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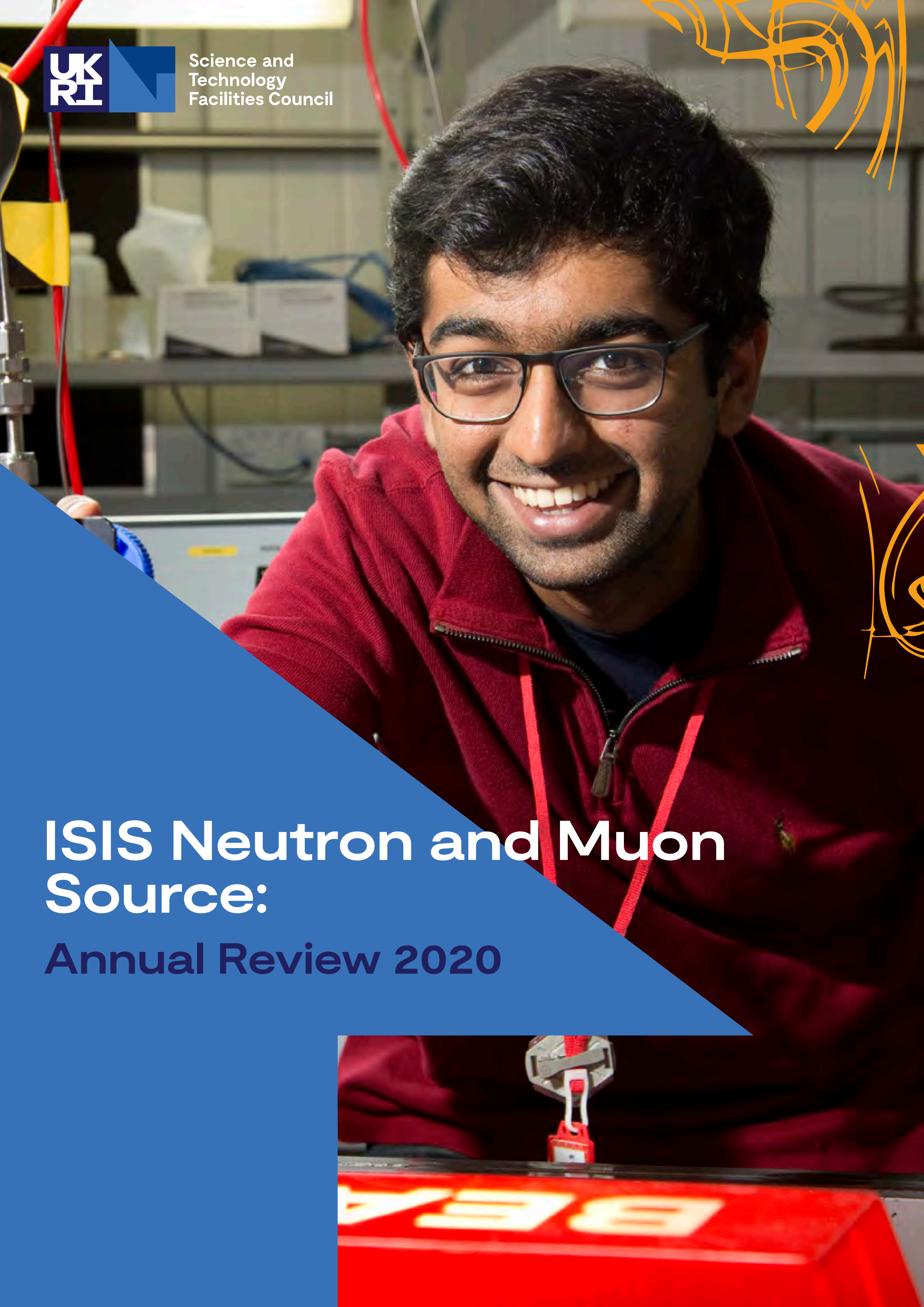

ISIS Neutron and Muon Source:

Annual Review 2020

ISIS Neutron and Muon Source Annual Review 2020 was produced for ISIS ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Oxford, Didcot, Oxfordshire, OX11 0QX

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Front cover: Mayank Jhalaria, Columbia University, USA, on the IRIS instrument.

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Foreword

Foreword

I never imagined that I would begin a foreword to an ISIS Annual Review by quoting from Forrest Gump, but this year it appears particularly apposite: "… life is like a box of chocolates; you never know what you're gonna get". In the 2018 foreword I suggested that we might miss the variety of collaborative fillings that we had enjoyed for several decades from the EU chocolate box, but at least we knew that was coming. This year, to use another popular culture analogy, we have been given a particularly bad bag of Bertie Botts Every Flavour Beans, without any warning.

However, although at the moment the bottom of the bag is not yet in sight, so far for ISIS the worst has certainly brought out the best in our staff. The business continuity plan that we had developed several years ago for pandemic flu was implemented. Within a very few days of the Covid-19 lockdown being announced in March we safely closed down ISIS operations and went from 500 staff on site to about 5.

> The business continuity plan that we had developed several years ago for pandemic flu was implemented. Within a very few days of the Covid-19 lockdown being announced in March we safely closed down ISIS operations and went from 500 staff on site to about 5.
> **– Robert McGreevy, ISIS Director**

Those who could moved rapidly to effective home working and frequent use of Zoom for keeping in touch, for both work and social purposes. Some of our technical staff, for whom remote working is less appropriate, were among the earliest volunteers helping VentilatorChallengeUK; others set up visor production supplying local health care organisations. But we also rapidly started the longer process of developing the safe methods of working to allow a future return to operation.

This work paid off. The majority of ISIS staff are now on site on a regular basis, with a mix of on-site and home working. The first cycle under Covid-19 constraints started and has proceeded remarkably smoothly, with accelerator records being set on several days. The science programme is running on most instruments at over 50% of 'normal' capacity and some users have been on site to do experiments. We believe that this mode of operation is sustainable unless prevented by government instructions.

Hopefully by the time that the foreword for the 2021 Annual Review is being written the beans will be finished and we will have some new chocolates to choose from. However, one thing is clear. The bad beans, whether pandemic or net zero-carbon flavour, can only be avoided or mitigated through scientific research and development. Facilities like ISIS, and researchers like our user community, will continue to be needed.

Left: STFC's Ventilator Challenge UK team tested and calibrated ventilators produced at Penlon's Abingdon facility as part of the Ventilator Challenge UK project Credit: STFC/Chris Pulker.

Overview

The ISIS Neutron and Muon Source is a world-leading centre for research at the STFC Rutherford Appleton Laboratory near Oxford. Our suite of neutron and muon instruments gives unique insights into the properties of materials on the atomic scale.

We are part of the global research infrastructure, providing tools for almost 1700 scientists a year to use our suite of 34 instruments.

Our science spans a wide range of disciplines, from magnetism to cultural heritage, engineering to food science, chemistry to environmental science.

We contribute to inspiring the next generation of scientists by welcoming over 1900 school pupils, teachers and general public to the facility as part of our public engagement programme as well as supporting training for apprentices, year-in-industry students, work experience students and graduates.

5 Muon instruments

29 Neutron instruments

1620 proposals received from **37** countries

300 Xpress proposals

4272 Visitors

Members of the public, schools and other visitors

new users **35%**

3361 user visits

unique research visitors **1680**

775 PhD students visited as users

(413 UK, 362 Intl)
4800 days of student training

108 Companies

Represent a variety of industrial areas, including chemicals, healthcare, automotive, materials, aerospace, engineering, energy and other high-tech companies.

561 Journal publications

The ISIS Neutron and Muon Source

Science at ISIS

64 Bioscience

11 Electronics

35 Engineering

561 Total Publications

163 Advanced materials

29 Energy

165 Chemistry

118 Physics

51 Life science

8 Heritage

Some papers fall into multiple categories

Left: ISIS users Adriana Mamede and Ana Batista De Carvalho, University Coimbra, Portugal, loading a sample for an experiment on the OSIRIS instrument.

Introduction

Industrial Use of ISIS

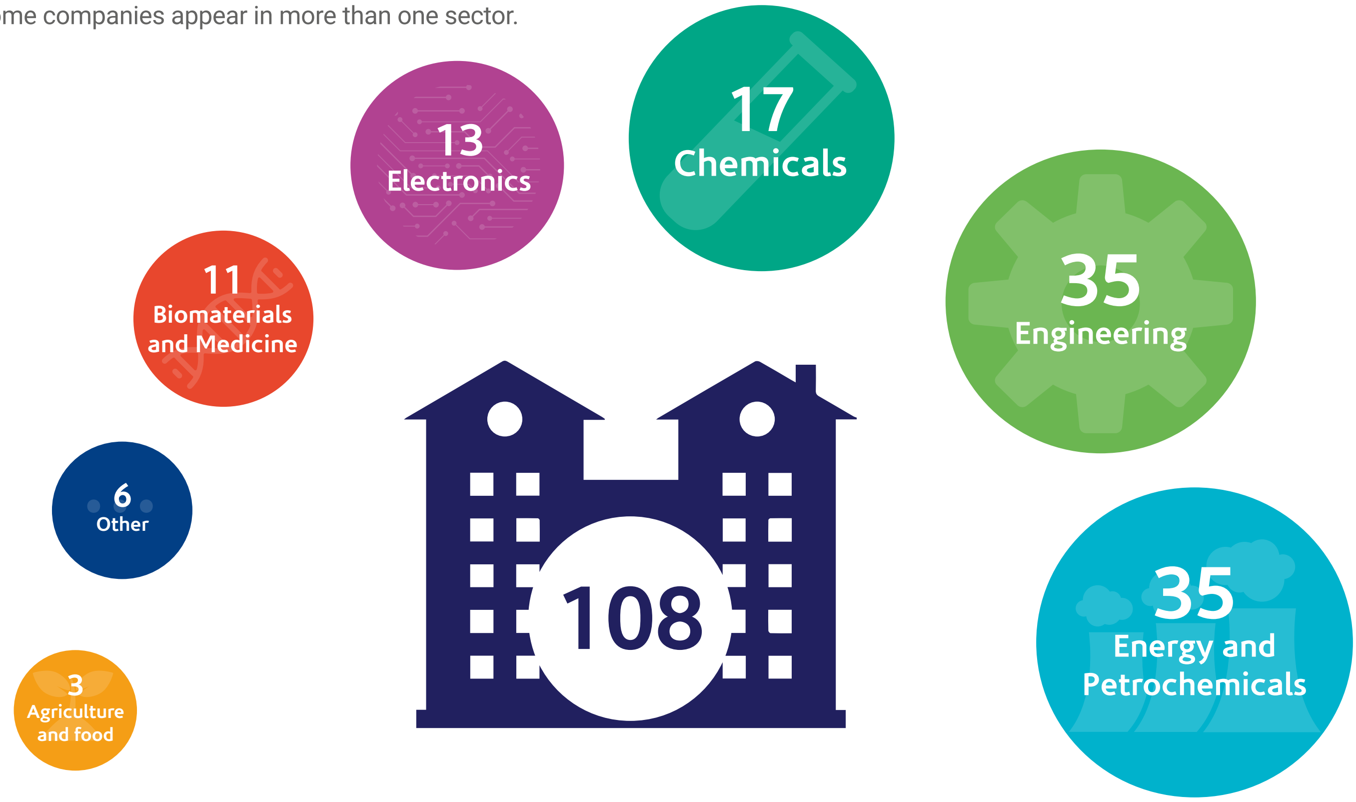
The number of industrial companies engaging with ISIS per year hit a new high of 108 in 2019, a record that shows that the properties of neutrons and muons can deliver key results and insights that translate into real economic benefit and impact. What is perhaps most impressive is that alongside the growth of the industrial use of ISIS we are also seeing a marked increase in the diversity of industries that are now using neutrons. Driven largely through partnerships with our academic users, neutrons have expanded from solving industrial problems in engineering, materials science and chemistry to solving problems within the agriculture and food sector, delivering key insights in the emerging areas of biomaterials and sustainable energy technologies and helping the electronic and avionic sectors deal with problems of reliability.

> Many companies already recognise the benefits of using neutrons, and we are seeing new companies using ISIS each year. - **Graham Appleby**

Investment by ISIS in new techniques and instrumentation and its development of new ways of accessing neutrons and muons, such as the Industrial Collaborative R&D scheme, are also helping to attract new industrial researchers and communities to neutron and muon science. The further potential of our collective community's expertise in the use of neutrons and muons for a whole variety of industrial and societal problems is something that the new ISIS Business Development Manager, Graham Appleby, is looking forward to fostering. "With my background in both neutron science and in industrial use of large scale photon sources in Europe, I am really excited by the potential that neutrons and muons have and how we can work with ISIS's academic and commercial users, to enhance ISIS industrial engagement across the UK and internationally."

Companies Engaging

Some companies appear in more than one sector.



Allergan plc.

Neutrons reveal water clusters that could explain the behaviour of amorphous pharmaceuticals

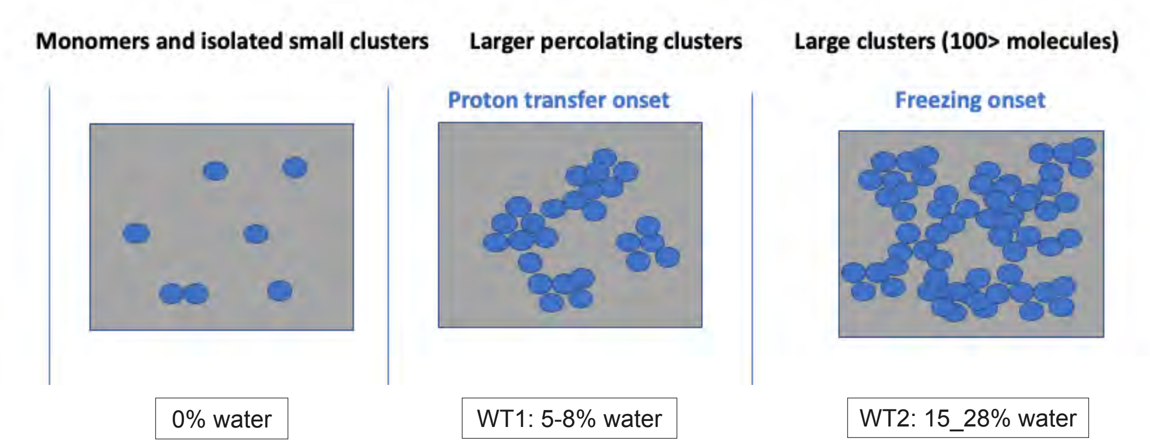
Amorphous solid (glassy) states are ubiquitous in both nature and industrial pharmaceutical products. For example, protein molecules are usually embedded in a freeze-dried amorphous sugar matrix to improve stability and shelf life.

The ability of molecules to move within the structure, or 'molecular mobility', has been traditionally thought of as the key property to consider when explaining the physical and chemical stability of diverse pharmaceutical systems. Although increased research efforts have begun to build up a comprehensive picture of the molecular mobility landscape, the relationship between molecular mobility and critical properties of amorphous pharmaceuticals is not straightforward.

The properties investigated in this study were the incomplete freezing leading to the existence of unfrozen water in aqueous solutions at sub-zero temperatures and the role of water in the chemical stability of amorphous pharmaceuticals. Using wide angle neutron scattering, the researchers observed nano-sized water clusters in aqueous pharmaceutical glasses and proposed that these clusters influenced both of the properties studied.

They demonstrated that the inhibition of freezing can be a direct consequence of the confinement of these water clusters in a solidified matrix of an amorphous solute. Considering the importance of proton transfer in many chemical processes, they suggest that the water cluster formation could catalyse proton transfer, promoting chemical instability.

> "Fundamental research at ISIS is essential in building scientific basis for development of novel pharmaceutical and biopharmaceutical products." *Dr Evgenyi Shalaev, Executive Director, Pharmaceutical Sciences, Allergan plc.*



Instrument: Sandals

Related publication: "Freezing of Aqueous Solutions and Chemical Stability of Amorphous Pharmaceuticals: Water Clusters Hypothesis." *J Pharm Sci., 108(1), 36-49 (2019)*

DOI: 10.1016/j.xphs.2018.07.018

Funding: EPSRC, Allergen Plc

Authors: E Shalaev (Allergan plc.), A Soper (ISIS), JA Zeitler (University of Cambridge), S Ohtake (Pfizer BioTherapeutics Pharmaceutical Sciences), CJ Roberts (University of Delaware), MJ Pikal (University of Connecticut), K Wu (Allergan plc.), E Boldyreva (Boreskov Institute of Catalysis SB RAS)

NVIDIA

Assessing the safety of driverless cars using Chiplr

Driverless vehicles rely on deep neural networks (DNNs) to respond to changes in the environment, and control the vehicle accordingly. Graphics processing units (GPUs) are used to provide the computational performance needed for these networks to dynamically detect and classify objects during autonomous driving operation.

The successful detection of obstacles, traffic and pedestrians is crucial when considering the safety implications of autonomous vehicles. It is therefore important to understand how vulnerable these networks are to hardware faults, when run on GPU-based platforms.

Faults can be permanent or transient, and caused by physical defects, the local environment or cosmic radiation. Any fault can impact the safety of the vehicle, and therefore it is crucial to understand the resilience of the neural networks used to these faults.

A group from NVIDIA used Chiplr at ISIS, and the Los Alamos Neutron Science Center, to perform accelerated neutron beam experiments to evaluate the sensitivity of such object detection networks to transient faults alongside investigations into the impact of permanent faults. Between the two testing sites, the group were able to test multiple GPU boards under the equivalent of 2000 years of exposure to ground-level neutron flux.

Using these results, they developed a methodology for determining the criticality of faults on the networks, and analysed the chip-level protection mechanisms in GPU architectures to test how effective they are at providing adequate coverage to faults. They found that the object detection networks are vulnerable to random hardware faults, but that existing chip-level protections successfully mitigate against the damage caused by transient faults.

"Measurement of the resilience to atmospheric neutron radiation is an important factor in meeting safety metrics for our automotive safety products; facilities such as ISIS help us accomplish that." *Dr Richard Bramley, GPU Architecture Group, NVIDIA*

Instrument: Chiplr

Related publication: "Resiliency of automotive object detection networks on GPU architectures." 2019 IEEE International Test Conference (ITC)

DOI: 10.1109/ITC44170.2019.9000150

Funding: NVIDIA

Authors: A Lotfi, S Hukerikar, K Balasubramanian, P Racunas, N Saxena, R Bramley, Y Huang (NVIDIA)

AkzoNobel

Beetle scales could hold the key to sustainable white paint

The beetles *Cyphochilus* and *Lepidiota Stigma* have scales on their wings that are exceptionally white. They are also thin and highly reflective, properties that do not occur often in nature. The colour is not due to pigmentation, but the complex nanostructure of the scales on the beetles' wings, which reflect light in a very special way. Similar effects are responsible for the iridescent colour of some bird feathers, and give polar bear fur its white appearance.

In collaboration with the coatings company AkzoNobel, the team investigated how to replicate the optical properties of the beetle scale nanostructure. Currently white paint contains nanoparticles of titanium dioxide, TiO_2. The industrial process to refine this nanomaterial has a significant carbon footprint and therefore a huge environmental impact. TiO_2 is responsible for around 75% of the embedded energy in a pot of paint, and is the most expensive component. Replacing it with a renewable bio-based polymer would make white paint much less damaging to the environment.

This study used the material cellulose acetate, from wood pulp, to recreate the nanostructure found in the beetle scales, and the technique of spin-echo small-angle neutron scattering (SESANS) on Larmor to confirm that the structure was equivalent to that within the beetle scale. Larmor's unique ability to directly measure real-space correlations at large length scales, and determine the material density of a porous structure, made it unequalled for investigating the properties of the amorphous network structures that give the beetle wings their structural white colour.

Dr Stephanie Burg (from the University of Sheffield) "Larmor's unique capabilities allowed us to determine the network properties of these incredibly fragile structures and draw important comparisons between the synthetic and biological specimens that would not have been possible otherwise."

In future, the ability to replicate structural colour in a paint using waste plastic or bio-derived materials could see titanium dioxide be replaced for much lower energy intensive materials and so reduce the impact and carbon footprint of all paint.

Dr Adam Washington (ISIS Neutron and Muon Source) said: "The structures we studied in these beetle scales are only accessible through a small number of techniques. Out of those techniques, only Larmor and the brightness of the ISIS source would let us examine hundreds of these scales in just a few days, instead of months".

Credit: University of Sheffield

Instrument: Larmor

Related publication: "Liquid-liquid phase separation morphologies in ultra-white beetle scales and a synthetic equivalent", *Commun Chem* 2, 100 (2019)

DOI: 10.1038/s42004-019-0202-8

Funding: Innovate UK in partnership with AkzoNobel and the University of Sheffield

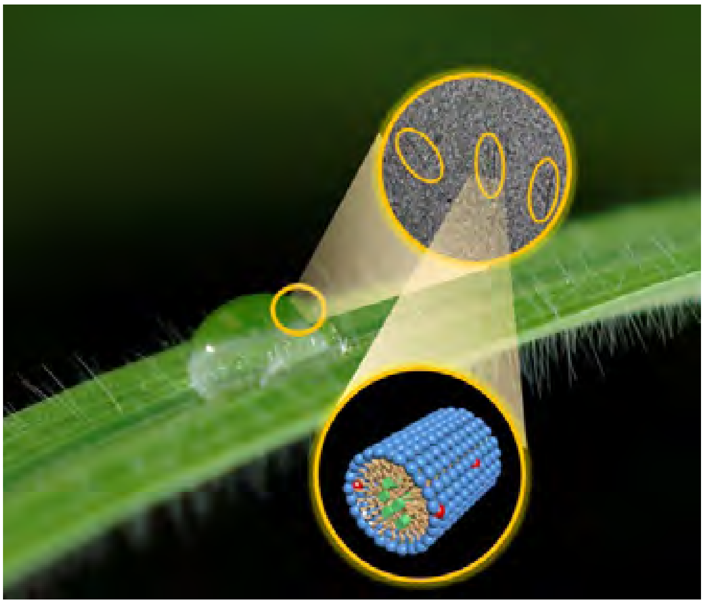
Authors: SL Burg (University of Sheffield), A Washington (University of Sheffield, ISIS), DM Coles, A Bianco (University of Sheffield), D McLoughlin (Akzo-Nobel), OO Mykhaylyk (University of Sheffield), J Villanova (ESRF), AJC Dennison, CJ Hill (University of Sheffield), P Vukusic (Exeter University), S Doak, SJ Martin, M Hutchings (Loughborough University), SR Parnell (Delft University of Technology), C Vasilev, N Clarke, AJ Ryan, W Furnass, M Croucher (University of Sheffield), RM Dalgliesh (ISIS), S Prevost (ESRF, ILL), R Dattani (ESRF), A Parker (University of Oxford), RAL Jones, JPA Fairclough, AJ Parnell (University of Sheffield)

Syngenta

Uncovering the effect of pesticides on the waxy layer of plants

Surfactants decrease the surface tension of the droplets in the agri-spray, increasing the contacting area on the spraying surface. They also absorb onto, and penetrate, the plant surface, creating a pathway for pesticides to diffuse into the plant itself. As a large proportion of pesticides have an extremely low water solubility, surfactants can also be used to improve their mobility by forming micelles, which act as capsules containing the pesticide.

When sprayed, the micelles come into contact with the thin wax layer on the outer surface of the plant. These waxes are predominantly hydrophobic, but contain polar alcohol and ester end groups that offer some weak hydrophilicity. Their amphiphilic nature may explain why the micelles take up wax molecules when they land on the plant surface. However, there is little knowledge about the exact molecular processes involved, and the impact on the pesticides when this happens.



Combining techniques such as proton nuclear magnetic resonance (H-NMR) and cryogenic transmission electron microscopy (Cryo-TEM) with SANS techniques using LOQ at ISIS, the research group examined the changes in micelles saturated with fungicide before and after wax solubilisation. Their study confirmed that the micelle nanostructures are heavily influenced by wax solubilisation and pesticide release. These initial findings have shown that agrochemical sprays are capable of dissolving the waxy layers on leaves, which may trigger surfactant micelles to release pesticides.

> "ISIS provides users with state of the art instruments that can provide us, as researchers, methods to probe deeper into our pesticide delivery and uptake system", *said Xuzhi Hu, from the University of Manchester*. "Our research is driven by both academic and industrial relevance which is enabled by the ISIS research facility; their incredibly helpful support staff and world leading experts provide a service that is second to none."

An image showing wheat waxes (green) solubilised inside a nonionic surfactant micelle in order to allow for the release of pesticides (red), provided by Xuzhi Hu & Jian Lu from the University of Manchester.

Instrument: LOQ

Related publication: "How does solubilisation of plant waxes into nonionic surfactant micelles affect pesticide release?" *J. Colloid Interface Sci.*, 556, 650-657 (2019)

DOI: 10.1016/j.jcis.2019.08.098

Funding: Syngenta, University of Manchester and the Chinese Scholarship Council

Authors: X Hu, H Gong, Z Li, S Ruane, H Liu, P Hollowell, E Pambou, C Brown (University of Manchester), S King, S Rogers, K Ma, P Li (ISIS), F Padia, G Bell (Syngenta), JR Lu (University of Manchester)

Will Jamieson

From sandwich student, to EngD, to industry

> As well as technical skills, my placement gave me valuable experience in learning patience, and using diplomacy to work with others.

Sandwich placement

During his Chemical Physics degree, Will Jamieson spent one year on a placement in the Materials Characterisation Lab at ISIS. This was the fourth year of his five-year integrated Masters from the University of Edinburgh. "My course required me to complete and write up a stand-alone project, which I did by synthesising and analysing a series of potential multiferroic materials," he explains.

"Almost all of the investigation techniques were new to me, which meant I learnt a lot during the placement. I also got to meet the users who used the lab, and collaborated on some of their projects." Will was even able to get his first publication based on work completed during his placement.

From the interview stage (which involved an overnight sleeper train from Edinburgh!) the placement caught his attention. "I find my skills are best applied when I have a lot of variety in my work, and the placement in the ISIS lab seemed the most interesting and varied of those I applied for. This was definitely the case – during the year I enjoyed working on many different user-led projects."

EngD studies

Will especially enjoyed seeing the mix of academic and industrial users come into the lab, and ISIS more generally. This encouraged him to look for industrially focussed PhD positions, and he began his EngD studies in 2014 at the Industrial Centre for Doctoral Training (CDT) in Offshore Renewable Energy (IDCORE), based out of Edinburgh.

The CDT saw him complete training modules for the majority of the first year, and work with an industrial partner for the remainder of the four years. "My project involved developing composites for wave energy systems at Zyba Ltd.; it was very much more like being in a company than a university. My placement gave me a good understanding of how companies work, and made me much better at managing my time, which was particularly helpful in dealing with deadlines for commercial projects."

"I was also able to look back on the experiments I'd seen being done at ISIS involving stress and strain measurements, and link these to the work I was doing. This really helped to put my work in context." He adds, "my time at ISIS was probably the first time I'd done any proper data analysis. I developed this during my EngD, and it's now really useful in my current role."

Working in industry

Will now works for the Energy Saving Trust as an Insight and Analytics Consultant. "I work within a team on a variety of projects, looking at how individuals, businesses and other organisations can reduce their emissions, maximise their energy efficiency and ultimately help deliver a more sustainable society. Having worked almost exclusively on the generation side of things during my EngD, it's good to be working on projects looking at technologies that are, or will become, a direct part of our everyday lives." Despite missing the lab, Will admits that computer-based working has its advantages during lockdown, as he can continue almost as normal.

"As well as technical skills, my placement gave me valuable experience in learning patience, and using diplomacy to work with others. I was very grateful for having an excellent manager, who I still keep in touch with." While at RAL, Will joined the Rec Soc Aunt Sally team, the Abingdon hockey club and Oxford University orchestras. The placements students got to know each other, and have met up a few times since. "It's interesting to see where everyone has ended up – the placements at RAL can lead you anywhere!"

Impact Awards

ISIS Impact Awards 2020

The third ISIS Impact Awards for facility users were presented in 2020, celebrating the socio-economic impact generated by the user community.

Science

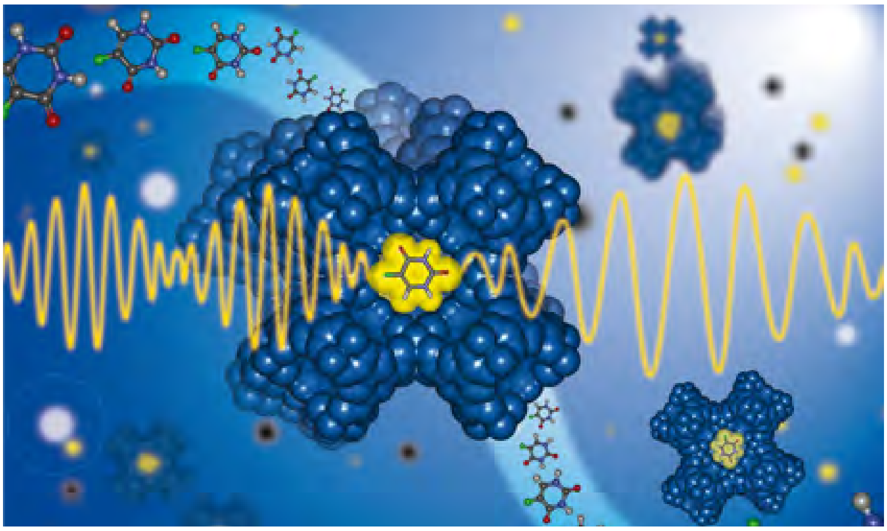
Professor Jin-Chong Tan, for his group's work on lattice dynamics in Metal-Organic Frameworks, and how this affects the way they absorb and release gases and drug molecules.

The winner of the Science Award is Professor Jin-Chong Tan from the University of Oxford, who leads the Multifunctional Materials & Composites Laboratory in the Department of Engineering Science. Since 2012, Jin-Chong's research group has used neutron vibrational spectroscopy at ISIS to investigate the distortions of Metal-Organic Framework (MOF) materials that enable them to absorb and release target molecules.

The way that a MOF framework distorts to enable the adsorption and release of molecules is important to understand, as controlling this could lead to a greater ability to direct the functionality. By studying the vibrational spectra of the MOFs using inelastic neutron scattering, and combining this with computational studies, Jin-Chong and his research group have been able to determine the behaviour of the MOF structure under low-frequency terahertz (THz) vibrations.

Their work revealed that the vibrational modes in the THz range are linked to the "gate opening" and pore "breathing" mechanisms of the framework, paving the way to an expanding area of research towards understanding of the role of THz vibrations in framework materials. This understanding has helped to identify ways the material could collapse under mechanical stress, and to develop new materials that are less prone to this kind of detrimental distortions. A deeper understanding of the THz modes also reveals opportunities for engineering new molecular sensors.

Building on this work, the group have investigated the low-frequency lattice vibrations of MOFs that have a molecule inside them, known as guest-encapsulated systems, including those containing anti-cancer drugs. The work has also led to the development of smart luminescent sensors that can detect toxic chemical compounds non-invasively, and sense changes in physical stimuli such as temperature and pressure.



An illustration of THz vibrations used to unravel the detailed behaviour of guest-host interactions by tracking the precise changes in its lattice dynamics.

Left: Alberto Viani, Centre of Excellence Tech, Czech Republic, and Heloisa Bordallo, University of Copenhagen, Denmark, on the IRIS instrument.

Society

Professor Paolo Rech, for his work developing artificial intelligence frameworks to improve the reliability of a driverless car's ability not to confuse a person with a post-box.

The winner of the Society Award is Paolo Rech, Associate Professor at the Institute of Informatics of the Federal University of Rio Grande do Sul, for his work investigating the effect of neutrons on the computing behind autonomous vehicles, and hence developing ways to improve the computing reliability.

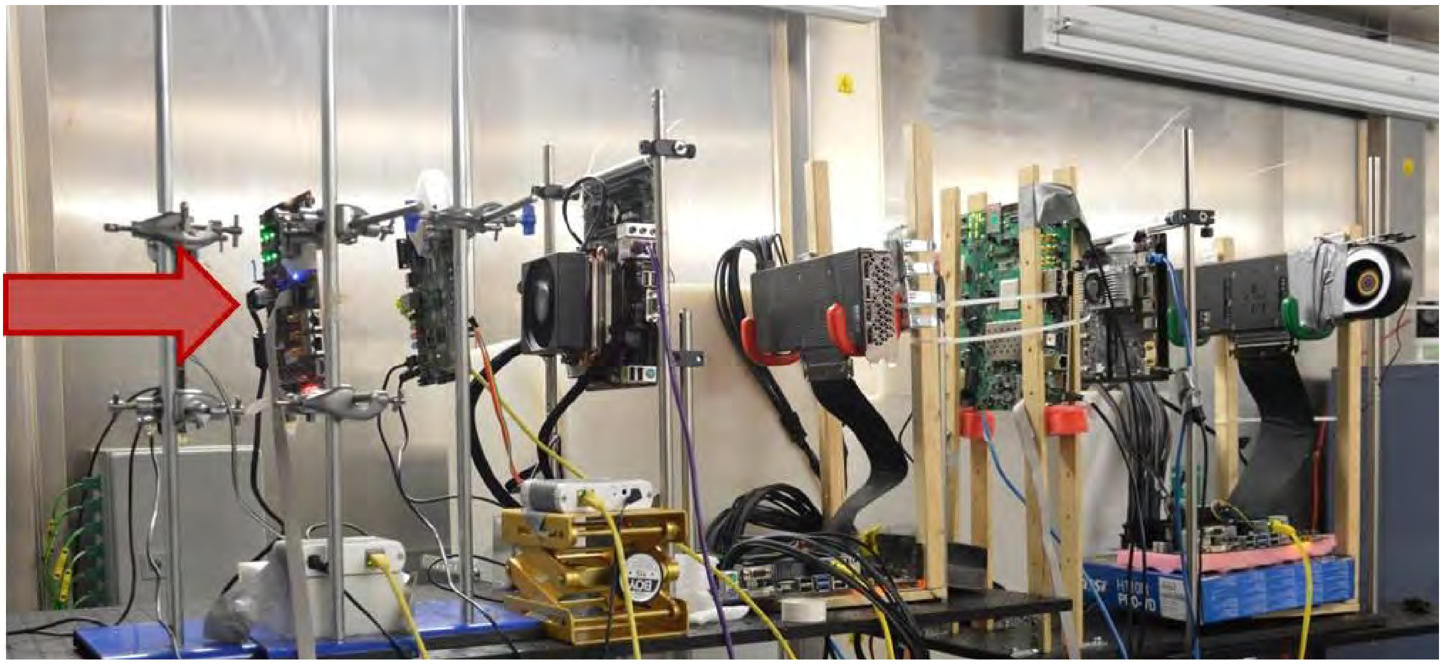
Atmospheric neutrons are known to generate faults in computing devices. The detection of objects is the most computationally demanding task for these vehicles, and is the task where the presence of errors causes the majority of accidents.

For a vehicle to detect objects such as pedestrians or other cars, images need to be processed in real-time. This requires cutting-edge hardware computing platforms that Paolo and his research group have found, through experiments on ChipIr, to have a failure rate of hundreds to thousands of times higher than the limit imposed by industry dependability standards.

The traditional solutions to these errors, such as hardware or software replication, are costly and disfavoured by the competitive automotive market. Paolo has worked with advanced devices designed by NVIDIA, AMD, ARM, Intel, and Xilinx using ChipIr to identify the errors that changed the computing behind the vehicle behaviour: the artificial neural networks.

By redesigning the artificial intelligence (AI) software that is used in object detection, Paolo and his group have managed to significantly reduce the probability of incorrect identification and detection. Testing their AI software on ChipIr, they found a reduction of more than 90% of errors with an overhead lower than 20% (0.01% in the best case).

Besides the automotive industry, their work has also had an impact on the space industry through a collaboration with the European Space Agency and NASA's Jet Propulsion Laboratory in the USA, using ChipIr to investigate the use of autonomous vehicles for space exploration.



Electronic samples being tested in ChipIr.

Economic

Dr Peter Albers, for his work over the last thirty years using neutrons alongside other methods to investigate materials with commercial applications, including catalysis.

The winner of the Economic Award is Peter Albers from Evonik Operations GmbH Technology & Infrastructure. Peter's work combining neutron scattering, electron microscopy and surface science (XPS, SIMS) to investigate materials of commercial relevance spans three major areas: carbons, silica and catalysts.

Peter has contributed significantly to the knowledge of the surface behaviour of precious metal catalysts, particularly platinum and palladium based materials. As an industrial user, his studies are carried out on commercial carbon supported palladium and platinum catalysts and the metal blacks that are used in industry every day, not model systems. The aim of his catalysis work has been to characterise the nature of hydrogen present on, or in, these catalysts.

Palladium (Pd) is well-known for absorbing hydrogen gas to form PdH, with the structure dependant on the concentration of hydrogen in the material. Using TOSCA and IN1-Lagrange, confirmed by density functional theory, Peter was able to observe an additional subsurface site for the hydrogen atoms, which was previously unreported. To detect hydrogen on this site for the first time, Peter used direct geometry spectrometry on MAPS and MERLIN. This work, alongside further experiments on SANDALS, enabled Peter and his research group to determine the mechanism of the hydrogen absorption by palladium. As this is the last site to be populated, it is likely they are the most reactive, and provide easy access for reactants.

Peter's well-established work at ISIS has provided the scientific community with the most detailed understanding currently available of the surface of palladium and platinum-based catalysts. By using ISIS, his employer Evonik gains a commercial advantage by being able to show that they have cutting-edge technical support for their products. Their continued use of neutron scattering for over twenty years is an illustration of its importance.

Dr Peter Albers (AQura GmbH, Germany), working in the Chemsistry Laboratory preparing hydrogen peroxide samples.

Science Highlights

MAPS

Iron Selenide: not as unique as expected

Previously thought of as a distinctive superconductor, researchers have used ISIS and other international facilities to show that iron selenide (FeSe) operates in the same way as other iron-based superconductors.

In FeSe, the iron atoms form a two-dimensional sheet sandwiched between two sheets of selenium. In other iron-based superconductors, these sheets are made of different elements. When the other elements are from Group 15 of the periodic table, the same as selenium, they are known as iron-pnictide superconductors. In some cases, including iron selenide, they exhibit a slight structural shift below a characteristic structural transition temperature, where the iron atoms move slightly further apart. This transition is associated with an anisotropic (directionally dependent) behaviour of electronic and magnetic properties, such as resistivity and spin fluctuations.

It has previously been impossible to measure the intrinsic anisotropy of these electronic and magnetic properties below the material's structural transition temperature. This is because of a property known as twinning, which occurs when layers of randomly oriented two-dimensional crystals are stacked and their individual differences are averaged.

Using a complex process involving gluing tiny FeSe crystals to larger crystals, the researchers were able to apply sufficient pressure to detwin the samples, finding that the spin fluctuations in FeSe are anisotropic, as in other iron-pnictide superconductors. This is evidence that superconductivity in different families of iron-based superconductors are of the same microscopic origin, suggesting that magnetism plays a critical role in unconventional superconductivity.

Tong Chen, a Rice PhD student, "detwinned" iron selenide crystals by gluing them atop much larger crystals of barium iron arsenide. Credit: Jeff Fitlow/Rice University.

Related publication: "Anisotropic spin fluctuations in detwinned FeSe." *Nat. Mater.* 18, 709–716 (2019)

DOI: 10.1038/s41563-019-0369-5

Funding: US Department of Energy, Robert A. Welch Foundation grant, National Natural Science Foundation of China and the Carlsberg Foundation

Authors: T Chen (Rice University), Y Chen (John Hopkins University), A Kreisel (Universität Leipzig), X Lu (Beijing Normal University), A Schneidewind (Jülich Center for Neutron Sciences at MLZ), Y Qiu (NIST Center for Neutron Research), JT Park (Heinz Maier-Leibnitz Zentrum), TG Perring, JR Stewart (ISIS), H Cao (Oak Ridge National Laboratory), R Zhang, Y Li (Rice University), Y Rong (Beijing Normal University), Y Wei (Chinese Academy of Sciences), BM Andersen (University of Copenhagen), PJ Hirschfeld (University of Florida), C Broholm (John Hopkins University, NIST Center for Neutron Research), P Dai (Rice University, Beijing Normal University)

Left: Nico Konig, University of Oslo, Norway, preparing a sample on the SANS2d instrument.

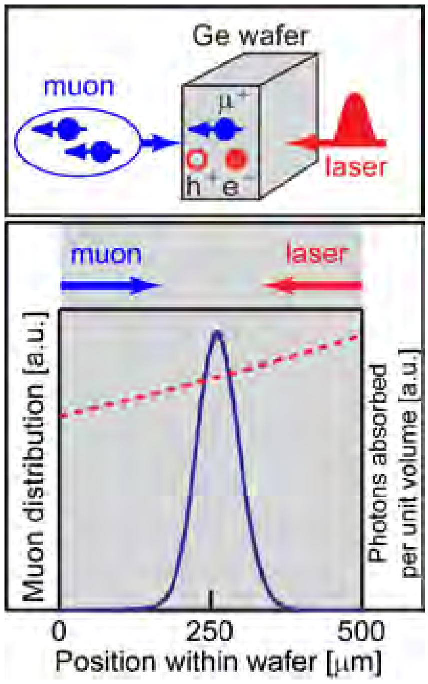
HiFi

Photoexcited μSR used to measure carrier kinetics in semiconductor materials

Knowledge of the kinetics of excess charge carriers (electrons and holes) in semiconductors is crucial when determining the performance of electronic devices such as solar cells or computer chips. The excess carrier recombination lifetime is a key figure of merit in photovoltaics applications that governs the efficiency of solar cells. However, traditional lifetime spectroscopy techniques currently used for characterisation only provide a bulk average for the material. The method described in this study, using photoexcited muon spin spectroscopy (photo-μSR), allows the carrier lifetime to be probed at a specific position within a wafer, giving a better picture of carrier dynamics.

When a positively charged anti-muon is implanted into a semiconducting material and localised in its crystalline lattice, it captures an electron to form muonium, a hydrogen-like species that can undergo spin and carrier exchange interactions with free electrons and holes. If there are more charge carriers present, then more of this exchange can occur, and the faster the measured muon spin relaxation. By combining this muon spin spectroscopy with optical carrier injection, the dynamics of the charge carriers can be investigated.

In this study, the researchers used the photo-μSR pump-probe technique on HiFi to measure the temperature dependence of the lifetime and mobility of the charge carriers inside germanium. Their results are in agreement with those using other methods, proving that photo-μSR can successfully be used to measure these kinetics. Based on the fact that muonium is a common state of implanted muons in a wide range of semiconductor materials, the method could contribute to the characterization of emerging functional materials, such as perovskite-structured compounds and wide-bandgap semiconductors.



Top: Schematic diagram of the experimental geometry. Bottom: Muon distribution (blue solid line) and photon flux (red broken line) as a function of depth measured from the surface on which muons are incident. The muon distribution has been calculated using a Monte Carlo simulation package based on GEANT4. Credit: K Yokoyama.

Related publication: "Muon probes of temperature-dependent charge carrier kinetics in semiconductors" *Appl. Phys. Lett.* 115, 112101 (2019)

DOI: 10.1063/1.5115596

Funding: STFC, Texas Research Incentive Program and the NMU Freshman Fellows Program

Authors: K Yokoyama, JS Lord (ISIS), PW Mengyan (Northern Michigan University, Texas Tech University), MR Goeks (Northern Michigan University), RL Lichti (Texas Tech University)

MuSR, EMU

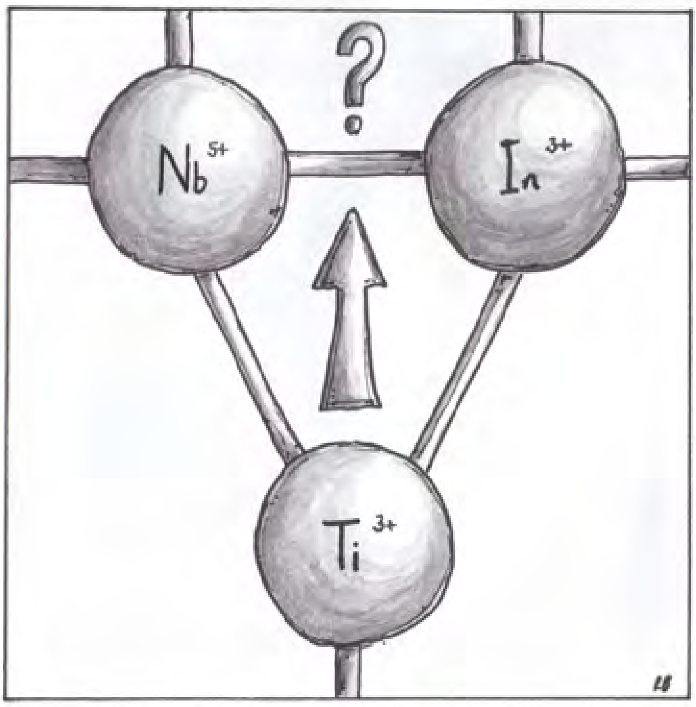
Muons show weak magnetism in a high capacitance, low loss dielectric material

For real world application in technological devices, materials are needed that show the novel dielectric behaviour of both high permittivity and low loss. This becomes even more interesting when they also exhibit magnetism. This coupling of electrical and magnetic properties is part of the recipe for multiferroics, which have great potential for use in future data storage devices.

Indium (In) and niobium (Nb) co-doped rutile (TiO_2) is one such compound that shows high permittivity and low loss that would make it ideal for capacitive devices. The inclusion of both In^{3+} and Nb^{5+} ions into the structure creates Ti^{3+} defects, each with a single electron localised within it. Although the dielectric properties of this material have been investigated, the magnetic behaviour has previously been overlooked.

This work used muon spin relaxation (μSR), which is an ideal probe of weak magnetism, on both the MuSR and EMU instruments to study the magnetic properties of the material for the first time. The researchers found that magnetic ordering, associated with spin freezing, occurred at room temperature and below, with the precise temperature dependence being related to the level of doping. From the μSR measurements, evidence was found for the doping and associated spin freezing being confined to the grain boundaries, the place at which the defects preferentially occur.

This location of ordering suggests that the formation of the magnetically ordered state could be prompted to occur at a higher temperature by introducing more boundaries into the material in the form of nanoparticles or thin films. Therefore, doped nanoparticles could be the next step towards the formation of materials that could offer even more technological impact.



Artists impression of an induced defect in In(III), Nb(V) co-doped rutile.

Related publication: "Understanding the role of electrons in the magnetism of a colossal permittivity dielectric material" *Mater. Horiz.*, 7, 188-192 (2020)

DOI: 10.1039/C9MH00983C

Funding: STFC

Authors: A Berlie (ISIS), I Terry (Durham University), SP Cottrell (ISIS), W Hu, Y Liu (Australian National University)

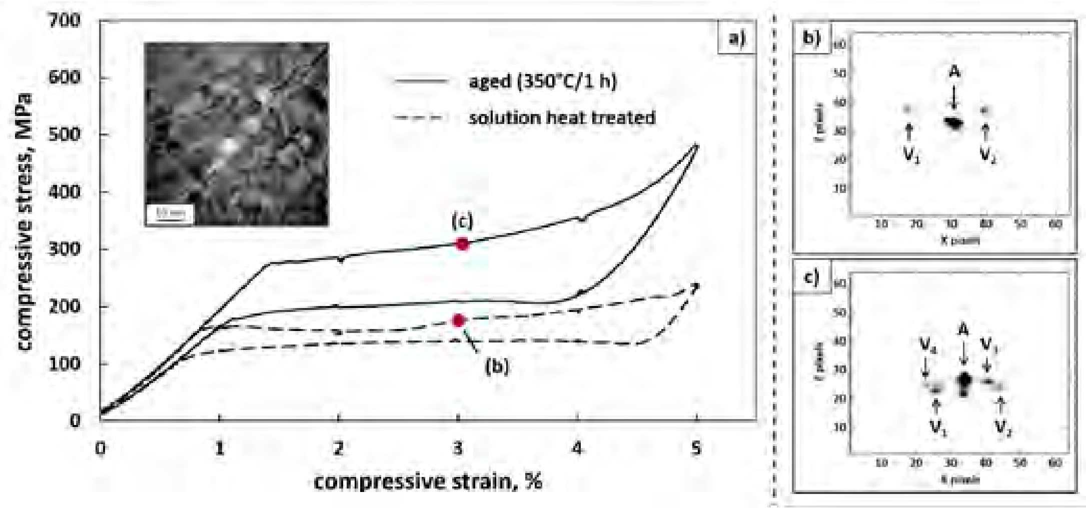
SXD

Nano-particles´ influence – how shape memory alloys behave under stress

A shape memory alloy (SMA) is one that can be shaped when cold, but then returns to its previous, "remembered", shape when heated. For the cobalt-nickel-gallium (Co-Ni-Ga) alloys, this transition is between an austenite structure and a tetragonal martensite structure. During the transformation, the austenite crystal lattice undergoes shearing in a particular direction. The 'martensite variants' are the different potential orientations of the shearing.

Co-Ni-Ga alloys have potential for higher-temperature applications due to their promising functional properties at elevated temperatures and good formability. To understand the morphology of martensite variants as they form, and their influence on the functional properties, this study used *in situ* optical microscopy and neutron diffraction on SXD to study the stress-induced martensitic transformation of $Co_{49}Ni_{21}Ga_{30}$ single crystals whilst they were undergoing compression cycles.

As well as studying a solution heat treated crystal, they studied an aged equivalent containing nano-sized particles, and discovered a big difference in the phase transition behaviour. In the solution heat treated crystal, the transition occurred via a single set of stress-induced martensite variants, whereas the presence of nano-particles caused the formation of two types of internally twinned variants. On applying further strain, they found that one was forming at the expense of the other, a process known as detwinning.



(a) Stress-strain curves of a ⟨001⟩-oriented Co-Ni-Ga crystal, solution heat treated (lower hysteresis) and subsequently aged (upper hysteresis), under compressive load at 100 °C. Spheroidal nanometric particles formed after aging are shown by the HRTEM image in the inset. (b,c) In situ neutron diffraction analysis of the solution heat treated (b) and aged (c) material at -3% compressive strain during the loading path as marked by the red points in (a).

Related publication: "Effect of nanometric γ'-particles on the stress-induced martensitic transformation in ⟨001⟩-oriented $Co_{49}Ni_{21}Ga_{30}$ shape memory alloy single crystals" *Scripta Materialia,* 168, 42-46 (2019)

DOI: 10.1016/j.scriptamat.2019.04.003

Funding: Deutsche Forschungsgemeinschaft and the Ministry of Science and Education of Russian Federation.

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Tosca

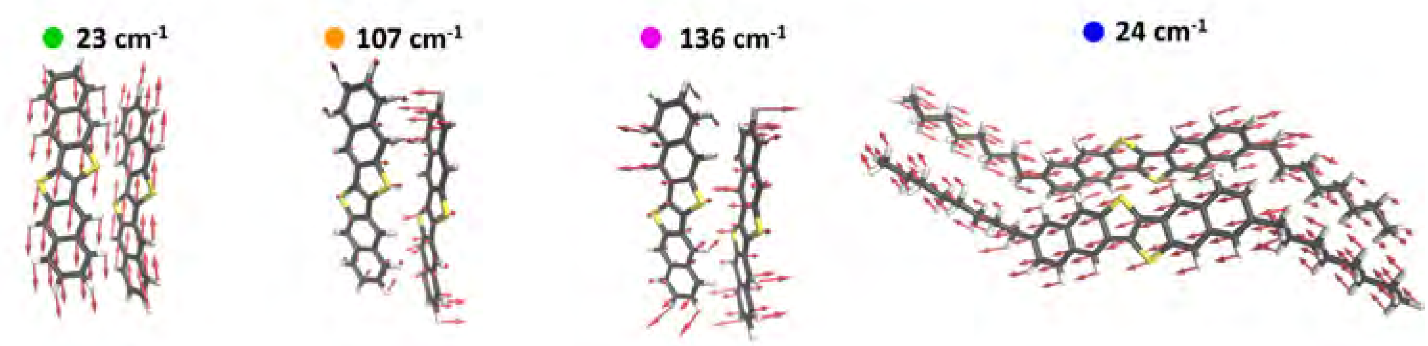
Discovery of "killer" phonon mode informs the search for new organic semiconductors

The electronic properties and the environmental and operational stability of organic semiconductors (OSCs) have improved considerably over the last ten years. The goal remains to find new materials that have higher carrier mobilities as this will enable faster operation and lower power consumption for use in advanced liquid crystal and organic light-emitting diode displays.

For high carrier mobility, the thermal molecular disorder needs to be minimised, as should the sensitivity of the carrier motion to this disorder. The sensitivity can be tuned through engineering of the molecular packing, but little is known about whether it is possible to influence the thermal disorder by molecular design. This results from the complexity of the unit cell of molecular crystals, typically containing on the order of 1000 atoms.

The vibration of these crystals can align in many different ways to produce hundreds of possible phonon modes, which can couple to the charge motion and contribute to thermal disorder. This study used terahertz time-domain spectroscopy and inelastic neutron scattering on TOSCA, coupled with computational modelling, to assess the contributions that individual modes make to the total thermal disorder in the OSCs pentacene, rubrene and a group of thienoacenes.

The researchers wanted to discover whether all the modes make important contributions to the disorder, or if there were specific "killer" modes that are responsible for the majority. Their results revealed that this was the case: a single sliding mode appears to be a "killer" mode: responsible for a large fraction of the total coupling. By considering the structural properties of the molecule that influences this sliding mode, the group's work will inform the quest for higher mobility semiconductors.



Relative displacements of neighbouring molecules associated with specific modes that contribute strongly to the energetic disorder.

Related publication: "Chasing the "Killer" Phonon Mode for the Rational Design of Low-Disorder, High-Mobility Molecular Semiconductors" *Advanced Materials,* 31, 43, 1902407, 2019

DOI: 10.1002/adma.201902407

Funding: EPSRC, Royal Society, German Research Foundation, European Research Council, ARCHER UK National Supercomputing Service, Belgian National Fund for Scientific Research

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Surf

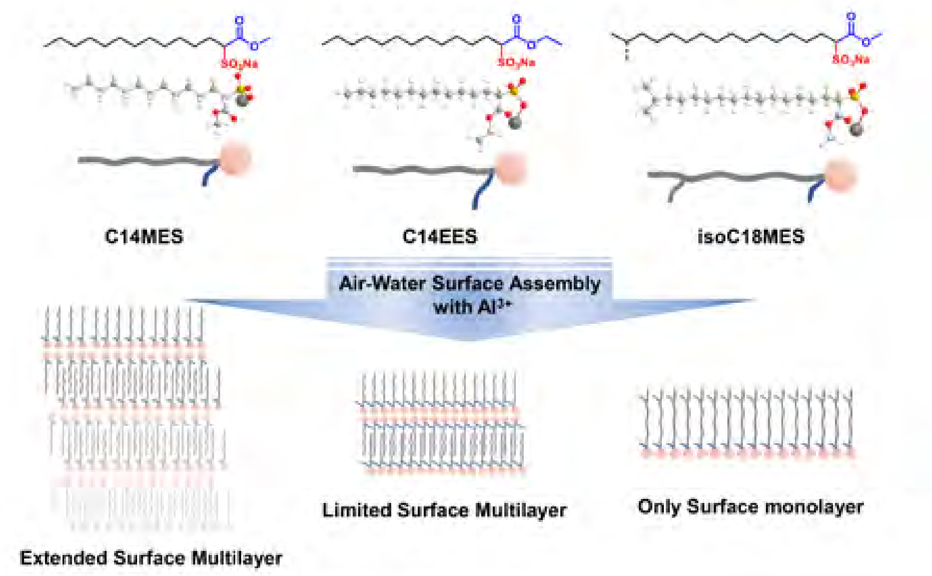
The effect of the headgroup and chain structure on surfactant behaviour at the surface

Anionic surfactants are the major surface active ingredient in most home and personal care products. The ester sulfonate surfactants are a class of anionic surfactants that exhibit increased tolerance to hard water, with a reduced tendency to precipitation in the presence of multivalent counterions. However, the addition of multivalent counterions results in the formation of multilayer structures at the air-solution interface, and is accompanied by advantageous wetting properties.

Changing the surfactant geometry, by altering the headgroup or the structure of the alkyl chain, can have a significant impact upon the nature of the surface adsorption induced by multivalent counterions. This study further investigated the impact of the changes in geometry by comparing surfactants with a branched isostearic alkyl chain to a linear saturated alkyl chain, and by modifying the headgroup from methyl- to ethyl-ester, in the MES (methyl ester sulfonate) surfactant.

Using neutron reflectivity on the SURF reflectometer the researchers found that, for the surfactants studied, in contrast to MES, more limited surface multilayer formation is observed with the addition of Al^{3+} counterions. This implies that the original Na^+ surfactant counterions are more strongly bound, and are therefore less readily displaced by the Al^{3+} ions.

Their results provide a crucial insight into how these subtle changes in surfactant geometry and structure can be used to manipulate their interaction with cations, and their associated surface properties.



Structure of the anionic ester sulfonate surfactants and its adsorption surface structures at the air water interface.

Related publication: "Impact of molecular structure, headgroup and alkyl chain geometry, on the adsorption of the anionic ester sulfonate surfactants at the air-solution interface, in the presence and absence of electrolyte" *JJournal of Colloid and Interface Science* 544, 293–302 (2019)

DOI: 10.1016/j.jcis.2019.03.011

Funding: China Scholarship Council. Samples were prepared at the ISIS deuteration facility

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LoQ

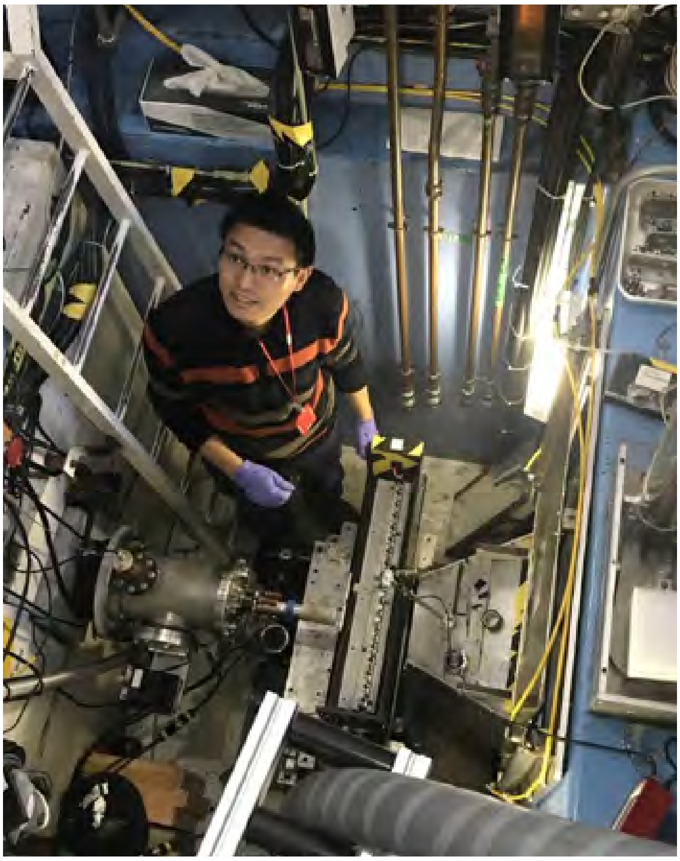
Cryo-SANS used for characterizing micellar structures at sub-zero temperatures

Some surfactants with specific architecture can self-assemble into wormlike micelles (WLMs) that show viscoelastic response macroscopically due to the entanglement of the WLMs. These surfactants are also called viscoelastic surfactants (VES) and they have been used in applications from oil production and drag reduction to personal care. Most of the documented results on VES are obtained at room temperature or high temperature.

However, few studies have been reported on the WLMs formed under sub-zero temperatures, cryo-VES fluids, mainly due to the limitation of the instruments available for use in freezing environment. In this study, the researchers made a series of cryo-VES fluids and found from rheological testing that they showed viscoelastic behaviours sub-zero temperatures, and increased viscosity upon decreasing the temperature.

To gain insight into the microstructures of these cryo-VES, with the aim of explaining these macroscopic responses, deuterated versions of these fluids were characterised by the ISIS deuteration facility, and small angle neutron scattering (SANS) experiments were designed and performed on Loq between 20 and –20 °C. The cryo-SANS results revealed that WLMs could still be formed at extremely low temperature, and the viscosity change is due to the transformation from spherical to worm-like micelles that occurs when decreasing the temperature.

This study is the first to describe cryo-WLMs, and the first to characterise micellar microstructures using cryo-SANS. These cryo-VES fluids may find potential use in hydro-fracking operations in arctic areas and aircraft de-icing fluids, replacing traditional polymer-based counterparts.



Dr Hongyao Yin, Sichuan University, working on the cryo-SANS cells of LoQ instrument.

Related publications: "Cryogenic viscoelastic surfactant fluids: Fabrication and application in a subzero environment." *J Colloid Interface Sci.*, 551, 89-100 (2019), "Cryogenic wormlike micelles." Soft Matter, 15, 2511-2516 (2019)

DOI: 10.1016/j.jcis.2019.05.011, 10.1039/c9sm00068b

Funding: National Natural Science Foundation of China, Sichuan University Postdoctoral Sustentation Fund. Samples were prepared at the ISIS deuteration facility

Authors: H Yin, Y Feng (Sichuan University), P Li, J Doutch (ISIS), Y Han, Y Mei (The Second Research Institute of Civil Aviation Administration of China (CAAC))

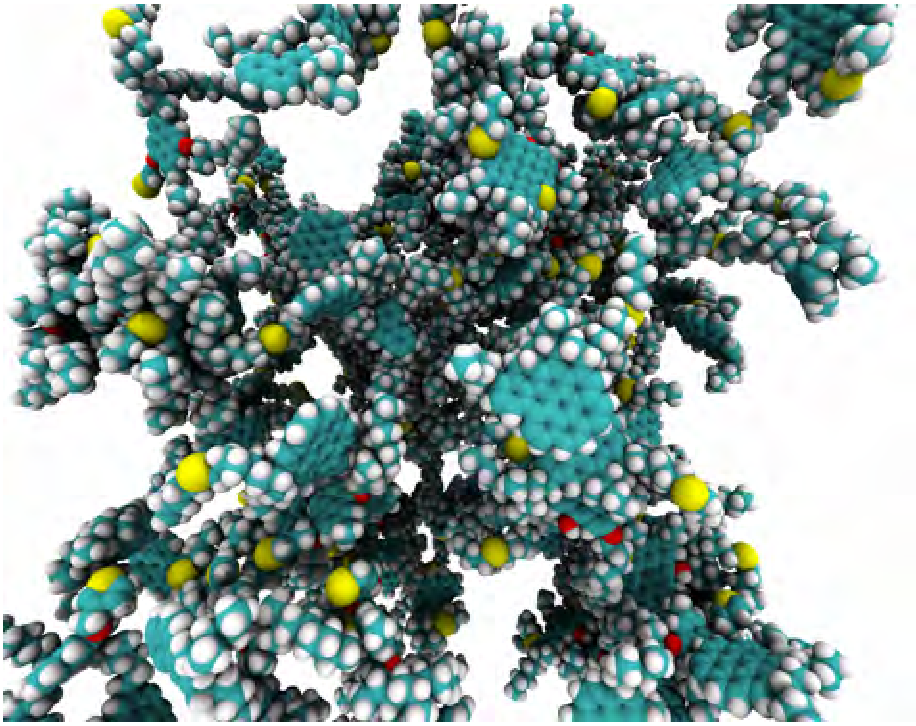
Nimrod

Verifying the molecular dynamics calculations of asphaltene aggregates

Asphaltenes are the most complex fraction of crude oil, accounting for a number of undesirable properties such as high viscosity, wettability alteration, and precipitation from the oil leading to fouling of equipment and blockage of pipelines. Computational modelling of a crude oil holds the promise of being able to predict if an oil is likely to precipitate, or perform a wide scan of potential chemical inhibitors, using only a small amount of experimental data. Correctly modelling the structure and behaviour of asphaltenes at the molecular level is therefore key for ensuring the validity of these computational studies. Neutron total scattering data can be directly calculated from the structures observed in molecular simulation, and provides a vital experimental yardstick of these computational methods and models.

This study looked at asphaltene solutions and solids using small-angle and wide-angle scattering on Nimrod and was, for the first time, compared directly to the results of widely used molecular dynamics models. The simulation correctly predicted the form of the scattering curves, however the study highlighted areas where the modelling could be improved.

In particular, the researchers found that the size of the system a simulated needs to be increased to accurately compare the simulation outputs. Analysis of the wide-angle regime highlights the need to refine the molecular structural models of asphaltenes or modify the simulation approaches as the predicted intermolecular structure deviated significantly from experimental observations. The team are now actively pursuing methods to increase the simulation size, within computational constraints, which will allow for a much more detailed and valuable comparison to experiment.



A snapshot from a molecular dynamics simulation of asphaltenes in 1-methylnaphthalene (solvent not shown for clarity). Credit: Tom Headen.

Related publication: "Predicting Asphaltene Aggregate Structure from Molecular Dynamics Simulation: Comparison to Neutron Total Scattering Data." *Energy Fuels, 33, 5, 3787–3795 (2019)*

DOI: 10.1016/j.ces.2019.07.023

Funding: EPSRC, US National Science Foundation

Authors: TF Headen (ISIS), MP Hoepfner (The University of Utah)

EMU

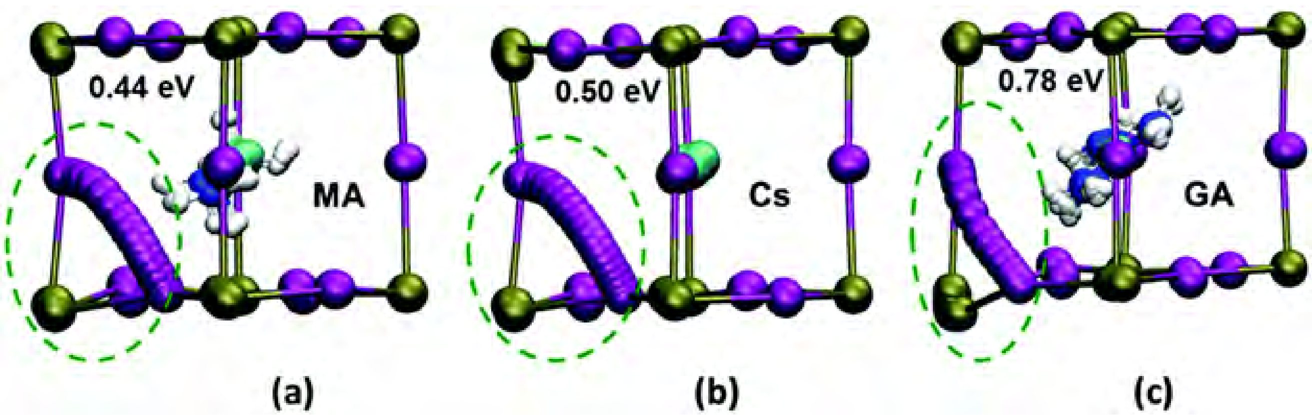
Insight into the impact of iodide ion movement in solar cells

Muon experiments have helped researchers study the movement of iodide ions within a new family of solar cell materials; reducing this movement could improve the efficiency of the devices. Halide perovskites are a series of materials that are used to make solar cells, and have developed rapidly over the last ten years to have high power conversion efficiency. The cells have the potential be made more cheaply than other competing technologies, but suffer from time dependent changes in the standard 'current-voltage' curves which are used to characterise cell efficiency, a process known as hysteresis.

The study investigated lead (Pb) iodide perovskites with the formula $MAPbI_3$, where 'MA' is methyl ammonium. They focussed on the iodide ion transport inside the material by partially substituting the MA with other cations, ranging in size from small rubidium to large guanidinium. They also studied how well solar cells of these substituted materials performed.

Computer modelling was used to study the paths that iodide ions would need to take through the material. Muon Spin Relaxation on EMU was used to detect ions moving inside the material, and Impedance Spectroscopy showed how well ions could (or couldn't) move within the material at different temperatures.

The results from all three techniques showed strong agreement: swapping just 5% of the MA for the larger GA ion increased the activation energy for iodide ion transport relative to pure $MAPbI_3$ as, when a bigger cation is present and distorts the structure, the iodide has to follow a more difficult curved path. This combined study has enhanced the fundamental understanding of mixed-cation perovskites, and provides a design strategy for reducing iodide ion transport that has important implications for improving solar cell performance.



Iodide ion transport paths and energetics. Ab initio simulations of the ion transport paths (using 18 intermediate images), the activation energies and the lattice ion displacements in (a) $MAPbI_3$ (b) $MA_{0.75}Cs_{0.25}PbI_3$ and (c) $MA_{0.75}GA_{0.25}PbI_3$. (Key: Pb, green; I, purple.) Local lattice relaxations near the diffusion path are highlighted by green circles, showing greater structural distortion in the GA-substituted material. Displacement values of the adjacent Pb ion in $MAPbI_3$, $MA_{0.75}Cs_{0.25}PbI_3$ and $MA_{0.75}GA_{0.25}PbI_3$ are 0.2, 0.2 and 0.6 Å respectively.

Related publication: "Partial cation substitution reduces iodide ion transport in lead iodide perovskite solar cells." *Energy Environ. Sci.*, 2019, 12, 2264-2272

DOI: 10.1039/C9EE00476A

Funding: EPSRC, University of Bath, EU Horizon 2020

Authors: DW Ferdani, SR Pering, D Ghosh, P Kubiak, AB Walker, SE Lewis, AL Johnson (University of Bath), PJ Baker (ISIS), MS Islam, PJ Cameron (University of Bath)

HiFi

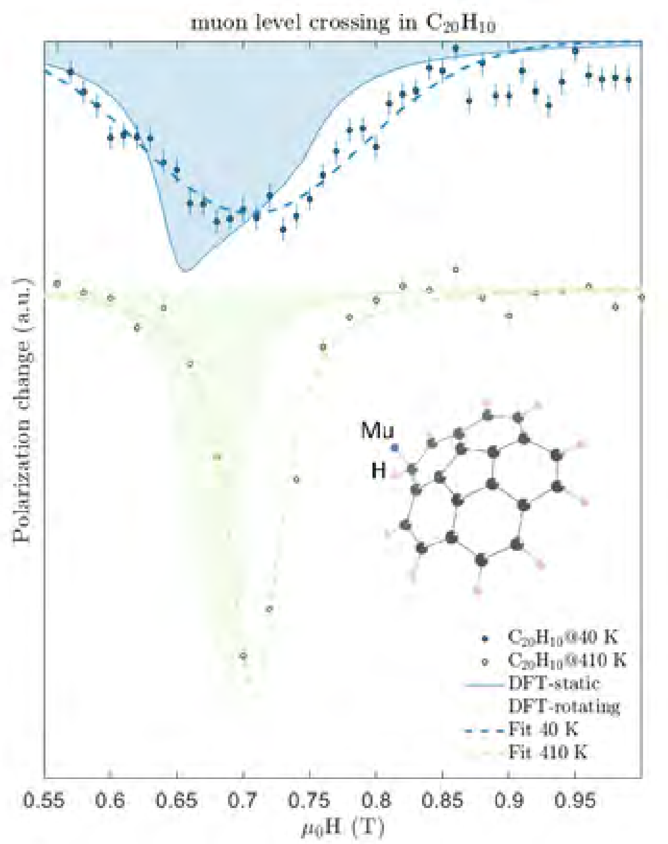
Corannulene shows promise as a hydrogen store

Carbon nanostructures such as fullerene buckyballs have shown potential for use as hydrogen storage systems. The presence of a curved structure enables the reversible formation of covalent bonds with atomic hydrogen as well as coordination with molecular hydrogen, H_2. Corannulene ($C_{20}H_{10}$) has a cup-like shape, and so could show the same possible storage potential.

This study used muon-spin spectroscopy on HiFi in combination with physisorption analysis to investigate the possible interactions between corannulene with both molecular and atomic hydrogen. The use of muonium as proxy for atomic hydrogen enables the collection of valuable information about the behaviour of atomic hydrogen, while the gas-physisorption analysis was able to measure the hydrogen diffusion through the crystal.

The results indicate that hydrogen molecules are able to diffuse through the bulk of the open crystal structure of corannulene and that there is a high affinity for the hydrogen atoms to form covalent bonds, illustrated by the formation of stable muonium adducts at all possible active sites of the corannulene molecule.

Their results suggest that corannulene could be exploited as a novel platform for hydrogen capture and storage, when combined with a suitable catalyst to promote H_2 dissociation, and that doping with alkali ions could bring this storage into a practical temperature range.



Muon resonance (μLCR) signal at 40 and and 410 K for the outer hydrogen-like adduct radical in Corannulene. Solid and dashed lines represent respectively the DFT-modelled polarization and fitting to Gaussian (40 K) or Lorenzian (410 K) lineshapes. Peak narrowing at 410 K suggests an activated dynamics in the high temperature phase.

Related publication: "The interaction of hydrogen with corannulene, a promising new platform for energy storage." *Carbon,* 155, 432-437 (2019)

DOI: 10.1016/j.carbon.2019.08.087

Funding: EPSRC

Authors: M Gaboardi (Elettra, ISIS), F Pratt (ISIS), C Milanese (Universitá Degli Studi di Pavia), J Taylor (ISIS), J Siegel (Tianjin University), F Fernandez-Alonso (ISIS, University College London)

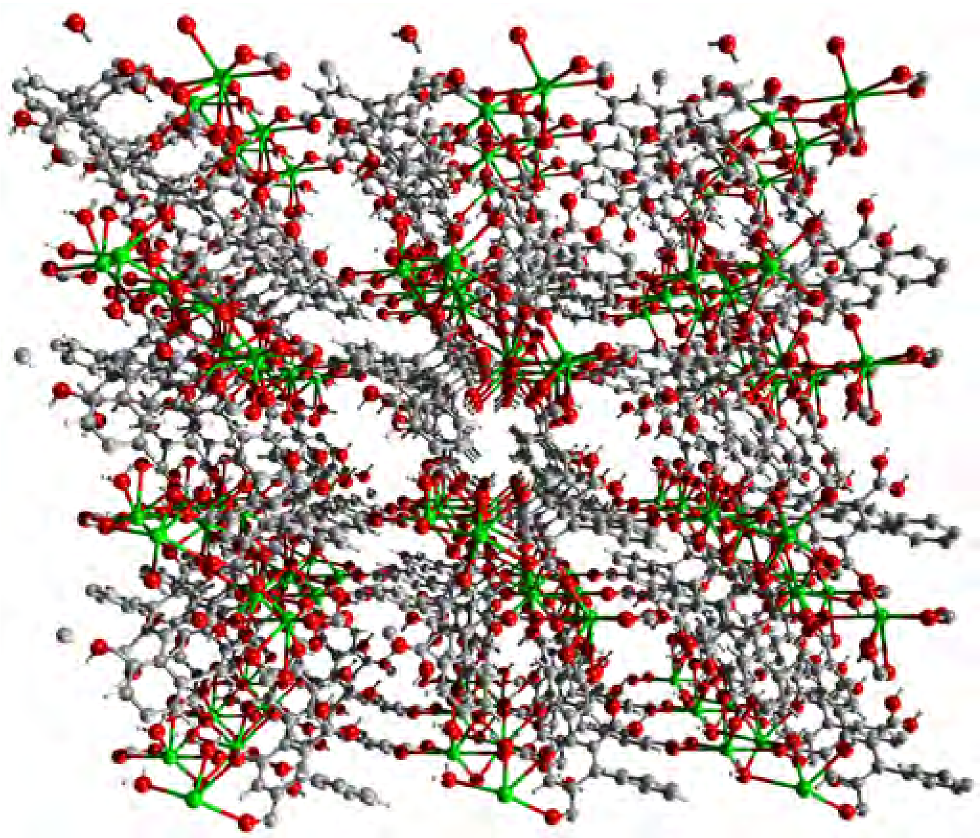
Iris

Manipulating MOFs to improve proton conduction

Proton exchange membrane fuel cells have the potential for widespread use in a hydrogen-based economy. Crucial to their design is the presence of a material to act as the membrane that efficiently transfers protons from one side of the cell to the other. The polymer Nafion is currently the most widespread membrane material but, in recent years, hybrid metal organic framework (MOF) materials have been made that show efficient proton transfer.

In this study, the group of researchers designed and synthesised three organic linkers, which they used to build three new MOFs. By measuring their proton conductivity, and comparing it to the structure, they were able to show that, by incorporating free and accessible carboxylic acid groups into the MOFs, proton conductivity can be increased.

Looking to further analyse their findings, and to understand the mechanism behind this increase in conduction, they measured one of their new MOFs, MFM-512, on Iris using quasi-elastic neutron scattering. Using neutrons, they were able to study the movement of the hydrogen atoms, and determine that the proton conduction is mediated by the model of "free diffusion inside a sphere" rather than "jump diffusion between sites".



The structure of MFM-512, Credit: Sihai Yang.

Related publication: "Modulating proton diffusion and conductivity in metal–organic frameworks by incorporation of accessible free carboxylic acid groups" *Chem. Sci.*, 10, 1492-1499 (2019)

DOI: 10.1039/C8SC03022G

Funding: EPSRC, ERC, Royal Society and University of Manchester

Authors: P Rought, C Marsh, S Pili (University of Manchester), IP Silverwood, V Garcia Sakai (ISIS), M Li (University of Nottingham), MS Brown (University of Manchester), SP Argent (University of Warwick), I Vitorica-Yrezabal, G Whitehead (University of Manchester), MR Warren (Diamond Light Source), S Yang, M Schröder (University of Manchester)

Tosca

Sulfur Dioxide: from toxic gas to industrial ingredient

An international team, led by scientists from the University of Manchester, have developed a new material that can reversibly adsorb sulfur dioxide from waste gas streams. The group developed a metal-organic framework (MOF), MFM-170, that can selectively take in toxic sulfur dioxide (SO_2) gas at record concentrations and preserve it for use in chemical production.

Using inelastic neutron scattering on Tosca, infrared and X-ray diffraction experiments at Diamond Light Source, and other facilities in the USA, the research group was able to do comprehensive studies *in operando*. This enabled them to observe the adsorption of SO_2 in real time, and determine the precise host-guest binding of the sulfur dioxide within MFM-170 at a molecular level.

The group found that MFM-170 showed a higher adsorption of SO_2 than any other porous material known to date. This is unprecedented as, unlike many other metal-organic frameworks, MFM-170 is remarkably stable to SO_2 exposure, even in the presence of water. The adsorption is also fully reversible at room temperature.

The publication also describes the scale-up of MFM-170 and its successful implementation for dynamic separation of SO_2 from gas mixtures that replicate those found in industry.

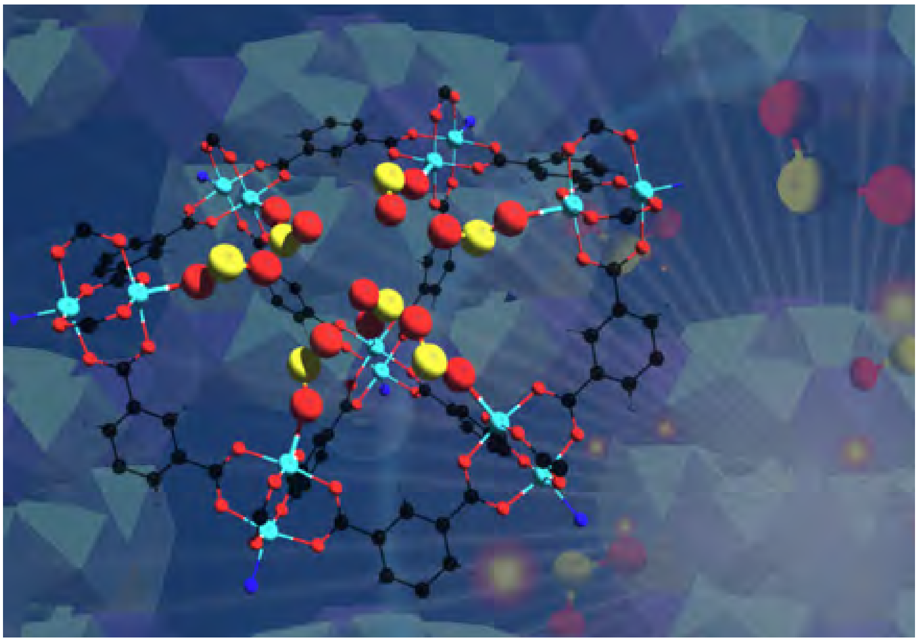


Illustration of sulfur dioxide captured within the material, MFM-170.

Related publication: "Reversible coordinative binding and separation of sulfur dioxide in a robust metal–organic framework with open copper sites." *Nat. Mater.* 18, 1358–1365 (2019)

DOI: 10.1038/s41563-019-0495-0

Funding: EPSRC (EP/I011870), ERC (AdG 742041), the Royal Society and University of Manchester

Authors: GL Smith, JE Eyley, X Han, X Zhang, J Li, NM Jacques, HGW Godfrey (University of Manchester), SP Argent (University of Nottingham), LJ McCormick McPherson, SJ Teat (Advanced Light Source), Y Cheng (Oak Ridge National Laboratory), MD Frogley, G Cinque, SJ Day, CC Tang (Diamond Light Source), TL Easun (Cardiff University), S Rudić (ISIS), AJ Ramirez-Cuesta (Oak Ridge National Laboratory), S Yang, M Schröder (University of Manchester)

Nimrod

New lanthanide liquids for greener materials

Deep eutectic solvents (DES) are mixtures of molecular and ionic compounds that melt at a temperature lower than their constituent parts, forming a partially ionic liquid phase. They are often based around choline chloride or urea, and are potentially a more environmentally friendly replacement for traditional organic solvents.

The inclusion of lanthanide ions has the potential to produce a DES that is task specific, and that could be used as a precursor to lanthanide-containing materials such as magnets, lasers and superconductors. This study describes the synthesis of the first lanthanide DES based on a mixture of urea and lanthanide nitrate hydrates, and its structural resolution using X-ray diffraction and neutron scattering.

The researchers found that in their cerium (Ce) based DES, the nanostructure is dominated by Ce-O interactions, forming a variety of [-Ce-NO_3-] networks. The formation of this ionic pseudophase causes the co-creation of a molecular rich pseudophase alongside it. This insight into the structure of these liquids helps to explain some of their unusual properties, and challenges the definition of what makes a DES.

Photographs of the lanthanide DES have colours dependent on the cation: (a) clear: 3.5 Urea : 1 $Ce(NO_3)_3.6H_2O$, (b) green: 3.5 Urea : 1 $Pr(NO_3)_{3.6}H_2O$, and (c) purple: 3.5 Urea : 1 $Nd(NO_3)_{3.6}H_2O$ LnDES, taken under Hg-vapor fluorescent strip lighting.

Related publication: "Structure and Properties of "Type IV" Lanthanide Nitrate Hydrate: Urea Deep Eutectic Solvents" *ACS Sustainable Chem. Eng.*, 7, 5, 4932–4940 (2019)

DOI: 10.1021/acssuschemeng.8b05548

Funding: STFC, EPSRC

Authors: OS Hammond (University of Bath), DT Bowron (ISIS), KJ Edler (University of Bath)

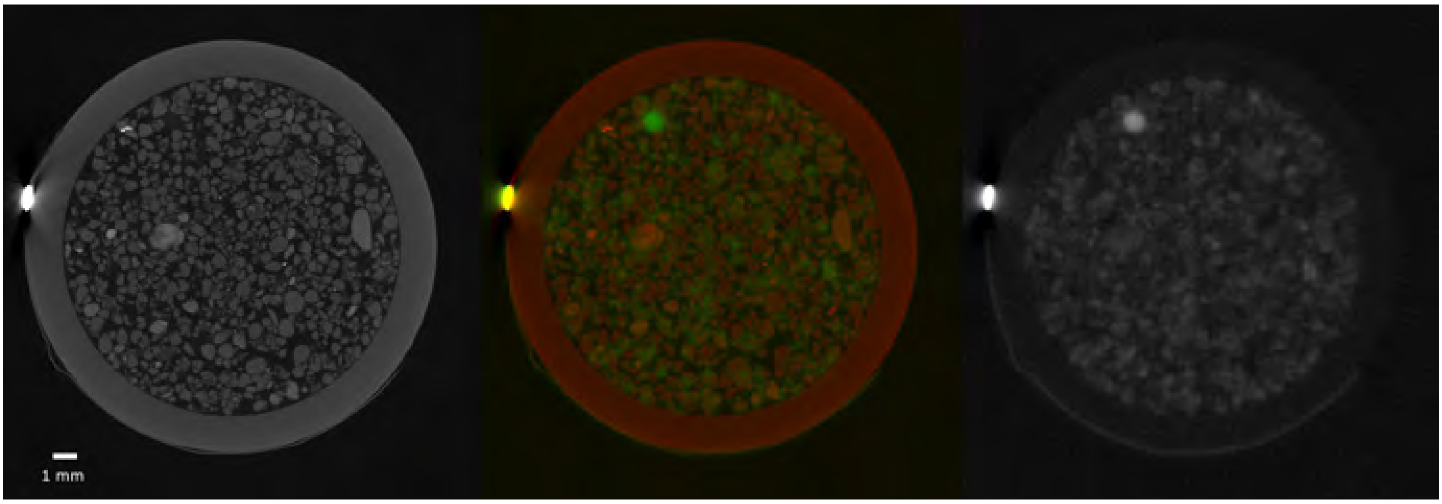
Imat

Getting to the root of it using X-rays and neutrons

The root system is key to plant functions such as water and nutrient uptake, anchorage and symbiotic interactions, with processes occurring at the root-soil interface strongly controlling plant performance. Improved traits below the ground could lead to enhanced plant performance and an increase in crop yield, helping to address global food security challenges and meet the demands of a growing population.

Tomographic imaging is ideal for plant root studies since it is non-invasive and allows for *in vivo* investigations. However, no single imaging technique is well suited to capture the whole system, with X-ray imaging giving insight into soil composition and structure, and neutrons offering a complementary view where water and biological matter are clearly distinguished, allowing water dynamics around the roots to be investigated.

To align the datasets from the two different modes of imaging, an object, known as a fiducial marker, can be attached to a sample as a point of reference. This study used cadmium fiducial markers in plant samples on IMAT and the X-ray imaging facility at the University of Southampton, and demonstrated that more information can be collected by combining imaging techniques than using either in isolation. Although cadmium's high attenuation introduced artefacts in the images that were shown to have a negative impact on data alignment, this work clearly demonstrates the value of combining neutron and X-ray tomography for studying plant root systems.



A slice from a plant root sample with X-ray data on the left and in red in the middle image, and neutron data on the right and in green in the middle image. This slice shows the match of a fiducial marker and the complementarity of the different modes of imaging. Credit: Thomas Clark.

Related publication: "Correlative X-ray and neutron tomography of root systems using cadmium fiducial markers." *Journal of Microscopy*, 277, 170-178 (2019)

DOI: 10.1111/jmi.12831

Funding: ISIS, University of Southampton, Diamond Light Source

Authors: T Clark (University of Southampton), G Burca (ISIS), R Boardman, T Blumensath (University of Southampton)

Iris

Fibre formation in meat analogues measured using neutron spectroscopy

Calcium caseinate (a micellar dairy protein) forms fibrous structures, that are a promising material for next-generation meat analogues. Better insights into the formation of these fibrous structures provides valuable insight for developing these, and plant-based, meat analogues. Fibre formation has been shown to be strongly influenced by whether the solvent is hydrogen or deuterium based water, suggesting the protein-water interactions are dominated by a subtle solvent effect. The structure of the fibrous materials also depends on the powderisation method, with spray drying and roller drying producing different fibre structures.

This investigation used quasi-elastic neutron scattering on IRIS to reveal the structuring potential of spray dried and roller dried food powders both when dry, and when solvated with H_2O and D_2O. The researchers found that the drying method did influence the protein dynamics. As roller drying involves more intense heating of the calcium caseinate, it allows the proteins to arrange into a more thermodynamically stable formation, making the material less susceptible for fibre formation.

The deuteration experiments disclosed the large impact caused by changing the solvent. Whereas the H_2O solvated fibres formed intact and homogenous gels, the use of D_2O resulted in a paste with an inconsistent texture. The neutron studies support these observations by revealing a clear difference in dynamics. The difference is not limited to the external hydrophilic protein groups of the protein, but also extends to the internal hydrophobic groups. Consequently, this work establishes a clear correlation between the microscopic protein dynamics and the bulk fibre structure formation, providing insight into the formulation of new meat replacement processing methods.

Example of a plant based meat replacement. Credit: Niko Koffeman

Related publication: “Fibre formation in calcium caseinate influenced by solvent isotope effect and drying method – A neutron spectroscopy study.” *Chemical Engineering Science* 207, 1270-1277 (2019)

DOI: 10.1016/j.ces.2019.07.023

Funding: SSCANFoods and the Netherlands Organisation for Scientific Research

Authors: B Tian (Delft University of Technology), V Garcia Sakai (ISIS), C Pappas (Delft University of Technology), AJ van der Goot (Wageningen University), WG Bouwman (Delft University of Technology)

RIKEN-RAL Port 4

Muons probe beneath the surface without leaving a scratch

Understanding the quality of ancient Roman silver coins can provide an indication of the financial condition of the state that issued them. Any surface analysis of the silver-copper alloy will be influenced by the surface-enrichment used to give the coins an appearance of being made of more valuable solid silver, but it is often difficult to gain permission from museums to take physical samples from within the bulk of such coins. This study used negative muons on the RIKEN-RAL muon facility to study a denarius of Julia Domna from 211–217 CE, shown below, completely non-destructively.

When a negative muon is captured by an atom (creating a muonic atom), it cascades down to the lowest energy state and causes the atom to emit energy in the form of X-rays (and maybe γ-rays), unique to the atom that emitted them. This makes it possible to identify the elements inside the sample. Elemental analysis using negative muons can therefore enable a full non-destructive analysis to take place. The composition of the inside of the coin studied was 51 ± 1.8% copper and 49 ± 1.9% silver, which is compatible with results from similar coins derived from destructive analyses. Surface measurements were also taken that confirmed surface enrichment with silver.

(a) Obverse of the Julia Domna coin analysed: IVLIA PIA FELIX AVG, draped bust right; (b) Reverse of the same coin: VESTA, Vesta seated left. RIC IV.1 391; BMCRE V 31. Reproduced from Heritage 2019, 2(1), 400-407.

Related publication: "Using Negative Muons as a Probe for Depth Profiling Silver Roman Coinage." *Heritage,* 2(1), 400-407 (2019)

DOI: 10.3390/heritage2010028

Funding: STFC, University of Warwick and RIKEN

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Iris

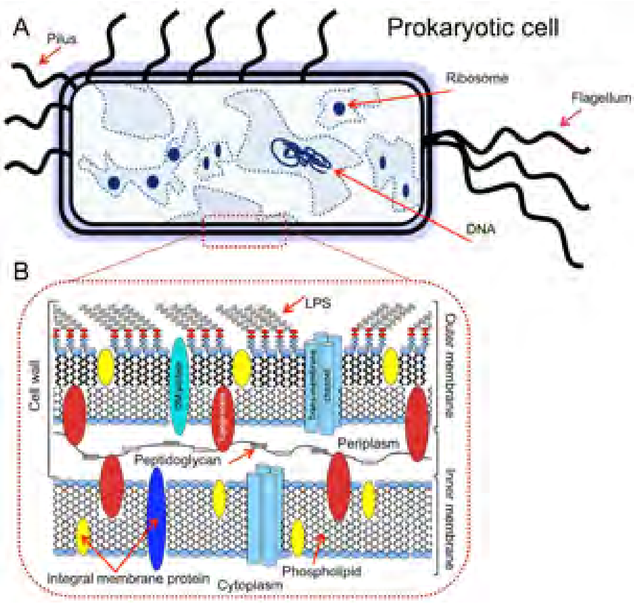
Understanding the dynamics of intracellular water in bacteria under high pressures

Understanding the biochemical reactions and transport processes within cells, which are determined by the intracellular water pressure, could lead to a better understanding of how bacteria behave under different conditions. This study investigated how water management occurs inside organisms without a nucleus (prokaryotes), and how dissolved ions, metabolites and macromolecular species would affect the mobility and transport properties of water in a macromolecular environment containing these molecules.

The research collaboration studied the diffusion and rotational relaxation of water in live *Shewanella oneidensis* bacteria at pressures up to 500 MPa using quasi-elastic neutron scattering (QENS). They found that the intracellular water dynamics exhibit significantly greater slowdown compared with bulk water and aqueous electrolyte solutions of compositions comparable to cytoplasm.

Classic interpretations of prokaryotes present the intracellular cytoplasm as a gel-like medium containing dissolved ions and macromolecules such as lipids and proteins. However, the findings suggest a more structured internal environment, with cooperatively organised "superclustered" arrangements of proteins and macromolecular complexes, separated by channels enabling transport of the water-based electrolyte solution.

The pressure-induced viscosity increase and slowdown in ionic/macromolecular transport properties within the cells affect the rates of metabolic and other biological processes. The findings of this investigation lend further support to emerging models for intracellular organisation that could lead to new insights into biological functioning of organisms under ambient and high pressure conditions.



A) Schematic drawing showing a prokaryotic cell; the cytoplasm is represented according to the model presented by Spitzer & Poolman [FEBS Lett. 587 (2013) 2094]. B) Schematic drawing showing: IM, OM and periplasmic space for G- bacteria. Credit: F Foglia.

Related publication: "*In Vivo* Water Dynamics in *Shewanella oneidensis* Bacteria at High Pressure." *Sci Rep* 9, 8716 (2019)

DOI: 10.1038/s41598-019-44704-3

Funding: Leverhulme Trust, Deep Carbon Observatory (Sloan Foundation), EPSRC, European Union's Seventh Framework Programme, Swiss National Science Foundation, French ANR within the Blanc International programme PACS

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Surf, Inter

Reflectivity studies the interactions between nanogels and skin models

Delivering drugs by applying the active ingredient to the skin offers many potential benefits in pharmaceutical, dermatological, and cosmetic applications, and yet the interactions and transport mechanisms across the skin barrier are not yet thoroughly understood at the molecular level. Nanogels have attracted particular interest as possible carriers, because of their high surface-to-volume ratio, ability to form stable colloidal systems and the fact that their chemical structure can be tailored to achieve particular physiochemical properties, and to respond to stimuli.

In this study, a team of researchers used neutron reflectivity to study the interactions between thermo-responsive N-isopropylacrylamide (NPAM) based nanogels, cross-linked with 10%, 20% and 30% N,N'- methylenebisacrylamide (MBA), and skin lipid multi-bilayer models. They also investigated the effect of the penetration enhancer benzyl alcohol on these interactions.

The results show the importance of membrane free acids, enhancing the ability of nanogels to associate with skin lipids to form water-dispersible complexes. This association increased with the percentage of the MBA cross-linker and temperature. The researchers concluded that the nanogels mainly associate with skin lipid molecules through hydrophobic interactions.

The observed enhancement effect could be a result of weakened neighbouring molecule interactions and the changes in the conformation of lipid bilayers. This work provides important advances in understanding the mechanism by which NIPAM-based nanogels are able to interact with multi-bilayers, which can ultimately contribute to the development of novel nanoparticles able to interact and penetrate biological barriers.

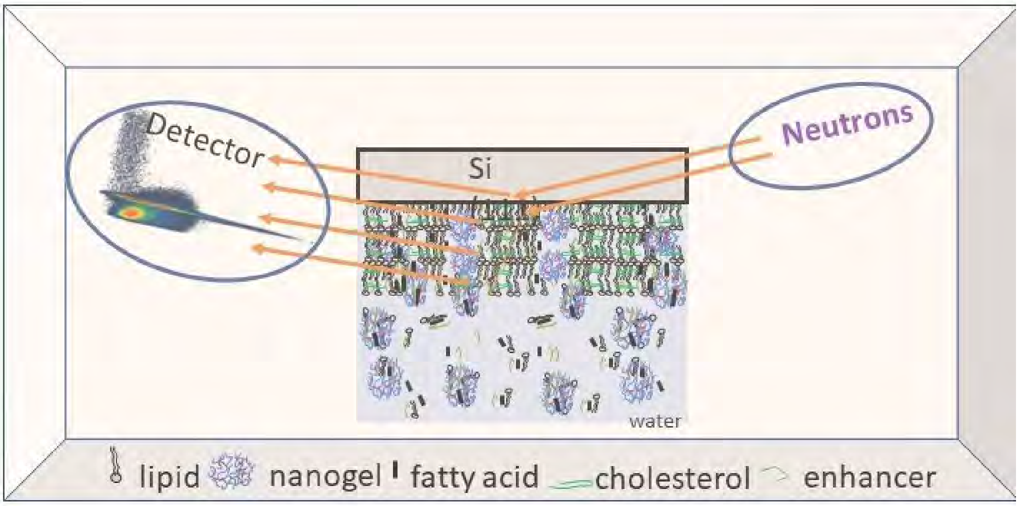

Figure showing the structure of the skin, and the lipid multi-bilayer model.

Related publication: "Interactions of NIPAM nanogels with model lipid multi-bilayers: A neutron reflectivity study." *Journal of Colloid and Interface Science* 536, 598-608 (2019)

DOI: 10.1016/j.jcis.2018.10.086

Funding: European Commission, the Chinese Scholarship Council and Queen Mary, University of London.

Authors: H Sun, K Zielinska, M Resmini, A Zarbakhsh (Queen Mary, University of London)

MAPS, Tosca

First analysis of ancient burned human skeletal remains probed by neutron and optical vibrational spectroscopy

As a result of fire, or funerary practices, archaeological and paleontological sites often contain burned skeletal remains. Studying bones in this state can be challenging due to the changes in the atomic structure of the bone caused by burning. This study uses, for the first time, an integrated approach, combining complementary vibrational spectroscopic techniques including inelastic neutron scattering, to study ancient burned bones.

By comparing their analysis to modern human bones that had been subjected to controlled burning, the researchers were able to identify the conditions that the ancient bones had been subject to. The group studied human and animal bones from different Italian archaeological sites from distinct historical periods: Neolithic, Copper Age, Roman, and the Middle Ages.

They were able to gain information about the difference in cremation practices in the Copper Age, which occurred mainly in home fires, and in the Roman age, where the bodies were cremated inside their graves, unwrapped, in direct contact with the soil. Their work provides archaeologists and anthropologists with new insights into past civilizations, including their burial, and cooking practices.

Giulia Festa and Luís Batista de Carvalho in ISIS target station 1.

Related publication: “First analysis of ancient burned human skeletal remains probed by neutron and optical vibrational spectroscopy.” *Sci Advances,* 5, 6, (2019)

DOI: 10.1126/sciadv.aaw1292

Funding: The Portuguese Foundation for Science and Technology and the CNR (Italy) within the CNR-STFC Agreement

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Sans2D

Studying the clinical markers for blocked arteries

The disease atherosclerosis is the leading cause of death in the western world. It occurs when plaques accumulate in blood vessels, which can lead to the hardening of arteries and eventually heart disease and stroke. There are several lipoproteins present that transport cholesterol through the blood plasma. Amongst these, high-density lipoprotein (HDL) and low-density lipoprotein (LDL) are used as biomarkers, and understanding their mechanism is likely to inform the understanding and treatment of the disease.

The accuracy of using the total amount of HDL and LDL in the blood as a predictor of atherosclerosis is low. Therefore, to understand the role that HDL and LDL play in the build-up of arterial plaques, their lipid exchange with the cellular membranes lining the artery wall needs to be carefully studied. This study uses selective deuteration, in combination with time-resolved small angle neutron scattering (TR-SANS), to investigate the molecular lipid exchange between human lipoprotein particles and model cell membranes.

The TR-SANS experiments suggest a multi-action mechanism for lipid exchange that includes diffusion, collision and tethering, leading to novel insights into the roles of different molecules present in the lipoprotein particle. The development of this method provides the research community with a way to begin to understand the molecular mechanisms underlying plaque build-up and therefore the onset of atherosclerosis. With developments in deuteration science, it could also lead to the systematic study of other complex biological protein-lipid systems.

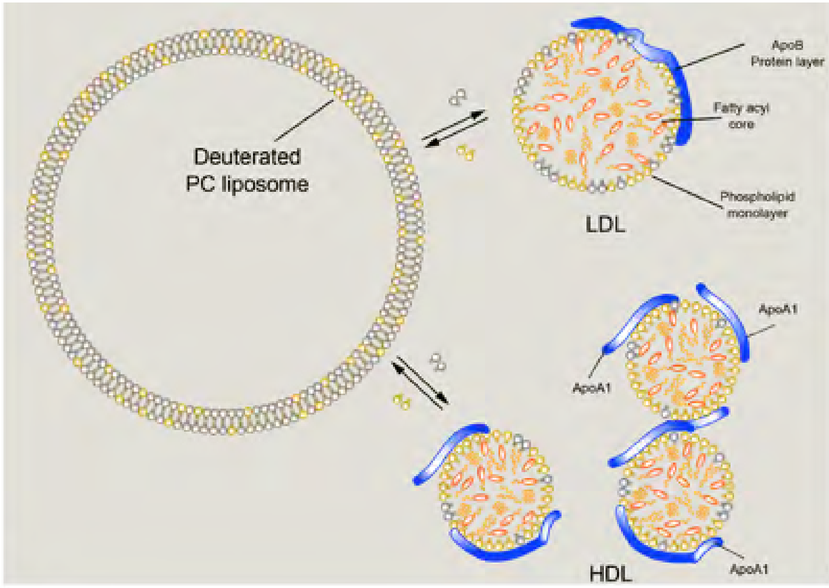


Illustration of the multi-action mechanism for lipid exchange.

Related publication: "Time-resolved small-angle neutron scattering as a probe for the dynamics of lipid exchange between human lipoproteins and naturally derived membranes." *Scientific Reports,* 9, 7591 (2019)

DOI: 10.1038/s41598-019-43713-6

Funding: Swedish Research Council, ESS & MAX IV: Cross Border Science and Society and the UNIK research initiative of the Danish Ministry of Science, Technology and Innovation

Authors: S Maric, TK Lind (Malmö University), MR Raida (National University of Singapore), E Bengtsson, GN Fredrikson (Lund University), S Rogers (ISIS), M Moulin, M Haertlein (ILL), VT Forsyth (ILL, Keele University), MR Wenk (National University of Singapore), TG Pomorski (University of Copenhagen, Ruhr University Bochum), T Arnebrant (Malmö University), R Lund (University of Oslo), M Cárdenas (Malmö University)

Sans2D

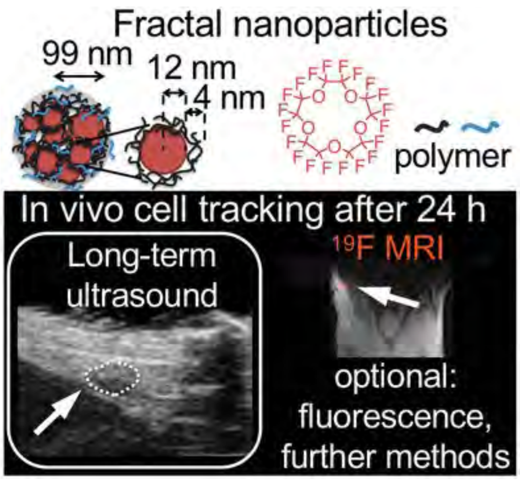
Neutrons investigate novel nanoparticle used in cell therapy imaging

Ultrasound is a powerful technique for medical imaging. However, the short lifetime and large size of the gas-filled microbubbles used as clinical contrast agents limits its use for long-term applications and, in particular, for tracking of cellular therapies. Recently, 19F MRI, has become an established technique for cell imaging. It provides direct quantification of cell numbers by imaging the 19F nuclei inside the contrast agent. Using the same contrast agent for both techniques could streamline the imaging process and enable fast screening with ultrasound along with quantification by ^{19}F MRI.

This study revealed that nanoparticles consisting of a liquid perfluorocarbon and biodegradable polymer are suitable for imaging with both ^{19}F MRI and ultrasound techniques. They remain stable for more than 48 hours during repeat ultrasound imaging sessions and, unlike microbubble-based contrast agents, they can enter the therapeutic immune cells without damaging them.

Due to the small size and high stability of the nanoparticles, the mechanism behind their visibility using ultrasound was not clear. Small angle neutron scattering measurements provided the researchers with an important insight. They found that the nanoparticles had an internal structure atypical for perfluorocarbon-loaded nanoparticles that could potentially explain the unusual imaging characteristics. The nanoparticles contain 12 nm core-shell building blocks, inside which highly hydrophobic perfluorocarbon was hydrated.

These nanoparticles provide exciting prospects for long-term imaging with ultrasound and ^{19}F MRI. They can be further tailored to other imaging or therapeutic applications, and could aid the movement towards personalised medication and the desired flexibility in clinical imaging. These nanoparticles are translatable to humans and have been approved for a pilot clinical trial. The research has also led to the foundation of a spin-out company, Cenya Imaging B.V.



The figure shows the schematic of the internal structure of nanoparticles on the upper panel, and dendritic cells labelled by the nanoparticles that migrated to a draining lymph node in a mouse using both ultrasound and ^{19}F MRI (^{19}F signal in false colour, superimposed over anatomic ^{1}H scan in grayscale).

Related publication: "Multicore Liquid Perfluorocarbon-Loaded Multimodal Nanoparticles for Stable Ultrasound and ^{19}F MRI Applied to In Vivo Cell Tracking" *Advanced Functional Materials,* 29, 19 (2019)

DOI: 10.1002/adfm.201806485

Funding: Netherlands Organization for Scientific Research, European Research Council, Netherlands Institute of Regenerative Medicine, EU FP7 program ENCITE and NanoNextNL

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Wish

Ambidextrous magneto-electric textures: the future of data storage?

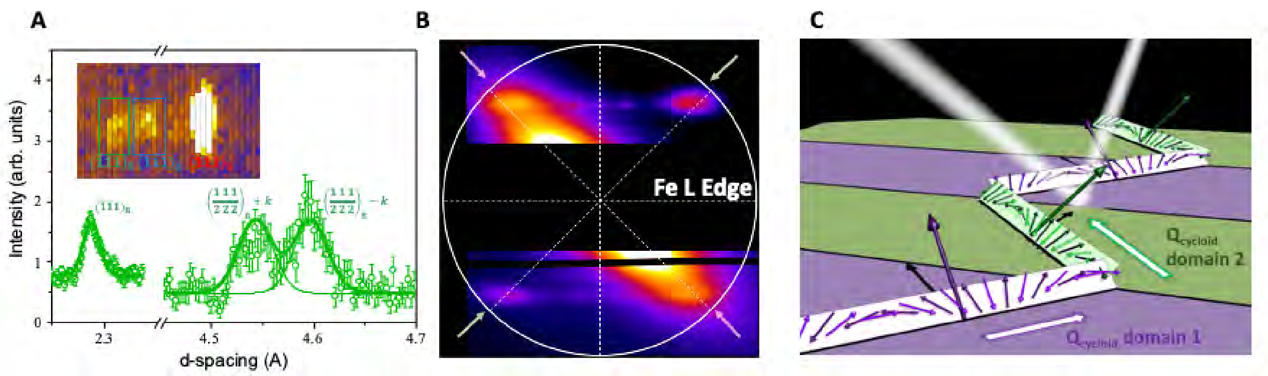
Combining the stability, dynamics and scalability properties of skyrmions, and the low susceptibility to interference with an external magnetic field of antiferromagnetic materials to create an antiferromagnetic skyrmion is very appealing for possible applications in quantum computing. In a skyrmion, the orientation of spins rotates progressively from the up direction at the edge of the circular texture, to the down direction at the centre, and the direction of the rotation determines whether the skyrmion is left- or right-handed.

Multiferroics, such as $BiFeO_3$, display magnetic order such as antiferromagnetism, as well as ferroelectricity; they have a spontaneous electric polarization that can be reversed by the application of an external electric field. $BiFeO_3$ is one of very few materials that exhibit both spin and dipole ordered phases above room temperature.

The boundaries between the regions in the material that have different spin and electric orientations, the domain walls, are of particular interest. A group of researchers from France studied $BiFeO_3$ on WISH to determine the magnetic structure for each ferroelectric variant throughout the whole sample.

The high resolution and high flux of the diffractometer were essential to detect subtle splitting and be able to measure such thin samples.

Combining this technique with resonant X-ray scattering, they observed, for the first time, both antiferromagnetic and electric chiral textures at domain walls in $BiFeO_3$ at room temperature. The appearance of both magnetic and electric chirality opens a new avenue for the creation and control of skyrmion systems. Future research on the interplay of these unusual spin textures with spin currents and light will enable further development of these materials for spintronic applications.



Non-collinear magnetic structure in ferroelectric domains by neutron and resonant X-ray scattering. (A) Neutron scattering measurements (2D and integrated intensity) showing the splitting of the Bragg peaks confirming the cycloidal arrangements. Open circles are experimental data and solid lines are fits assuming a bulk-like spin cycloid with a k vector giving a wavelength of 80 nm. (B) X-ray diffraction at the Fe L edge (709 eV) for the 71° periodic ferroelectric patterns. The four spots (marked with arrows) particularly visible in (B) stem from the two families of cycloids sketched in (C) (one in each polarization domain) and correspond to a cycloidal period of about 80 nm. The spots on the horizontal line (in B) indicate the chiral windings at domain walls.

Related publication: “Electric and antiferromagnetic chiral textures at multiferroic domain walls.” Nat. Mater., 19, 386–390 (2020)

DOI: 10.1038/s41563-019-0516-z

Funding: European Research Council, EU Quantum Flagship project, French Agence Nationale de la Recherche (ANR), PIAF and SANTA well as the ‘Programme Transversal CEA ACOSPIN and ELSA’.

Authors: J Chauleau (Université Paris-Saclay, Synchrotron SOLEIL), T Chirac, S Fusil, V Garcia (Université Paris-Saclay), W Akhtar (Université de Montpellier and CNRS), J Tranchida, P Thibaudeau (CEA – DAM le Ripault), I Gross, C Blouzon (Université Paris-Saclay), A Finco (Université de Montpellier and CNRS), M Bibes, B Dkhil (Université Paris-Saclay), DD Khalyavin, P Manuel (ISIS), V Jacques (Université de Montpellier and CNRS), N Jaouen (Synchrotron SOLEIL), M Viret (Université Paris-Saclay)

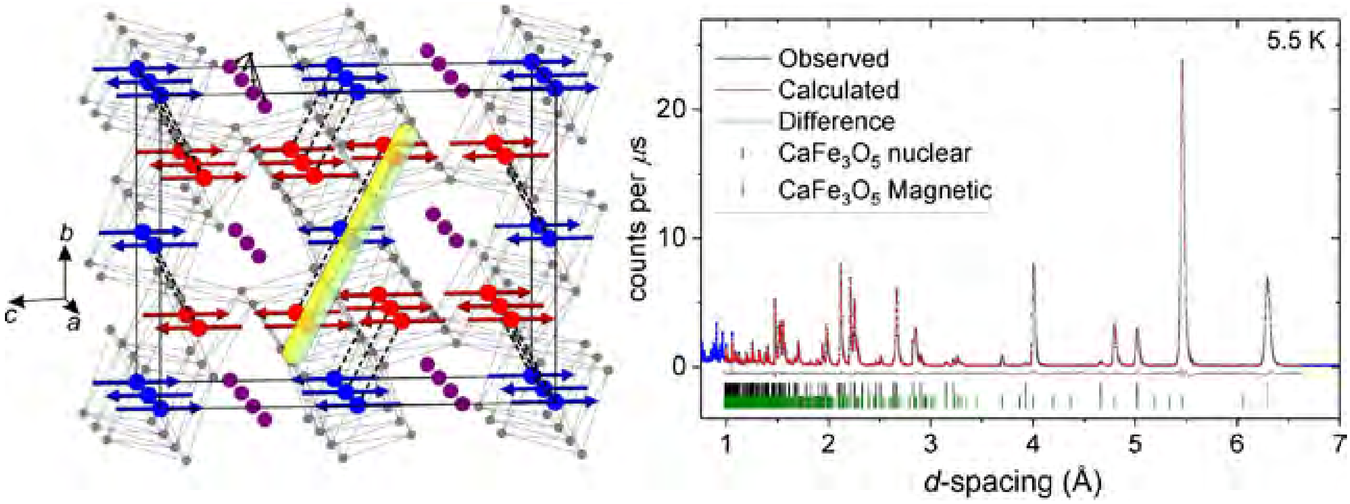
Wish

Stoichiometry changes influence magnetic behaviour

Mixed-valent compounds of iron and other transition metals show a wide range of physical and chemical properties. Understanding the complexities of their structures and magnetism provides insights that can be used to design materials with specific desirable properties.

CaFe3O5 is a mixed-valent compound that exhibits charge ordering with the formation of ferromagnetic trimers of the form Fe3+–Fe2+–Fe3+. These dictate the low temperature magnetic structure, as shown below in the figure. This investigation used neutron powder diffraction on WISH, Monte Carlo simulation and symmetry analysis to probe the magnetic ordering in perfectly stoichiometric CaFe3O5, including the observation of an incommensurate magnetic phase forming at the onset of long range magnetic ordering.

Previous work on a sample that was slightly off-stoichiometric [*Nat. Commun.* 9, 2975 (2018)] had shown phase separation on cooling into a charge-averaged phase with a different magnetic structure, and the charge-ordered phase. This new study shows that the phase separation is not found in stoichiometric $CaFe_3O_5$ and, together, the works emphasise the subtleties of these mixed-valent phases, and indicate that changing the material's exact composition and microstructure could lead to subtle control of its physical properties.



Left, structure of $CaFe_3O_5$, highlighting the ferromagnetic trimers. Right, neutron powder diffraction pattern of the sample.

Related publication: "Single phase charge ordered stoichiometric $CaFe_3O_5$ with commensurate and incommensurate trimeron ordering." *Nat Commun* 10, 5475 (2019)

DOI: 10.1038/s41467-019-13450-5

Funding: EPSRC

Authors: SJ Cassidy (University of Oxford), F Orlandi, P Manuel (ISIS), SJ Clarke (University of Oxford)

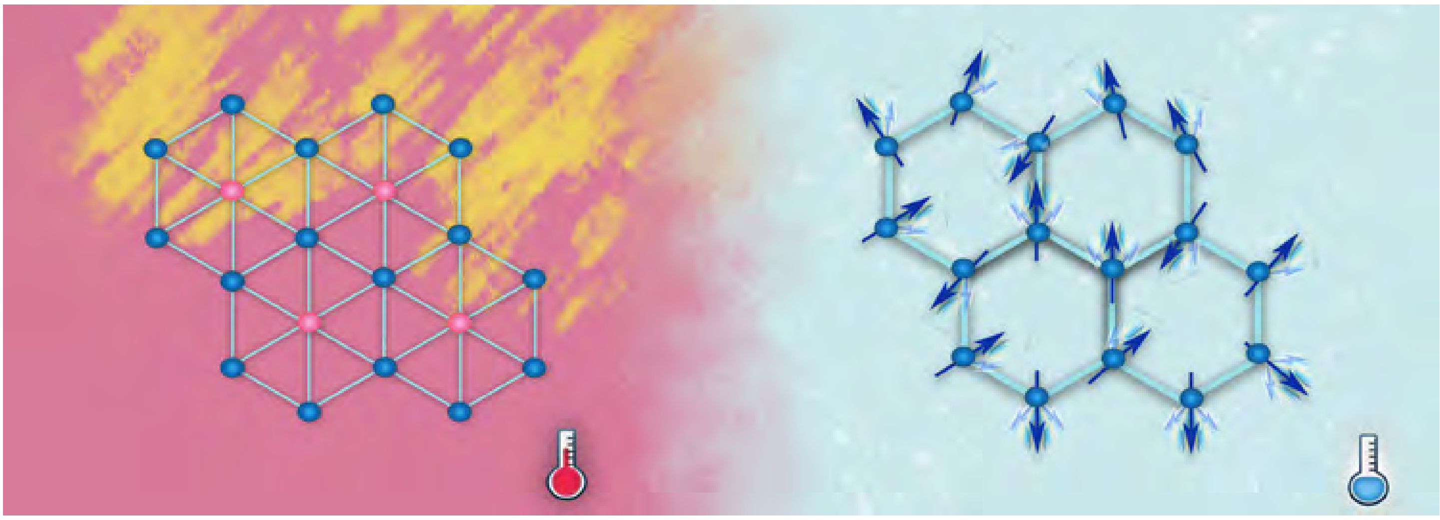
HRPD, EMU, MuSR

Thinking outside the triangle: quantum spin liquid formed in an unexpected way

In a quantum spin liquid, the magnetic moments of a material act like a liquid and remain disordered even at absolute zero. Materials that can form a quantum spin liquid have the potential for applications in quantum computing, data storage and high temperature superconductivity.

Many quantum spin liquids are based on magnetic atoms arranged in triangular planes, with magnetic interactions that are frustrated by this arrangement. Even at temperatures approaching absolute zero, the magnetic frustration and quantum fluctuations of the atomic magnetic moments cannot arrange themselves into a magnetically ordered state.

This study focussed on $TbInO_3$, and used HRPD to measure the neutron diffraction from the sample at temperatures down to 0.46K. The group saw a lack of magnetic Bragg scattering from the sample, indicating the absence of long-range magnetic order in the material. This demonstrates that $TbInO_3$ forms a much more exotic structure where the magnetic atoms sit on two interpenetrating sites that ultimately form a honeycomb lattice, rather than a simple triangular one. Their experiments on MuSR and EMU enabled them to show that this lack of long-range magnetic order, and therefore the exotic structure, was present down to 0.1 K.



The triangular to honeycomb transition within the two-dimensional layers of the quantum spin liquid candidate, $TbInO_3$, upon cooling. Artwork Credit: E. H. Driscoll, University of Birmingham (@EHDriscoll).

Related publication: "Two-dimensional spin liquid behaviour in the triangular-honeycomb antiferromagnet $TbInO_3$" *Nat. Phys.* 15, 262–268 (2019)

DOI: 10.1038/s41567-018-0407-2

Funding: NSERC of Canada, US Department of Energy, STFC

Authors: L Clark (University of Liverpool, McMaster University), G Sala (McMaster University, Oak Ridge National Laboratory), DD Maharaj (McMaster University), MB Stone (Oak Ridge National Laboratory), KS Knight (UCL, Natural History Museum, ISIS), MTF Telling (ISIS), X Wang, X Xu, J Kim (Rutgers University), Y Li (Rutgers University, Shandong University), S Cheong (Rutgers University), BD Gaulin (McMaster University, Brockhouse Institute for Materials Research, Canadian Institute for Materials Research)

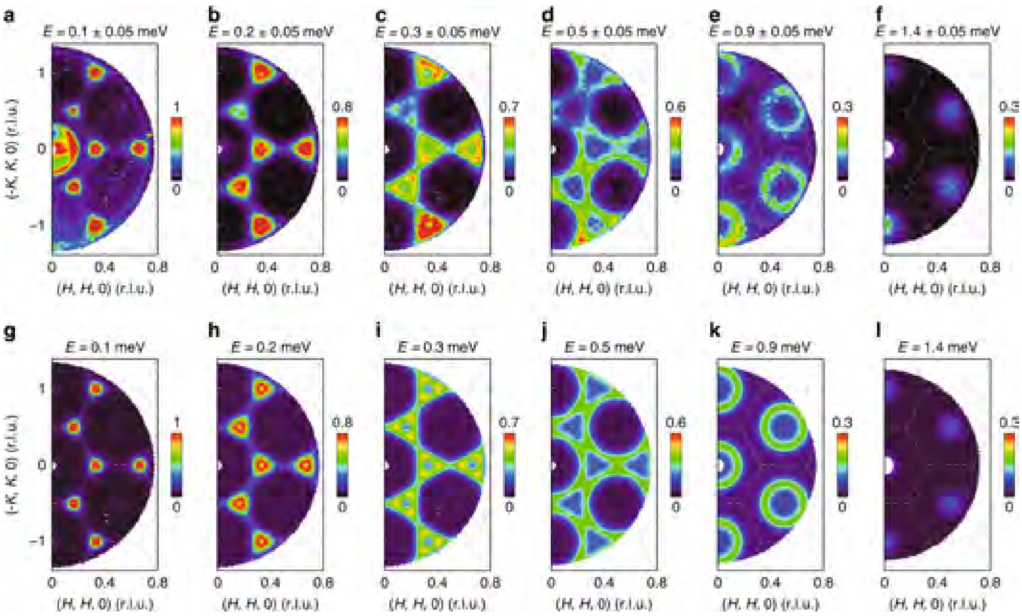
Let

Understanding hidden magnetic phases

Some magnetic materials show hidden order phases, where the order parameters are not observed using conventional magnetic measurements. The hidden order phase transition is usually accompanied by changes in the bulk properties such as heat capacity, but identification and understanding of the phases is very difficult when they cannot be observed microscopically.

This study focusses on the recently discovered rare-earth triangular-lattice magnet $TmMgGaO_4$. Bulk measurements show that a phase transition occurs at low temperature, but this is the first study to look at the microscopic measurements. The researchers used neutron scattering and thermodynamic measurements to study the phase transitions and spin correlations of single crystals of $TmMgGaO_4$.

They observed clearly in the elastic neutron diffraction patterns that the longitudinal component of the effective spins is dipolar. However, they also observed spin excitations that were not present in the elastic diffraction patterns, corresponding to the transverse components. Their calculations demonstrate that this behaviour can be described by a transverse field Ising model on the triangular lattice, with an intertwined dipolar and ferro-multipolar order.



Measured and calculated momentum dependence of the spin excitations in $TmMgGaO_4$ at the indicated energies and T = 0.05 K. a–f Raw contour plots of the constant energy images at T = 0.05 K. The signals near Q = (0, 0, 0) in a are due to the elastic contamination from the sample environment close to the direct beam. g–l Calculated spin excitations using the model specified in the text. The dashed lines indicate the zone boundaries. The measurements were performed on LET spectrometer with Ei = 4.8 meV. The color bars indicate scattering intensity in arbitrary unit in linear scale.

Reproduced from **DOI:** *10.1038/s41467-019-12410-3.*

Related publication: "Intertwined dipolar and multipolar order in the triangular-lattice magnet $TmMgGaO_4$." *Nat Commun* 10, 4530 (2019)

DOI: 10.1038/s41467-019-12410-3

Funding: Innovation Program of Shanghai Municipal Education Commission, the Ministry of Science and Technology of China, the National Key R&D Program of the MOST of China and Hong Kong's Research Grants Council

Authors: Y Shen, C Liu, Y Qin, S Shen (Fudan University), Y Li (Fudan University, University of California Santa Barbara), R Bewley (ISIS), A Schneidewind (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ)), G Chen (The University of Hong Kong, Fudan University, Nanjing University), J Zhao (Fudan University, Nanjing University)

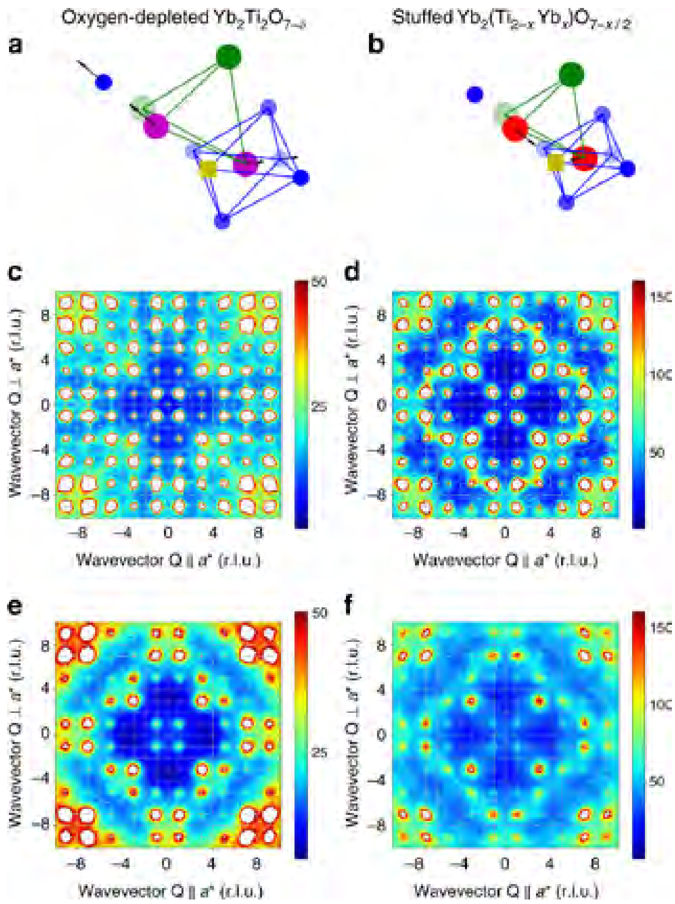
SXD, Merlin

One material: two ground states?

The pyrochlore system $Yb_2Ti_2O_7$ has attracted both experimental and theoretical interest as a model geometrically frustrated magnet with large quantum fluctuations. These studies have identified two possible ground states for the material, where the state formed is dependent on the individual sample, and its pressure. This suggests that low-level structural disorder could be causing the change in ground state preference.

By using neutron scattering on SXD, which is very sensitive to the vacancies and displacements of oxygen ions, the researchers were able to determine the structure of the defects in single crystals of $Yb_2Ti_2O_7$. They found that isolated oxygen vacancies on the O(2) site stabilise the formation of the spin liquid ground state, whereas ideal defect-free samples exhibit long-range order, with a ferromagnetic ground state.

Understanding the impact of these defects on the functionality of the pyrochlore system, and the competition between classically ordered systems and quantum states, could enable the development of novel quantum spin liquid phases.



The structure of defects in $Yb_2Ti_2O_7$. a For oxygen-depleted $Yb_2Ti_2O_{7-\delta}$ the oxygen vacancies (gold) are located on the O(2) sites (blue), and neighbouring Ti^{4+} (green) are replaced by charge compensating Ti^{3+} (purple) ions that are slightly displaced away from the vacancy. b For stuffed $Yb_2(Ti_{2-x}Yb_x)O_{7-x/2}$ neighbouring Ti^{4+} ions are replaced by Yb^{3+} (red) ions that are displaced towards the O(2) vacancy. The diffuse neutron scattering measured at $T \sim 30$ K in the (hk7) plane in c for oxygen depleted and d for stuffed samples is compared with the simulated scattering in e and f, calculated using the models shown in a and b, respectively. The contour diagrams are on a hot scale with an arbitrary maximum.

Related publication: "Role of defects in determining the magnetic ground state of ytterbium titanate." *Nat Commun* 10, 637 (2019)

DOI: 10.1038/s41467-019-08598-z

Funding: EPSRC

Authors: DF Bowman (Royal Holloway, University of London), E Cemal (Royal Holloway, University of London, ILL), T Lehner (Royal Holloway, University of London), AR Wildes, L Mangin-Thro (ILL), GJ Nilsen (ILL, ISIS), MJ Gutmann, DJ Voneshen (ISIS), D Prabhakaran, AT Boothroyd (University of Oxford), DG Porter (Diamond Light Source), C Castelnovo (University of Cambridge), K Refson, JP Goff (Royal Holloway, University of London)

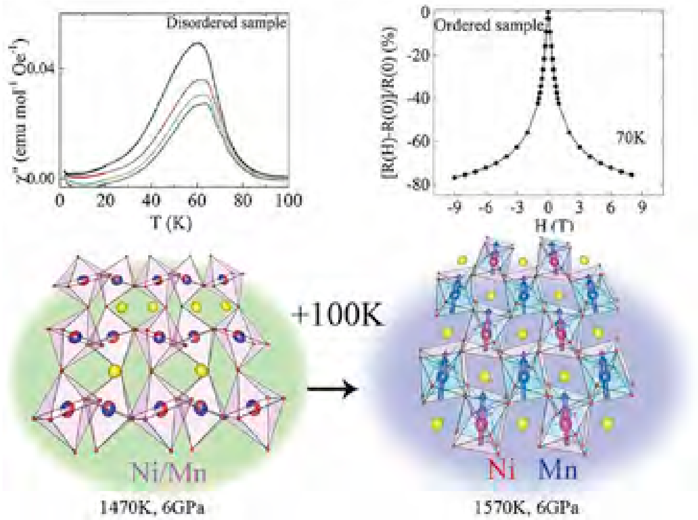
Wish

New double perovskite shows novel colossal magnetoresistance

Ordered double perovskites have the chemical formula $A_2BB'O_6$, where A is a rare earth or alkaline, and B and B' are transition metals or, in some cases, post-transition and non-metals. Within the structure, the B and B' cations generally form either a rock-salt or layered type superstructure. Some double perovskites show colossal magnetoresistance (CMR), which enables them to dramatically change their electrical resistance in the presence of a magnetic field, due to the half-metallic nature of their electronic structures.

This study introduces the double perovskite Tl_2NiMnO_6. As the B (Ni^{2+}) and B' (Mn^{4+}) cations have similar radii, they can partially occupy the sites of the other, depending on the temperature and pressure used during synthesis. This work is dedicated to investigating the crystal, magnetic and electronic structures by a combination of neutron diffraction experiments on WISH, magnetic, heat capacity and magneto-transport measurements, and density functional theory calculations.

The group discovered that the extent of cation ordering has a large impact on the magnetic properties of the material. By reducing the degree of ordering of the cations from 70% to 31%, the long range ferromagnetic order is suppressed, resulting in short range spin correlations and glass-like behaviour. The ordered sample exhibits a low-field CMR: the first example of a ferromagnetic insulating double perovskite showing CMR. These results open new avenues for material design for functional magnets in the family of double perovskites.



The magnetic and transport properties of the ordered and disordered Tl_2NiMnO_6 samples with the ordered one showing colossal magnetoresistance near the Curie temperature.

Related publication: "Colossal magnetoresistance in the insulating ferromagnetic double perovskites Tl_2NiMnO_6: A neutron diffraction study." *Acta Materialia 173, 20-26 (2019)*

DOI: 10.1016/j.actamat.2019.04.044

Funding: EU Horizon2020, Rutherford International Fellowship Programme, ISIS co-funded studentship

Authors: L Ding, D D Khalyavin, P Manuel (ISIS), J Blake (Royal Holloway, University of London and ISIS), F Orlandi (ISIS), W Yi, A A Belik (National Institute for Materials Science, Japan)

Anna Herlihy

From Diamond Sandwich student to ISIS Facility Development Student

> "Since my placement year, my dream job has been to be an instrument scientist, and I've not been put off yet!"

Sandwich placement at Diamond Light Source

Anna studied Materials Chemistry at the University of St Andrews and wanted to use her year in industry to do research, to find out more about what it's like to be a full-time researcher. She applied to the year-in-industry placement scheme at Diamond Light Source, despite not being that sure what the placement would involve. "It was a lot better than anything I expected", she explains. "Everything involved in the placement was new to me, but it felt really good to be working on a project that was completely mine."

Her placement year at Diamond was spent on the I11 beamline, working on a sol-gel synthesis for silica frameworks, and comparing these to their equivalents that would be formed in space. "I spent a lot of time in the lab, and was able to run my samples on I11 if there was available beamtime. The team also had beamtime allocated on I22 during my placement, and I was able to join them and measure my samples." Anna also had the opportunity to present at the British Crystallography Association conference on her work, and to be part of the outreach activity "Project M", run by one of her Diamond supervisors.

The placement prepared Anna well for her final year at university, and convinced her that she would like to continue in research. "I had a better understanding of how research happens, and how it can be slower than you might expect!" Seeing all the visiting scientists come in and use the facility made her keen to do a PhD that involved both a university and a central facility.

Facility Development Studentship

It was one of these users, Dr Mark Senn from the University of Warwick, who Anna contacted towards the end of her final year, asking if he had any PhD positions available. He did – including one working with ISIS, which she started in October 2018. Working on the PEARL beamline, with Nick Funnell, Anna is now in her second year of the project, studying pressure-induced functional properties of materials.

Her PhD sees her mainly based at the University of Warwick, with travel down to ISIS for beamtime allocations, or meetings with her supervisor. These trips to ISIS provide Anna with the majority of her data, "then I go back up to Warwick to do all the analysis."

Every ISIS-funded PhD studentship has an element of facility development: Anna's is developing a method for local structure determination in crystalline materials. This can already be done on PEARL for glasses, and Anna is investigating the best way to subtract the additional peaks in the pair distribution function to enable the same experiments to be carried out on crystalline materials.

Student meetings, and the future

During her placement year, Anna found it easy to settle in at RAL, thanks to a large cohort of summer and sandwich students. "When the summer students left, I found myself becoming part of the group on I11, as well as staying in touch with the other placement students," she says; "During my PhD, I have met other students at the ISIS student meetings, and through a Crystallography Student Day held jointly with Diamond."

As for the future, Anna explains; "Since my placement year, my dream job has been to be an instrument scientist, and I've not been put off yet!"

Right: Giuseppe Paterns, Italian Institute of Technology, preparing a sample for an experiment on the IRIS instrument.


Science & Technology
Facilities Council
EXIT
NITROGEN

A year around ISIS

ISIS during lockdown

From instrument support to supporting frontline workers

The Instrument Support team adapted during the pandemic to move from upgrading beamlines and detector systems to producing visors for local NHS services, pharmacies and care workers.

After an appeal from a local GP who was finding it difficult to source visors, the ISIS support team decided to use their expertise to help. Within four days, an open source "badger shield" was designed by technician Josef Lewis. A short training video showed the team how to assemble the visors at home, and how to keep assembly areas clean. The technicians were also given guidance on wearing masks and gloves, and immediately sealing visors into zip lock bags for collection.

Over 2000 visors had been distributed by the small, 15-strong team, with fantastic feedback from clinicians and healthcare workers. While the visors are not medical grade, they provide an extra layer of protection that frontline workers find very valuable.

As Josef said, "Our ability to react in the moment, and deliver an end product, is something we need to do regularly in our roles, and that has really helped. It means a great deal to me to be able to support our country in this way and it makes me very proud."

Josef Lewis, from the ISIS Instrument Support team, and the bundles for distribution.

Visits go online

ISIS has an extensive visits programme, with over 4000 visitors every year. As we went into lockdown and visits and tours to the facility were cancelled, ISIS quickly transitioned to virtual events, where school and university students, and members of the public could tour the facility remotely. Our engagement activities usually centre on tours of the facility and hands-on activities, so adapting to online activities was a huge challenge.

Nonetheless, the ISIS Impact Team rose to the challenge to find new and exciting ways to engage with audiences during a time of social distancing and home learning. A 360 degree tour of the facility and new hands-on "science at home" and "kitchen science" activities were developed, allowing ISIS to continue their public engagement and student programmes, reaching over 400 students, teachers and members of the public across the UK in the first few months of the lockdown.

> "I liked having multiple speakers; that was really nice to see diversity of staff delivering the tour."
>
> **ISIS Exploring Engineering virtual event attendee**

Quote from a parent about the ISIS Exploring Engineering virtual event, "It is a great way of showing students what is happening in the world around them and that exciting projects are taking place so close by. It makes students excited about being involved in contributing to a better world using scientific research."

Left: Avinash Mahajan, Indian Institute of Technology, Bombay, on the MuSR instrument.

Ventilators

STFC staff were part of a national collaboration producing ventilators for the NHS, developing and delivering the training needed for others (including more STFC members) to carry out the necessary testing and calibration.

One of the major challenges for the UK when facing the Covid-19 pandemic was the production of ventilators, to keep patients with respiratory difficulties out of intensive care. The medical equipment manufacturer Penlon, based in Abingdon, already supplied the NHS with machines used by anaesthetists in operating theatres. After it was clear that the demand for ventilators was going to increase dramatically, the company developed a simpler device that can be mass-produced and used on a ward as a ventilator, breathing for a patient when they are unable to do it themselves.

Penlon was part of the consortium, VentilatorChallengeUK, of over 20 companies including Airbus, Ford and McLaren, who produced the ventilators on a large scale. Before the tens of thousands of ventilators could be used by the NHS, they needed to be tested and calibrated, to ensure they could be delivered under the company's medical licence.

With their high level of technical skill, STFC staff delivered training in how to test the ventilators to some 300 staff from the other companies in the collaboration, who then carried out the testing at Penlon's facility, and others nearby.

ISIS 'super trainer', John Crawford explains, "Our part in this huge project was to facilitate the testing and commissioning. It was daunting and initially overwhelming, like climbing a mountain, but it's a great thing to be involved with, and very satisfying to get to the top."

ISIS 5K Lockdown Challenge raises £830 for local charity

ISIS staff and their families recently took part in a virtual 5K challenge to raise funds for SOFEA, a charity based in Didcot who are supplying free food packages to the vulnerable and low income families across Oxfordshire.

Lots of staff and their families took part in the challenge, spread over nine days in May, sticking to social distancing and daily exercise rules. Challenges included leisurely countryside walks, first-time 5 km runs, 5 km PBs, and even a mega 50 km static cycle. We exceeded our £600 target, raising a grand total of £830 by the last day of the challenge; that's 276 free food packages for families who really need it at this challenging time.

Support labs - hand sanitiser

During the early stages of the COVID-19 pandemic within the UK, procuring hand sanitising solution was very difficult. With dwindling supplies on supermarket shelves and limited supplies through other commercial routes, the Support Labs Group decided to produce their own hand sanitiser for the use across RAL. Following a World Health Organisation based formulation, containing only 4 ingredients and a minimum of 70% alcohol, the team have been producing batches of 100L, whilst working under socially distanced conditions. Dispensing bottles and automatic dispensing units have appeared at the entrances to ISIS buildings as well as other buildings across the RAL site. The task of producing the sanitiser also served as a pilot task for working within our prep labs, and informed the group how best to set up the labs for use for the ISIS user programme.

Support laboratory milestones

This year, the ISIS deuteration facility celebrated the measurement on WISH of a sample made using the 500th compound synthesised in the lab.

In 2013, the decision was made to move the lab, originally based at the University of Oxford, 'in house' to ISIS. The original primary demand was from the Small Angle Scattering and Reflectometry beamlines, but there have been increasing numbers of requests for organic synthesis and ionic liquids. Some compounds are very routine and take a few hours to make, whereas others can take months, or even years.

A recent type of request has been for deuterated ligands to make Molecular Organic Frameworks (MOFs): porous structures than can be used for gas storage, catalysis but also exhibit unconventional physical phenomena such as superconductivity. The 500th compound was an example of one of these materials; 1,2-bis(4pyridyl)ethane and 1,2-bis(4-pyridyl)ethylene ligands (below) were sent to the University of Liverpool where PhD student Kate Tustain used it to make the MOF material for her magnetic investigations on WISH.

The group has grown from the two post-doctoral researchers who moved from Oxford to four full time members of staff, a graduate and a sandwich student, as well as taking on summer students for 6-8 week-long placements every year. In addition to the complex requests for compounds such as ionic liquids, and electrolytes for battery materials, the team is also looking at different synthesis routes they could use to make the 'day to day' deuterated compounds.

D-lab staff.

Ten years after its development, the Experimental Risk Assessment (ERA) process at ISIS has reached the milestone of giving out the 10,000th ERA.

A collaboration between the ISIS Support Labs Group and the ISIS Computing division began developing the ERA system back in 2009. The previous 'sample risk assessment sheet' completion was manual and time consuming, and relied on one person carrying out a risk assessment for each experiment based on the proposal submitted. With the number of proposals continuing to increase, the group saw the opportunity to develop something new that would make a real change.

Led by Marek Jura and Hannah Griffin, the group developed a system to make the process more efficient and streamlined. After carrying out a trial, and using feedback forms and workshops to develop the user interface, they were able to develop a system that worked for everyone.

The type of experiments taking place at ISIS has increased in complexity since 2009: from measuring powder/crystalline samples in a simple experimental process to those that involve in situ experiments and/or multiple techniques. This leads to more complexity in the sample environment - gas flow and pressure changes for example - and therefore more consideration required during the ERA process.

The recipients of the milestone 10,000th ERA were Wasiu Abdullahi and Professor Peter Griffiths from Greenwich University. They were studying the nanoscale structures that are present in air-in-water foams using ISIS' newest beamline, ZOOM.

> Reaching the 10,000th ERA is a big milestone; it was hard to get the process of the ground, but it has been very successful, and I am proud of what we have done. - **Marek Jura, ISIS**

Wasiu Abdullahi and Professor Peter Griffiths from Greenwich University, ZOOM users, with the 10,000th ERA.

International

International

ISIS has significant, long-standing agreements with several countries which provide support for ISIS instruments for all users whilst allowing particular access for researchers from the partner countries.

ISIS has had a partnership with RIKEN in Japan for the operation of the RIKEN-RAL Muon Facility for several decades. The first formal agreement was signed in 1990 – so 2020 marks 30 years of continuous collaboration. The current agreement runs until 2023 and will see the refurbishment of the facility to ensure its ongoing use for many years to come.

ISIS has an ongoing agreement with the Italian CNR which has involved development of several instruments across ISIS and includes operation of the INES instrument focused on cultural heritage studies. ISIS has also been working in partnership with Italian colleagues on development of an instrument for the European Spallation Source. A new agreement to continue the ISIS-Italy partnership is currently under discussion.

Italian users Giulia Marcucci (below), University of Milano-Bicocca, Italy, with sample on the INES instrument and Piernicola Oliva (above), University of Sassari, Italy, setting up historical artefact, a Nuragic Bronze Age Votive boat from the Tomba delle Tre Navicelle, Vetulonia, Tuscan, on Port 4, RIKEN-RAL.

ISIS has a very successful ongoing partnership with the Indian Nanomission which, together with Newton Programme funding, has seen a significant increase in proposals from India to use ISIS instruments. An extension of the current agreement is in place whilst a further agreement is considered.

Amitava Bhattachayya from Vivekaranda University, India, loading a sample on the MuSR instrument.

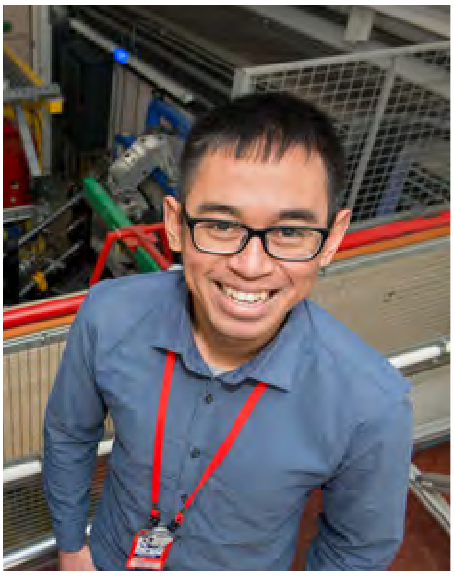
ISIS has ongoing Newton funding to support researchers from Malaysia, Indonesia and Thailand to use the facility. A successful call for proposals for ISIS time by the Malaysian Ministry of Education in 2019 has led to a variety of experiments due to be run this year. Battery and catalysis research is the focus of Indonesian experiments, whilst Thai experiments are focused on polymer studies.

ISIS is a founding member of LENS, the League of Advanced European Neutron Sources. LENS supports the collaboration between neutron facilities on matters of policy and funding, as well as technical work such as polarisation, detectors and software.

Left: Dr Philip King (ISIS) with Dr Toshiyasu Ichioka Director, RIKEN Europe Office in TS2.

Ranggi Ramadhan

From ISIS Facility Development Student to post-doctoral researcher at ILL



> “I am very grateful for the chance to have the experience of both university, and time at a large-scale internationally renowned research facility.”

“Not expecting to use neutrons!”

Ranggi did his undergraduate degree in Mechanical Engineering at the University of Indonesia. His five-year course included a master’s project that involved him using neutron radiography at the research reactor in Indonesia. “I just used it as a tool: I was not expecting to use neutrons again!”, he explains.

His interest in aerospace led him to do a one-year master’s project at Sheffield and, while in the UK, he saw an advertisement for a PhD project based at Coventry University and ISIS, working on IMAT testing materials for aerospace applications.

ISIS Facility Development Studentship

During his studentship, Ranggi spent most of his time at Coventry, but with about one week every month down at ISIS. “This worked well,” he says, “as I was doing an engineering PhD, all of my colleagues at Coventry were engineers, and my time at ISIS gave me the opportunity to learn more about the science.” Ranggi found this a good way to break up the routine of PhD life in Coventry: “It made sure I never got bored!”

While at ISIS, Ranggi stayed at Ridgeway House, finding that a fellow Sheffield alumnus was also doing an ISIS studentship, and joining them to take part in the occasional match for the Harwell Campus football league. “I enjoyed my time at ISIS; I had a good relationship with my supervisor, and using other instruments meant that I got to know some of the other instrument scientists, and users from a wide range of backgrounds.”

His project on IMAT was to develop the technique of strain imaging using neutron transmission. “The technique was not well established when I started but, by the end of my project, I was able to help users to answer their research questions. In particular, I spoke at a conference in Singapore and one of the attendees was very interested in the technique. We worked together to write a proposal, and then did the measurement together. It was really good to see that the technique could be so useful for them.”

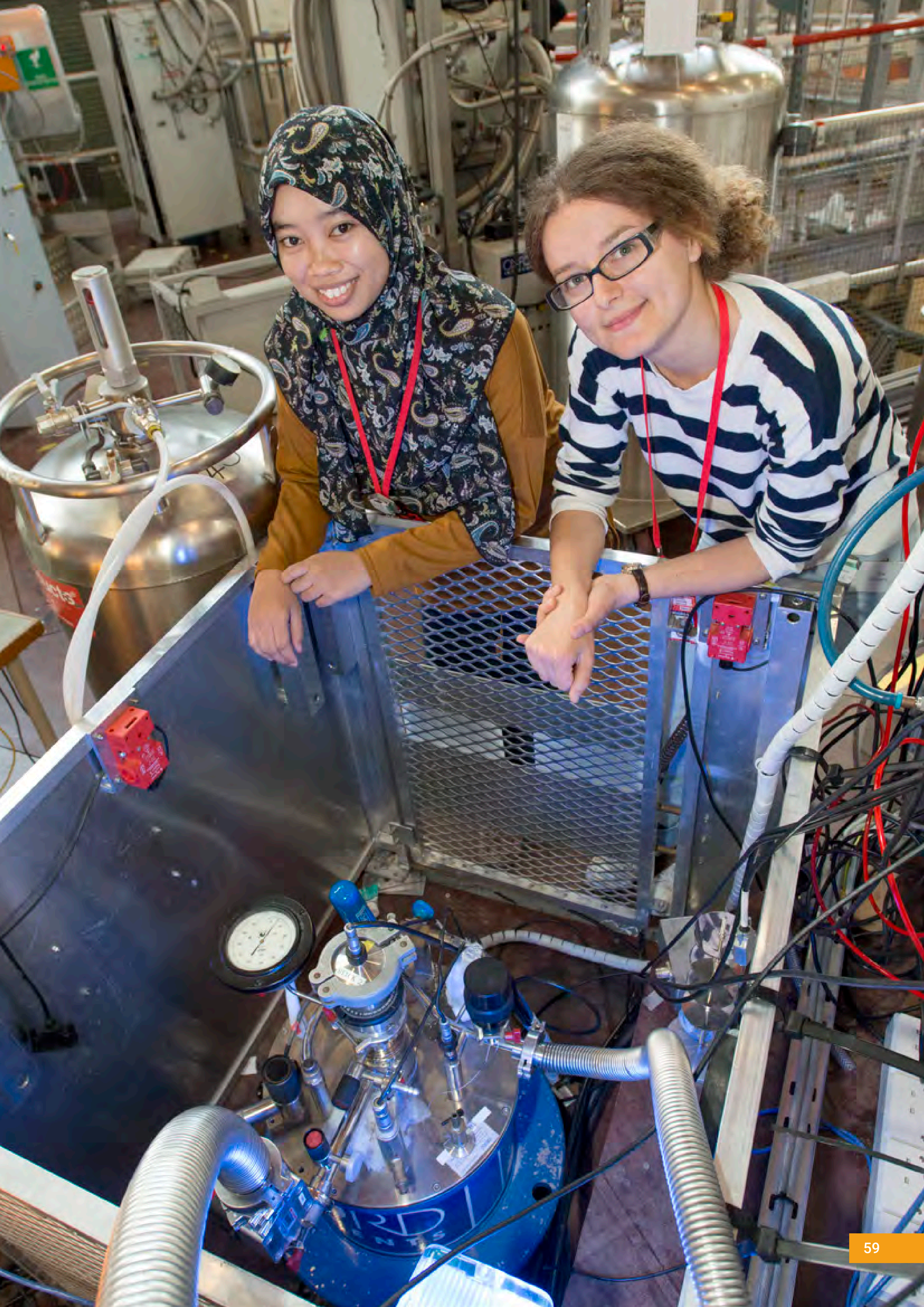
Networking and international travel

This conference was one of many Ranggi attended during his PhD, the studentship giving him many opportunities to travel, including some beamtime in Japan that was very useful. As well as international conferences, Ranggi attended the ISIS student meetings, engineering group user meetings and NMSUM. He found that this networking really added value to the studentship. Whilst writing up his PhD, he saw a post-doctoral position available at ILL and, having met the group at NMSUM, and being familiar with the techniques needed, decided to apply.

He got the position and is now working at ILL as part of a European project standardising strain scanners across different neutron facilities. This has involved taking measurements at Engin-X, as well as at the ILL and in Munich. “Luckily I managed to get a lot of these measurements in before lockdown, and so I have plenty of analysis to keep me busy. Although likely travel restrictions mean that it’s likely I will be sending samples to South Africa rather than going there myself.”

On the Facility Development Studentship scheme, Ranggi says, “It was really enjoyable, and the people were great and supportive. I am very grateful for the chance to have the experience of both university, and time at a large-scale internationally renowned research facility.”

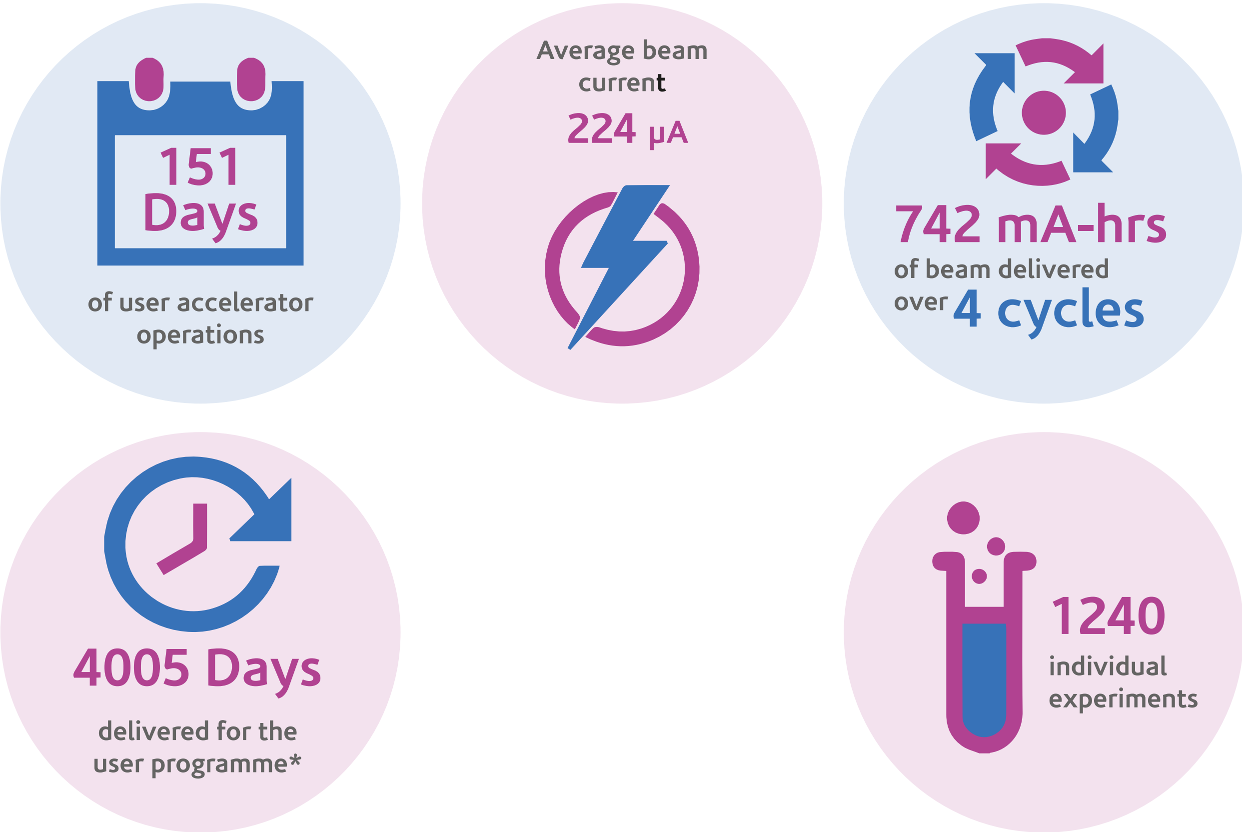
Right: Saidah Sakinah Mohd Tajudin, University Sains, Malaysia & RIKEN and Oana Ciubotariu, Babes-Bolyai University, Romania, working on the EMU instrument.



Technology

Technology

Cutting edge science at ISIS must be underpinned by cutting edge technology. ISIS has an ongoing programme of developments on its accelerator complex and instruments, extending capabilities and improving performance.



*Taking into account instrument down-time, plus calibration and commissioning time.

Table 1.1: Performance in 2019 Cycle by Cycle

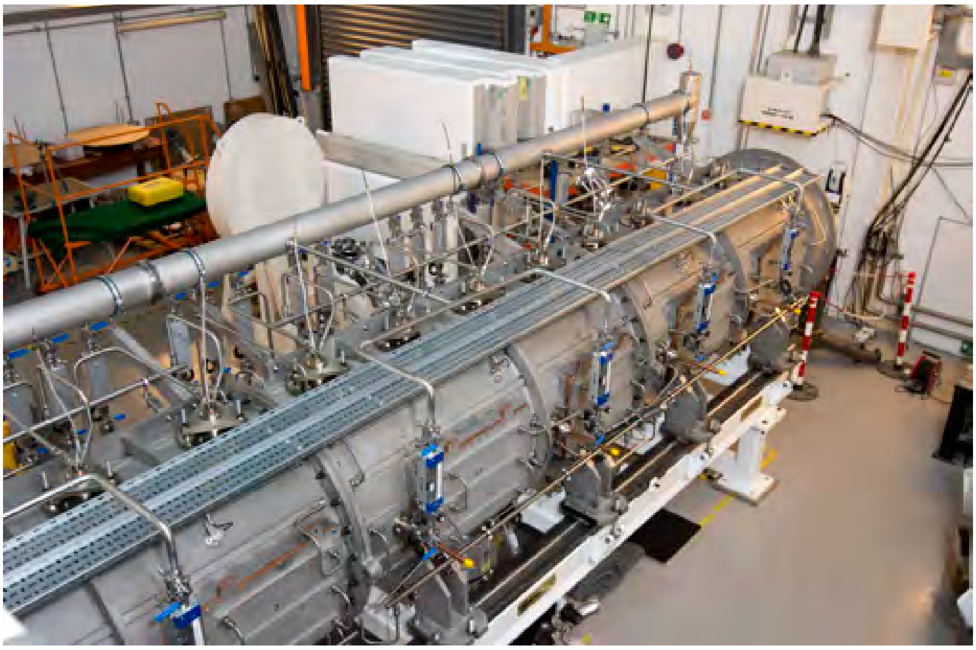
Cycle	2019-1	2019-2	2019-3	2019-4
Beam on time (h)	931.5	830.4	792.5	776.9
Availability (%)	89.5	89.8	91.2	94.9
Total Beam (mAh)	214.3	166.6	173.9	187.0
Mean current when beam on				
Synchrotron (uA)	232	203	221	241
TS1 (uA)	191	164	181	200
TS2 (uA)	41	40	40	40
Highest daily beam total (mAh)	5.64	5.15	5.48	5.84

Left: Galen Amar inspecting the conical drift tubes within the new Linac tank 4.

Major Projects

Linac Tank 4

Linac tank 4 is nearing readiness for full power testing ahead of planned installation on ISIS during the forthcoming long shutdown. Now populated with drift tubes and having received its external water cooling pipework, tuning adjustments can be made and remaining electrical connections attached prior to end plates and hatches finally enclosing the cavity and permitting it to be brought under vacuum. A High-power amplifier has been commissioned ready to deliver up to 2 MW pulses for conditioning. Plans and trials with a full size mock-up have also been carried out to develop and refine the method for physical removal and disposal of the old tank.



TS1 Project

The ISIS first target station (TS1) has been in operation for 36 years without any major refurbishment. In order to keep the facility operating for many more years to come, the target and moderator assembly, together with all the plant and operating systems behind the target station, will be replaced during the ISIS long shutdown in 2021. This is a large project that has been many years in the planning, but which will see TS1 able to operate more efficiently and for longer.

Reflectors

A major milestone for the TS1 project was the safe delivery of the new reflector assembly, which took place in December 2019. This valuable, accurately machined and delicate critical component was transported from the supplier in Spain in four custom-made reinforced boxes. The design of the new reflector is similar to that used in Target Station 2: a modular solid beryllium block design with external cooling that makes it easier for moderator changes, future development and end of life disposal. Replacing the moderators, which used to take about a week, should take less than a weekend to complete.

Having been in manufacture for approximately 18 months, it was a relief to finally get it on site to allow the next stages of testing, alignment and preparation.

Pipework

Work on the services trolley that sits behind the TRaM providing fluids and controls to keep it operating safely, and performing optimally, is one of the largest parts of the project. Since the summer of 2019, an external supplier has been working on site to weld up and fit the many metres of pipework that go into creating all the water and gas circuits. Completion was only a few weeks away when the COVID-19 lockdown was enforced but, through careful planning and a lot of hard work, the work has restarted, although at a slower pace.

The water systems are being built in a modular fashion so future changes can be made more easily and quickly. This also enables testing of a lot of the equipment off-line, minimising impact on shutdown timescales.

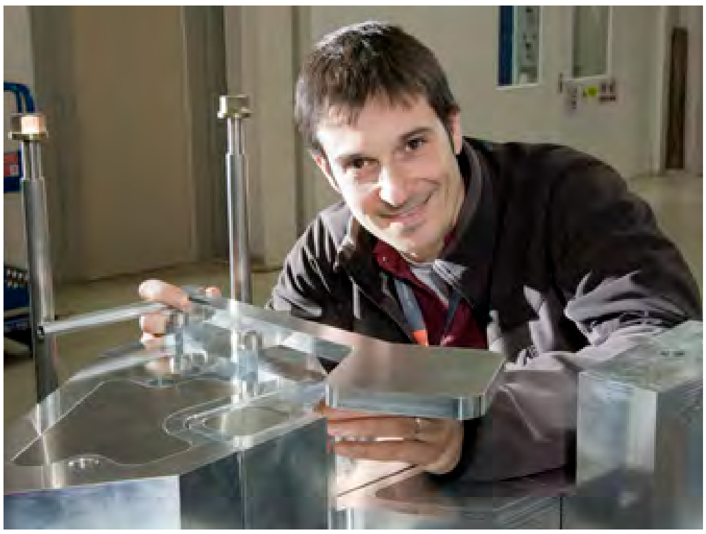
Flasks

During the long shutdown the TS1 project will be removing the majority of items that are based, and operate, in the void vessel. To safely contain, transport and store these items on-site requires a selection of radiologically shielded flasks. Four of these flasks have been specifically designed in-house for the TS1 project: the Reflector Flask, Cantilever Frame Flask, Hardened Rail Flask, and a Moderator Flask. These items are physically large and very heavy (>10T), even if some of the items going in them are much smaller and lighter.

Manufacture of these flasks had started when the coronavirus pandemic hit, and virtual factory acceptance testing enabled the team to continue despite being unable to visit the manufacturers. The approved flasks were then able to continue their manufacturing journey, with the first arriving on site at the beginning of June 2020.

Phillip Lester about to perform a TIG weld on pipework.

Gary Hatliff, left, and Phillip Lester installing a non-return valve on the ISIS TS1 project services trolley in building R106.



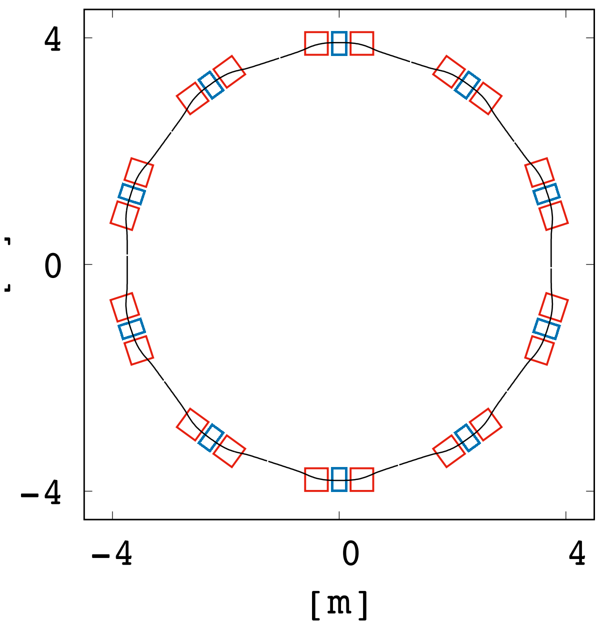
Dan Blanco Lopez working on the pre-moderators on the ISIS TS1 TRaM mock up.

ISIS II

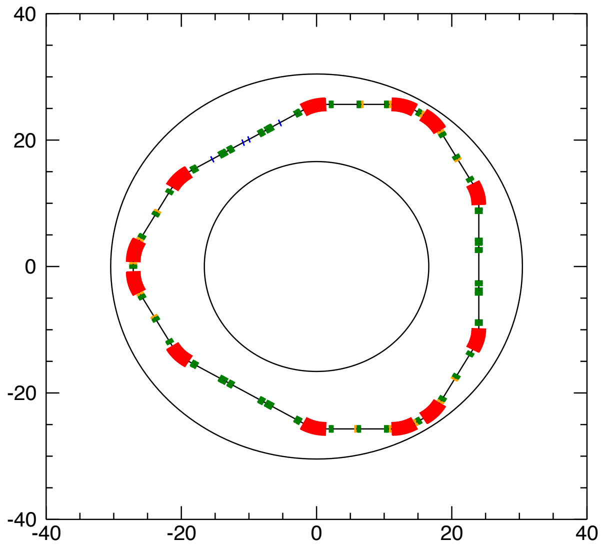
ISIS-II is the proposal for a next-generation neutron source as the successor for ISIS. Although ISIS will continue to operate for many years to come, plans for a new facility will be developed over the next decade in order to be ready for construction sometime after 2030. This will maintain and enhance the UK's neutron provision, in a way complementary to the ESS, in order to continue to support the UK research community.

A project has been established to consider the requirements for an ISIS-replacement facility, and to explore the technologies that might underpin this. This work includes considering the science drivers for neutrons and muons over coming decades and how these will influence the design of new neutron and muon instrumentation. In turn, these considerations affect the nature of the source and hence the accelerator characteristics. Feasibility work on accelerator possibilities is ongoing, with the aim of ramping this up over coming years. Alongside this, we will be developing the science case in consultation with the ISIS user community.

The UK research community is at the forefront of neutron scattering through having ISIS as a national source in addition to access to the ILL and the ESS in the future. ISIS-II will maintain the UK's position and provide many more years of pure and applied studies using neutrons and muons.



ISIS-II FFA Prototype Propose layout: A plan view of a proposed Fixed-Field Alternating-Gradient Accelerator (FFA) design for a small-scale prototype to prove the technology for a later potential full-scale ISIS-II design. Main bending magnets are shown in blue and red.



ISIS-II RCS Proposed Layout: A plan view of a proposed Rapid Cycling Synchrotron (RCS) design for ISIS-II showing the main dipole magnets in red and focusing quadrupoles and accelerating cavities in green and blue.

Accelerating Cavity Prototype: A 3D render of an accelerator cavity design to be used on the proposed FFA prototype. A rectangular beam pipe is visible in the centre and is surrounded by ferrite material cores (in grey) tuned for the appropriate frequency performance. Cooling and structural components are shown in orange and yellow.

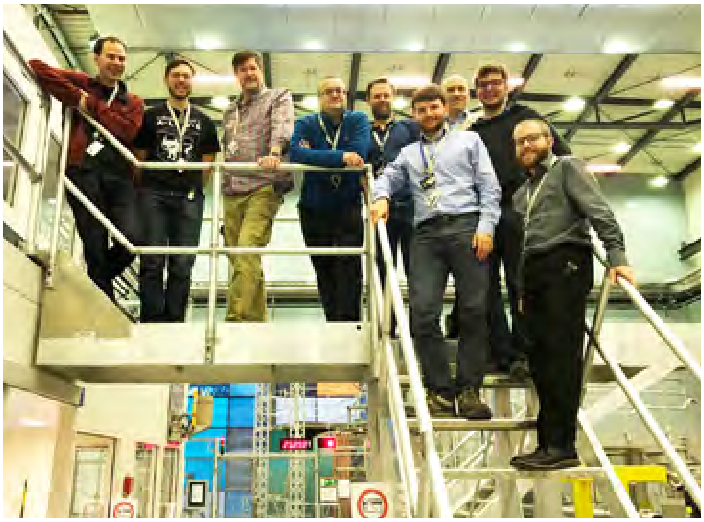
European Spallation Source (ESS)

ISIS staff continue to be involved with the UK's contribution to the ESS in Lund, Sweden. The ESS has moved further into its installation and commissioning phase alongside ongoing construction and deliveries. ISIS staff are engaged in delivering two instruments: LoKI and FREIA, as well as expertise for laboratory design and installation, and data reduction/streaming software development. Staff are also supporting colleagues in Italy (CNR) to deliver the VESPA spectrometer.

LoKI is a versatile small angle neutron scattering instrument and will be one of the first instruments operational at ESS (alongside DREAM and ODIN from other ESS partners). Freia is a liquid reflectometer and is planned to be operational as part of the second tranche of instruments. Many areas of the detailed designs are complete and the projects are in the procurement phases. Sections of LoKI are being pre-built at ISIS to test some of the operational procedures and ensure that the instrument can be efficiently constructed once it arrives in Lund.

The UK-ESS Programme Office (PO) is also part of ISIS and is responsible for managing and overseeing the whole £165m UK construction contribution to ESS. This includes the above projects that fall within ISIS; projects in other STFC departments (Technology, AsTEC); and projects in other organisations (University of Huddersfield and UKAEA). The UK-ESS PO also forms a valuable bridge between the project delivery and the UK-ESS governance Board. All of the UK-ESS work was recently show-cased at the Daresbury Laboratory and Rutherford Appleton Laboratory with the project teams giving presentations and holding poster sessions.

Jon Elmer presenting his poster at the UK-ESS Day held at Rutherford Appleton Laboratory in December 2019.



Developers and Instrument Scientists from ESS and partners (including STFC), conducting testing at the ESS test facility in Berlin.

Participants of the handover ceremony form the layout of the instrument suite inside the Long Instrument Hall.

Endeavour: next generation instruments for ISIS

ISIS seeks to continually update and develop its suite of neutron and muon instruments, in order to respond to current research needs and to ensure it remains a world-leading neutron and muon source.

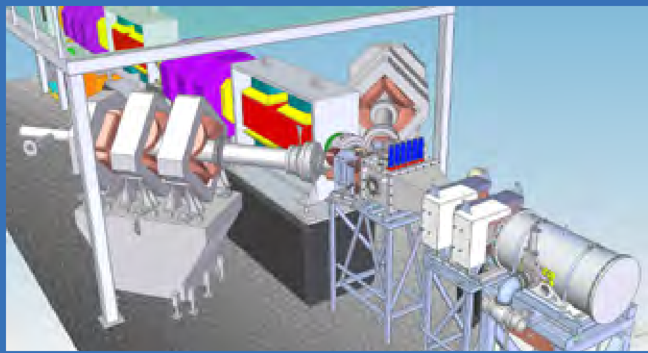
Over recent years the first and second phases of instruments on the Second Target Station have been completed, with the latest, Zoom, coming into the user programme over the past year.

ISIS is now seeking its next phase of new instruments and significant instrument developments: a portfolio of projects that has been called the Endeavour programme. Endeavour will see the ISIS instrument suite developed to meet current and future challenges in areas such as Materials for the Future; Smart, Flexible and Clean Energy Technologies; Advanced Manufacturing; and Biosciences and Healthcare.

A proposal for Endeavour has just been submitted to the UKRI Infrastructure programme. A variety of large instrument projects is included within the Endeavour suite – examples include:

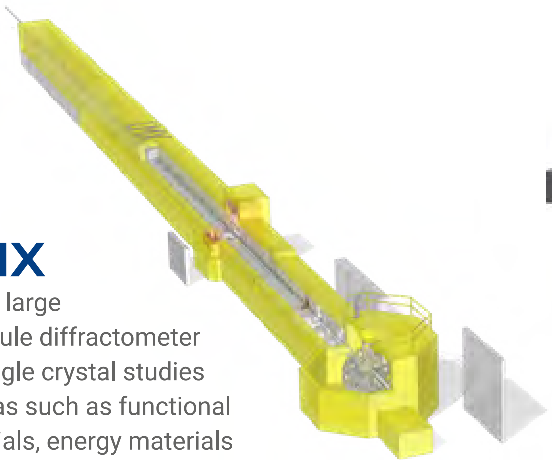
Super-MuSR

Enhanced time resolution and flux for next-generation muon studies.



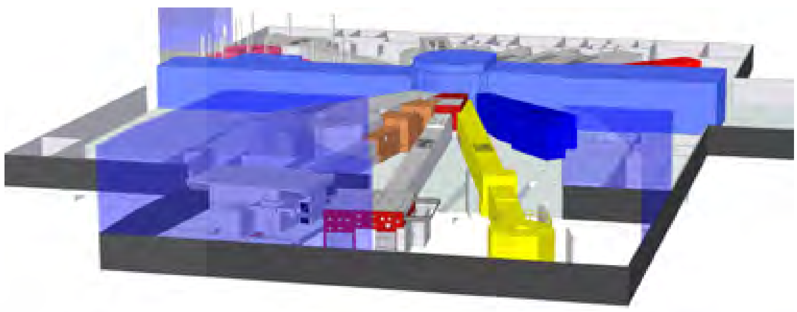
HRPD-X

A next-generation high-resolution powder diffractometer enabling enhanced studies of MOFs and Zeolites amongst other materials.



LMX

A new large molecule diffractometer for single crystal studies in areas such as functional materials, energy materials and biomolecular science.

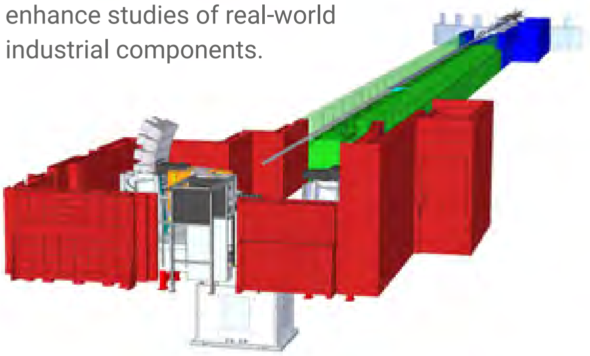


Tosca+

An order of magnitude more flux through development of the Tosca secondary spectrometer for vibrational spectroscopy studies in catalysis and energy materials.

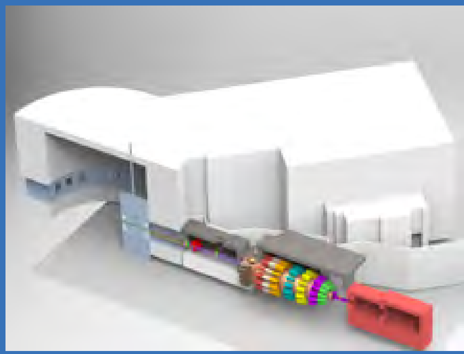
e-map and Engin-x

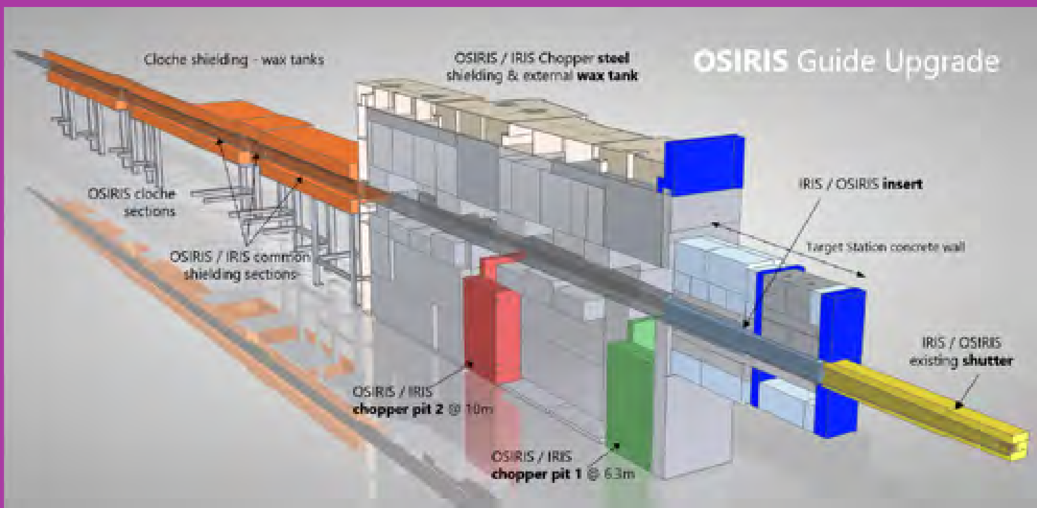
Advanced engineering capability through upgrading the existing Engin-x and construction of e-map, a new instrument to enhance studies of real-world industrial components.



Sandals-II

A diffractometer for chemical engineering in amorphous and liquid samples providing information on multi-component samples used in catalysis, drug release, hydrogen storage, oil industry systems and polymers.





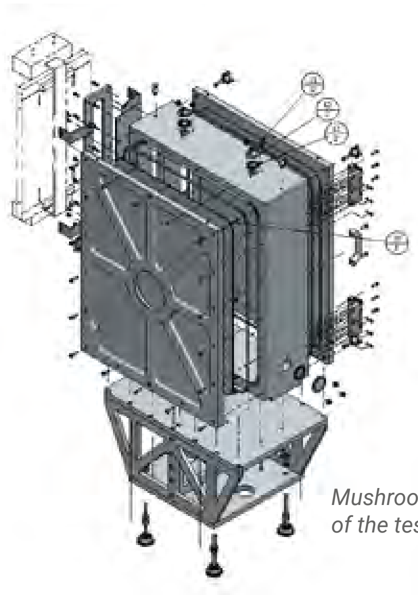
Osiris+

A high-resolution spectrometer and diffractometer for studies of atomic and molecular-level motions. This upgrade will enable studies in catalysis and energy materials, enhancing exiting industrial work.

Mushroom

An entirely novel concept that will be transformative for inelastic neutron scattering. Mushroom will enable use of much smaller samples, more detailed parametric studies, and new types of sample environment and in-situ equipment, in areas such as thin magnetic films, thermo-electrics, magneto-resistive materials, ionic conductors and battery materials.

Mushroom: manufactured test vessel. It's a vacuum vessel used to investigate the relative position of crystal analyser and position sensitive detector of the Mushroom beamline.



Mushroom - 3D drawing of the test vessel.

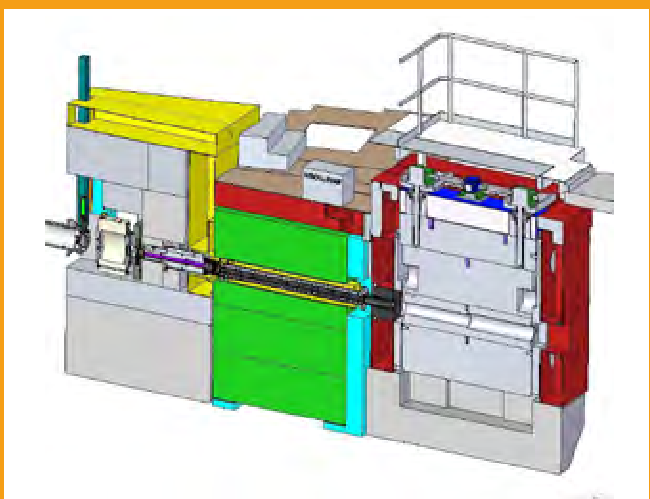
Instrument Updates

RIKEN-RAL muon beamline refurbishment

The RIKEN-RAL muon beamlines were constructed by the Japanese RIKEN institute, but ownership and operation have now passed to ISIS under a new five-year agreement signed with RIKEN in 2018. As part of this agreement, the beamlines are being refurbished to enable them to continue to operate for many years to come. This year has seen detailed planning work for cabling and water-circuit replacement, together with placement of an order for new power supplies for all beamline magnets. The refurbishment work will take place during the long shutdown.

ALFRed – ALF Redesigned

Preparations are accelerating all around ISIS for work that will take place in the long shutdown. For the Excitations group the most significant project is called "ALFRed". It is the completion of a steady programme of improvements to our alignment diffractometer ALF. This final step, which will be done in parallel with a major upgrade to the next-door beamline SANDALS, will be to remove all of the remaining components from the old PRISMA beamline (long since decommissioned) from upstream of ALF and install better shielding and evacuated collimation tubes. The collimation to be used is actually being recycled from old parts of MAPS that we removed for its guide upgrade project a couple of years ago. By removing about 4 metres of air from the ALF flight line we expect to increase the flux by about 50%, and the extra shielding should improve the background both on ALF and on neighbouring beamlines SANDALS and SURF.



Cross-section through the ALFRed beamline (beam goes left to right) from choppers to entry into the blockhouse. The green area is currently a large void.

Polaris induction furnace

A new induction furnace has being developed on Polaris as the result of a collaboration between Aarhus University, ISIS Crystallography Group, the ESS and Chalmers University of Technology. A water-cooled copper coil generates an oscillating magnetic field and this couples with electrons in the sample tube for quick and efficient heat transfer. Unlike other ISIS standard furnaces, which require their own ultra-high vacuum vessel, the induction furnace can sit directly in the vacuum of the detector tank, reducing background scattering from the sample environment.

Many different sample geometries are possible using this furnace, as the coils can be made in different shapes and sizes. A long-term objective is adding uniaxial compression, to take measurements during compaction of powders to form dense pellets. This would be the first induction press compatible with neutron scattering experiments.

The group has also been in discussions with other ISIS instrument teams (PEARL and Engin-x) regarding potential applications. The electronics from the Polaris set-up will apply to a range of coil designs that could be used in different neutron experiments, or even in synchrotron environments.

Neutron and Muon Instrumentation Development Group

The aim of the new Neutron and Muon Instrumentation Development Group (NMIDG) is to act as a support for scientists and technology groups in the development of new, state of the art instrumentation at ISIS. The group will advise, give training and help scientists with instrument simulations and design as well as conducting technical reviews of new instrumentation prior to approval for construction.

The group will act as a link to advanced instrumentation teams at other facilities and software providers in order to continually enhance ISIS's capabilities in relevant areas. To improve people's instrumentation knowledge and capabilities, NMIDG will organise internal and external meetings and workshops. In addition, the group will work to develop new instrumentation concepts and ideas through internal and external collaborations.

Polref

A new Ferromagnetic Resonance (FMR) setup in the ISIS Materials Characterisation Lab has been put together to develop *in-situ* FMR for the polarised reflectometer program, allowing for additional characterisation while the neutron reflectivity is being taken on the sample.

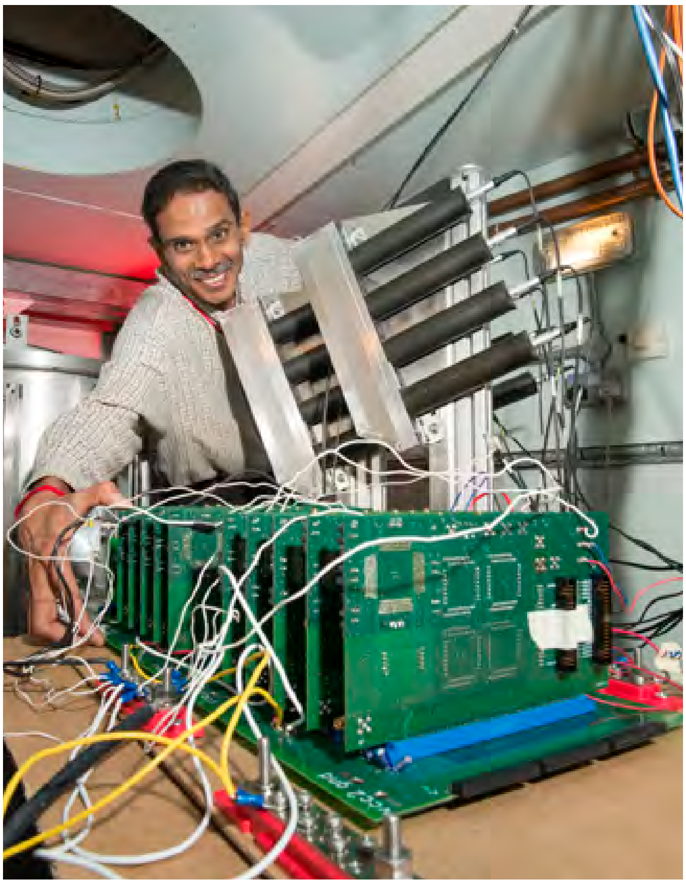
This is useful for samples where there is a specific area of phase space – i.e. temperature and field – where something interesting could be going on. For example, if a user sees an interesting effect in their FMR from the MCL, and wants to know the magnetic depth profile of the sample, we can use the on-beamline FMR setup to replicate their lab conditions before measuring with neutron reflectivity. This will enable more targeted studies, where we can reliably measure at the correct point in a phase space, rather than having to map around the temperature and field values observed in the user's home laboratory.

There is a broad range of science in the magnetism community where this will be useful; specifically in the spintronics community. For example, skyrmions only exist in certain materials at very specific field and temperature values. FMR could allow us to confirm the sample is in the correct state when measuring. It could also be used for investigating other spintronic technologies such as the spin Seebeck effect; a potential new way of energy harvesting from waste heat.

The first publication resulting from measurements used this setup to investigate the spin Seebeck effect in Yttrium iron garnet. In addition to the FMR, SQUID measurements were used to extract the magnetic properties as well as to extract the spin wave damping parameter. *G Venkat et al. Spin Seebeck effect in polycrystalline yttrium iron garnet pellets prepared by the solid-state method. Europhys Lett 126, no. 3 (2019): 37001. doi:10.1209/0295-5075/126/37001.*

High-throughput Transmission Measurements on VESUVIO

Recent upgrades on VESUVIO make it a world-leading instrument to perform neutron transmission experiments and obtain accurate thermal neutron cross-sections. Commissioning of a new neutron-Gas-Electron-Multiplier (nGEM) 2D detector is underway in collaboration with colleagues from Univ. Milano Bicocca (Italy) and Nuclear Instruments s.r.l. It has a ca. 100-fold efficiency gain with respect to the traditional beam monitor, thus allowing faster measurements and high-throughput parametric investigations. The new detector will allow measurements with a 2D spatial resolution of ~3mm over the entire VESUVIO beam size (ca. 4.5cm diameter). This new addition, together with the installation of a lower-background beam pipe in the blockhouse, and a new incident foil changer for optimal calibration and background subtraction, which took place over the last two years, will boost the scientific programme around the measurement of neutron total cross sections. For further information, the instrument capabilities for neutron transmission experiments have been recently summarised by Robledo et al. (Nucl. Inst. Meth. A, 971, 164096, 2020).

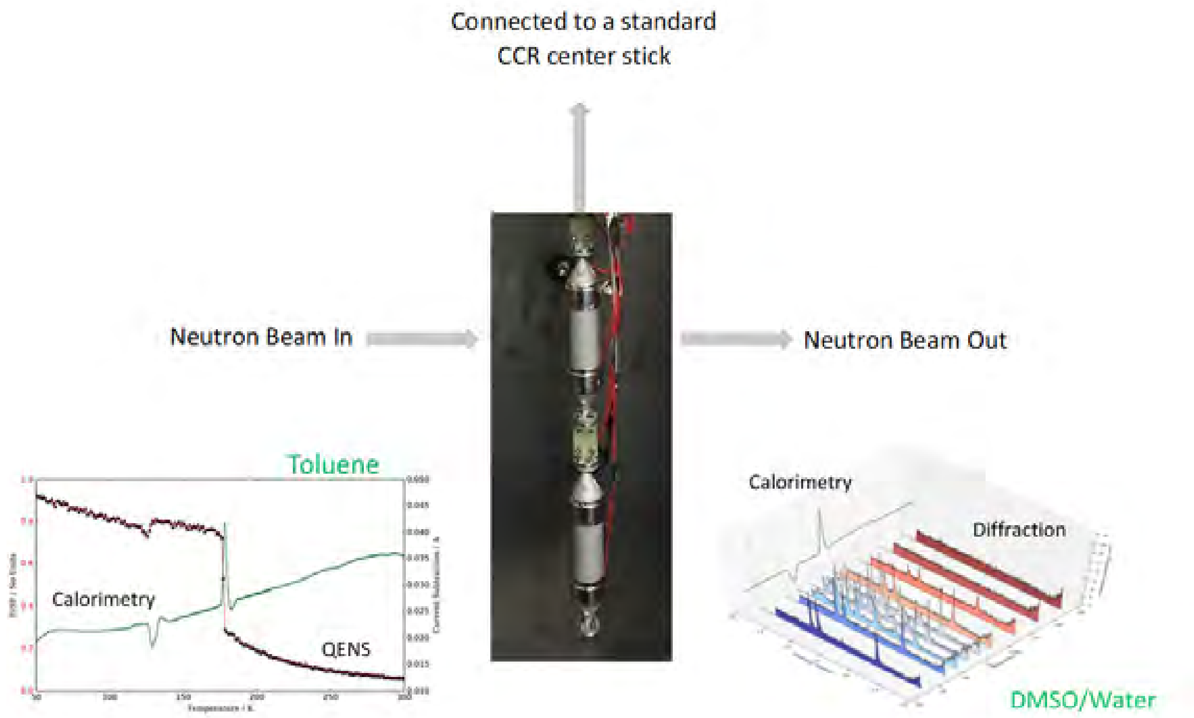


Professor Bharat Bhuva, Vanderbilt University, USA, on the VESUVIO instrument.

In-situ calorimetry with quasi-elastic neutron scattering on IRIS for liquids

Differential Scanning Calorimetry (DSC) is an analytical technique commonly used to probe phase transitions and quantify enthalpy changes that occur in materials. These changes are typically associated with structural rearrangements and/or dynamics at the molecular level. Quasi Elastic Neutron Spectroscopy (QENS) allows for an insight into the molecular dynamics (MD) and stochastic motions occurring in materials, thereby providing complementary information to that obtained using DSC. Performing the two measurements simultaneously can therefore be a powerful tool, allowing for a more complete understanding of a material's characteristics with good accuracy.

The first ever working prototype has been realised on the IRIS spectrometer to measure thermodynamic changes in parallel with QENS neutron data (and diffraction data using the auxiliary bank). Initial proof-of-concept has been carried out with specially designed aluminium cells that can accommodate liquids, with measurements currently limited to room temperature and below using a standard closed-cycle refrigerator (CCR). The next step includes cells for powders and higher temperature measurements.



In-situ calorimetry + QENS cell set-up on IRIS. Left figure shows combined measurement of thermal transitions and elastic fixed window scan for toluene. Right figure shows combined measurement of thermal transitions with diffraction patterns for a DMSO/water mixture.

Harry Nolan

From work experience student to apprentice, and now undergraduate.

> My original attraction to ISIS was the fascinating work that happens here, and the large scale of the engineering.

Work experience at ISIS

Harry began his apprenticeship at ISIS in 2014. During the application process, he also applied for a work experience placement, and spent a week with the electrical design team. "My original attraction to ISIS was the fascinating work that happens here, and the large scale of the engineering", explains Harry. "The work experience placement gave me a chance to look around a bit more, and meet the staff. Seeing how the engineering can be used to support the amazing science projects made me sure about taking up the apprenticeship."

During his apprenticeship, Harry had placements at Diamond Light Source, the Central Laser Facility, RAL Space and even ILL and CERN. During his penultimate placement, he spent time in the electrical design team at ISIS. "I was back in the same desk that I'd been sat at during my work experience!" Harry remembers, "I enjoyed being part of that team, and especially like the design aspect of the work."

Finishing an apprenticeship, and starting a degree

When given a number of offers for work after his apprenticeship had finished, Harry chose to join ISIS as an Electrical Design and Projects Engineer. Not content with full-time employment, he wanted the opportunity to keep expanding his knowledge and started a part-time BEng in Electrical Engineering sponsored by STFC, based out of London South Bank University.

"It's intense, but I wanted to push myself", he says. "I spend one day a week in London, with sessions running 9am-9pm, and then also have university work to do in my evenings and weekends. I've also enjoyed meeting the other students, who are from companies including TFL and UK AEA."

Studying under lockdown

Now two years into his four-year degree, Harry has the Covid-19 lockdown to contend with. "I'm trying to keep my normal routine, doing university work on a Tuesday. As most of my design work is on the computer, I'm not struggling too much with not being able to go onto site. Although it's not as easy to talk to people over Zoom as it is in the office, and I miss that!"

He also has exams to sit this summer. "The University has made all the exams open book. They will release the exam questions in the morning and expect the hand-written answers scanned in and submitted by the evening. It's a very different way of doing it, but I'm looking forward to exams being over so I can get my evenings and weekend back."

Not all apprentices go on to complete part-time degrees, but Harry knew it was for him. "I knew I wanted the qualification, so I'd rather do it straight away than have a gap between studies. My ISIS supervisor has been very supportive and, in my fourth year, I will be able to use my work at ISIS as part of my Final year Project."

As for the next step, Harry hasn't written off further study, but thinks, "it would be nice to have fewer pressures, and just have a normal job!"

Accelerator

Accelerator and Electrical Systems

Modernising the Ion Source

The particle beam in the ISIS accelerator starts at the H^- ion source. The existing ion source has served ISIS well for nearly 40 years, but requires replacement and maintenance every two weeks. A project is underway to develop a new type of ion source using modern technology which should last months or years rather than weeks.

One of the key components of the new ion source is a radio-frequency (RF) amplifier that delivers power into a plasma, from which the particle beam emerges. The amplifier is highly powerful, yet rugged enough for long-term maintenance-free operation on the accelerator. The team looks forward to the installation and commissioning of the system by the end of 2020.

Members of the Low Energy Beams Group with the new ion source RF amplifier: Tim Stanley, Tiago Sarmento, Scott Lawrie, Rob Abel, Dan Faircloth and Olli Tarvainen (left to right).

Upgrading the Synchrotron RF High Power Drives

The fundamental frequency high power RF systems in the ISIS synchrotron have been accelerating protons largely unchanged for over thirty years. Due to end of life and obsolescence issues with much of the equipment, major upgrades are now necessary to ensure continued operation.

A new RF drive system has been installed in superperiod seven of the synchrotron, proving technology for a full upgrade of the system. The installation has performed flawlessly, operating without fault throughout cycle 2019/4. The remaining fundamental RF drives are currently scheduled to be upgraded in the ISIS long shutdown, promising a modern system that is more reliable, sustainable and efficient.

Retired member of the RF Group, Derek Bailey, inspects the new high power drive and driver during testing.

New Injector Phase Monitoring System

Synchronisation of the ISIS linac's accelerating RF fields with particle arrival times is key to ensuring efficient acceleration through the linac and synchrotron. This synchronisation of phase has traditionally been carried out empirically, consuming valuable set-up time during the machine physics and run-up periods.

The Diagnostics Section have developed a new phase monitoring system, by connecting newly developed signal processing electronics to existing linac hardware. The new system will provide a direct measurement of the relative phase changes, reducing set-up time and providing a reference for future optimisation. Consequently, beam output can be improved whilst reducing activation of components, making the facility safer and easier to maintain. Following the success of the initial prototype, the first operational devices are now being produced.

Left: Asim Yaqoob, Performance Improvement Engineer working on a synchrotron dipole magnet.

Upgrading the Injection Dipole Magnet Power Supply

The injection dipole magnet steers the H¬– beam through the stripping foil at the end of injection. The resulting protons fill the synchrotron over ~140 turns, after which the magnet is switched off and the beam is allowed to pass by on a normal orbit. The magnet is driven by a power supply, which can switch from delivering 15 kA to fully off in just 100 µs.

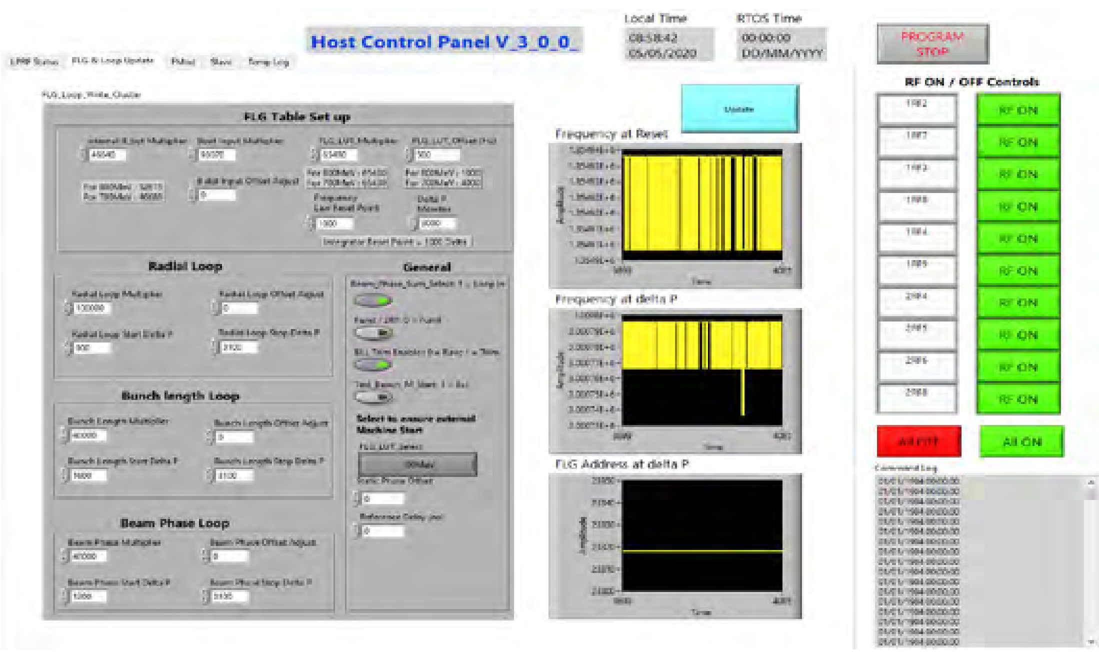
Prior to decommissioning, the power supply had been operational for over 30 years, making it the oldest magnet power supply in ISIS. It was also the cause of around three days of beam downtime per year. A three-year project was thus commenced to replace it, which was completed in January 2020. The new power supply is of a modular construction, has better diagnostics and spare parts are readily available. These key benefits should help to improve the availability of ISIS.

Jonny Ranner of the Magnet Power Supplies Group configuring the new injection dipole magnet power supply.

Enhancements to Digital Low Power RF

The PXI-based digital low power RF system has been used for several years to provide the frequency sweep that drives each of the ten RF cavities. This year, the digital system has been upgraded to include a feedback mechanism around each cavity, enabling greater control of the voltage that accelerates the synchrotron beam. Feedforward beam compensation has also been implemented to reduce the adverse effect of the beam on each cavity during acceleration.

These improvements, coupled with the introduction of the UPS-driven filament power supplies have led to much greater stability, particularly during the crucial stage of beam injection into the synchrotron. This has played a key role in enabling ISIS to produce the record beam currents seen in Cycle 2019/4.



The new low power RF software control panel, which plays a key role in the improved performance.

Enabling Access to Data and Trends

The accelerator control system monitors and controls over 30,000 settings across the injector, synchrotron and related systems. However, all of this data has never been logged in a centralised data repository, making it difficult to draw meaningful trends and insights.

Ivan Finch and Gareth Howells of the Controls Group have installed a new messaging system and InfluxDB time-series database, which combined provide a permanent record of large volumes of machine data. This facilitates fault finding in the event of machine downtime, and enables trend analysis to improve reliability. This new focus on data is also driving developments in machine learning to predict component lifetimes better, providing ISIS with predictive maintenance capability for the future.

The new InfluxDB time-series database, which enables access to data and trends that were previously unavailable.

Maximum Beam Current Achieved

Physicists in the Synchrotron Group continually optimise over 10,000 machine parameters to maximise the beam current provided to users. Over 35 years of operation the beam current has been limited by the number of particles lost as they are accelerated. Beam loss cannot be avoided completely due to engineering limitations and physical phenomena but it must be carefully controlled to prevent damage to equipment and high radiation levels such that components cannot be repaired safely.

In 2020, new beam loss diagnostics and improvements to magnet power supplies and RF system stability has enabled the physics team to achieve 245 μA, the maximum beam current the targets can take (205 μA to TS-1 and 40 μA to TS-2). The team will work to retain this level to enable users to complete more experiments more quickly.

Members of the Synchrotron Group optimising the beam in the ISIS Main Control Room: Hayley Cavanagh, Bryan Jones and Peter Hicks (left to right).

Skills

Placements and visits

Developing the skills of our staff and wider scientific community is vital to maintaining our status as a world-leading research facility. We also have a key role to play in inspiring the scientists and engineers of the future. We offer a wide range of hands-on training, offer around 150 placement opportunities and have an active public engagement programme.

25 on Graduate training programme

22 vacation students

42 work experience placements

43 Apprentice placements

30 undergraduate sandwich students

Higher education: 30 visits; 812 visitors

11 new co-sponsored students

862 Business visitors

Total visitors: 4272
School students, teachers and public visitors: 2598

Left: Students from Willink school during a visit to ISIS.

Developing the student community

The student community continues to lie at the heart of ISIS Neutron and Muon Source. More than 50 vacation and sandwich students worked at the facility in 2019/20, and another 11 students began co-sponsored PhD studentships. In addition, there were visits from 775 PhD students to ISIS for experiments. The facility seeks to encourage and grow the student community through training courses, direct supervision and on the job training.

PhD student training and events

The ISIS Neutron Practical Training Course ran from 18-27 June for around 35 students, giving them first-hand experience of using ISIS neutron instruments. The Oxford School of Neutron scattering ran from 2-13 September 2019 for around 60 attendees, and ISIS ran an Advanced School in Muon Spectroscopy (jointly with PSI and the universities of Oxford and Durham) from 15-22 August 2019 for 45 attendees.

These courses are always extremely popular and enable students to get a hands-on experience of work at the facility, gaining skills to help them when they come back as users and when they take the data back to their institution.

Each year ISIS organises two student-specific meetings: the ISIS Student Meeting held in October and a satellite student day at the UK Neutron & Muon Science and User Meeting (NMSUM). These provide opportunities for students to present their research to their peers, chair the meeting sessions and challenge them to ask questions of each other, as well as network with other students who also spend significant time at large scale facilities. 2019/20 saw increased attendance at the October event, and excellent presentations showcasing the diverse research with the ISIS student community. Due to the cancellation of NMSUM, there was no student conference in the spring.

Facility Development Studentships

ISIS has an annual call for Facility Development and Utilisation Studentships. These are co-funded studentships, normally 50% funded by ISIS and 50% by a university, which contain an element of facility development - for example development of equipment, software or experimental processes. Studentships have an ISIS supervisor and a university supervisor who work in partnership throughout the student's project. Over recent years, ISIS has funded around 60 of these studentships across a wide range of topics and university partners.

James Annis, University of Warwick, taking part in the ISIS Neutron training course on the GEM instrument.

Visits to ISIS

In addition to beamtime allocation, many groups of students at both undergraduate and postgraduate level visit ISIS through the year. This year saw 30 academic visits to the facility, with over 800 attendees able to view the facility for themselves. After the facility was no longer able to host visitors in person, these events were hosted online.

ISIS Student Meeting held at Milton House on 28 October 2019.

Sandwich student scheme

In 2019/20, ISIS hosted 30 undergraduate students for twelve-month placements as part of their degree. The students are a crucial resource to the facility, offering new ideas and perspectives. It also gives them an introduction to work outside of academia and to the range of careers available at ISIS and STFC more widely.

ISIS Sandwich students took part in the new FameRAL science communication challenge, where they were tasked to explain their placement work to a general audience in only three minutes. Isobel Adamyk was awarded Highly Commended as the highest scoring ISIS student.

> “I am doing a PhD next academic year in Atmospheric Chemistry at the University of York. I am very grateful for this placement opportunity as I feel it has really helped me decide what to do in the future and has enabled me to achieve it so thank you!” **- Loren, 2019/20 Sandwich student**

Fame RAL
A year on placement...
...in 3 minutes

Sandwich student Loren Temple presenting at the ISIS Student Meeting.

Inspiring the next generation

This has been another great year for public engagement at ISIS, with the facility welcoming over 2500 school students, teachers and members of the public for talks, workshops and tours of the experimental halls.

Our events span a wide range of activities and themes, to reach and captivate new audiences. 2019 saw the 50th anniversary of the Apollo moon landings, with over 400 school students and members of the public visiting ISIS as part of the RAL Apollo@50 events, discovering the research in space science that ISIS contributes to. These and other public and education access days are extremely popular, and feedback consistently show that tours of ISIS are a highlight at these events. At school events such as Chemistry@Work, Particle Physics Masterclass, Schools Accelerator Day, Exploring Engineering Days, Atomic Afternoons and Space Explorer days, we demonstrate the vast range of science and engineering that goes on at ISIS and the interdisciplinary nature of our work, allowing students to explore STEM and STEM careers beyond the classroom.

As well as school events, ISIS opens its doors to the general public several times a year for events such as Stargazing at RAL, where hundreds of visitors come to explore our cutting-edge science and engineering, meet our staff, hear our stories, and discover the world-leading research that goes on, from superconductors and soaps to Martian meteorites and fossilised skulls.

Visitor to ISIS as part of RAL Stargazing event.

In addition to visits from school students, teachers and members of the public, ISIS also hosted 42 work experience students for 1-2 weeks over the summer in 2019, offering unique insights into the facility and opportunities to work alongside ISIS staff in our experimental halls, workshops, labs and design offices. ISIS continues to play a leading role in the Engineering Development Trust's Engineering Education Scheme, during which ISIS staff mentor a group of local school students for 6 months on a real engineering challenge. This year, A-level students from Willink School in Reading were tasked with designing a device to lift radioactive waste baskets from a highly radioactive area.

A further 4000 members of the public have engaged with ISIS science and engineering at off-site events, with ISIS staff venturing out to local schools, community centres, festivals and fairs, reaching new and diverse audiences and inspiring the next generation of scientists and engineers. At events such as the Oxford Science and Ideas Festival, Family Science Day at Cornerstone Didcot, Cowley Road Carnival, Harwell STEAM festival, Wantage Museum STEM Day and Space Day@The Hive, we reach new and diverse audiences.

March 2020 saw the start of the lockdown and a very rapid transition to virtual school and public events. See P51 "ISIS during the lockdown" for more information on how ISIS adapted during the crisis, developing new and exciting ways to engage with school students, teachers and the general public during a time of social distancing and home learning.

School students visit ISIS as part of the Apollo 50, Chemistry @ Work, and RAL Stargazing events.

Chloe Johnson

From ISIS Sandwich Student to Research fellow, and future user?

> "The skills I developed during the year were just as important as the ones I would have gained from a lab-based placement."

Science communication placement

Chloe studied biomedical sciences at the University of Kent and, during her second year, was persuaded by a careers talk into taking time out of her studies to do a year in industry. She applied for some lab-based placements and, because of an opportunity in sixth form to go in to a primary school and speak to the children about science, she was also encouraged to apply for a science communication placement here at ISIS.

For a year, beginning in September 2014, Chloe worked as part of the Impact Team at ISIS, writing industry case studies, helping with the site Open Week and editing the website pages. "I loved being a placement student," she explains; "it was very different to university studies – and very interesting being exposed to real scientists doing science! We built a community between the sandwich students, which was nice." She says, "The skills I developed during the year were just as important as the ones I would have gained from a lab-based placement."

From placement to PhD

During her second year, Chloe discovered a love of research, and decided during her placement that she wanted to include science communication as much as she could. In her final year project, she worked with a group looking at myosin, a muscle protein. She enjoyed this and continued in the group as a PhD student, investigating myosin in the heart, and its effects on inherited heart disease. "But even after a PhD-worth of research, we still don't know the answers!"

During her PhD, Chloe kept up her science communication by teaching undergraduates and developing a demonstration to out to a local school. "The presentation skills I gained during my placement were not just valuable for outreach activities, but also for presenting my work to the department and at international conferences." Chloe explains; "there are lots of times you need to be able to explain your work to non-scientists, or write for a general audience. My placement gave me a chance to develop these skills."

Chloe really noticed a difference in herself when coming back to university after her year at ISIS. "I had definitely got much better at time management! I worked my final year at university as if it was a job, which made me much more efficient. I even used the same skills when writing my PhD thesis up in 2019."

The favourite part of Chloe's placement came towards the end, when she went the RADECS conference in Moscow. "Having been part of the conference build up, it was great to see my work go full circle. To be trusted to represent the organisation made me realise how much I'd grown into the role during the year."

Research fellowship

After finishing her PhD, Chloe has been successful in applying for a research fellowship at the University of Cambridge to study non-muscle myosin. She has gone into the fellowship knowing the value of using neutrons at ISIS in her work, and aiming to share her knowledge of ISIS with her new colleagues.

Chloe has advice for those considering a placement: "Do it! A year feels like a long time, but it's worth it. Being at ISIS, I got to experience large-scale science at a really early stage in my career. If you come into the placement with a goal of what you want to get out of it, that really helps focus your mind and your motivation while you're there."

Events

UK Neutron & Muon Science and User Meeting

The UK Neutron & Muon Science and User Meeting (NMSUM), a joint meeting held by ISIS and the Institut Laue Langevin (ILL), has been postponed to April 2021. However, as an alternative during lockdown, we held a series of online discussions on the science applications of neutrons and muons, with members of the community presenting their work. The first of these online meetings took place on place on Tuesday 9 June 2020 and was based around the Functional Materials session that would have taken place at NMSUM, with the second on 20 July focussing on Soft Matter and Biomaterials.

> I would not have attended the 'physical' meeting as it's not in my specific research interests but I learned new things and got new ideas for proposals after ISIS reopens.

> The format of such short online meetings is perfect. I, being located in New Zealand, had no chance to join in person, but the online format makes this all possible.

The 2019 meeting attracted over 300 attendees in Warwick, who then split into groups for the parallel sessions. In 2020, over 150 participants were present in each of the online meetings, treble the number of people who would have been able to attend one of the parallel sessions during the conference in its usual set up. Attendees joined in from across the UK and Europe, and as far away as Australia.

TwinCAT for Motion Control Development Workshop

A new workshop took place on 1-4 April 2019 aimed at developing innovative software for motion control. It brought together engineers from ISIS, the European Spallation Source (ESS) in Sweden and the Jülich Centre for Research with Neutrons (JCNS) in Germany. While general motion control workshops already exist, participants saw a need for a workshop specific to software.

Motion control is the automated movement of objects, most commonly used in applications for remote controlled cars and industrial robots. Motion control systems are capable of extremely precise speed and positioning. The team's development of this next generation of software will move ISIS towards more advanced motion applications that will speed up the process of aligning instruments and improve the science capability of some of ISIS' instruments.

The collaboration hopes to develop best practice principles that all three facilities can use in terms of software and project management. For all the facilities represented at the workshop, this should improve the quality of user experiments and provide technical expertise to solve common problems.

High-Pressure Neutron Diffraction: Current and Future Prospects

On the 13-14 May 2019, a meeting organised by ISIS brought together a group of UK, European and US researchers with a joint interest in performing neutron scattering experiments at extreme pressure and temperature conditions.

The application of pressure can have a dramatic effect on the physical state of a material and its physical properties (for example, by compressing liquid water to a pressure ~22000 times that experienced on the surface of Earth, it will have a melting point of around 100˚C). Therefore, studying the behaviour of materials at the extremes of pressure and temperature is of interest to both academic and industrial communities.

Neutron scattering under these conditions is particularly challenging as there is an inherent need for large sample volumes, which brings difficulties in reaching the temperatures and pressures, required by the user community.

The aim of the meeting was to hear about the current status of the high-pressure user programme at ISIS, and at other international neutron facilities, and the science performed within them. It is expected that the meeting will open up new and exciting areas of research at high pressure using neutron scattering techniques and develop further international collaborations within the user community.

ISIS-Diamond Crystallography Student Day

The Crystallography Groups at Diamond and ISIS held a student meeting to give their early career stage researchers a chance to present their work. The day, held at Diamond, saw presentations from students on their work in research areas including toxic gas storage, pharmaceuticals, minerals and experiments under high pressures. The students ranged from undergraduates on their placement year to PhD students in their final year of study, and many in between.

As well as those presenting, there were other student and instrument scientists from both ISIS and Diamond attending, who asked useful questions after the talks, and contributed to the lively coffee and lunch breaks.

As ISIS-funded PhD studentships include an element of facility development, it was especially interesting to see the technologies developed that they would be leaving behind to the ISIS user community, including sample set-ups on both Polaris and PEARL.

Anna Herlihy presenting at the ISIS-Diamond crystallography student day.

Workshop on Neutron and X-Ray Imaging Applications in Life Sciences and Biology

On 18 and 19 February 2020, ISIS and Diamond Light Source collaborated to hold, the first, international workshop focussing on the use of neutron and X-ray imaging to provide a new approach for research into life sciences, palaeontology, geoscience and biology.

By showcasing the large variety of research that uses the IMAT instrument at ISIS, Diamond imaging beamlines I12 and I13, and CLF laser-driven accelerators for neutron and X-ray imaging, instrument scientists were able to promote the benefits of using these imaging techniques to users.

The novelty of the research and the wealth of results already acquired showed the potential of interdisciplinary research projects which brought together scientists from different fields. The necessity of developing new imaging techniques was another important topic addressed during the workshop. All participants agreed that the potential of neutron and X-ray imaging applications in life sciences is huge, opening the way for a new and exciting cutting-edge research.

Electrochemistry workshop

Diamond Light Source and ISIS jointly organised a two day workshop on electrochemistry on 4-5 November 2019. The workshop covered a wide range of subjects within electrochemistry including energy production and storage, corrosion, electrolyte interfaces as well as characterisation methods and instrumentation.

SINO-UK Workshop on Science and Cultural Heritage

The SINO-UK workshop in January 2019 brought together British and Chinese researchers focussing on interdisciplinary and multi-disciplinary research using cutting edge technologies for the protection, restoration, preservation of cultural heritage artefacts.

The scientific study of cultural heritage artefacts is particularly challenging, as breaking them apart to see inside simply isn't an option. However, over the past decade there has been significant interest in what non-destructive techniques, such as neutron scattering or muon spectroscopy, can add to our existing knowledge. These techniques allow researchers to see what is happening beneath the surface without damaging the artefact.

The SINO-UK workshop covered examples of successful research carried out at the ISIS neutron and muon source, including a neutron study of Oxford's famous Sheldonian Heads, and a muon spectroscopy study on Roman coins. Researchers from China spoke about some of the challenges faced in conserving cultural heritage sites, for example Dunhuang's famous Magao Grottoes. It is hoped the meeting will strengthen existing collaborations between Chinese and UK researchers and opening up novel and exciting opportunities in understanding our cultural heritage.

ISIS Deuteration for Neutron Science Meeting – Milton Hill House on 16th-17th May 2019

The attendees of NMSUM 2019. We're looking forward

to seeing you all in person again soon!

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