

Ex/SC/PHY/PG/CBS/TH/203/2025

M. Sc. EXAMINATION, 2025

[2nd Year 1st Semester (Day)]

PHYSICS

PAPER : PHY/TH/203

[X-Ray Crystallography (I)]

Time : Two Hours

Full Marks : 40

Answer *any four* questions. (4×10)

1. (a) What does ‘structure factor’ mean? Deduce the general form of it from the scattering of the unit cell.
- (b) Determine the structure factor of β -ZnS and indicate the cases where intensity can be observed. The atomic positions of Zn and S in the unit cell are

$$\text{Zn} \quad (000) \quad \begin{pmatrix} 1 & 1 \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 \\ 2 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 \\ 2 & 2 \end{pmatrix} \quad 0$$

$$\text{S} \quad \begin{pmatrix} 1 & 1 & 1 \\ 4 & 4 & 4 \end{pmatrix} \quad \begin{pmatrix} 1 & 3 & 3 \\ 4 & 4 & 4 \end{pmatrix} \quad \begin{pmatrix} 3 & 1 & 3 \\ 4 & 4 & 4 \end{pmatrix} \quad \begin{pmatrix} 3 & 3 & 1 \\ 4 & 4 & 4 \end{pmatrix}$$

$$[(1+3)+6]$$

2. (a) What do you mean by ‘Phase problem’ in crystallography? How is Patterson’s method useful in overcoming the phase problem?

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[Turn Over]

(2)

- (b) Derive the Patterson function and show how this function shows each peak in the Patterson map. How can an origin peak be assigned to the Patterson map?
[(2+2)+(4+2)]

3. (a) What is 'Normalized Structure Factor'? Derive an expression for it and correlate it with the 'Unitary Structure Factor'.

- (b) Derive the 'Triplet Relation' from Sayre's equation and show how the tangent formula is useful in the Direct Method of structure solution [5+5]

4. (a) What is atomic scattering factor? Plot its variation with the scattering angle (for any given element). What factors influence the scattering ability of an atom?

- (b) Why is it not possible to determine the fractional coordinates inside a unit cell from the information of crystal structure factor, F_{hkl} ?

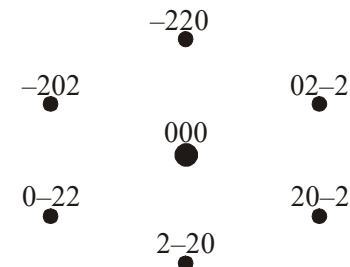
(c) A unit cell of tetragonal system has identical atoms at fractional coordinates: $0\frac{1}{2}\frac{1}{4}$, $\frac{1}{2}0\frac{1}{4}$, $\frac{1}{2}0\frac{3}{4}$ and $0\frac{1}{2}\frac{3}{4}$. By considering the expression for crystal structure factor, F_{hkl} , calculate the diffraction intensity for the following class of reflections: mixed (110), unmixed even (222) and unmixed odd (111). [(1+1+1½)+2+4½]

5. (a) Why is copper chosen as the most preferred wavelength in X-ray diffraction experiments?

(3)

- (b) What is the concept of a zone in crystallography? Also explain the Weiss Zone law using a clean diagram.

- (c) For the indexed diffraction pattern given below, identify the following :



- (i) the zone axis
(ii) the crystal type with explanation
(iii) the significance of 000 spot [2+(2+2)+2+1+1]

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