$

Where a_o is a constant and r is the distance from the nucleus.

i. Write an equation for the probability density. What is the location with maximum probability? (15 mark)

ii. What is the probability of finding the electron in a volume element δ_V which is small even on the scale of the atom? (10 mark)

iii. Find the mean potential energy and the mean kinetic energy of the electron in terms of a_o, its charge, e, and mass, m_e.

$\left\{ \text{You may use, } \int_0^\infty x^n\ e^{-ax} = \frac{n!}{a^{n+1}} \right\}$ (35 mark)

b.

i. Obtain an expression for the average linear momentum of a particle described by the wave function e^{ikx}.

(30 mark)

ii. Calculate the probability that a particle will be found between 0.49 ℓ and 0.51 ℓ in a box of length, ℓ when it is in

I. ground state n= 1 level
II. first excited state n= 2 level (10 mark)

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4. a.

i. Write down the Schrödinger equation for a particle in two-dimensional box described below.

$V = 0, \quad 0 \le y \le L$

$V = \infty \quad$ elsewhere

(5 mark)

ii. Derive the expressions for the wave function and the energy for a particle of mass 'm' which is confined in the above mentioned potential box. Clearly state the boundary conditions.

(35 mark)

iii. Calculate the percentage change in energy, in a given energy level of a particle in an infinite potential box when the length of the cube is decreased by 15%.

(15 mark)

b.

i. Assuming that the vibrations of a $^{35}Cl_2$ molecule are equivalent to those of a harmonic oscillator with a force constant k= 329 N m^{-1}, find the zero point energy of vibration of this molecule. The mass of a ^{35} Cl atom is 34.9688 amu.

(10 mark)

ii. Compare the following briefly.

I. Translational motion of a particle

II. Vibration motion of a particle

(05 mark)

iii. Calculate the wave length of a photon required to excite a transition between neighboring energy levels of a harmonic oscillator of mass equal to that of an oxygen atom (16.0 amu) and force constant 544 N m^{-1}.

(20 mark)

iv. Write down the canonical partition function Z, of a pure ideal gas of N- molecules in terms of its molecular partition function q.

(1[illegible]

5. a.

i. Write the Boltzmann distribution law for non interacting particles in terms of the partition function. Define all the terms in it.

(05 mark)

ii. Use the Boltzmann law to indicate that the relative population of an upper state with energy E_2, decreases exponentially with its energy above the lower state which has an energy E_1.

(25 mark)

iii. The boat conformation of cyclohexane lies 22 kJ mol^{-1} higher in energy than the chair conformation. Find the relative populations of two conformations in a sample of cyclohexane at 20 °C.

(20 mark)

b.

i. Calculate the partition function for cyclohexane molecule confining attention to the chair and boat conformations mentioned in above (a) (iii) at 0 °C and at 20 °C. Comment on your results. Take the energy of the lowest state to be zero.

(15 mark)

ii. Show that the internal energy (U) of a system is related to the canonical partition function (Z) by $\boldsymbol{U = kT^2\left(\frac{\partial \ln Z}{\partial T}\right)_{V,N}}$

(15 mark)

iii. The translational partition function for a molecule of mass 'm' confined in a flask of volume V at a temperature T is given by $\boldsymbol{Z = \frac{(2\pi m k T)^{3/2}}{h^3} V}$. Using the equation in (b) (ii) above, show that the molar internal energy is given by $\boldsymbol{\frac{3}{2} kT}$.

(20 mark)

6. a.

i. Briefly explain the energy band theory of single crystal materials indicating the energy band splitting, and the formation of allowed and forbidden bands.

(25 mark)

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ii. Using your answer above indicate what is meant by the valence band and the conduction band?

(05 mark)

iii. The electronic configuration of an element 'X' which results in an n atomic crystal was found to be [core electrons] $4s^2$ $4p^1$. Find the number of energy levels, number of electrons in terms of n (only considering the valence electrons), for the whole crystal.
Hence deduce an expression for the number of energy levels filled in the crystal composed of *n* number of X atoms.

(20 mark)

b.

i. Illustrate the variation of Fermi Dirac Probability function with energy at
T= 0 K, for
(I). energy greater than the Fermi Energy
(II). Energy lower than the Fermi Energy

(20 mark)

ii. Using the answer provided for part (b) (i), give a value for the probability of the Fermi level being occupied by an electron at T= 0K.

(05 mark)

iii.

I. State differences between intrinsic & extrinsic semiconductors.

(05 mark)

II. Describe how free electrons and holes are generated in p type and n type semiconductor materials, using energy levels of conduction band, valence band and the donor atom energy levels.

(20 mark)