

Answer all the questions. All questions carry equal marks each.

1. Estimate the % ionic character of the inter-atomic bonds in the following compounds:

- a) TiO_2
- b) ZnTe
- c) CsCl
- d) InSb
- e) MgCl_2

2. The potential energy (E) of a system of two atoms varies as a function of their distance of separation 'r' as follows:

$$E = -\frac{A}{r^n} + \frac{B}{r^m}$$

Determine the equilibrium bond length (r_0) and the bond strength (or bond energy) in terms of the parameters A, B, m and n .

3. Name three elements of symmetry and illustrate them using relevant examples. List the crystal systems and describe the characteristics of each in terms of the cell parameters.
4. Molybdenum has a BCC lattice with an atomic radius of 1.36 Å. Calculate the lattice parameter of BCC Mo.
5. What is the difference between a diamond crystal structure and a zinc blende crystal structure? Use figures to illustrate.
6. A diffraction pattern of a cubic crystal of lattice parameter $a = 3.16 \text{ Å}$ is obtained with a monochromatic x-ray beam of wavelength 1.54 Å. The first four lines of this pattern were observed to have the following values.:

Line	θ (in degrees)
1	20.3
2	29.2
3	36.7
4	43.6

Determine the interplanar spacing (d) and the Miller indices (hkl) of the reflecting planes.

7. Use diagrams to illustrate how close packed structures (like fcc or hcp) can be formed and calculate the packing density (atomic volume by unit cell volume) for an fcc structure.

8. Distinguish between quartz, fused silica and glass. What experiment can you perform to determine if a piece of material is quartz or fused silica? Briefly describe.
9. What is polydispersity index (PDI)? What are the implications of the PDI for a polymer sample having a value of 1?
10. Classify crystal defects based on their dimension. Calculate the ratio of the number of vacancies in equilibrium at 300 K in aluminium to that produced by rapid quenching from 800 K.

Constants

Boltzmann constant: $8.65 \times 10^{-5} \text{ eV/K}$
 Avogadro's number: $6.023 \times 10^{23} \text{ /mole}$
 Permittivity in free space ϵ_0 : $8.854 \times 10^{-12} \text{ F/m}$
 Charge on an electron: $1.602 \times 10^{-19} \text{ C}$
 Mass of electron: $9.11 \times 10^{-31} \text{ kg}$
 Planck's constant $6.626 \times 10^{-34} \text{ J-s}$
 Velocity of light in vacuum: $2.998 \times 10^8 \text{ m/s}$
 Lattice parameter of Aluminium: 4.04958 \AA
 Structure of Aluminium: FCC
 Atomic Weight of Aluminium: 26.98 g/mol

$$\chi_{\text{Ti}}=1.54$$

$$\chi_{\text{O}}=3.44$$

$$\chi_{\text{Zn}}=1.65$$

$$\chi_{\text{Te}}=2.1$$

$$\chi_{\text{Cs}}=0.79$$

$$\chi_{\text{Cl}}=3.16$$

$$\chi_{\text{In}}=1.78$$

$$\chi_{\text{Sb}}=2.05$$

$$\chi_{\text{Mg}}=1.31$$

Formulae

$$n = N \exp\left(-\frac{E_v}{k_B T}\right)$$

$$U = -\frac{a}{r^m} + \frac{b}{r^n}$$

$$2d \sin \theta = \lambda$$

$$\frac{1}{d} = \frac{\sqrt{h^2 + k^2 + l^2}}{a}$$

$$\% \text{ covalent character} = 100 \exp\left[-0.25(\chi_A - \chi_B)^2\right]$$