

Course Objectives:

1. Introduce the concept of diffraction with X-rays and electrons to the student
2. Briefly describe the use of X-rays to determine crystal structures, construct phase diagrams and analyse phase transitions and particle agglomeration in materials; a topic on refinement methods is also introduced
3. Introduce the student to conventional transmission electron microscopy (TEM) and its utility to analyse crystal structures, analyse line and planar defects and grain boundaries in materials
4. Qualitative treatment of phase contrast (High Resolution) TEM

UNIT I: Properties of X-rays and description of crystals

Production and detection of X-rays; Directions and intensities of diffracted beams; Detectors and measuring intensities of X-rays; Methods of X-ray diffraction; Penetration of X-rays; Grain size, particle size and crystal perfection and orientation.

UNIT II: X-ray analysis

Determination of phase diagrams; Order-disorder phase transitions; Chemical analysis by diffraction - Hanawalt method, direct comparison and internal standard methods; Chemical analysis by fluorescence and absorption.

UNIT III: Precise lattice parameter measurements - Rietveld refinement methods

General methods of precise lattice parameter measurement: Least Squares method, Cohen's method, Calibration method; Hugo Rietveld's method of full pattern refinement; Introduction and practice of refinement using the FullProof software (open source).

UNIT IV: Transmission Electron Microscopy

Comparison of scattering by electrons and X-rays; Elastic and Inelastic electron scattering; Basic instrumentation and imaging modes in the TEM; Obtaining and indexing parallel beam electron diffraction patterns; the Kikuchi lines and use of Convergent Beam Electron Diffraction (CBED) techniques.

UNIT V: Phase Contrast Imaging and HR-TEM

Different contrast mechanisms in the TEM - Amplitude, Mass-thickness, Z-contrast, STEM diffraction contrast; Analysing defects - two beam condition, weak beam dark field imaging, thickness and bending effects, planar defects, strain field imaging; High resolution TEM.

Reference Books:

1. B. D. Cullity and S.R. Stock, *Elements of X-ray Diffraction*, 3rd Edition, Pearson Education India, 2014.
2. Vitalij Pecharsky and Peter Zavalij, *Fundamentals of powder diffraction and structural characterization of materials*, 2nd Edition, Springer, 2005.
3. David B. Williams and C. Barry Carter, *Transmission Electron Microscopy – A textbook for Materials Science*, 2nd Edition, Springer, 2011.

Course Outcomes:

On completion of this course students will be able to:

CO1. Understand fundamental concepts of X-ray diffraction

CO2. Apply diffraction techniques to study materials

CO3. Understand electron diffraction and the instrumentation of the TEM

CO4. Understand how to index 2D electron diffraction patterns.