CH986-10 X-ray and Neutron Techniques

26/27

Department
Chemistry
Level
Taught Postgraduate Level
Module leader
Lydia Barnes
Credit value
10
Module duration
10 weeks
Assessment
100% coursework
Study location
University of Warwick main campus, Coventry

Description

Introductory description

X-ray and neutron diffraction and scattering techniques, as well as X-ray spectroscopies will be described. The course will cover the underlying theory of the experiments as well as practical aspects of recording data and their interpretation. The importance of X-ray and Neutron methods across science, in e.g., material chemistry, pharmaceuticals and proteins will be demonstrated.

Module web page

Module aims

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Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

Outline Syllabus:

1. Introduction: Scattering factors for X-ray and neutrons. Production of x-rays and neutrons. Types of facilities.

2. Diffraction: X-ray and Neutron.
   Material characterisation of systems with long range order. Topics might include: symmetry, form factor, structure factor in addition to texture and orientation; differences between X-ray and neutron cross section; powder diffraction, single crystal diffraction; thin film diffraction as well as PDF and protein crystallography. Possible extensions include resonance and incommensurate structures (magnetism, Jahn-Teller, structural domains). Also to include Particle size (Scherrer) and strain analysis (Williamson-Hall).

3. Grazing Incidence.
   Scattering around the origin of reciprocal space. Reflectivity, interfaces. Optical theorem (scattering from refractive index rather than crystal structures). Extension to include patterned arrays and nanostructures.

4. SAX/SANS: Extension of previous topics, but now looking at mesoscopic length scales. Contrast matching in SANS. Guinier and Porod plots.

5. Spectroscopy: Moving away from scattering to looking at core-hole excitations. Topics might include: XRF and GI-XRF; Elemental mapping and quantitative analysis of compositions; XAS (NEXAFS, EXAFS) and radial functions (materials characterisation on nearest neighbours); chemical/species analysis (states of oxides etc.). Possible extensions to include XPS and XMCD.

Learning outcomes

By the end of the module, students should be able to:

- Understand the physical basis of X-ray and Neutron diffraction and scattering experiments and be familiar with the different analytical techniques involving those phenomena
- Appreciate the wide applicability of techniques involving X-ray and Neutron scattering and diffraction
- Be able to interpret experimental data from a range of techniques

Interdisciplinary

Cross-disciplinary techniques applicable in Chemistry, Engineering, Physics and other fields, co taught by Chemistry and Physics.

Subject specific skills

Understand the physical basis of diffraction, refractions and absorption experiments
Acquire familiarity with the range of techniques and the role of the different elements of

instrumentation
Interpretation of experimental data
Use relevant databases and prediction programs
Appreciate the wide applicability of X-ray and Neutron techniques

Transferable skills

Problem solving and Critical thinking developed during data analysis workshops and follow-up assignments.
Literature review and Scientific Writing developed during Mock Beamtime Application assignment.

Study

Study time

Type	Required
Lectures	20 sessions of 1 hour (20%)
Practical classes	4 sessions of 2 hours (8%)
Private study	72 hours (72%)
Total	100 hours

Private study description

72 hours self study (reading, preparation, data analysis, write-ups)

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group A2

Assessment component	Weighting	Study time	Eligible for self-certification
Practical data analysis assignments	66%		Yes (extension)

	Weighting	Study time	Eligible for self-certification
Assessment based on practical workshops (x2)			

Reassessment component is the same

Assessment component

Mock beamtime application	34%	Yes (extension)
Submission of mock beamtime application		

Reassessment component is the same

Feedback on assessment

Written work will be annotated and returned to students. Feedback on workshop presentation will be provided verbally.

Availability

Courses

This module is Core optional for:

- Year 1 of TCHA-F1PL Postgraduate Taught Molecular Analytical Science

This module is Optional for:

- Year 1 of TCHA-F1PY Postgraduate Taught Analytical Science and Instrumentation
- Year 1 of TCHA-F1PX Postgraduate Taught Analytical and Polymer Science
- Year 1 of TCHS-F1PK Postgraduate Taught Polymer Chemistry
- TCHA-F1PW Postgraduate Taught Polymer Science
    - Year 1 of F1PW Polymer Science
    - Year 2 of F1PW Polymer Science

This module is Unusual option for:

- Year 3 of TCHA-F1PW Postgraduate Taught Polymer Science

This module is Option list A for:

- Year 1 of RCHA-F1P9 Postgraduate Research Analytical Science