2022

PHYSICS

Paper : PHY 522

(Material Physics)

Full Marks : 50

The figures in the margin indicate full marks.

Candidates are required to give their answers in their own words as far as practicable.

Answer ***any five*** questions.

1. (a) Establish that substitutional diffusion process may be analysed with Fick's first law, even though bulk motion of the atoms occur. Comment on the nature of the diffusion coefficient.

   (b) Show graphically that small composition fluctuations are favoured inside the spinodal points.

   (c) Compare between diffusion controlled growth and interface controlled growth.

   (d) Comment on the coherent boundaries observed in a crystal lattice. (3+1)+2+2+2

2. (a) Consider a tri-layer, where two ferromagnetic half metallic layers are separated by a non-magnetic layer. Illustrate the Density of State (DOS) of the tri-layer system with the help of schematic diagram and show that the resistance of this tri-layer system will decreases in presence of magnetic field.

   (b) Consider Lanthanum Manganite system. State how the electronic configuration of five fold degenerate 3d Mn^{3+} changes when divalent alkali earth ion substitutes for trivalent La (La^{3+}). Now, qualitatively explain the origin of negative magnetoresistance observed in lanthanum manganites with the help of double exchange (DE) mechanism.

   (c) State with an example the working principle of a Field Emission source used in an electron microscope. (2+2)+(1+3)+2

3. (a) Compare the performance of Energy Dispersive (EDS) and Wave Dispersive (WDS) spectrometer.

   (b) Draw schematic diagram of an electromagnetic lens used in TEM and indicate electron ray path. State how focusing is achieved in an electromagnetic lens used in TEM.

   (c) How are Bright Field (BF) and Dark Field (DF) images formed in TEM? Show schematic ray diagram only.

   (d) Consider the intensity profile of X-Ray Diffraction (XRD) pattern and Neutron Diffraction (ND) pattern. The intensity of diffraction peaks decreases with increasing angle in an XRD pattern, whereas it remains almost unchanged in ND. Indicate the reason. 2+(1+2)+2+3

4. (a) Show that the thermodynamic properties are identical for ferromagnetic as well as anti-ferromagnetic spin-spin interaction in a bipartite lattice. Why the spin susceptibility of a material can never be negative?

(b) Consider the asymmetrical dependence of potential energy of atomic separation of the form

$$U(s)=\frac{1}{2}k_0 s^2-\frac{1}{3}\mu s^3,\ s=r-r_0,\ \mu \ll k_0^2,$$

where r_0 is the equilibrium distance. Show that the thermal expansion coefficient is independent of temperature and is given by $\frac{\mu k_B}{r_0 k_0^2}$.

(c) The pressure P of a system of N particles contained in a volume V at a temperature T is given by

$$P=nk_BT-\frac{1}{2}an^2+\frac{1}{4}bn^4,$$

where n is the number density and a and b are temperature independent constants. If the system exhibits a gas-liquid transition, find the critical pressure in terms of a and b. (2+2)+3+3

5. (a) Between (9, 0) and (8, 0) SWCNT, which one is a semiconductor and why? Estimate the Young's modulus of (9, 0) SWCNT using Lennard-Jones potential. In this model, how does Young's modulus of (9, 0) SWCNT vary with temperature? (Assume U_0 = 4.5 eV).

(b) The Bloch Hamiltonian of the electrons in graphene under tight-binding approximation can be written as

$$H=\begin{pmatrix} 0 & f\left(\vec{k}\right) \\ f^*\left(\vec{k}\right) & 0 \end{pmatrix},$$

where $f\left(\vec{k}\right)=-t\left(e^{-ik_x a}+2e^{ik_x a/2}\cos\left(\frac{k_y a\sqrt{3}}{2}\right)\right)$.

(The symbols have their usual meanings).

Find out the eigenvalues of the above Hamiltonian and hence, obtain the positions of Dirac points. What is the energy dispersion relation of the electrons near these Dirac points? (2+2+1)+(2+2+1)

6. (a) Estimate the fraction of electrons in 3d free electron gas at $T=0$ between $E_F-\epsilon$ and E_F $(\epsilon \ll E_F)$. Hence, explain the magnitude and variation of the specific heat of metal at low temperature.

(b) Write down two important differences between the direct and the indirect band gap of semiconducting materials. Explain inspite of having an indirect band gap, why Si is used in solar cell.

(c) Define absorption coefficient $\alpha(\omega)$ of a material. Show that $\omega\alpha(\omega)\propto\left(\hbar\omega-E_g\right)^2$ for a direct band gap (E_g) 3d material with parabolic band edge. (2+1)+(2+1)+(1+3)

7. (a) State and prove Hohenberg-Kohn theorem in density functional theory.

(b) Explain the meaning of exponential wall experienced in the wave function of nitrogen molecule. Assume that the wave function is expressed on a grid with 100 points along each spatial direction. How is this problem solved in case of Kohn-Sham density functional theory?

(c) The exchange energy of a homogeneous electron gas is given by :

$$E_X(n,V) = -\frac{1}{2} \times 2 \sum_{i,j} \int d^3r \int d^3r' \frac{\phi_i^*(r)\phi_i(r')\phi_j^*(r')\phi_j(r)}{|\vec{r} - \vec{r}'|}.$$

Show that $E_X(n, V)$ satisfies the following equation :

$$n\frac{\partial \log E_X}{\partial n} + V\frac{\partial \log E_X}{\partial V} = \frac{7}{3}$$

(1+3)+(2+1)+3