

M.SC. 2ND YEAR 1ST SEMESTER, 2017

Subject: X-RAY & CRYSTALLOGRAPHY -I

Time: Two hours

Full marks:40

Answer any four questions

1. (a) Write down the expression for electron density function and structure factor function so that they are Fourier Transform of each other. What do you mean by structure factor?
(b) Show that the structure factor for C-centered orthorhombic and body centered orthorhombic are the same.
(c) Explain phase problem in crystallography.

[3+4+3]

2. (a) Show that Patterson functions have a centre of symmetry in the origin irrespective of whether the crystal is centrosymmetric or not.
(b) Discuss whether an R-factor of 0.0 can be attained practically or not.
(c) Why a weighted R-value is more important than ordinary R-value?

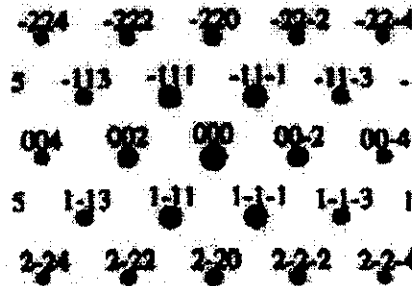
[6+2+2]

3. (a) Explain what is the point group symmetry for crystals.
(b) Which crystal system exhibits highest number of point groups?
(c) Draw the stereographic projections of the following point groups
(i) $2mm$ (ii) $4/mmm$ (iii) $\bar{4}$
(d) Explain with a neat diagram how a third mutually perpendicular 2-fold axis is automatically generated when two 2-fold axes are placed perpendicular to each other.

[2+1+4.5+2.5]

4. (a) What is Weiss Zone law?

(b) For the given indexed diffraction pattern below, identify the following (consider only ZOLZ):



- (i) determine the zone axis
- (ii) identify the crystal class
- (iii) the significance of 000 spot

(c) Sketch and explain the diffraction intensity profile according to Ewald's construction for an **ideal** polycrystalline material at **any** Bragg angle. Assume arbitrary scale for both intensity and Bragg angle. What deviation is observed for **real** polycrystalline materials and why?

[1.5+(2+1+1)+(2+3)]

5. (a) What is reciprocal lattice of a crystal? What are the common steps for constructing the reciprocal lattice of a crystal? Construct the reciprocal lattice for a monoclinic crystal system.

(b) Show that reciprocal lattice vector σ_{hkl} is normal to the crystal plane (hkl).

[(1.5+2+4)+2.5]

6. (a) Derive the relation between interplanar spacing (d_{hkl}) and the crystal axes for an orthorhombic and hexagonal system.

(b) Find the expressions for reciprocal lattice parameters (a^* , b^* , c^*) in terms of crystal unit cell parameters (a , b , c).

(c) Derive the Laue equations and show that these equations are equivalent to Bragg's reflection condition.

[3+2.5+4.5]

7. Write short notes on any *two* :

[2×5=10]

(a) Herker sections and Herker lines.

(b) Frideal's law (discuss including statesman and prove)

(c) Miller-Bravais indices