Provisional Programme of Lectures and key Learning Outcomes

Introduction to Diamond and ISIS

Diamond Light Source and ISIS Neutron Source are examples of modern accelerator-based facilities for studying a vast range of materials and complex phenomena. While the CDT Introductory School focusses on how the facilities can be used for diverse science applications, this session gives a very basic introduction to the facilities and the science behind them.

Introduction to Diamond Light Source

- What is Diamond Light Source?
- How does Diamond make X-rays?
- Why is Synchrotron Radiation important for Science?
- What's on a Diamond Beamline?
- The Future of Accelerator-based Light Sources

Introduction to ISIS Neutron Source

- What is ISIS?
- What is a neutron and why use them?
- How Does ISIS Make Neutrons?
- Why are neutrons important for science?

Imaging and tomography

Synchrotron X-ray imaging can provide two- or three-dimensional, spatially resolved images of a wide range of samples that are temporally resolved and hence can reveal the kinetics of reactions, deformation, flow, etc. This enables new insights into the underlying mechanisms for a range of applications in scientific and technological areas from biological to aerospace.

The theory behind X-ray imaging and tomography are reviewed first, with a focus on understanding the benefits and limitations of the method, and when other techniques from electron microscopy to neutron imaging should be used. This includes an overview of the key algorithms needed to quantify the results and how to deal with the 'big data' produced. A number of example applications of in situ, time resolved, synchrotron x-ray tomography are then covered to demonstrate how the technique can best be used.

Neutron imaging methods are introduced with a focus on the main application areas: non-destructive testing and mapping of light elements, especially hydrogen. Novel neutron imaging methods such as energy-dependent radiography and magnetic imaging reveal phase changes, grain orientations and magnetic domain distributions in engineering materials. Special attention is given to the comparison and complementarity with X-ray methods.

Talk contents & Learning Outcomes

Synchrotron X-ray imaging, how does it work?

- Introduction to synchrotron imaging
- Theory of tomography
- Theory of reconstruction algorithms
- Simple guidelines on what it does well, and when it is unlikely to work
- Examples of what works well, and what doesn't

Imaging functional materials with X-rays

- Functional materials: why use X-ray imaging?
- Designing experiments for in situ X-ray imaging
- Imaging chemical and structural changes related to battery performance

How does neutron imaging work?

- Why use neutron radiography and tomography for material analysis?
- How does neutron imaging compare to X-ray imaging?
- Applications of neutron imaging in materials sciences

Visualizing the invisible: imaging magnetic fields with neutrons

- Introduction to Advanced neutron imaging with unpolarised and polarized neutrons
- How to visualize magnetic fields and magnetic domains with neutrons?
- Applications of magnetic imaging in physics and engineering science

Small Angle Scattering and Disordered Systems

Small Angle Scattering (SAS) provides essential information on the structure, and in some instances dynamics/kinetics, of large molecule systems and molecular assemblies having low degrees of order (non-crystalline systems). The technique is very well established, having first been put on a physical basis by Lord Rayleigh in the late 19th century. If you have ever witnessed a 'halo' around the moon, that is the small-angle scattering of light by ice crystals in the upper atmosphere. SAS is often considered to bridge the gap in length scales between optical or electron microscopy and crystallography. Equally it can tackle samples that the former techniques find difficult. For example, a bulk sample (or its container) may be opaque to light. Whilst the production of very thin slices for electron microscopy can often destroy the very thing that one wants to look at.

SAS is routinely performed with light (SALS), X-rays (SAXS) and neutrons (SANS). This talk will focus on the last two, whose capabilities are best viewed as complementary. SAXS looks at inhomogeneities in electron density in the sample, whilst SANS probes differences in neutron scattering length density. But both techniques investigate length scales ranging from angstroms (0.1 nm) to microns. These dimensions are characteristic of molecular conformation, microphase domain structures, crystallisation phenomena, network/gel formation, craze initiation, void distributions, polymers, proteins, nanoparticles, colloids, liquid crystals, and even bacteria.

The disordered materials component will briefly cover the basics of neutron diffraction in the context of non-crystalline diffraction (i.e., generally investigating shorter length scales than SAXS/SANS), with a focus on introducing key concepts within the framework of real-world scientific problems and the related diffraction experiments. Disordered materials cover an enormous range of materials, principally those composed of liquids and glasses, and they are characterised by having little (or no) long-range structural / atomic correlations, in direct contrast to crystalline diffraction. Nevertheless, the dynamically-averaged picture of the systems can be extracted via neutron diffraction, allowing structural properties to be calculated and related to macroscopic phenomena. Such studies are routinely performed on, for instance, pure chemical solvents, their mixtures, and amorphous glasses such *as silicates.*

Talk contents & Learning Outcomes

Introduction to Small Angle Scattering

- Introduction to SAS –Concepts
- How to obtain parameter information on semi-disordered systems
- Obtaining Shape information
- Obtaining structural information

- Anomalous Scattering (Contrast lengths and Absorption Contrast)

SAS Case Studies

- Time Resolved SAS
- Combining SAS with Sample Environments – examples from Raman/Pressure/Rheology SAS experiments
- Microfocus Mapping with SAXS
- Grazing Incidence Small Angle Scattering

Introduction to Disordered Materials

- What are disordered materials?
- How can the structure of a disordered material be described?
- How can you measure the structure of a disordered material?
- Basic examples of disordered materials (glasses, simple liquids etc.)
- What information can you obtain from studying disordered materials?

Case study: Aromatic Liquids

- Aromatics and the oil industry
- Using isotopic substitution in disordered materials
- Using simulation: 3 dimension structure of molecular liquids
- Looking at aggregation on the molecular level

Case study: Catalysis

- Confined liquids in heterogeneous catalysis – why so important?
- How can heterogeneous catalysis be investigated with neutrons?
- What can neutrons tell us about the kinetics in a dynamic system?

Surfaces, films, multilayers

X-ray reflectivity (XRR) is able to yield very accurate information on the structure of thin films at the interface with a supporting substrate, which can be either a solid or liquid. It is only sensitive to the film structure in the direction perpendicular to the surface. When X-rays are used as the probe, it gives information on the electron density profile in the film and can accurately give information on film thickness, interface and surface roughness and degree of intermixing. In multilayer samples it can show the quality of the layer structure and whether interface roughness is correlated across the different interfaces. It is also heavily used in 'soft condensed matter' systems where, for example, molecules may self-organise on a water surface and the layer thickness may be dependent on specific parameters such as surface tension, pH or gas composition above the layer. Many studies identify how the layer develops during changes of experimental parameters, which are often linked to other changes in the system e.g. enhanced magnetism or changes in chemical reactivity.

Talk contents & Learning Outcomes

A general introduction to Reflectivity from Surfaces and Interfaces.

- Highlight the geometry of the experiment and the instrumentation used.
- Outline the different parameters that can be investigated by these investigations

The complementarity of X-rays and Neutrons as probes of the surface or interface.

- Highlight the power of each probe and also of combined investigations.

X-ray and Neutron Reflectivity applied to model biological membranes.

- Outline the types of interface that can be studied.
- The application of reflectivity to understand a real world lipid interface

Single Crystal and Powder Diffraction

As the basic theories of diffraction and crystallography are applicable to both single crystal (SXD) and powder diffraction (PD) techniques, the two sessions are combined under the same general heading of Diffraction. Diffraction techniques, whether using X-rays or neutrons and with either SXD or PD methodologies, are a crucial pillar of research in both the physical and the life sciences. Scientists who use the beamlines at Diamond and ISIS, have access to state-of-the-art SXD and PD instrumentation that can support diverse research disciplines: in the physical sciences materials research in advanced energy storage systems, such as Li-ion batteries and metal-organicframeworks, other functional materials, such as multiferroics, high-Tc superconductors, superalloys and nano-composites, is supported; in archaeometry both neutron and X-ray diffraction techniques provide an unrivalled non-destructive means of studying historical artefacts; while in the life sciences the architecture of the molecular machinery within proteins and viruses can be studied at the atomic level, which is in turn a vital means of directing the synthesis of pharmaceutical molecules for their incorporation into the active regions of proteins.

In this session, the fundamentals of diffraction and crystallography will be introduced and this will be followed by an overview of neutron and synchrotron beamlines and their applications. The presentations will be illustrated with selected science case-studies which will provide an insight into how the PD and SXD techniques may be applicable to the research programmes of the school's participants.

Talk contents & Learning Outcomes

Diffraction and Crystallography (Part I)

Diffraction and Crystallography (Part II)

Synchrotron X-Ray Powder Diffraction (SXPD)

- Introduction – powder diffraction (basic concepts)
- Why powder diffraction?
- Powder diffraction methods – basic theory and diffraction process
- Why use Synchrotron X-rays?
- Synchrotron PD Beamlines
- What information do we get?
- Case studies

Neutron Powder Diffraction

Neutron Single Crystal Diffraction

- How single crystal diffraction is done at a pulsed neutron source
- What instrumentation is being used
- Examples of when neutrons are used and where they provide complementary information to X-rays

Synchrotron Single Crystal Diffraction (SXD)

- Single-crystal diffraction techniques

- Instrumentation for small-molecule crystallography
- A description of beamline I19 and the sample environment techniques it offers to users
- Some example studies

Synchrotron Macromolecular Crystallography (MX)

- Introduction to the relevance of macromolecular crystallography to biomedical science and biology
- Examples of high macromolecular structure providing insight to our fundamental understanding of biology
- Importance of synchrotron radiation and large facilities to macromolecular crystallography
- Diamond Light Source macromolecular crystallography beamlines
- Key areas of methods development

Single crystals from a diffraction point of view

- The specificity of single crystal diffraction
- Differences between neutron and X-rays diffraction
- Different techniques for different problems
- Instrumentation

Powder Diffraction is Amazing

Molecular Spectroscopy

Conventional spectroscopy using light can be used to investigate materials by encouraging transitions between the energy levels of components in a system. This is used extensively in fields such as diagnostic medicine, industrial process control, and cutting edge research. Neutron scattering can also be used as a form of molecular spectroscopy that correspond to how materials move within a system, complementing the optical techniques of infrared and Raman spectroscopy. These talks will introduce these powerful techniques and provide examples of their application in recent research

Talk contents & Learning Outcomes

Molecular Motions and calculations

- Translation, rotation and vibration
- Quantisation of motion
- Harmonic and anharmonic oscillators
- Selection rules
- Calculations and comparison with experiment

Inelastic Neutron Scattering

- Selection rules/hydrogen sensitivity
- Direct and indirect geometry instruments
- Q resolution
- Examples

Infrared spectroscopy

- Absorption spectroscopy basics
- Interferometers and microscopes principles
- Introduction to synchrotron IR Microprobe
- Research Examples

Raman spectroscopy

- Instrumentation
- The fluorescence problem
- Advanced techniques (SERS, resonance, Raman imaging, Kerr gating etc.)
- Examples

Quasielastic Neutron scattering

- Structure of the Quasielastic peak
- Elastic window scan
- Elastic Incoherent Structure Factor
- Quasielastic experiments and modelling
- Examples

Electronic spectroscopy

X-ray and neutron spectroscopies are a crucial part of the methods provided by synchrotron and neutron facilities. They provide chemical, electronic and vibrational state information that often cannot be obtained by any others means. The intense flux of these sources allows for studies of materials of a vast range including catalysis, thin films, transition metal oxides, magnetic materials and chemical and environmental samples. These lectures will give an introduction to the techniques and some examples of their use.

Photoelectron spectroscopies exploit differences in the ground state of core level electrons induced by the chemical environment of the sample, allowing the chemical composition of samples to be directly probed. Through the tuneable nature of synchrotron light, this chemical information can be utilised to understand processes occurring at the surface interface and at buried interfaces, and even to gain quantitative information on the geometric structure of the present chemically distinct species. We will look briefly at the theory that underlies photoelectron spectroscopy, before moving onto how to detect and utilise these photoelectrons. Finally we will discuss the recent advances aiming to bring photoelectron studies into more realistic environments, in order to gain greater understanding of catalytic interactions and device performance in ambient conditions.

Talk contents & Learning Outcomes

Measuring magnetic dynamics with neutron scattering

- What are strongly correlated electron materials and why they are interesting
- Why a knowledge and understanding of magnetic fluctuations is important

Introduction to X-ray Absorption Spectroscopy

- What is XAS: history and applications
- Information available and uses
- Beamline and sample environments
- Different methods: transmission, fluorescence, electron yield

Introduction to Photoelectron Spectroscopy

- Photoelectric effect
- Electron binding energies and chemical shifts
- Energy resolved detection of electrons
- Synchrotron x-ray photoelectron spectroscopy
- Ambient Pressure Photoelectron Spectroscopy

Introduction to Angle Resolved Photoemission and Resonant Inelastic X-ray Scattering

- Scientific Opportunities
- Beamline and Instrumentation
- Fermi Surface Mapping
- Resonant Inelastic X-ray Scattering: Instrumentation and Scientific Opportunities

Muons

Muon spectroscopy for condensed matter research has become a mainstream technique since its inception from an applied particle physics method only practised by a small number of specialists. It is now utilized by a wide user-base of scientists across the world. There are only four centres in the world, with one being the STFC ISIS facility in the UK. Recently, muon spectroscopy has provided invaluable information in a wide range of research areas such as: unconventional superconductivity, magnetism, semiconductors, ion diffusion, polymer dynamics and chemical reactions. In this talk we will give an overview of the technique and highlight some recent results.

Talk contents & Learning Outcomes

All in a spin – An introduction to muon spectroscopy

- An Introduction to Muons
- The μSR technique
- The ISIS μSR Facility
- Muons elsewhere in the world
- Science tasters

Overview of muons in magnetism

Overview of muons in Superconductivity

Overview of muons in Ion Transport

Overview of muons in Reaction Chemistry

Overview of muons in Soft Matter

Overview of muons in Semiconductors

Overview of muons in Elemental Analysis

Overview of muons in Electronic Irradiation