

PHY6180: MODERN SCATTERING METHODS IN MATERIALS SCIENCE

Effective Term

Semester A 2025/26

Part I Course Overview

Course Title

Modern Scattering Methods in Materials Science

Subject Code

PHY - Physics

Course Number

6180

Academic Unit

Physics (PHY)

College/School

College of Science (SI)

Course Duration

One Semester

Credit Units

3

Level

P5, P6 - Postgraduate Degree

Medium of Instruction

English

Medium of Assessment

English

Prerequisites

Nil

Precursors

Nil

Equivalent Courses

AP6180 Modern Scattering Methods in Materials Science

Exclusive Courses

AP8180/PHY8180 Modern Scattering Methods in Materials Science

Part II Course Details

Abstract

This course covers a range of experimental and applied-physics topics and methods in materials science that involve X-ray and neutron scattering in the laboratory and as well as at large-scale facilities like at synchrotrons, at research nuclear-reactors, or at spallation neutron-sources. Its central aims are: (1) to describe the fundamentals of scattering by condensed matter, (2) to introduce the different commonly employed scattering techniques available in the laboratory and at large-scale facilities, (3) to show the possible applications in discovering advanced materials and (4) to motivate the students for discovery and innovation in applying scattering techniques in materials science.

Course Intended Learning Outcomes (CILOs)

| CILOs | | Weighting (if app.) | DEC-A1 | DEC-A2 | DEC-A3 |
|-------|--|---------------------|--------|--------|--------|
| 1 | Explain the importance of modern scattering techniques and their applications in material research. | | x | | |
| 2 | Acquire the fundamental knowledge about different scattering techniques with special emphasis on neutron diffraction. | | x | | |
| 3 | Clarify the similarities and differences between X-ray and neutron scattering. | | x | | |
| 4 | Recognize the fundamental theory of scattering and its application to study the structures of different classes of materials. | | | x | |
| 5 | Apply the kinematical diffraction theory to materials science problems. | | | x | x |
| 6 | Master the basic knowledge of small-angle-X-ray-scattering (SAXS) and small-angle-neutron-scattering (SANS) for determining the large-scale structure of materials | | | x | x |
| 7 | Describe the basics of inelastic-neutron-scattering (INS) and quasi-elastic-neutron-scattering (QENS) for being able to study the dynamics of liquids and soft materials | | | x | x |
| 8 | Observe specific case-studies for better understanding the practical application of 1 to 7 | | | | x |

A1: Attitude

Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2: Ability

Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to real-life problems.

A3: Accomplishments

Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

Learning and Teaching Activities (LTAs)

| LTAs | | Brief Description | CILO No. | Hours/week (if applicable) |
|------|-----------|--|---------------------|----------------------------|
| 1 | Lectures | Explain the basic principles of modern theories related to diffraction, small-angle, inelastic and quasi-elastic scattering techniques | 1, 2, 3, 4, 5, 6, 7 | 2 |
| 2 | Tutorials | Problem solving related to scattering | 1, 2, 3, 4, 5, 6, 7 | 1 |
| 3 | Project | Analysis of neutron scattering data of small-angle x-ray/neutron scattering and/or quasi-elastic neutron scattering | 8 | 1 |

Additional Information for LTAs

The “Lectures” will be in the form of 2-hrs lectures each week, while the “Tutorials” and/or the "Laboratory demonstrations" will always follow the lectures.

Assessment Tasks / Activities (ATs)

| ATs | | CILO No. | Weighting (%) | Remarks ("- for nil entry) | Allow Use of GenAI? |
|-----|--------------|---------------------|---------------|----------------------------|---------------------|
| 1 | Assignments | 2, 3, 4, 5, 6, 7 | 10 | - | Yes |
| 2 | Project | 7, 8 | 20 | - | Yes |
| 3 | Midterm Test | 1, 2, 3, 4, 5, 6, 7 | 30 | - | Yes |

Continuous Assessment (%)

60

Examination (%)

40

Examination Duration (Hours)

2

Assessment Rubrics (AR)**Assessment Task**

Assignments (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

Explain key concepts of modern scattering methods

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not even marginal level

Assessment Task

Project (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

Basic understanding of data analysis of SAXS/SANS or QENS

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not even marginal level

Assessment Task

Midterm Test (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

Ability to explain concepts of different scattering methods

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not even marginal level

Assessment Task

Final examination (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

Ability to explain key concepts of diffraction, SAXS, SANS, INS, and QENS scattering methods

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not even marginal level

Assessment Task

Assignments (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion

Explain key concepts of modern scattering methods

Excellent

(A+, A, A-) High

Good

(B+, B) Significant

Marginal

(B-, C+, C) Moderate

Failure

(F) Not even marginal level

Assessment Task

Project (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion

Basic skills in data analysis of SAXS/SANS and QENS

Excellent

(A+, A, A-) High

Good

(B+, B) Significant

Marginal

(B-, C+, C) Moderate

Failure

(F) Not even marginal level

Assessment Task

Midterm Test (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion

Ability to explain concepts of different scattering methods

Excellent

(A+, A, A-) High

Good

(B+, B) Significant

Marginal

(B-, C+, C) Moderate

Failure

(F) Not even marginal level

Assessment Task

Final examination (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion

Understanding of fundamental concepts of different scattering methods, including diffraction, SAXS, SANS, INS, and QENS

Excellent

(A+, A, A-) High

Good

(B+, B) Significant

Marginal

(B-, C+, C) Moderate

Failure

(F) Not even marginal level

Part III Other Information

Keyword Syllabus

- Introduction

Basics of the structure of condensed materials: From atoms to the structures of crystalline, liquid and amorphous substances with showing materials of specific interest in modern life

- Fundamentals of scattering techniques: neutron diffraction, X-rays diffraction, scattering mechanisms, similarities and differences in X-ray and neutron scattering

- Fundamentals of the kinematical scattering theory, correlation between real and reciprocal space, and its relevance to understanding the structure of materials

- Small-angle-X-ray-scattering (SAXS) and small-angle-neutron-scattering (SANS), scattering by non-crystalline materials

- Inelastic-neutron-scattering (INS) and Quasi-elastic-neutron-scattering (QENS), atomic and molecular motion, and magnetic and crystal field excitations
- Specific case studies, atomic/molecular motion in liquids, the structure of bulk metallic glasses, magnetic shape-memory alloys, the dislocation density to strengthen metallic materials, internal stress measurements in engineering materials, interaction of water with biomolecules, etc.

Reading List

Compulsory Readings

| Title | |
|-------|---|
| 1 | B. E. Warren, X-ray diffraction, Dover Books on Physics, 1964 |
| 2 | G. L. Squires, Introduction to the Theory of Thermal Neutron Scattering, Cambridge University Press, 1978 |

Additional Readings

| Title | |
|-------|---|
| 1 | L. H. Schwartz & J. B. Cohen, Diffraction from materials, Academic Press, 1977 |
| 2 | G. E. Bacon, Neutron diffraction, Clarendon Press, 1975 |
| 3 | Ilias Michalarias & Dr. Jichen Li, Neutron Scattering Experiments of Water in Biomolecules, University of Manchester, 2005 |
| 4 | F. H. Chung & D. K. Smith Eds. Industrial Applications of X-ray Diffraction, Marcel Dekker, Inc. USA, 2000 |
| 5 | M. Bee, Quasielastic Neutron Scattering, Principles and Applications in Solid State Chemistry, Biology and Materials Science, Taylor & Francis; 1 edition (January 1, 1988) |
| 6 | Stewart F. Parker, Inelastic Neutron Scattering Spectroscopy, Wiley, 2006. |
| 7 | T. Egami and S. J. L. Billinge "Underneath the Bragg Peaks, Structure Analysis of Complex Materials," Elsevier, 2003. |
| 8 | Linan Tian, A Kolesnikov and Jichen Li. Ab Initio Simulation of Hydrogen Bonding in Ices under Ultra-High Pressure. J. Chem. Physics. 2012 |
| 9 | D. Ma, A. D. Stoica X.-L. Wang, Z. P. Lu, B. Clausen, D. W. Brown, "Moduli inheritance and the weakest link in metallic glasses," Phys. Rev. Lett., 108, 085501 (2012) |
| 10 | S. Cheng, A.D. Stoica X.-L. Wang, Y. Ren, J. Almer, J.A. Horton, C.T. Liu, B. Clausen, D.W. Brown, P.K. Liaw and L. Zuo "Deformation cross-over: from nano to meso scales," Physical Review Letters 103, 035502 (2009) |
| 11 | P. Cordier, T. Ungar, L. Zsoldos G. Tichy Dislocation creep in MgSiO ₃ perovskite at conditions of the Earth's uppermost lower mantle, Nature, 428 (2004) 837 |
| 12 | S. M. Chathoth E. Mamontov Y. B. Melnichenko and M. Zamponi Diffusion and adsorption of methane confined in nano-porous carbon aerogel: a combined quasi-elastic and small-angle neutron scattering study, Mesoporous and Microporous Materials 132, 148 (2010) |