ISIS 40th Science Roadshows: Manchester Stop

10th – 11th September 2024

Alan Turing Building, University of Manchester, UK

Speakers Abstracts

Understanding complex fluids and catalysis using Total Neutron Scattering (TNS)

Chris Hardacre

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The drive to net zero is being accelerated significantly with governmental targets to reach this over the next 20 years. However, in order to achieve this aim, a detailed understanding of molecular interactions within complex systems, for example within a heterogeneous catalyst or during the solvation of biomolecules, is critical to be able to design more efficient systems. Total neutron scattering has the ability to probe these structures and provide invaluable information which can be used to model and develop relevant processes. In this presentation, the use of total neutron scattering for the examination of ionic liquids, particularly those associated with the conversion of biomass, and catalytic systems will be presented. As the structural information obtained the talk will demonstrate how technique development has been used to enhance the information provided and its relevance to the reactions being undertaken. In particular, the incorporation of additional spectroscopic techniques can enable detailed kinetic information to be elucidated. More recently, modulation excitation with phase sensitive analysis has been also applied to TNS for the first time and the preliminary data investigating fuel cell electrocatalysis will be shown.

FlowSANS and RheoSANS to investigate soft matter structure

Bana Shriky

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Understanding structure-property relationships is critical for the development of new soft matter systems for various applications. This study investigates the properties of Pluronic-based smart hydrogel formulations for future use as injectable controlled drug carriers. The smart hydrogels promise to enhance patient compliance, decrease side effects and reduce dose and frequency. Pharmaceutically, these systems are attractive due to their unique sol-gel phase transition in the body, biocompatibility, safety and injectability as solutions before transforming into gel matrices at body temperature. We quantify the structural changes of these complex fluids under controlled temperature, flow, and extension as experienced during real bodily injection. The structural transitions measured in-situ by small angle neutron scattering reveal mixed oriented structures that can be exploited to tailor the load release profile and optimise processing.

Defective MOF Materials for Clean Air and Sustainable Energy

Yujie Ma

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The presence of active sites in porous materials can control and affect significantly their performance in adsorption and catalysis. However, fine tuning of the active sites and revealing the interactions between substrate and active sites in porous materials with atomic precision remains a challenging task. Metal-organic framework (MOF) materials adopt uniform and well-defined structures, are designable, and can show exceptional structural diversity, enabling the control of active sites at atomic precision. Here, we report a comprehensive investigation of the structures and the roles of atomically dispersed defects and metal sites in MOFs for adsorption of environmental pollutants and catalytic conversion into value-added chemicals, including ammonia (NH_3), nitrogen dioxide (NO_2), benzene and nitrate species.[1-5] Our studies provide valuable insights into the relationship between structure and adsorption/catalysis activity, and will inspire the further design and study of new efficient MOF sorbents/catalysts by targeted control of active sites.

References

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2. Ma, Y.; Lu, W. et al. Direct Observation of Ammonia Storage in UiO-66 Incorporating Cu(II) Binding Sites. *J. Am. Chem. Soc.* 2022, 144, 8624–8632.
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How Neutron Based Methods Have Augmented the Ability to Develop New Applications/Formulations

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Over the years since their inauguration, the methods based on neutrons, scattering and reflectivity, have become the undisputed "golden standard" when it comes to structural characterisation at molecular level. The availability of such methods has made possible to advance our understanding of how the building blocks of a formulation or the aggregation behaviours of newly synthesised molecules evolve at different conditions.

A very important lesson we have learnt over the years is, that neutrons should be the final test that brings answers to our hypothesis usually built upon more conventional techniques, e.g. surface tension, ellipsometry, QCM-D, Dynamic Light Scattering, etc. There are occasions when only neutrons are able to reveal some extraordinary phenomena, e.g. multilayering near an interface, that otherwise one cannot envisage only based on "conventional" techniques results.

In this talk an attempt will be made to manifest both the power and versatility of neutrons and how they have helped progressing certain hypothesis.

Solid-State Phase Transformations in Steels and their Effects on Weld Residual Stresses and Distortion

John Francis

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For safety-critical engineering components such as those that are employed in nuclear power plants, it is crucial to account for residual stresses that reside in the vicinity of welded joints. The development of these stresses and associated weld distortion is made more complex by the solid-state phase transformations that take place in many power-plant steels. Over the past 15 years or so, significant advances have been made in our understanding of the role that phase transformations in steels have on the development of weld residual stresses and distortion. This talk will provide an overview of the author's research on this topic and will highlight the crucial role that neutron scattering has played in enabling this research.

Unravelling the Structure of Glass with Neutrons

Paul A. Bingham

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The structure and properties of glasses and glassy materials have long fascinated physicists, solid state chemists, engineers and philosophers alike. Glasses now play a fundamental role in modern society, from mobile phone screens to toothpaste, windows, containers, optics and radioactive waste immobilisation. Indeed, arguably we are living in The Glass Age, and 2022 was designated the United Nations Year of Glass to celebrate the heritage and importance of glass in our lives. Yet, the fundamental composition-structure-property-application nexus of glass remains elusive to full understanding, and much research continues to be undertaken to make glasses stronger, better, cheaper, safer, more sustainable, with new or enhanced properties and performance. Neutron diffraction is a vital tool to better understand the atomic structure of glasses, being ideally suited in many ways to this task. Here we will explore our group's use of neutrons to better understand the fundamental atomic structure of different glasses relevant to commercial manufacture and radioactive waste immobilisation. Neutron diffraction has enabled us to develop greater understanding of mechanisms behind solubility in the glass network of components such as sulphate [1], and the role of network modifier ions such as sodium [2]. We will discuss the research presented in these papers and explore future possibilities for neutrons in the pursuit of knowledge and understanding of glassy materials.

References

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A perfect spy: how muons reveal the secrets of topological magnets

Tom Lancaster

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Muons have proven a valuable probe of exotic magnetic materials, such as one- and two-dimensional systems, and compounds hosting exotic excitations that can be described using topology - the study of shapes of objects and spaces. Here I will discuss investigations of topological magnetic excitations where we have used the muon beam at ISIS to probe the magnetism. These include the study of spinons in one-dimensional molecular spin-chain materials and searches for skyrmions. These examples demonstrate how the facilities hosted at ISIS allow powerful insights into the underlying magnetism of the materials.

Neutron scattering in materials design and discovery

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The need for new materials to tackle societal challenges in energy and sustainability is widely acknowledged. As demands for performance increase while resource constraints narrow available options, the vastness of composition, structure and process parameter space make the apparently simple questions of where to look for and how to then find the materials we need a grand challenge to contemporary physical science. This talk will emphasise that discovery synthesis of new inorganic materials is at the extreme forefront of this endeavour, and highlight the role that neutron scattering has played in determining the structures that underpin our understanding.

Using Muon Spectroscopy to probe solar cell materials

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Spin polarised muons are essentially heavy positive electrons, which act as tiny little magnetic gyroscopes, when implanted into materials. They are used to probe a range of different behaviours including superconductivity, quantum spin states and electronic transport. One research field they are utilised in is solar cell materials, where transport mechanisms and spin dynamics can be studied as a function of temperature, electric and magnetic field. This presentation overviews the work we have done on two different solar cell materials: conjugated polymers and metal-halide perovskites. The majority of the research was carried out on the HiFi beamline performing avoiding level crossing (ALC) measures as a function of magnetic field and temperature. These measurements allow us to determine the electron spin relaxation (eSR). For the conjugated polymers (polythiophenes), we investigated the effect of chain length, morphology and light on the eSR. It was determined that the eSR had two different characteristic energies associated with the intra-chain and inter-chain processes. While for the metal halide perovskites, we studied the change in eSR as a function of temperature for three different phases of NH2-CH2=NH2PbI3 (FALI) and determined that the solar active phase had a large change in eSR as a function of temperature compared to the other two non-active phases. Further for the metal halide perovskites (CH3NH3PbI3 (MALI) and FALI), we used the EMU beamline to study the hopping mechanism and relaxation rate as a function of magnetic field and temperature. It was found that the changes in the relaxation rate for MALI coincided with the structural phase transitions, and agreed with the published modelling for two different dynamic regimes.

A Journey Through Space and Time

Jayne Lawrence

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The structures of aggregates formed by amphiphilic lipids and surfactants have, for many years, been used to prepare a range of drug delivery vehicles. These vehicles vary from micelles and emulsions through to vesicles or liposomes, and to the lipid nanoparticles that were used for the delivery of the BioNTech/Pfizer vaccines, and which are now being examined in clinical trials to provide new treatments for cancer. It is important to note that these structures cannot be considered as inert and can be affected by the payload they carry and/or the biological environment they encounter when administered to a patient. This is particularly true if the drug itself is amphiphilic, as indeed many drugs are. Furthermore, the range of aggregate structures that can be formed by lipids/surfactants is enormous, although there are certain principles that can be uniformly applied to their design. For example, a knowledge of the amphiphilic tendency of molecules can predict the likely aggregate structure(s) that a lipid/ surfactant can form. If a drug delivery vehicle is to be effective, then it is essential to have a detailed knowledge of how lipid/surfactant structure can influence the nature of the vehicle formed. The presentation will detail how neutron scattering studies have enabled an understanding of how the structures of the lipid/surfactants influence the properties of the vesicles, microemulsions and LNPs they form and show how it has informed the design and manufacture of medicines and vaccines.

From thin films to polycrystals: using neutrons to probe magnetic structure in functional materials

Kelly Morrison

Physics, Loughborough University, UK

Neutrons are a useful tool for probing key properties of magnetic materials such as: whether the underlying magnetic structure is ferro- ferri- or antiferromagnetic; charting magnetic excitations such as magnons or spin fluctuations; or measuring the magnetisation as a function of depth in a thin film heterostructure.

In this talk I will be present some examples of using neutron techniques to understand fundamental properties of functional magnetic materials. This will include: (1) an investigation of magnetic excitations in a potential magnetocaloric material ($La(Fe,Si)_{13}$) measured by inelastic neutron scattering; and (2) a study of the spin Seebeck effect of a Fe_3O_4/Pt bilayer and the impact of Fe nanodroplet inclusions at the interface measured by neutron and x-ray reflectometry.

The Impact of Neutron Scattering in Understanding and Improving Engine Lubricants

David Growney

Research Chemist, Lubrizol, UK

The environmental impact of the internal combustion engine (ICE) is now under significant scrutiny. Using the correct engine lubricant formulating strategy is imperative for increased efficiency and reduced emissions, while the electrification of vehicles is also becoming more prevalent. In hybrid-electric vehicles, the ICE often operates at lower temperatures since work is shared with the electric motor. This can promote lubricant water and fuel ingress. On the other hand, the ICE is often smaller, meaning higher engine speeds and temperatures are possible, leading to increased potential for lubricant oxidation. Such extremes in temperature therefore impact lubricant requirements.

Overbased detergents are a class of engine lubricant additive that perform the primary role of acid neutralisation. They consist of an inverse micelle stabilising an amorphous metal carbonate (MCO_3) core (usually calcium or magnesium), acting as a supply of hard base. The MCO_3 particles are typically spherical (~5 nm radius), and surfactants are typically alkyl benzene sulfonic acids or alkyl salicylic acids which salt at the MCO_3 surface, stabilising the particles in the oil phase. Sulfuric and nitric acids can ingress with water in the combustion zone, and organic acids are formed from lubricant and fuel oxidation. Such acids must be neutralised to prevent engine corrosion, which can lead to reduced efficiency, increased emissions and potentially total engine failure. At the same time, overbased detergents contribute towards undesirable ash build-up in the vehicle exhaust aftertreatment system, and so additive concentration must be optimised. This presentation will showcase how small angle neutron scattering has enabled us to gain valuable structural and mechanistic understanding of overbased detergents, enabling formulators to optimise additive concentrations to meet today's needs.

Using Neutron Scattering to see the biology other techniques cannot reach.

Jeremy Lakey

Biosciences Institute, Newcastle University, UK

My research interests have generally involved membranes and those of the outer surface of Gram-negative bacteria in particular. How are they constructed, how do the membrane proteins and lipids interact, how do antibiotics cross them, and how can we make vaccines out of them? After understanding the proteins better, we used them to develop a series of nanoscale devices for sensing and also create a business. Neutrons are good for these studies in two ways. Firstly, they see inside the physical structures we use to make membrane models e.g. cuvettes, silicon blocks, metal housings. Secondly, and this is the big one, they allow us to use different contrasts to separate the complex components of these membranes. My talk will describe how this enabled us to study critical structures and dynamics invisible to other methods.

The Development Road Map for the ISIS Pulsed Neutron and Muon Source

Roger S Eccleston

ISIS Pulsed Neutron and Muon Source, Harwell, Oxfordshire, UK

The ISIS Pulsed Neutron and Muon Source has been operating for nearly 40 years. Through continuous development and significant upgrades, including the addition of a second target station, ISIS has continued to provide world-leading capability to a thriving international user base and deliver world-leading productivity.

The next wave of development of the instrument suite, the Endeavour Programme, which involves five significant instrument upgrades and the construction of four new instruments, is now underway and will be completed within ten years. A further wave of instrument development is proposed which will maximize the capacity and optimise capability.

Throughout 2021 and 2023 the synchrotron and high-power target station (Target Station 1) underwent a significant refurbishment to improve performance and serviceability. This extensive project is now complete and both target stations are fully operational. The ISIS Accelerator Strategy focuses on maximizing the performance of the source in terms for both beam current and reliability.

A feasibility study for a MW class source to replace ISIS, ISIS-II, is in progress, which includes a detailed analysis of technical options and the scientific specification.

An overview of plans for the future development of ISIS will be presented, including the Endeavor Programme and ISIS-II