

Course Code	Course Name	Credits
26PH605	X-RAY CRYSTALLOGRAPHY	04

Course Objectives

- To present the basic concepts needed to understand the crystal structures of materials.
- To cover the theory of x-ray diffraction by crystalline matter along with the experimental x-ray methods to determine the crystal structure of materials.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Becomes familiar with the types of information that x-ray diffraction can provide on the structure of wide variety of samples.
- Gain an understanding of the underlying principles and greater insight into their own characterisation problems.

Unit 1 – X-Ray and Crystals (12 Hrs.)

Origin of X-rays – conventional generators-construction and geometry sealed tuberotating anode generator-choice of radiation-Synchrotron radiation - Lattice planes-Miller indices - X-ray diffraction - Crystal systems and symmetry – unit cell – space lattices- non primitive lattices – point groups-space groups – analysis of space group symbols - Crystallization – growing crystals – choosing a crystals – crystal mounting- alignment – measurement of crystal properties.

Unit 2 Data Collection Techniques For Single Crystals (12 Hrs.)

Laue method- single crystal diffraction cameras: rotation and Oscillation method – Ewald construction - Single crystal diffractometers: Instrument geometry-crystal in a diffracting position – Data collection strategy: determination of unit cell – orientation matrix - Intensity Data collection - Unique data –equivalent reflections – selection of data.

Unit 3 - Data Reduction (12 Hrs.)

Integration of intensity - Lorenz and Polarization corrections – absorption – deterioration or radiation damage – scaling – Interpretation of Intensity. Structure factors and Fourier syntheses: Structure factor –Friedel's Law – exponential and vector form – generalized structure factor.

Unit 4 – Fourier System (12 Hrs.)

Fourier synthesis –Fast Fourier transform – Anomalous scattering and its effects. Calculation of structure factors and Fourier syntheses— Relationship between Fourier and Least squares – Practical consideration in least squares methods – Random and systematic errors.

Unit 5 - Phase Problem (12 Hrs.)

Methods of solving Phase Problem: Direct methods – Patterson methods –Heavy atom methods. Refinement of crystal structures: Weighting – Refinement by Fourier syntheses – Locating Hydrogen atoms identification of atom types – least squares – goodness of fit –least square and matrices-correlation coefficients.

Reference Books:

1. X-ray Structure Determination, Second Edition, Stout and Jensen, John Wiley Publications.
2. Fundamentals of Crystallography, Second Edition, C. Giacovazzo, Oxford Press.
3. Structure Determination by X-ray Crystallography, Second Edition, Ladd and Palmer.

Websites and eLearning Sources:

1. <https://nptel.ac.in/courses/112106227>
2. https://youtu.be/_8BNoavI_bQ?si=QAvk4U7t-6cH4yYv
3. https://youtu.be/2F9NEoXvkQE?si=dKJBwu__z8Hkubml

COs and Bloom's Taxonomy Mapping – 26PH605

Course Outcomes	On successful completion of this course, students will be able to	BTL
CO1	Recall and explain the origin of X-rays, crystal systems, lattice structures, and symmetry elements in crystals.	K1, K2
CO2	Apply X-ray diffraction principles and data collection techniques to determine crystal structures.	K3
CO3	Analyze diffraction data using intensity corrections, structure factors, and Fourier synthesis methods.	K4
CO4	Analyze phase determination techniques and refinement methods for accurate crystal structure analysis.	K5
CO5	Evaluate and design crystal structure models using advanced computational and analytical methods.	K6

BTL (Bloom's Taxonomy Level) - K1 – Remembering, K2 – Understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6 - Create

Relationship Matrix – 26PH605

Course Outcomes	Programme Outcomes (POs)						Programme Specific Outcomes (PSOs)						Mean Score of Cos
	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	
CO1	3	2	1	1	1	1	3	2	1	1	1	1	1.58
CO2	3	3	2	2	1	1	2	3	2	2	2	1	2.00
CO3	3	3	3	2	1	1	2	3	3	2	2	2	2.25
CO4	3	3	3	2	2	1	2	3	3	2	2	2	2.33
CO5	3	3	3	3	2	2	3	3	3	3	2	2	2.58
Total													2.15

Mean Score: 3- High, 2- Medium/Moderate, 1-Low

