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|  | **University of Management and Technology****School of Science****Department of Physics** |

**Course Code: PH-7277**

**Course Title: X rays Diffraction**

**Program: MS (Physics)**

**Course Outline (Spring 2023)**

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| **Lecture Schedule** | Wednesday 6:30-9:30Sunday 3:30-6:30 | **Pre-Requisite** | N/A |
| **Course Coordinator** | Dr. Muhammad Tahir | **Contact** | muhammad.tahir@umt.edu.pk |
| **Course****Description** | The objective of this course is to present the basic concepts needed to understand the crystal structure of materials. Fundamental concepts including lattices, symmetries, point groups, and space groups will be discussed and the relationship between crystal symmetries and physical properties will be addressed. The theory of X-ray diffraction by crystalline matter along with the experimental x-ray methods used to determine the crystal structure of materials will be covered. |
| **Course Outcomes** | Having successfully completed this module you will be able to:* Be aware off advanced techniques such as X-ray reflectivity, texture analyse and high-resolution measurements.
* Complete a Rietveld refinement and extract crystallographic and sample information.
* Apply the concepts of unit cells and lattices to describe observed diffraction patterns in reciprocal space.
* Perform basic calculations relating to crystal planes, lattice parameters and sample characteristics.
* Process data, solve/refine and interpret a single crystal structure.
* Setup data collection strategies and collect data on both a single crystal and powder samples.
* Understand solid-state matter in terms of crystallinity and bonding.
* Interpret data using line positions and profiles.
* Understand and apply the various types of powder diffraction experiment and appreciate the importance of sample preparation.
* Evaluate the differences and synergies of powder and single crystal diffraction.
* Understand the basics of X-ray diffraction theory in terms of X-rays, diffraction and Bragg’s Law.
* Be aware of and use various crystallographic databases.
* Understand point and translational symmetry elements and derive symmetry from measured data.
* Have an understanding of the advantages of synchrotron and neutron diffraction and the additional information they can provide.
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| **Text Book** | 1. “Elements of X-ray Diffraction-4th Edition”, B. D. Cullity, Addison-Wesley Publishing Co. Inc. 2014.
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| **Reference Books**  | 2. “Interpretation of X-ray Powder Diffraction Patterns”, H. Lipson, H. Steeple, Macmillan London, 1970.3. “Essentials of Crystallography-2nd Edition”, D. Mckie, Christine Mckie, Blackwell Scientific Publications Oxford, 1986.4. “Crystallography” R. Steadman, Van Nostrand Reinhold Company Ltd. New York, 1983.5. “X-ray diffraction and Crystallography” by Y. Waseda, E. Matsubara and K. Shinoda, Springer-Verlag, Germany, 2011. |
| **Assignment& Projects** | Problems will be assigned at regular intervals as an assignment. | **Quizzes** | * All quizzes will be announced well before time.
* No make-ups will be offered for missed quizzes.
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| **Mid - Term****Examination** | A 60-minutes exam will cover all the material covered during the first 15 lectures. | **Final****Examination** | A 120-minutes exam will cover all the material covered during the semester. |
| **Attendance****Policy** | Attendance is mandatory. Every class is important. All deadlines are hard. Under normal circumstances late work will not be accepted. Students are required to take all the tests. No make-up tests will be given under normal circumstances. Students missing more than 20% of the lectures will receive an “SA” grade in the course and will not be allowed to take final exam.  |
| **Grading****Policy** | Assignment and Quizzes: 25%Mid-Term Examination: 25%Final Examination: 50% |

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X-rays Diffraction (PH-7277)

* **BASICS OF CRYSTALLOGRAPHY:**

Basis and lattice points, Lattice types in 2D and 3D, Planes and Directions, Miller’s and Weber’s indices, Directions in planes, Zone of planes, Atomic/fractional Coordinates, Crystal systems and Crystal structures, Twinned crystals, Real and reciprocal lattices, Reciprocal lattice and Bragg’s law

* **CRYSTAL SYMMETRY:**

Axes of symmetry, Point groups, Crystal classes, Crystal system and Stereographic projection

* **PRODUCTION AND PROPERTIES OF X-RAYS:**

Production, Absorption, Characteristics, Filters, Detection, Coherent and Incoherent scattering

* **DIFFRACTION OF X-RAYS:**

Diffraction, Bragg’s Law, X-ray Spectroscopy, Diffraction directions, Diffraction methods

* **INTENSITIES OF DIFFRACTION BEAMS:**

Scattering by an electron, an atom and a unit cell, Structure factor calculations, Application to Powder Method, Multiplicity factor, Temperature factor, Intensity calculations

* **EXPERIMENTAL METHODS:**

Laue Methods, Rotating Crystal Method, X-ray Powder Diffractometry (θ- θ, θ-2θ), X-ray Reflectometry (XRR), Grazing Incidence Angle X-ray Diffraction (GIXRD)

* **DETERMINATION OF CRYSTAL STRUCTURE:**

Treatment of Data, Indexing of cubic and non-cubic crystals, Direct Method, Determination of number of atoms in a unit cell, Determination of atomic position, Introduction and Applications of Crystal Structure Determination - Computer Programs, Refinement of Diffraction data using Rietveld’s approach

**Recommended Books:**

1. “Elements of X-ray Diffraction-4th Edition”, B. D. Cullity, Addison-Wesley Publishing Co. Inc. 2014.

2. “Interpretation of X-ray Powder Diffraction Patterns”, H. Lipson, H. Steeple, Macmillan London, 1970.

3. “Essentials of Crystallography-2nd Edition”, D. Mckie, Christine Mckie, Blackwell Scientific Publications Oxford, 1986.

4. “Crystallography” R. Steadman, Van Nostrand Reinhold Company Ltd. New York, 1983.

5. “X-ray diffraction and Crystallography” by Y. Waseda, E. Matsubara and K. Shinoda, Springer-Verlag, Germany, 2011.

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| **Week No.** | **Topic** | **Reading Material (s)****such as (PDF/PPTS/Videos/Research Papers/Articles/Web-links/)** | **Course Learning Outcomes (CLOs)** | **Activities (Group Discussion, Presentation, Assignment etc.)** | **Reference (Additional Reading Material, Web-links etc.)** |
| **Week 1** | Basis and lattice points, Lattice types in 2D and 3D, Planes and Directions, Miller’s and Weber’s indices  | PDF/PPTS/Research Papers  | 1-5  |  Group Discussion  |  https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link |
| **Week 2** | Directions in planes, Zone of planes, Atomic/fractional Coordinates  |  PDF/PPTS/Research Papers  | 1-5  |  Group Discussion | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 3** | Crystal systems and Crystal structures, Twinned crystals, Real and reciprocal lattices, Reciprocal lattice and Bragg’s law  | PDF/PPTS/Research Papers   |  1-5 | Group Discussion/Assignment  | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 4** | CRYSTAL SYMMETRY  | PDF/PPTS/Research Papers   | 1-5  | Group Discussion/Quiz  | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 5** | PRODUCTION OF X-RAYS  | PDF/PPTS/Research Papers   | 1-5  | Group Discussion/Assignment   | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 6** | PROPERTIES OF X-RAYS:  | PDF/PPTS/Research Papers   | 1-5  | Group Discussion/quiz | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 7** | Diffraction, Bragg’s Law,  | PDF/PPTS/Research Papers   | 1-5  | Group Discussion  |  https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link |
| **Week 8** | **Mid Exams** |
| **Week 9** | X-ray Spectroscopy   | PDF/PPTS/Research Papers   |  1-5 | Group Discussion |  https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link |
| **Week 10** | Diffraction directions, Diffraction methods  | PDF/PPTS/Research Papers   | 1-5  | Group Discussion/Assignment   | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 11** | Scattering by an electron, an atom and a unit cell, Structure factor calculations  | PDF/PPTS/Research Papers   | 1-5  | Group Discussion/Quiz  | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 12** | Application to Powder Method, Multiplicity factor Temperature factor, Intensity calculations | PDF/PPTS/Research Papers   |  1-5 | Group Discussion/Assignment   | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 13** | EXPERIMENTAL METHODS  | PDF/PPTS/Research Papers   | 1-5  |  Group Discussion/Quiz |  https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link |
| **Week 14** | Treatment of Data, Indexing of cubic and non-cubic crystals, Direct Method, Determination of number of atoms in a unit cell, Determination of atomic position  | PDF/PPTS/Research Papers   |  1-5 |  Group Discussion/Assignment  |  https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link |
| **Week 15** | Introduction and Applications of Crystal Structure Determination - Computer Programs, Refinement of Diffraction data using Rietveld’s approach  | PDF/PPTS/Research Papers   | 1-5  | Presentation   | https://drive.google.com/file/d/1jatWS8I4OVaohTSUt7-SCPIKzecQPLUp/view?usp=share\_link  |
| **Week 16** | **Final Exams** |

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|  | **University of Management and Technology****School of Science****Department of Physics****Lecture Plan (Spring 2022)** |

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| **Sixteen Week Lecture Plan** | **Week** | **TOPICS** | **Chapter** |
| 1 |  |  |
| 2 |  |  |
| 3 |  |  |
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| 5 |  |  |
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|  | **Mid Term** |  |
| 8 |  |  |
| 9 |  |  |
| 10 |  |  |
| 11 |  |  |
| 12 |  |  |
| 13 |  |  |
| 14 |  |  |
| 15 | **Final Term** |  |

CONTRIBUTION OF COURSE LEARNING OUTCOMES (CLOs) TO PROGRAMME LEARNING OUTCOMES (PLOs)

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| **BS Physics** | **Digital Electronics** |
| **Serial #** | **Program Learning Outcomes** | **Course Learning Outcomes** |
|  |  | **1** | **2** | **3** | **4** |
| **1** | Knowledge |  |  |  |  |
| **2** | Problem analysis |  |  |  |  |
| **3** | Design/Development of solutions |  |  |  |  |
| **4** | Investigation |  |  |  |  |
| **5** | Modern tool usage |  |  |  |  |
| **6** | Environment and sustainability |  |  |  |  |
| **7** | Individual and Team work |  |  |  |  |
| **8** | Lifelong learning |  |  |  |  |