

Part II

Answer FIVE (05) Questions only.

Answer at least 01 (ONE) question from each of the parts A, B and C.

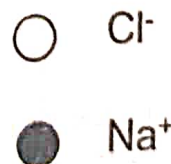
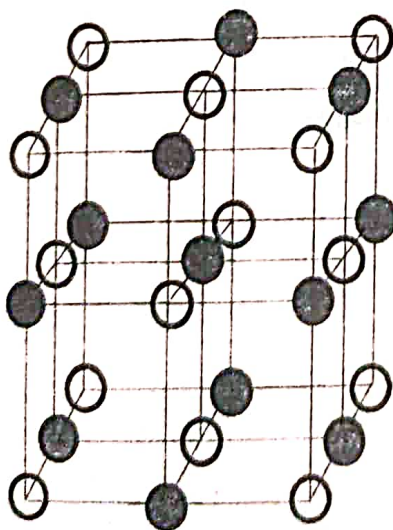
(All symbols have their usual meaning)

Planck's constant ( $h$ ) =  $6.626 \times 10^{-34}$  Js  
Avogadro's number ( $N_A$ ) =  $6.022 \times 10^{23}$   
Speed of light ( $c$ ) =  $3 \times 10^8$  ms<sup>-1</sup>  
1 eV =  $1.602 \times 10^{-19}$  J

Boltzmann constant ( $k_B$ ) =  $1.38 \times 10^{-23}$  JK<sup>-1</sup>  
Mass of an electron ( $m_e$ ) =  $9.1 \times 10^{-31}$  kg  
Rydberg constant ( $R$ ) =  $2.2 \times 10^{18}$  J  
1 a.m.u =  $1.66 \times 10^{-27}$  kg

PART A

- 1.
- (a) What is meant by the atomic packing fraction (APF)?
- (b) Sketch of a NaCl crystal is shown below. Show that a unit cell of NaCl contains 4 ions each of Na<sup>+</sup> and Cl<sup>-</sup>.



(c) Calculate the packing efficiency and density of NaCl using following data.

Radius of sodium ion =  $0.98 \text{ \AA}$

Radius of chlorine ion =  $1.81 \text{ \AA}$

Atomic mass of sodium = 22.99 a.m.u

Atomic mass of chlorine = 35.45 a.m.u

Lattice constant of the unit cell =  $5.58 \text{ \AA}$

(d) An X-ray beam of wavelength  $0.71 \text{ \AA}$  is diffracted by a cubic NaCl crystal. Calculate interplaner spacing for (200) planes and the glancing angle for second order Bragg reflection from these planes.

2.

(a) What are the basic types of crystal defects?

(b) Explain, briefly, Schottky and Frenkel defects.

(c) Derive an expression for the concentration of vacancies at equilibrium in a crystal having Schottky defect. Show that the concentration of vacancies increases as the temperature increases.

(d) The energy of formation of one vacancy by removing a copper atom from its lattice site and placing the same on the surface of the crystal is 0.7 eV. Find concentrations of vacancies at equilibrium at temperatures 300 K and 1250 K. Hence prove that the above statement in part (c).

3.

(a) Electrical conductivity of a metal is given by

$$\sigma = \frac{ne^2\tau}{m_e}$$

Where  $\tau$  - relaxation time of electrons  
 $e$  - charge of the electron  
 $n$  - mobile carrier density  
 $m_e$  - mass of the electron

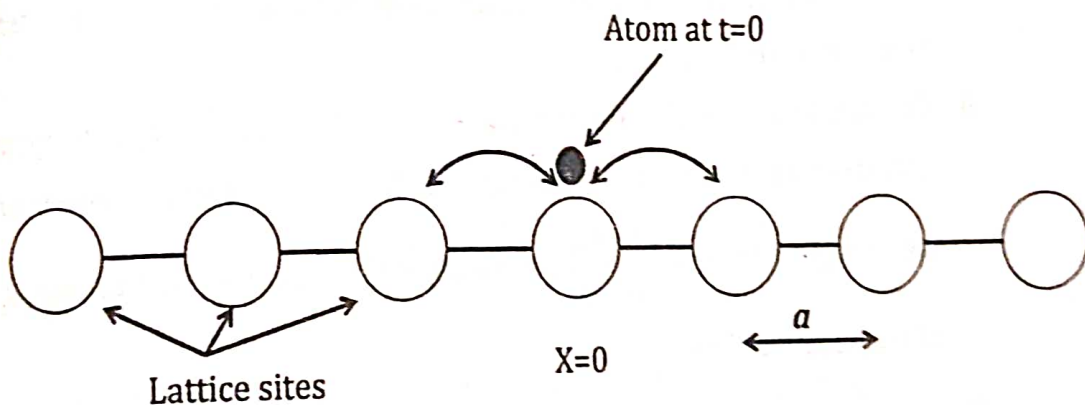
Use law of equipartition energy to show that the electrical conductivity is inversely proportional to the square root of the absolute temperature.

(b) A sample of Cadmium Sulfide displays a mobile carrier density of  $10^{16} \text{ cm}^{-3}$  and a mobility coefficient  $\mu = 10^2 \text{ cm}^2/\text{Volt sec}$ .

- (i) Calculate the electrical conductivity of this sample.
- (ii) If charge carriers have an effective mass equivalent to 10% of the mass of a free electron, what is the average time between successive scatterings?
- (iii) Calculate mean free path of mobile carriers at room temperature,  $27^\circ\text{C}$ .

### PART B

As shown in the figure below there exists a one-dimensional lattice with lattice constant  $a$ . An atom in the lattice transits from one site to a nearest-neighbor site in every second. The probability of transiting to the right and left sides are  $p$  and  $q(=1-p)$  respectively.



(a) Write down an expression for the probability of making  $n_1$  transition to right by making  $N$  total transitions.

(b) Calculate the mean number of transition to right.

(c) If  $p = 0.7$  and  $a = 20 \text{ nm}$ , calculate the average position ( $\bar{x}$ ) of the atom after 20 total transitions.

(d) The dispersion of  $n_1$  after  $N$  total transitions is given by  $Npq$ . By using it find the dispersion of position  $\overline{(\Delta x)^2}$  of the atom after 20 total transitions.



5. The energy levels of a rigid rotator is given by  $\epsilon_j = \frac{j(j+1)h^2}{8\pi^2 ma^2}$  where  $j=0,1,2,3,\dots$ . The degeneracy of each level is given by  $g_j = (2j+1)$ . Here  $m$  and  $a$  are constants with dimensions of mass and distance respectively.

(a) Write down the partition function ( $Z$ ) for the rigid rotator.

(b) Assume that at high temperatures the sum can be approximated by an integral. Show that

$$Z \approx \frac{8\pi^2 ma^2}{h^2 \beta}$$

(c) Obtain mean energy ( $\bar{U}$ ) and the heat capacity ( $C_V$ ) at high temperature and discuss the results.

(d) Show that at very low temperatures  $Z$  can be approximated as  $Z \approx 1 + 3e^{\frac{-2h^2}{8\pi^2 ma^2 kT}}$  and

$$C_V \propto \frac{e^{\frac{-2\theta}{T}}}{T^2} \quad \text{Here } \theta \text{ is a constant.}$$

6.

(a) Write down the differences among Maxwell-Boltzmann (MB), Bose-Einstein (BE) and Fermi-Dirac (FD) statistics.

(b) Consider a gas of  $N$  identical particles in volume  $V$  in equilibrium at temperature  $T$ . By neglecting the interaction between particles show that the average number of particles in state  $s$  is given by  $\bar{n}_s = -\frac{1}{\beta} \frac{\partial \ln z}{\partial \epsilon_s}$ .  $z$  is the partition function of the gas and  $\epsilon_s$  is the energy of the particle in state  $s$ .

(c) By using part (b) derive an expression for the average number of photons ( $\bar{n}_s$ ) with energy  $\epsilon_s$ .

(d) Consider a gas consists of three particles. Assume that each particle can be in one of three possible quantum states,  $S = 1, 2$  and  $3$ . Find the possible arrangement of these three particles into above states according to Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics.

## PART C

- (a)
- (i) What lead de-Broglie to suggest that material particles have wave characteristics?
  - (ii) State the de-Broglie equation for matter waves.
  - (iii) Derive de-Broglie wavelength of an electron in terms of potential difference  $V$  through which it is accelerated.
  - (iv) In a diode, the anode has a potential of 100 V relative to the cathode. Find the wavelength associated with the electron as it reaches the anode.
- (b)
- (i) State the Heisenberg's uncertainty principle. What is the practical importance of it?
  - (ii) The position and momentum of 0.5 keV electrons are simultaneously determined. If its position is located within 0.2 nm, what is the percentage uncertainty in its momentum?

- (a) A particle of mass  $m$  and energy  $E$  is travelling along  $x$ -axis towards right to meet a potential barrier defined as

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } 0 \leq x \leq a \\ 0 & \text{for } x > a \end{cases}$$

where  $E < V_0$ .

- (i) Solve the Schrödinger equation to obtain physically acceptable solutions for the particle. No need to apply boundary conditions.
  - (ii) Can the particle exist in the region  $x > a$ . Explain your answer.
- (b) Eigen functions for a particle in a 1-D potential well of width  $a$  is given as

$A \sin \frac{n\pi x}{a}$ ;  $n = 1, 2, \dots, \infty$ . Discuss the orthogonality of eigen functions, prove your argument.

9. (a)

- (i) What is meant by an operator and its expectation value?
- (ii) Write down the momentum operator and the corresponding expectation value.
- (iii) Calculate the expectation value of  $p_x^2$  for a particle having a wave function

$$\psi_n = \left(\frac{2}{l}\right)^{1/2} \sin\left(\frac{n\pi x}{l}\right) \text{ in the region } 0 < x < l.$$

(b)

- (i) All Hydrogen like atoms have one electron in the outermost orbit. However, their ionization energies are different. Explain.
- (ii) In a singly ionized Helium atom, the electron is found in the third orbit. A photon of energy 10.04 eV knocks out the electron. Calculate the energy of the ejected electron. Energy required to remove the electron in the ground state of the Hydrogen atom is 13.6 eV.
- (iii) What is the wavelength of a photon required to raise the ground state electron in the hydrogen atom to the first excited state?