

ISIS 2015

neutron and muon source annual review



Science & Technology
Facilities Council

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Left: Rt Hon Hugo Swire MP (Minister of State at the Foreign & Commonwealth Office) and His Excellency Roberto Jaguaribe (Brazilian Ambassador to the UK) with Brazilian students during their tour of ISIS in December.

Below: Prof Julie Williams (Chief Scientific Advisor for Wales) visiting Engin-x at ISIS in April.



Above: Prof CNR Rao, FRS Delegation Leader, JNCASR and Prof R McGreevy (ISIS Director) sign a MoU for collaboration in neutron science on 15th January 2015. With Prof A K Sood (Indian Institute of Science), Prof MK Sanyal (Head, Saha Institute of Nuclear Physics), S Kumar (Foreign Commonwealth Office), HE Ranjan Mathai (Indian High Commissioner), Dr S Shailesh Kumar Singh (Indian High Commission), Brigadier K Jha (Indian High Commission), Dr A Taylor (Executive Director, National Laboratories, STFC), Prof S Langridge and Terry Mawby (STFC).

Above: The Special Envoy of the President of the People's Republic of China, Mr Meng Jianzhu, exchanging gifts with Prof John Womersly (STFC Chief Executive Officer) during his visit to ISIS in July.

Right: Rt Hon Jo Johnson MP (Minister of State for Universities and Science) discussing engineering applications of neutrons with Shu Yan Zhang (ISIS) during his visit to ISIS in July.



Foreword

On December 16th 2014 ISIS celebrated its 30th birthday. In keeping with the times it was a restrained celebration, then back to work completing the long shutdown tasks. The main control room, on daily view for 30 years, has been reborn. The front end muon magnets, many of which were closer to pension age and hadn't been seen for 30 years, were replaced as were more of the TS1 extracted proton beam magnets. The TS2 reflector, an absolute youngster at only 6, was replaced to open up the moderator views for Larmor and ChipIr and to facilitate future moderator development. And much, much more... but most importantly it all went back together again and ISIS restarted operation on time.

With increased funding from several sources, this year we will be carrying out more experiments than ever before. As is evident from these pages, the variety and quality remain high. ISIS staff put an enormous amount of effort and dedication into achieving these results, both in shutdowns and in operations, much of it invisible behind the front stage of the user programme. This annual report is one way of recognising and celebrating their work, to which I would add my personal congratulations and thanks.

One of the aspects of ISIS I am most proud of is our external reputation for collaboration. This extends over all aspects of our work, but I will highlight two examples.

The International Collaboration on Sample Environment was originally seeded through EU funding as part of NMI3, but has since gone from strength to strength. ISIS is one of the driving forces and in 2014 hosted the annual meeting and ran a training course for cryogenics technicians. The DENIM workshops on instrument engineering were launched by ISIS in 2012 and are increasingly popular, this year attracting 139 participants from 16 countries. In hard times we are always encouraged to reduce travel, but I am convinced that the technical knowledge gained and given through such collaborations is worth far more than the cost of a few plane fares.

The neutron working group of the European Strategy Forum on Research Infrastructures and the European Neutron Scattering Association have independently concluded that the future health of ISIS is critical for neutron scattering in Europe, not just for the UK. With the UK going through its 5-yearly government spending review we have made the case for future support for ISIS. This is based not only on scientific excellence and strategic importance, but also the significant return on investment in terms of economic impact. I am hopeful of a funding outcome that allows ISIS to continue a vibrant user programme at the same time as developing its future potential. Watch this space ...

Robert McGreevy, ISIS Director

Sir William Castell LVO (Chairman, Wellcome Trust), Mr Tim Livett (Chief Financial Officer, Wellcome Trust) and Prof John Isaac (Head of Neuroscience and Mental Health, Wellcome Trust) visiting ISIS in December, with Prof Sir Michael Sterling (STFC Chair), Prof Robert McGreevy (ISIS Director), Prof John Womersley (STFC Chief Executive Officer), Mr Tim Bestwick and Dr Andrew Taylor (STFC Executive Directors).



An introduction to ISIS

ISIS is a world centre for research in the physical and life sciences at the Rutherford Appleton Laboratory near Oxford in the United Kingdom.

We support a national and international community of more than 3000 scientists for research into subjects ranging from clean energy and the environment, pharmaceuticals and health care, through to nanotechnology and materials engineering, catalysis and polymers, and on to fundamental studies of materials.

ISIS uses neutrons and muons to investigate how materials work at the atomic level. This enables us to understand every-day materials properties – and so make new ones tailor-made for particular applications.

Why use neutrons and muons?

The neutron is a powerful probe of the atomic-level properties of solids and liquids. Neutrons are able to study both structure and dynamics – where atoms are and how atoms are moving. The neutrons used at ISIS have wavelengths which are comparable to atomic spacings, and so can be used to study structures from the Ångstrom to the micron scale. At the same time they have energies similar to those of atomic and electronic processes, enabling lattice vibrations, molecular motions, diffusion and tunnelling to be explored.

Neutrons scatter from the nucleus of an atom rather than the electron cloud (which X-rays scatter from). This means that light atoms, such as hydrogen, can be seen

in the presence of heavier atoms. Neighbouring elements in the periodic table can be distinguished, and different isotopes of the same element can be used to label parts of molecules and enhance the technique's sensitivity. The relatively weak interaction of neutrons with matter makes them a penetrating probe, so that complex sample environment can be used. And neutrons have a magnetic moment, making them suitable for studying magnetic materials.

Muons are an alternative probe of the structure and dynamics of materials. Their applications span a broad range of science areas, and they often provide complementary information to that given by neutrons.

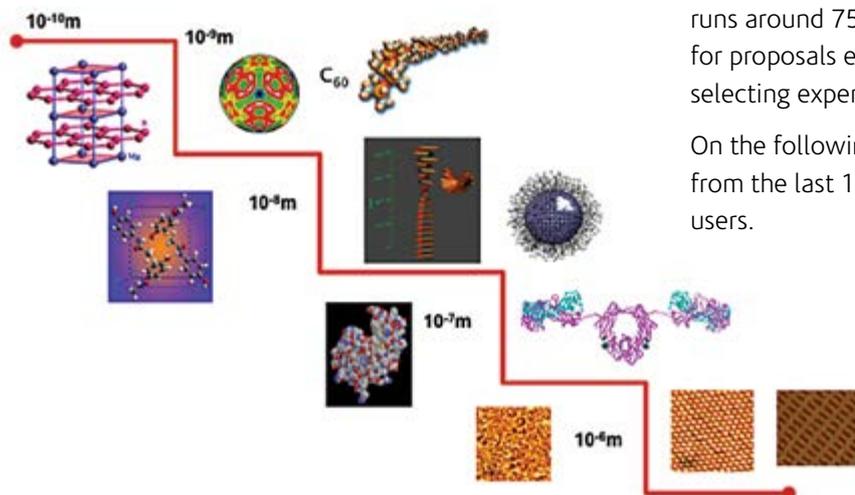
Producing neutrons and muons

Neutrons are produced at ISIS by the 'spallation' process. A heavy metal target is bombarded by an energetic proton beam from a circular, synchrotron accelerator, driving neutrons from the metal nuclei. The neutrons produced in the target are slowed to energies (wavelengths) useful for studying materials by hydrogenous moderators around the target. They are then directed to some 25 instruments, each optimised to explore different atomic-level properties. Muons are produced by the interaction of the proton beam with a thin carbon target and fed to seven experimental areas.

A user facility

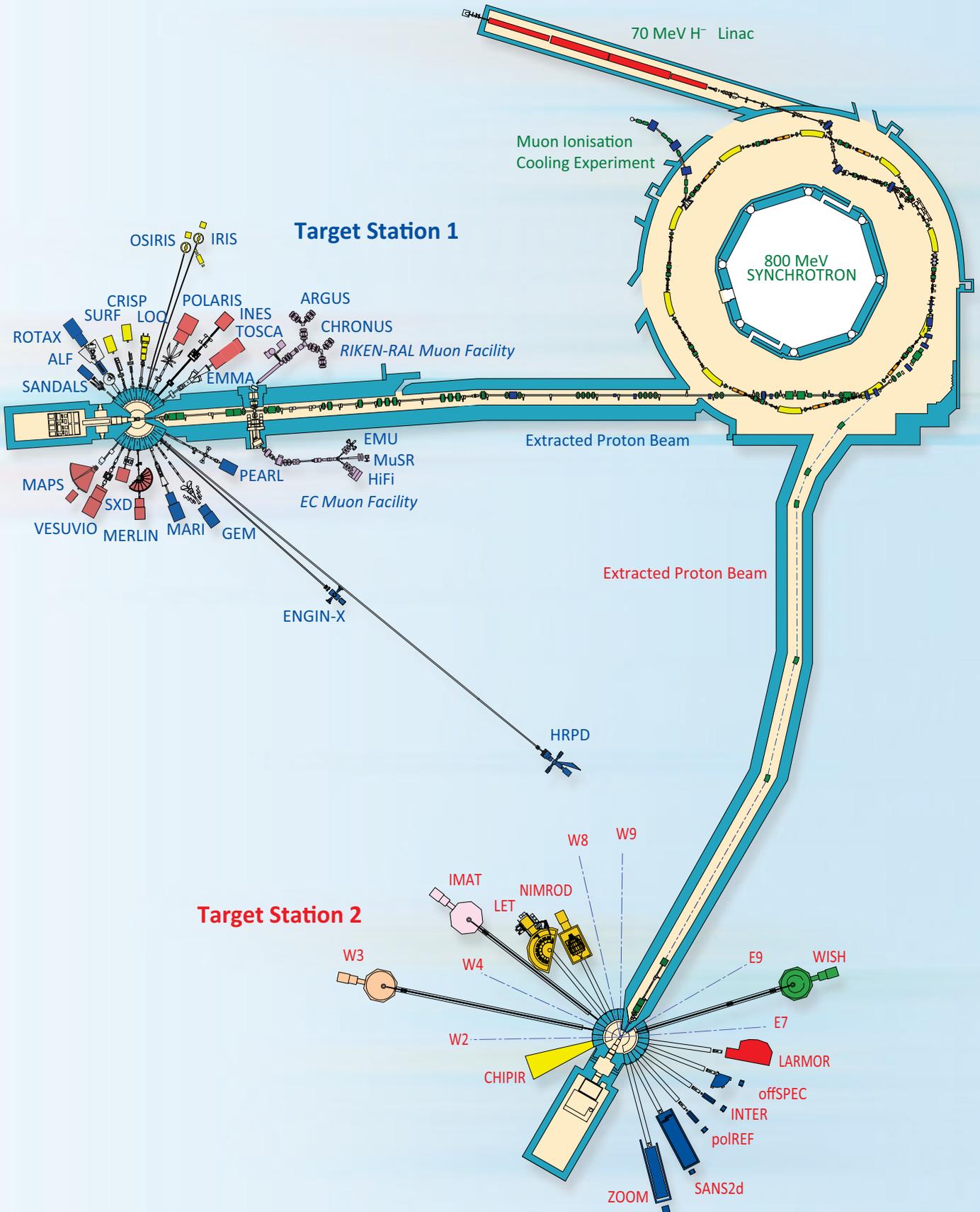
ISIS is a facility dedicated to enabling external researchers, from academia and industry, to use neutrons and muons in their research. ISIS receives around 3000 user visits and runs around 750 experiments per year. It holds two calls for proposals each year, with peer-review panels of experts selecting experiments based on scientific excellence.

On the following pages we described some of the highlights from the last 12 months of excellent science from our users.



Neutrons can be used to study a wide range of length scales – from the Ångstrom to the micron level.

The ISIS Facility



Science





Every year over 400 papers are published based on research at ISIS. These span a wide range of scientific disciplines, from pharmacology, cultural heritage and engineering to chemistry, magnetism and bioscience. This section gives a snapshot of ISIS research from some of these areas.

Applied materials

The dynamics of methyl ammonium ions in hybrid organic-inorganic perovskite solar cells

AMA Leguy (Imperial College London), J Moore Frost (University of Bath), A McMahon (Imperial College London), V Garcia Sakai, W Kockelmann (ISIS), CH Law, X Li, F Foglia (Imperial College London), A Walsh (University of Bath), BC O'Regan, J Nelson, JT Cabral, PRF Barnes (Imperial College London)

Instruments: Osiris, Gem.

Research support: EPSRC grants EP/J002305/1, EP/M023532/1, EP/I019278/1 and EP/M014797/1.

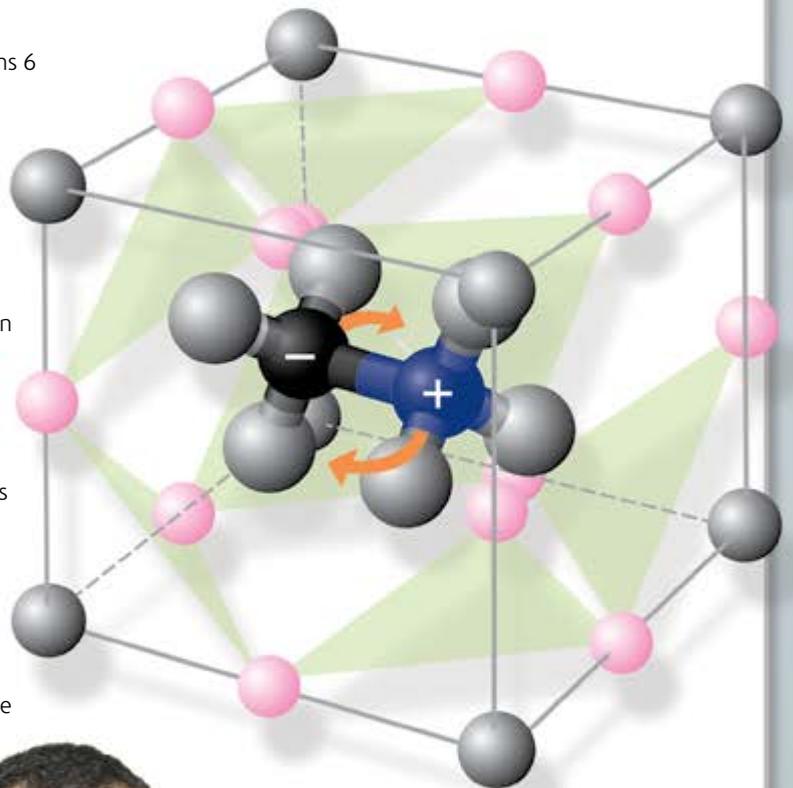
Contact: Piers Barnes, piers.barnes@imperial.ac.uk

Further reading: AMA Leguy et al., Nature Communications 6 (2015) 7124, doi:10.1038/ncomms8124 (2015).

The material methylammonium lead iodide (MAPI) which has a perovskite crystal structure is attracting massive attention because it makes very efficient solar cells from solution at low temperature from cheap ingredients. However MAPI solar cells show an unexplained hysteresis in their photocurrent, which represents a problem for commercialising the technology. One hypothesis to explain this is that the charged methylammonium ions in the crystal structure may rotate, giving rise to ferroelectric effects, which would change the performance of the solar cells.

To examine this we used neutron scattering measurements to show that these ions can jump between different orientations within the crystal lattice. This can give rise to regions of ordered ion directions in the material. However our calculations based on the measurements showed that the rearrangements in ionic direction are likely to be too fast to explain the hysteresis seen in solar cells. The reorientation of the ions is likely to be one of the reasons that MAPI screens electric fields very strongly.

Crystalline structure of methylammonium lead iodide (colour code: grey is lead, pink iodine, blue nitrogen, black carbon and white hydrogen).



Abdullah Mamun and Anas Achouni (Open University) using Engin-x to study stress in 316H steel during asymmetric cyclic loading.

Generation and control of a purely magnetic interface

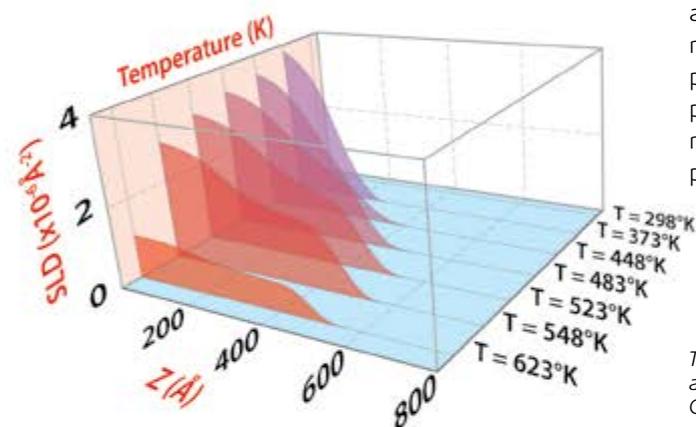
C Le Graët, M McLaren, SA Morley, RMD Brydson, CH Marrows (University of Leeds), TR Charlton, CJ Kinane, S Langridge (ISIS), M Loving, LH Lewis (Northeastern University, USA)

Instrument: Polref.

Research support: EPSRC: EP/G065640/1, NSF: DMR-0908767.

Contact: Christopher Marrows, c.h.marrows@leeds.ac.uk

Further information: C Le Graët et al. *APL Materials* 3 (2015) 041802, doi:10.1063/1.4907282.



FeRh is a fascinating and highly-tuneable functional material. It displays a transition between a high resistance antiferromagnetic state and a low resistance ferromagnetic one. This transition can be tuned to occur at a convenient temperature by numerous means including chemical doping. In this work we engineered a chemical doping gradient in a film of FeRh which resulted in a controllable and purely magnetic interface. To spatially resolve this interface we used polarised neutron reflectivity to extract the magnetic interface position. Given the different electrical behaviour of the two magnetic phases we could then relate this result to its transport properties. The controllable and tuneable nature of this functional material means that the system has potential for applications in magnetic field and temperature sensing.

*The magnetic profile of the ferromagnetic phase within the FeRh layer as a function of temperature. Modified with permission from C. Le Graët et al. *APL Materials* 3 (2015) 041802.*

In situ neutron diffraction studies of battery electrodes

JJ Biendicho (Catalonia Institute for Energy Research), D Noréus (University of Stockholm), U Lagerqvist (Nilar Svenska AB), S Eriksson, S Norberg (Chalmers University), C Offer, R Smith, S Hull (ISIS)

Instrument: Polaris.

Research support: Swedish Research Council Vetenskapsrådet.

Contact: Jordi Jacas Biendicho, jjacas@irec.cat

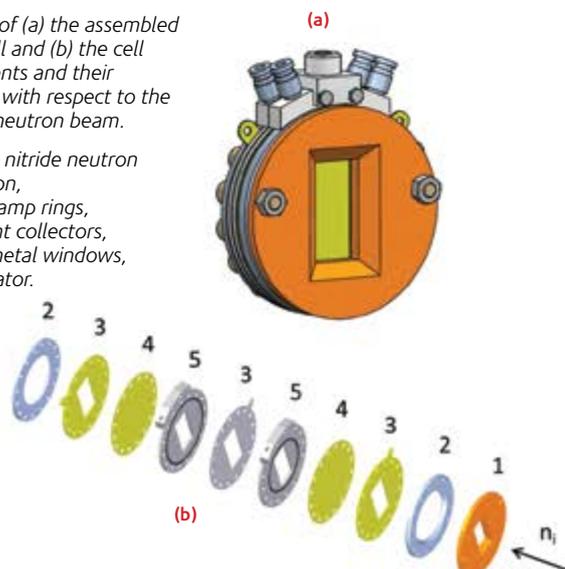
Further reading: JJ Biendicho et al., *J. Mater. Res.*, 30 (2015) 407.

To achieve better battery technologies, with improved power densities and more rapid charge and discharge times, we require new materials to fulfil the key roles of electrodes and electrolyte. A novel electrochemical cell has been constructed to allow in situ neutron powder diffraction studies of the changes that occur to the crystal structures of these components during operation and, hence, identify those factors which promote (or hinder) the essential electrochemical reactions. The cell's design is based on a commercial coin cell, but has larger dimensions to maximize the speed of collection of the neutron data. For example, a recent in situ study of a nickel-metal hydride system used 30 minute data collections to understand the phase changes that occur within the $\text{Ni}(\text{OH})_2^-$ and LaNi_5^- based electrodes. As part of the ongoing development project, the cell will shortly be used to probe the electrochemical processes which take place within lithium

batteries, to relate changes in the structural properties of cathode materials such as LiCoO_2 , LiMn_2O_4 and LiFePO_4 during charge-discharge cycling.

Diagram of (a) the assembled in situ cell and (b) the cell components and their positions with respect to the incident neutron beam.

(1) boron nitride neutron collimation,
(2) cell clamp rings,
(3) current collectors,
(4) thin metal windows,
(5) separator.



Applied materials

Local structure underlying anomalous tetragonal distortions in a new piezoelectric

I Levin, V Krayzman, JC Woicik (NIST, USA), MG Tucker (ISIS)

Instruments: Gem, Z23A2 at the National Synchrotron Light Source, USA.

Contact: Igor Levin, igor.levin@nist.gov

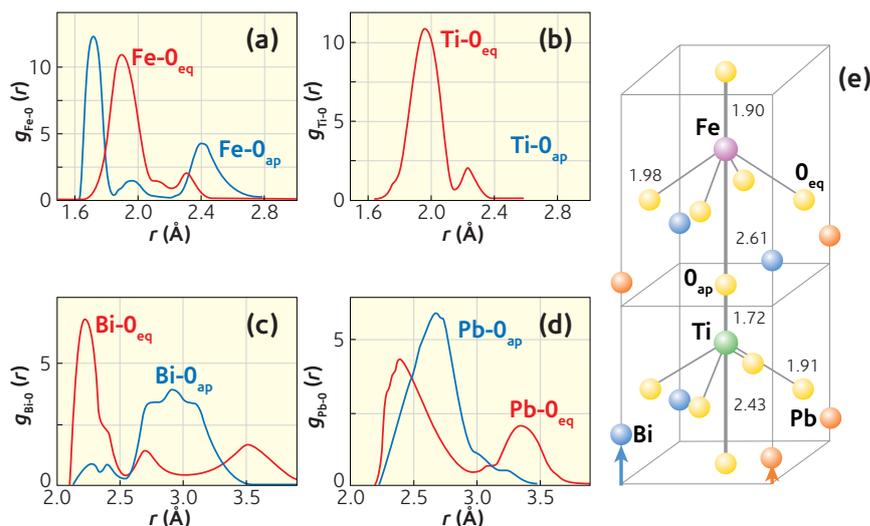
Further information: I Levin et al., Appl. Phys. Lett. 104 (2014) 242913.

Piezoelectric materials change shape with an applied electric field. Materials showing this property at high temperatures are actively sought for use in fuel injectors in diesel and direct-injection gasoline engines. Piezoelectrics enable much faster and precise injection than conventional electromagnets, yielding significant fuel economy and reduced emissions. New promising materials for these applications are being derived from lead titanate using partial replacement of lead by bismuth and of titanium by another metal. We investigated the atomic arrangements in a system with titanium substituted by iron, which exhibits an anomalously distorted crystal structure. The chemical disorder inherent to these materials introduces significant structural complexity because local structural distortions differ from the average. The detailed structure was elucidated using a new methodology that combines information from neutron scattering and X-ray absorption spectroscopy to probe

both local and average atomic order.

Our study found that on the local scale, the anomalous distortions, promoted by the displacements of bismuth and lead, are accommodated primarily by the oxygen coordination of iron, due to iron's ability to adopt five-fold coordination. This is suggested as the key for stabilizing the structure of these potentially useful materials.

Partial metal-oxygen pair-distribution functions and a schematic of the adjacent iron- and titanium-centered unit cells illustrating local lattice distortions around these atoms.



Elias Pambou (Manchester) using Surf to study adsorption of an egg shell membrane polypeptide at the oil-water interface.

Muon-induced single-event upsets in 28-nm static random access memories

BD Sierawski, BL Bhuva, RA Reed (Vanderbilt University), N Tam (Marvell Technologies Group), B Narasimham (Broadcom Corp.), K Ishida (RIKEN), A Hillier (ISIS), M Trinczek, E Blackmore (TRIUMF), SJ Wen, R Wong (Cisco Systems)

Instruments: RIKEN-RAL Port 4 muon beamline, TRIUMF muon beamline (Canada).

Research support: Industry and university funding.

Contact: Bharat Bhuva, Bharat.bhuva@vanderbilt.edu

Further information: B. Sierawski, et al., Proceedings of 2014 IEEE International Reliability Physics Symposium, pp. 2B.2.1 – 2B.2.5, June 2014.

Neutron- and alpha-induced soft errors are the most dominant failure mechanisms in microelectronic devices fabricated at advanced technology nodes. Leading-edge microelectronic circuits also exhibit sensitivity to lightly-ionizing singly-charged particles. For the older technologies, the transport of a singly-charged particle through semiconductor material did not generate sufficient charge to result in a soft error. However, recent experiments have shown that muons are capable of producing soft errors in Static Random Access Memories (SRAMs).

This work examined the sensitivity of SRAM cells fabricated at the 28-nm technology nodes to single positively-charged muons at TRIUMF and

ISIS. Experiments have shown that the muon-induced single event upset cross section increases due to reduced operating voltage over the range of muon momenta tested. Results aid our understanding of the relatively unknown effects of muon ionization. In addition, it was demonstrated that muon-induced upsets can be observed with packaged parts as well as unpackaged devices.

Dr Nelson Tam (Marvell Semiconductor) setting up for the muon experiment at ISIS.



Characterisation of a shamsheer from the late 18th or early 19th century made in India

E Barzagli, F Grazzi (CNR-ISC, Italy), Alan Williams, David Edge (The Wallace Collection, London), A Scherillo, J Kelleher (ISIS)

Instruments: Ines, Engin-x.

Research Support: ISIS-CNR agreement, University of Florence.

Contact: Elisa Barzagli, elisa.barzagli@fi.isc.cnr.it

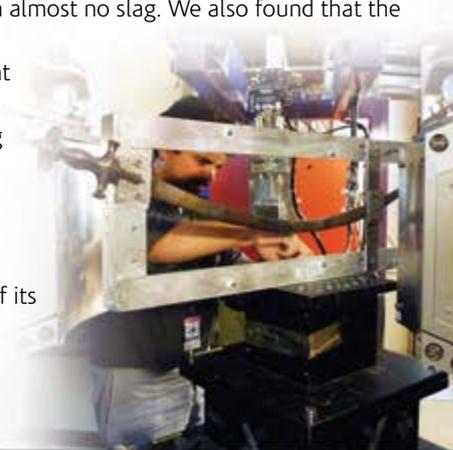
Further reading: E Barzagli et al., App. Phys. A 119(1) (2015) 97, doi 10.1007/s00339-014-8968-0.

Indian swords are really outstanding specimens to study the evolution of metallurgy, although they have not until now been investigated to any great extent. The most ancient artefacts are few in number and the best ones are in an excellent state of conservation, therefore traditional invasive analytical methods may not be applicable. Moreover, techniques that require sampling of the artefacts give insight only into a very limited area of the object, which is not always representative of the whole. To reveal more information on the raw material and production methods we used the non-invasive technique of time-of-flight neutron diffraction.

A series of experiments was performed using Ines and Engin-x which enabled us to determine the composition of the phases

present in the sample and hence the microstructure of the metal, differentiating the various areas, and also to construct maps of the distribution of residual strain in three directions. The analysis showed that this blade was made of very good quality high-carbon steel which had not been quenched or normalized, and with almost no slag. We also found that the forging method was substantially different in the upper and lower parts, resulting in an opposing strain distribution. There is some sign of cold working, which is probably the result of its use in battle.

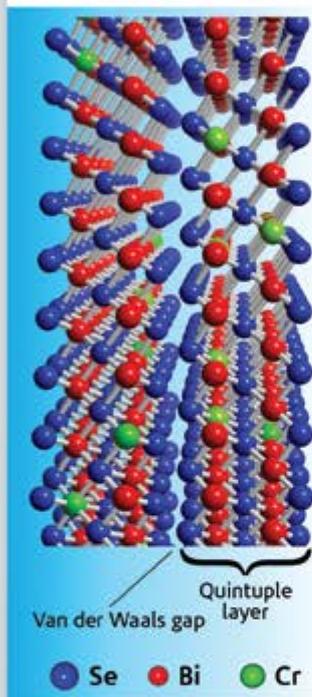
CNR scientist Francesco Grazzi aligning the shamsheer on Engin-x.



Applied materials

Creating magnetic topological insulators

LJ Collins-McIntyre (Oxford University), SE Harrison (Stanford University), P Schönherr (Oxford University), N-J Steinke, CJ Kinane, TR Charlton, D Alba-Venero (ISIS), A Pushp, AJ Kellock, SSP Parkin (IBM), JS Harris (Stanford University), S Langridge (ISIS), G van der Laan (Diamond Light Source), T Hesjedal (Oxford University)



Instruments: Polref.

Research support: John Fell Oxford University Press Research Fund, EPSRC, Studienstiftung des deutschen Volkes, Corpus Christi College, MesoDynamic Architectures Program (DARPA) and VPGE (Stanford University).

Contact: Thorsten Hesjedal, thorsten.hesjedal@physics.ox.ac.uk

Further information: LJ Collins-McIntyre et al., EPL 107 (2014) 57009, doi:10.1209/0295-5075/107/57009.

Topological insulators (TIs) are a new type of quantum material that promises dissipationless carrier transport

at room temperature. TIs are insulating in the bulk and show a conducting topological surface state (TSS). The TSS, which is not destroyed by normal scattering from crystal defects and lattice vibrations, is characterised by counter-propagating spin polarized electrons. The main method for making practical use of TIs is by combining them with ferromagnetic materials. Introduction of magnetic order can result in many interesting quantum phenomena.

We performed a combined structural and magnetic study of Cr-doped Bi_2Se_3 thin films grown by molecular beam epitaxy, using X-ray diffraction, magnetometry and polarized neutron reflectometry (PNR). We found that Cr-doping is possible up to a Cr concentration of 12% without loss of crystalline quality. PNR showed that the ferromagnetism is prevalent throughout the film with no evidence of an enhanced surface magnetic layer. Such studies offer a way to increase the Curie temperature, thereby paving the way for low-power electronic applications of TIs in the future.

Layered crystal structure of Bi_2Se_3 showing Cr substitutional dopants on Bi sites.

Optimising machining strategies for Boeing

R Bilkhu, S Ayvar (Sheffield University), J Caste (Boeing)

Instrument: Engin-x.

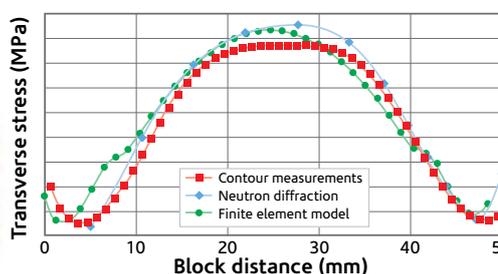
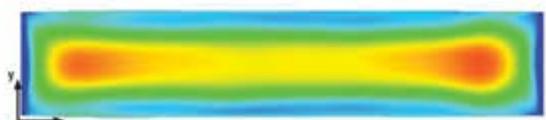
Contact: Ravi Bilkhu, r.bilkhu@sheffield.ac.uk

Understanding the development and distribution of residual stresses caused by machining is key to improving machining processes. Residual stresses can cause distortion in components meaning they are not fit for purpose or have a reduced lifetime, and require costly operator skill to identify and intervene in the machining process when distortion occurs.

The Advanced Manufacturing Research Centre (AMRC) at the University of Sheffield and Boeing have been using Engin-x to study the evolution of residual stresses in AA7050 – an aluminium alloy commonly used in aerospace structures – as it is heated and then machined. Alongside their experiments at ISIS the

team developed 3D finite element modelling to predict the residual stress resulting from quenching and machining. The combination of modelling, measurement and experiment allowed them to gain a clear understanding of how distortion occurs in the different manufacturing processes.

The ability of Engin-x to map residual stresses in three dimensions is unachievable by other means and allowed the team to see the hidden residual stresses prior to releasing them during the machining process. This understanding will enable them to reduce non-conformance in the manufacturing process and significantly reduce costs.



Simulated map of stress distribution across a section of a quenched aluminium block. The graph shows good agreement between simulated and measured (neutron diffraction and contour method) stress profiles along one of the central lines across the block.

Pharmaceuticals *and bioscience*

The mode of action of anticancer drugs: cisplatin's interplay with DNA

MPM Marques (University of Coimbra, Portugal), D Gianolio, G Cibir (Diamond Light Source), J Tomkinson, SF Parker (ISIS), R Valero, RP Lopes, LAE Batista de Carvalho (University of Coimbra, Portugal)

Instruments: Tosca, B18-Core EXAFS (Diamond), Raman and FTIR (Coimbra University), Advanced Computing Laboratory (Coimbra University).

Research support: Portuguese Foundation for Science and Technology – PEst-OE/UI0070/2014; EU FP7 funding for access to ISIS (NMI3) and Diamond (Calypso).

Contact: MPM Marques, pmc@ci.uc.pt

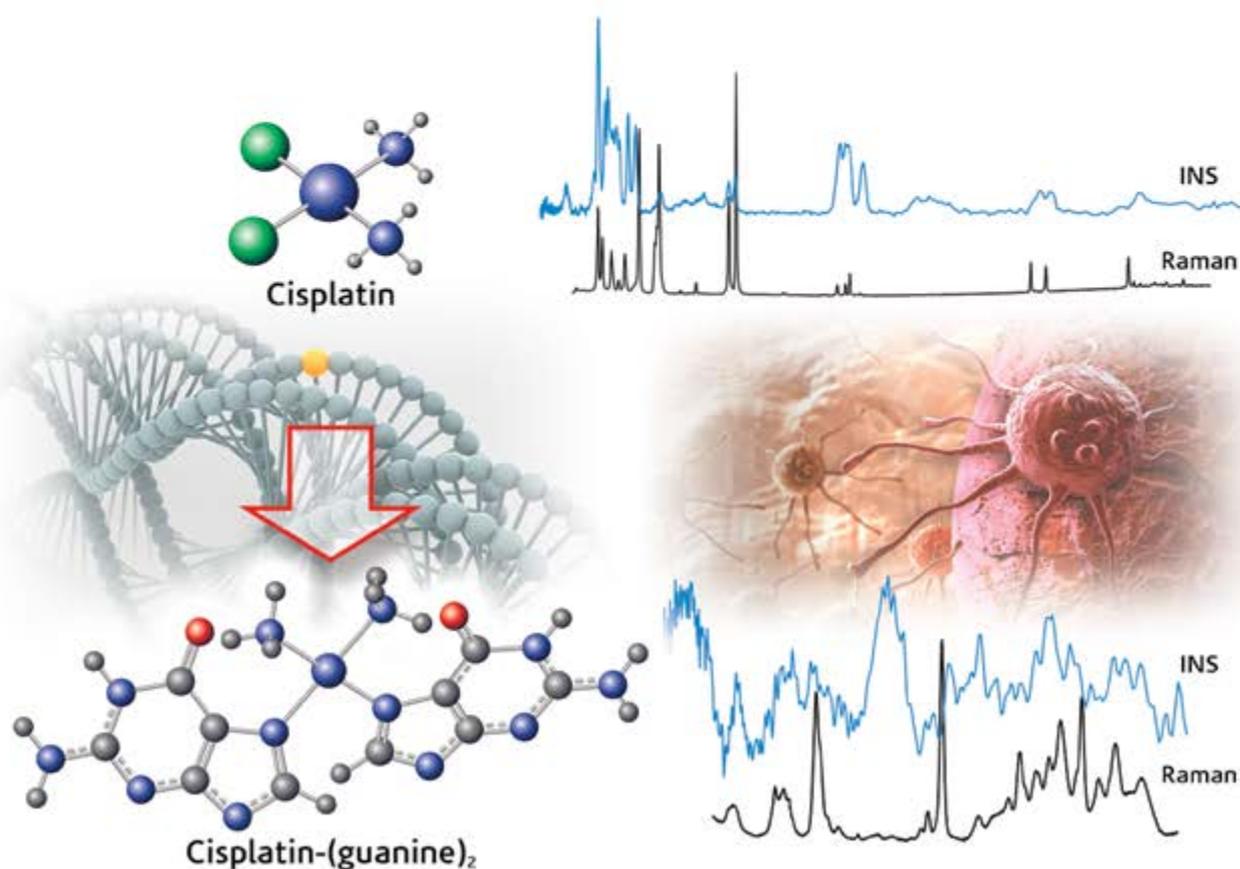
Further information: MPM Marques et al., Phys.Chem.Chem. Phys. 17 (2015) 5155, doi: 10.1039/C4CP05183A, URL: <http://rsc.li/1zVOE4T>

Cisplatin ($\text{cis}-(\text{NH}_3)_2\text{PtCl}_2$) is a widely-used anticancer drug for testicular, head and neck tumours, that exerts its effect through selective interactions with DNA within the cell nucleus. Despite the success of these Pt-based antitumour agents, acquired resistance is still one of the main limiting factors in their clinical application. In particular, compounds such as glutathione, a

ubiquitous antioxidant in mammary cells, is known to intercept these types of drugs and hinder them from reaching DNA in therapeutically significant amounts.

The present study aimed to elucidate cisplatin's interaction with DNA (purine and pyrimidine bases) using experimental techniques – EXAFS and vibrational spectroscopy (infrared, Raman and inelastic neutron scattering) – coupled to theoretical simulations (DFT/Plane-Wave). Detailed information was obtained by EXAFS on the local atomic structure around Pt(II) in the cisplatin-(DNA bases) and cisplatin-glutathione adducts. Simultaneous neutron and Raman scattering experiments enabled us to obtain a clear picture of the drug interplay with its main pharmacological target (DNA), at the molecular level.

Molecular picture of cisplatin's mode of action, from Raman and INS experimental data for cisplatin and cisplatin-DNA adducts.



Pharmaceuticals and bioscience

The role of cations in the stability of bacterial membranes

LA Clifton, MWA Skoda, F Ciesielski (ISIS), SA Holt, AP Le Brun (ANSTO), I Kuzmenko (APS), JH Lakey (Newcastle)

Instruments: Inter, Advanced Photon Source.

Research support: Wellcome Trust.

Contact: Luke Clifton, luke.clifton@stfc.ac.uk

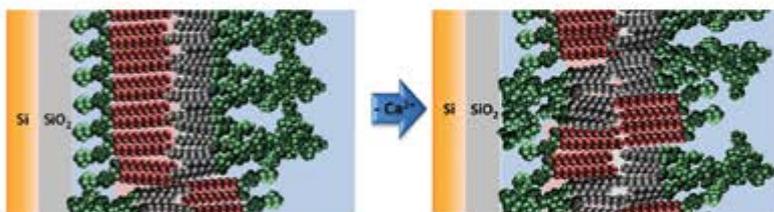
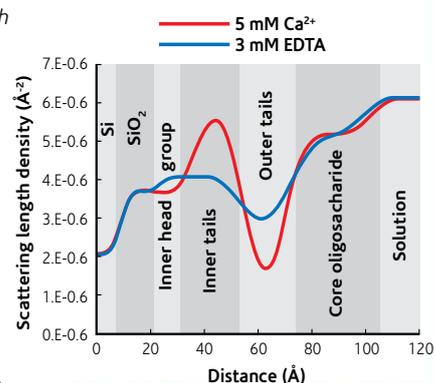
Further information: LA Clifton et al., *Langmuir* 31 (2015) 404–412.

The Gram-negative bacterial outer membrane (GNB-OM) is an important barrier to antibiotics. It is asymmetric in its lipid composition with a phospholipid-rich inner leaflet and an outer leaflet predominantly composed of lipopolysaccharides (LPS). A LPS is a polyanionic molecule containing numerous phosphate groups. The repulsive forces due to accumulation of the negative charges are screened and bridged by the divalent cations (Mg_{2+} and Ca_{2+}) that are known to be crucial for the integrity of the bacterial OM. Using advanced models of the GNB-OM and a combination of neutron and X-ray reflectometry we revealed the molecular details of how divalent cations stabilise the GNB-OM and the disruption to the bilayer caused by their removal.

The results revealed that divalent cations accumulate in the phosphate-containing inner core region of LPS. Removal of these was followed by rapid mixing between the phospholipid inner and LPS outer membrane leaflets. This was likely driven by strong

electrostatic repulsion between neighbouring LPS molecules. These biophysical measurements agree well with in vivo observations and provide new insights into the nature of the OM.

Neutron scattering length density profiles obtained from an asymmetric bilayer composed of deuterated 1,2-dipalmitoylphosphatidylcholine (DPPC, inner leaflet) and hydrogenous *Ra*-lipopolysaccharide (*Ra*LPS, outer leaflet) in the presence of calcium (red line) and EDTA (blue line). Representations of the interfacial structure before and after calcium sequestration are shown.



Using SAS and NR to understand the stability of drug delivery vehicles

M Wadsäter, T Nylander, F Tiberg (Lund University), J Barauskas (Camurus AB, Lund), S Rogers, MWA Skoda (ISIS), RK Thomas (Oxford University)

Instruments: Sans2d, Inter, I911-4 (MAX-lab).

Research support: Swedish Foundation for Strategic Research (SSF), Camurus AB.

Contact: T Nylander, Tommy.Nylander@fkem1.lu.se

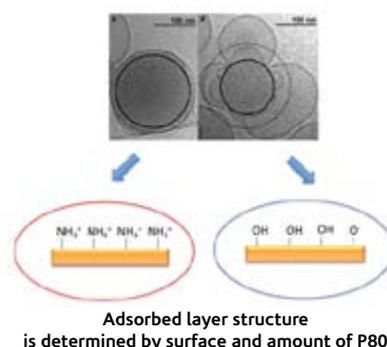
Further information: M Wadsäter et al., *Soft Matter* 11 (2015) 1140.

Reversed lipid liquid crystalline nanoparticles (LCNPs) have a large potential in drug delivery applications due to their good drug loading ability and small size, which allows them to penetrate tissue and reach targeted organs. In this study, well-defined, stable and highly-structured cubic micellar (I2) phase LCNPs of 50/50 (wt/wt) soy phosphatidylcholine (SPC)/glycerol dioleate (GDO) were formed without using high shear fields by using a low fraction (5–10 wt%) of the dispersing polymeric surfactant polysorbate 80 (P80). The location of the stabiliser within the particles largely controls their function. Contrast variation small-angle neutron scattering (cv-SANS),

small-angle X-ray scattering (SAXS) and neutron reflection (NR) were used, for the first time, to determine a detailed picture of the internal structure of the LCNPs and how they are stabilised by the P80. The results are relevant not only for the capability of LCNPs as drug delivery vehicles but also as means of preparing functional surface coatings.

Neutrons, X-rays and cryo-TEM reveal internal structure and adsorption of lipid liquid crystalline nanoparticles. The stabiliser (polysorbate 80) location within the particle determines their function.

Particle structure and LIPID/P80 distribution is determined by P80 amount (SANS, SAXS & CRYO-TEM)



Diffusion in membranes: toward a two-dimensional diffusion map

L Toppozini, MC Rheinstädter (McMaster University), V Garcia Sakai, R Bewley, R Dalgliesh, T Perring (ISIS)

Instruments: LET, Offspec.

Research support: NSERC of Canada.

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Further information: L Toppozini et al., EPJ Web of Conferences 83, 02019 (2015); L Toppozini et al., Soft Matter 11 (2015) 8354.

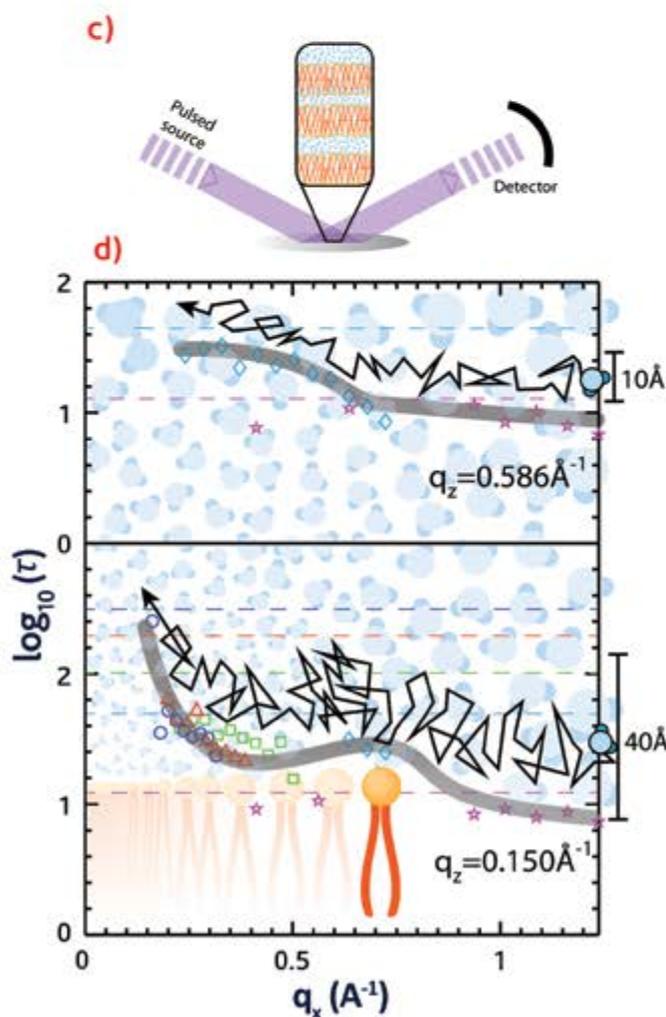
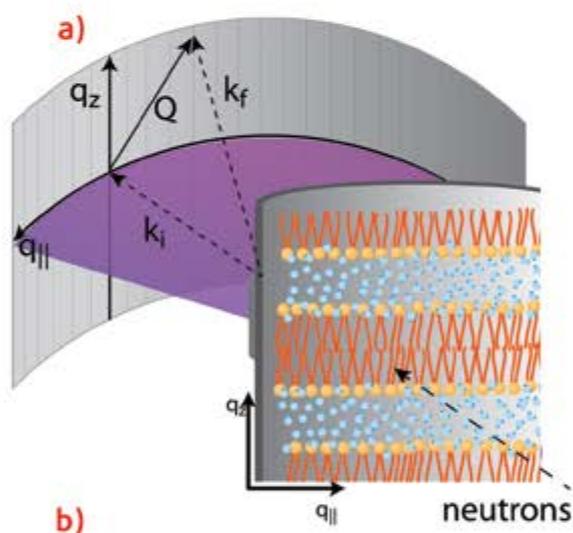
Our understanding of the behaviour of water in biological membranes is important as water is actively involved in membrane activity and function. We have studied nanoscale diffusion of membrane hydration water in fluid lipid bilayers using neutron diffraction and incoherent quasi-elastic neutron scattering. By using large, 2-dimensional detectors, lateral motions of water molecules and motions perpendicular to the membranes could be studied simultaneously. We found

experimental evidence for anomalous (sub-diffusive) and anisotropic diffusion of membrane hydration water molecules over nanometer distances. By combining molecular dynamics and Brownian dynamics simulations, the potential microscopic origins for the anomalous and anisotropy of hydration water have been investigated. Bulk water was found to show intrinsic sub-diffusive motion at time scales of several picoseconds, likely related to caging effects. In membrane hydration water, however, the anisotropy of confinement and local dynamical environments leads to diffusion anisotropy, indicative of anomalous dynamics.

Hydration water dynamics were studied on Let by analysing individual detector areas (a) & (b).

c) Water distribution was measured on Offspec.

d) Hydration water motions.



Rock and ice

Networks under pressure

A Zeidler, K Wezka, RF Rowlands, DAJ Whittaker, PS Salmon, A Polidori (University of Bath), JWE Drewitt (University of Edinburgh), S Klotz (Université Pierre et Marie Curie, France), HE Fischer (Institut Laue-Langevin), MC Wilding (University of Aberystwyth), CL Bull, MG Tucker (ISIS), M Wilson (University of Oxford)

Instruments: Pearl, D4c (ILL).

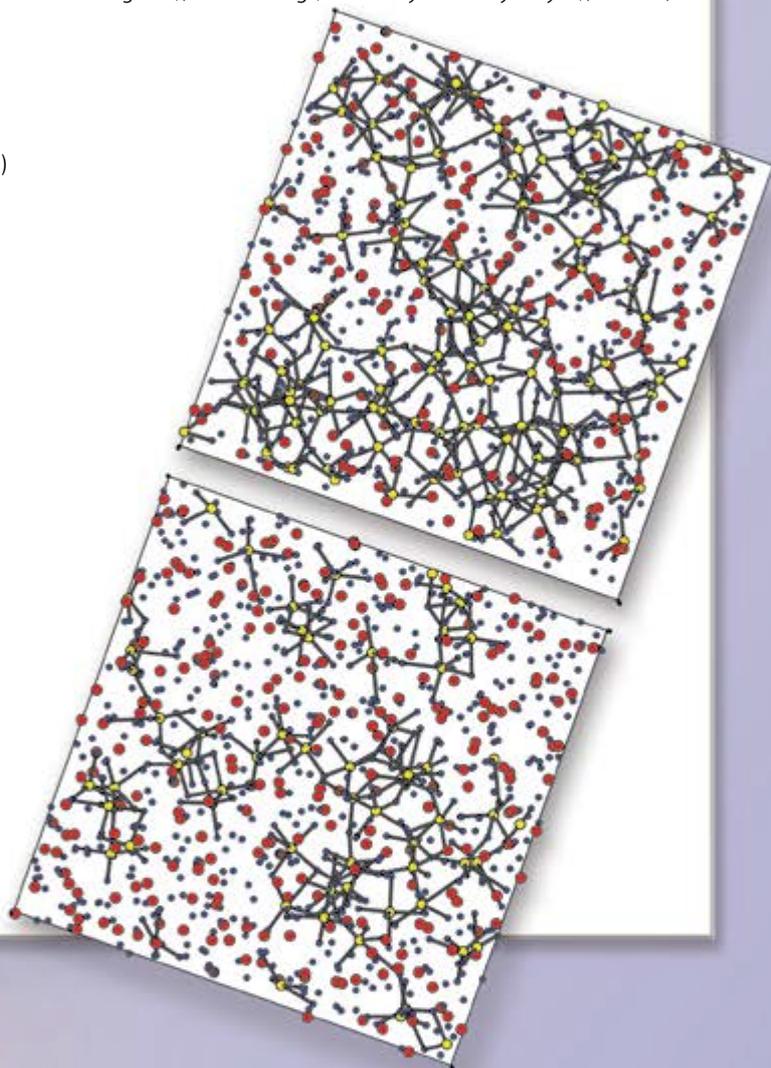
Research support: EPSRC, University of Bath, ILL.

Contact: Philip Salmon, P.S.Salmon@bath.ac.uk

Further information: A Zeidler et al., Phys. Rev. Lett. 113 (2014) 135501.

Silica is a major component in the sand on a beach and in the rocks below our feet, pointing to its widespread abundance on Earth. As a glass, the material is exploited to make the fibres used for optical telecommunication systems, and its behaviour under pressure serves as a reference for geophysically relevant silicates. At ambient conditions, the atomic-scale structure is built from a network of corner-sharing SiO_4 tetrahedral motifs that link to form open ring-like arrangements. But how does this network respond when high pressures are applied? We investigated this issue by combining neutron and X-ray diffraction experiments with molecular dynamics computer simulations. The results show that the network collapses via a process in which rings are 'zipped' by a pairing of higher-coordinated Si atoms, namely those at the centres of the SiO_5 and SiO_6 motifs that are coaxed into existence. The work provides a starting point for predicting how such changes to a network's connectivity govern its physical properties.

Right: As the pressure on SiO_2 glass is increased (bottom to top), 4-fold coordinated Si atoms (red) convert to 5-fold coordinated Si atoms (yellow) that cluster together.



Evolution of hydrogen dynamics in amorphous ice with density

A Parmentier (Università degli Studi di Roma Tor Vergata, Italy), JJ Shephard (University College London and Durham University), G Romanelli (Università degli Studi di Roma Tor Vergata, Italy, and ISIS), R Senesi (Università degli Studi di Roma Tor Vergata and CNR-IPCF Sezione di Messina, Italy), CG Salzmänn (University College London), C Andreani (Università degli Studi di Roma Tor Vergata, Italy)

Instruments: Vesuvio, Mari.

Research support: Royal Society (CGS, UF100144); Leverhulme Trust (RPG-2014-04); CNR-ISIS Agreement (2014-2020).

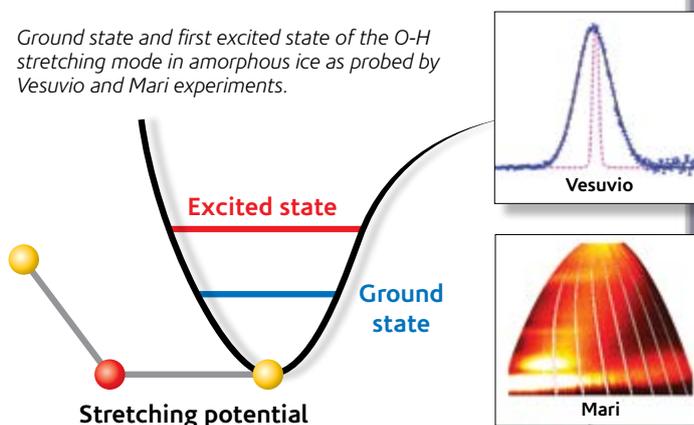
Contact: Dr G Romanelli, giovanni.romanelli@stfc.ac.uk; Dr CG Salzmänn, c.salzmänn@ucl.ac.uk

Further information: A Parmentier et al. *J. Phys. Chem. Lett.*, 6 (2015) 2038-2042.

In stark contrast to the crystalline state, amorphous materials display a complete lack of long range structural order. In the case of ice it came as a huge surprise that several different amorphous ices exist and they have been classified according to their densities. The water molecules in ice are held together through hydrogen bonds and we have set out to investigate how changes in density affect hydrogen bonding and nuclear quantum effects of the hydrogen atoms.

Data from the Vesuvio instrument showed a pronounced softening of the O–H stretching potential in the low-density ice compared with the higher-density ices. Moreover, the hydrogen mean kinetic energy was found to increase with increasing density indicating the weakening of hydrogen bonds

as well as steeper and more harmonic hydrogen vibrational potential energy surfaces. In a novel approach, we used data from both the Vesuvio and Mari instruments to determine the anharmonicity constants of the O–H stretching modes. We then arrived at a very simple conclusion: hydrogen bonding is the main cause for anharmonicity in amorphous ice.



Using fluoride analogues of MgSiO_3 to understand the core-mantle boundary of the Earth

DP Dobson, IG Wood, E Bailey, A Lindsay-Scott, L Vocablo, JP Brodholt (University College London)

Instruments: Polaris, Pearl, HRPD.

Research support: NERC grant.

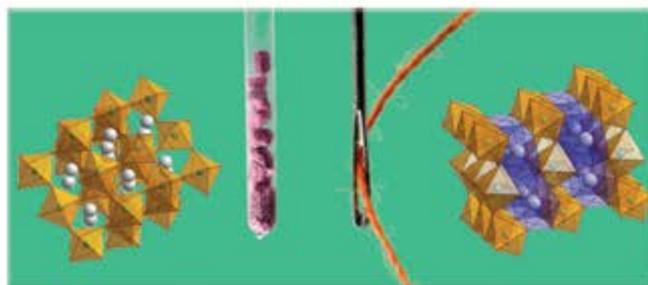
Contact: Ian Wood, ian.wood@ucl.ac.uk

Further information: D P Dobson et al., *Nature Geoscience* 6 (2013) 575.

At the bottom of the Earth's lower mantle, just above the liquid outer core, there is a roughly 300 km thick region, called the D'' zone, that is associated with a change in the crystal structure of the major lower-mantle mineral, MgSiO_3 perovskite, to a denser 'post-perovskite' (PPV) form. The D'' zone plays a crucial role in Earth's evolution as it regulates heat exchange from the metallic core to the silicate mantle. To understand D'' requires accurate knowledge of the physical properties of PPV- MgSiO_3 , many of which cannot be measured directly as it is stable only at million-atmosphere pressures. Computer simulations of PPV- MgSiO_3 have indicated that properties such as its diffusion coefficients have a surprisingly high directional dependence. In order to verify these predictions we are carrying out parallel

computational and experimental studies of isostructural analogue compounds, such as PPV- NaCoF_3 , which are stable at much lower pressures. Neutron powder diffraction at ISIS enables us to determine accurately the crystal and magnetic structures of these analogues from our necessarily small samples.

The perovskite (left) and post-perovskite (right) structures of NaCoF_3 , together with the powder sample of post-perovskite NaCoF_3 used in an experiment on the POLARIS diffractometer.



Industrial chemistry

Supramolecular binding and separation of hydrocarbons within a porous metal-organic framework

S Yang, R Newby, M Schröder (Nottingham University), AJ Ramirez-Cuesta, SI Campbell (ORNL, USA), V Garcia-Sakai, P Manuel, SK Callear (ISIS), CC Tang (Diamond)

Instruments: Tosca, Wish, Iris; Diamond; Oak Ridge National Laboratory.

Research support: EPSRC, Leverhulme, University of Nottingham.

Contact: Dr Sihai Yang, Sihai.Yang@nottingham.ac.uk

Further information: S Yang, et al., Nature Chem. 7 (2015) 121.

Crude oil is a raw material that is refined to produce fuel for cars, to heat homes, and to create polymers and other useful materials. It is made up of a complex mixture of hydrocarbons, of which certain components are especially commercially useful. The state-of-the-art industrial process used to achieve hydrocarbon separation is called 'cryogenic distillation'. It is operated at enormous scales worldwide and uses vast amounts of energy to generate the high pressures and cryogenic temperatures required to ensure efficient separation of hydrocarbon mixtures into pure components. Here, an innovative solution may have come in the form of a novel chemical sponge. This porous material, a metal-organic framework (MOF, denoted NOTT-300), has demonstrated the capability to separate hydrocarbon mixtures without the need

for high pressures or very low temperatures, and therefore tremendous amount of energy savings can be potentially gained. We used ISIS, Diamond and Oak Ridge National Laboratory to prove that this novel hybrid material works under real life conditions.

A representation of the mobility and binding dynamics of acetylene, ethylene and ethane guests within the NOTT-300 MOF host.



Revealing the physical phenomenon in promising next-generation materials

MR Ryder (Oxford University), B Civalleri (Turin University), TD Bennett, S Henke (Cambridge University), S Rudic (ISIS), G Cinque (Diamond), F Fernandez-Alonso (ISIS), JC Tan (Oxford University)

Instruments: Tosca, B22 (Diamond).

Research support: EPSRC.

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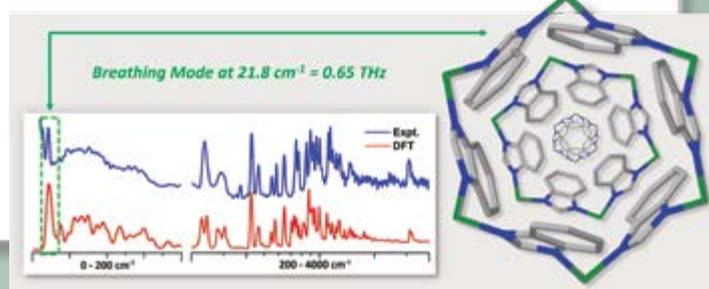
Further information: MR Ryder et al., Phys. Rev. Lett. 113 (2014) 215502.

Metal-organic frameworks (MOFs) are a class of nanoporous materials constructed of metal ions connected by organic linkers. These molecular 'building blocks' assemble to produce a variety of crystalline structures whose porosity and flexible design has resulted in them being named 'the most promising next-generation technology for carbon capture'. In addition, MOFs have also shown potential for other emerging applications, such as drug delivery and microelectronics.

State-of-the-art supercomputers were used to unravel the complete vibrational nature of three zeolitic imidazolate frameworks (ZIFs) at the molecular level. The theory was then

confirmed using high-resolution neutron and synchrotron spectroscopy. The work gave new insights into the mechanical response of MOFs, elucidating possible phase transition mechanisms and also showing how they can even 'breathe'. This has resulted in a better understanding of the mechanical properties which are intrinsically controlled by elastic responses and collective vibrations located in the low-energy THz region of the vibrational spectrum, important for the future development of next-generation framework materials.

Molecular vibration responsible for the breathing motion of ZIF-7.



How the surface structure determines the properties of CuH

EL Bennett, T Wilson, PJ Murphy (Bangor University), GA Chass (Queen Mary University of London), K Refson (ISIS and RHUL), AC Hannon, S Imberti, SK Callear, SF Parker (ISIS)

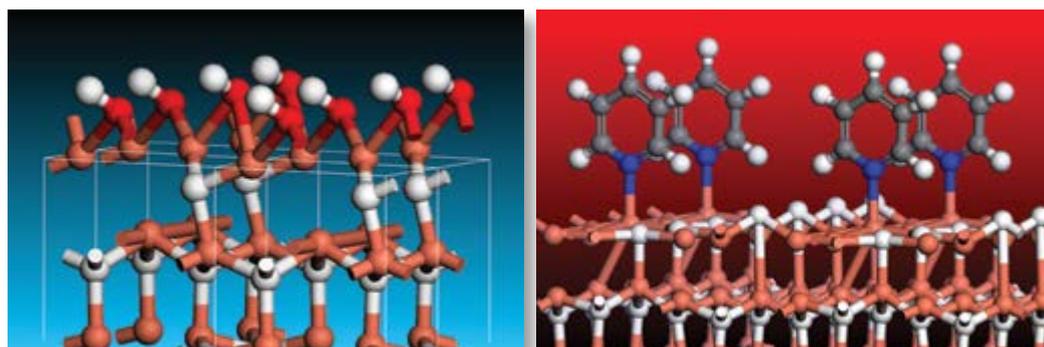
Instruments: Sandals, Tosca, Maps.

Contact: Stewart Parker, stewart.parker@stfc.ac.uk

Further information: E. L. Bennett et al., *Inorg. Chem.* 54 (2015) 2213-2220.

CuH is a material that appears in a wide variety of situations ranging from catalysis to electrochemistry to organic synthesis. There are both aqueous and non-aqueous synthetic routes to CuH, each of which apparently leads to a different product. We have used a combination of neutron spectroscopic, neutron diffraction and computational methods to characterise the

materials. Our results show that while all methods for the synthesis of CuH result in the same bulk product, the synthetic route produces distinct surface properties. The different properties of CuH obtained by aqueous and non-aqueous routes can be ascribed to a combination of significant differences in particle size and dissimilar surface termination: bonded hydroxyls for the aqueous routes and a coordinated donor for the non-aqueous routes. This work provides a particularly clear example of how the nature of an adsorbed layer on a nanoparticle's surface determines the nanoparticles' properties.



The different surfaces of CuH produced by aqueous (chemically bound hydroxyls, left) and non-aqueous (adsorbed pyridine, right) methods.

Polar stacking of molecules in liquid chloroform

JJ Shephard (University College London and Durham University), AK Soper, SK Callear, S Imberti (ISIS), JO Evans (Durham University), CG Salzmann (University College London)

Instrument: Sandals.

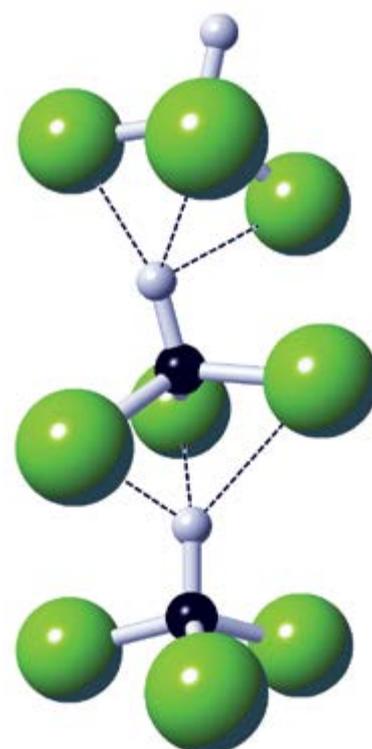
Research support: EPSRC.

Contact: Christoph Salzmann, c.salzmann@ucl.ac.uk

Further information: JJ Shephard et al., *Chem. Comm.* 51 (2015) 4770.

Chloroform is a powerful solvent capable of dissolving a vast range of chemicals such as vitamins, antibiotics, polymers and dyes at high concentrations. It is therefore frequently used as a reaction medium in the lab and a wide range of natural products can be extracted from plant materials using chloroform. We set out to study the structure of liquid chloroform using the Sandals instrument with the aim of establishing a link between the structure of chloroform and its performance as a solvent. A very strong tendency for chloroform molecules to stack on top of each other was found. The dipole moments of the molecules within those stacks all point in approximately the same direction which leads to a very large overall dipole moment. It was proposed that the interactions of these 'super-

dipoles' with dissolved molecules in chloroform enhance dissolution and extraction processes. The aim is now to replicate this effect in other liquids in order to design new and more environmentally friendly high-performance solvents.



Polar stack of three chloroform molecules.

Fundamental magnetism

Another dimension: designing magnets to explore fundamental physics

T Lancaster (Durham University), P A Goddard (Warwick University), S J Blundell, FR Foronda, S Ghannadzadeh, JS Möller (Oxford University), PJ Baker, FL Pratt (ISIS), C Baines (PSI), L Huang, J Wosnitza (Dresden High Magnetic Field Laboratory) RD McDonald, KA Modic, J Singleton, CV Topping (National High Magnetic Field Laboratory, Los Alamos), TAW Beale, F Xiao (Durham University), JA Schlueter (Argonne National Laboratory), AM Barton, RD Cabrera, KE Carreiro, HE Tran, JL Manson (Eastern Washington University)

Instruments: HiFi; SmuS (PSI); National High Magnetic Field Laboratory (USA).

Research support: EPSRC, US National Science Foundation.

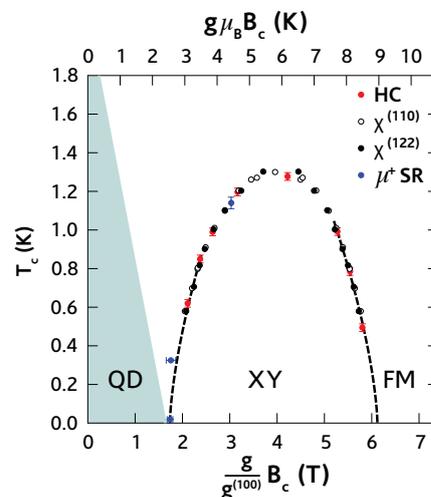
Contact: Tom Lancaster; tom.lancaster@durham.ac.uk

Further information: T Lancaster et al., Phys. Rev. Lett. 112 (2014) 207201.

The experience of a creature that lives in the flat-land of two dimensions is very different to that of one living in the line-land of one dimension. Quantum mechanics also tells us that two-dimensional magnets show vastly different properties to one-dimensional ones. In this work we have made magnetic materials out of molecular building blocks - effectively nanoscale LEGO - and have shown, using a range of probes including ISIS muons, that it is possible to tune the number of dimensions of the system. This demonstrates the design and manipulation of magnetic materials that act as if they are made from two-dimensional planes, one-dimensional chains or even zero-dimensional points. Moreover, it turns out that these

materials may be used to simulate the behaviour of still more quantum mechanical systems. The physics of Bose-Einstein condensation, for example, is very similar to that of our zero-dimensional magnet, and opens up the possibility of building magnets that simulate other exotic, quantum states.

The magnetic field-temperature phase diagram for zero-dimensional [Cu(py₂z)(gly)](ClO₄).



Fractionalisation of magnetic quasi-particles in a two dimensional magnet

B Dalla Piazza (EPFL), M Mourigal (EPFL and ILL), NB Christensen (Technical University of Denmark and PSI), GJ Nilsen (Edinburgh University and EPFL), P Tregenna-Piggott (PSI), TG Perring (ISIS), M Enderle (ILL), DF McMorro (University College London), DA Ivanov (ETH Zürich and Zürich University), HM Rønnow (EPFL)

Instruments: Maps, IN20 (ILL)

Contact: Henrik Rønnow, henrik.ronnow@epfl.ch

Further information: B Dalla Piazza et al., Nature Physics 11 (2015) 62-68.

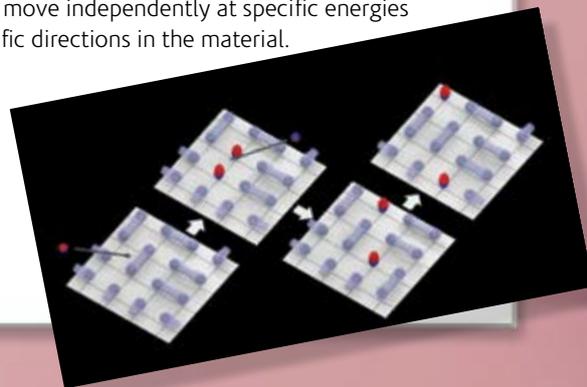
Fundamental particles are indivisible into smaller entities. Isolated electrons are fundamental particles that carry both a charge and a magnetic moment. In an interacting system, such as inside certain magnetic insulating materials, the electrons take on a different guise, breaking up or 'fractionalising' into quasi-particles. Quasi-particles act like electrons, but with modified properties that arise due to the strong interactions between them.

An extreme form of quasi-particle fractionalisation is observed in one-dimensional conductors, where the magnetic and electrical properties of the electron quasi-particles part company completely. However observing such phenomena in

higher-dimensional systems, particularly in magnetic materials, has proven to be elusive.

However, in this recent study using Maps at ISIS and IN20 at ILL, an international team of scientists observed fractionalisation in a two-dimensional quantum magnet. This work, including a new theoretical framework, demonstrated that the magnetic quasi-particles, known as magnons, split into two halves ('spinons'), that move independently at specific energies and along specific directions in the material.

Illustration of the creation of fractional excitations out of singlets by scattering neutrons on the square lattice antiferromagnet.



High field spin-density-wave phases in a metal

C Lester, SM Hayden, TP Croft (University of Bristol), S Ramos (University of Kent), EM Forgan (University of Birmingham), RS Perry (UCL), P Manuel, DD Khalyavin, RI Bewley, T Guidi (ISIS)

Instruments: Wish, Let.

Research support: EPSRC: EP/J015423/1.

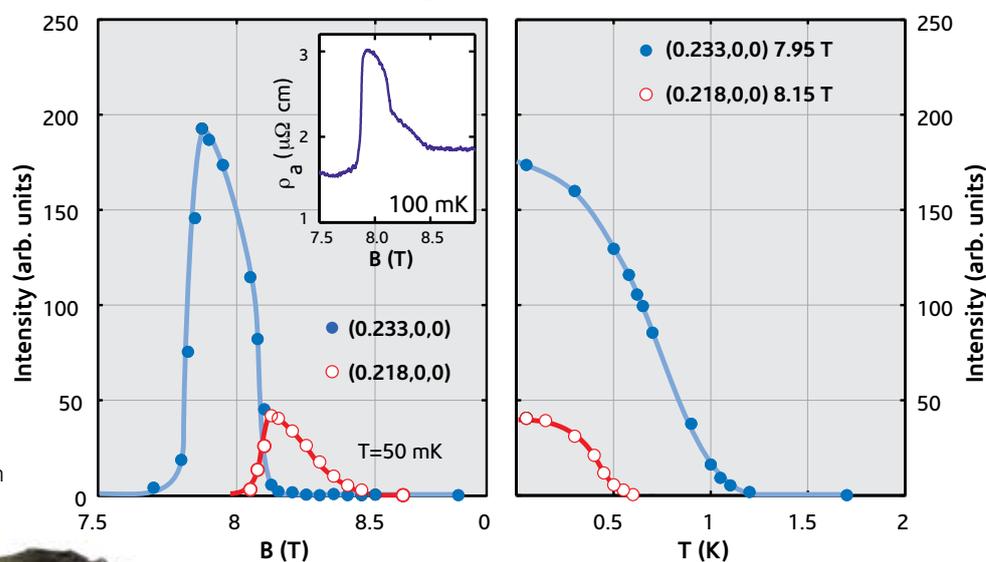
Contact: Stephen Hayden, s.hayden@bristol.ac.uk

Further information: C Lester et al., Nat. Mat. 14 (2015) 373.

A phase transition between two electronic states is often accompanied by profound changes in physical properties, for example resistance or heat capacity. It has been known for some time that at low temperatures ($T < 1$ K), the application of a large (8 T) magnetic field causes large changes in the resistivity of $\text{Sr}_3\text{Ru}_2\text{O}_7$ over a narrow range in field. While it was assumed that the material must enter a new electronic phase, the microscopic details of this new phase remained unknown for a number of years. Following initial experiments made on Let, recent diffraction measurements made on the Wish diffractometer have shown that the high-field resistivity anomaly of $\text{Sr}_3\text{Ru}_2\text{O}_7$ is due

to a cascade of two distinct spin density wave phases at low temperatures. This research has demonstrated a novel way to control the resistance of a metal by tuning the magnetic ground state with an applied field.

Field- and temperature-dependence of magnetic Bragg peak intensities (measured on WISH) of two magnetically-ordered phases in $\text{Sr}_3\text{Ru}_2\text{O}_7$. Inset: high field resistivity data.



Thomas Croft (Bristol University) exploring the electronic ground states of $\text{Sr}_3\text{Ru}_2\text{O}_7$, using Let.

Technology





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

Advances in instrumentation & techniques

New Second Target Station instruments



A small project board oversees the project to build four more instruments on the ISIS second target station. Here members of the board are viewing the new Larmor instrument. Image shows (left to right) Matt Fletcher (ISIS), Andrew Taylor (STFC), Kevin Jones (ISIS), Sean Langridge (ISIS), Adrian Hillier (ISIS), Jim Kay (Diamond), Robert McGreevy (ISIS) and Paolo Radaelli (Oxford University).

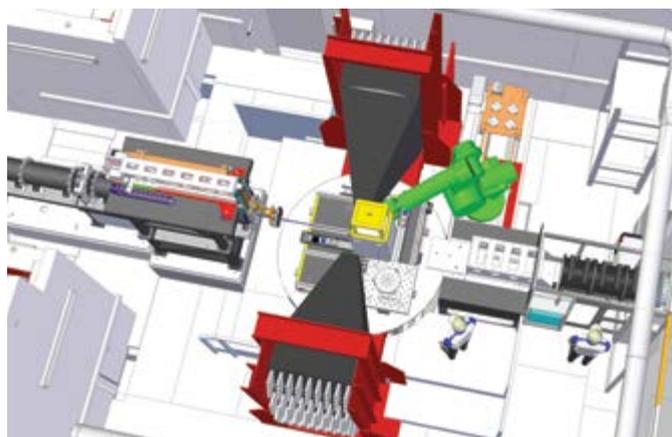
Imat



Chopper development and installation team with the three IMAT double-disk and TO neutron beam choppers.

Installation of the Imat neutron imaging and diffraction instrument is nearing completion. Imat will be applicable to a diverse range of disciplines ranging from Engineering Sciences to Earth Sciences, Archaeology and Heritage Science, to Soft Matter and Biomaterials. It will provide non-destructive and in-situ testing, including white-beam neutron radiography and tomography, as well as energy-dependent neutron imaging. The IMAT beam shutter was

opened for the first time in July 2015 for radiation shielding tests, and scientific commissioning will start in Autumn 2015.



Schematic of the Imat sample area.

Chiplr

Chiplr reopened its shutter on the 25th March 2015 following modifications to the target and reflector on the Second Target Station. These modifications were designed to provide Chiplr with many more of the very fast neutrons (in the mega-electron-volt regime) to closely mimic the energy spectrum of those generated in the atmosphere by cosmic rays which are proving so problematic to modern electronics and avionics. A fast neutron irradiation instrument like Chiplr has not been built on a spallation source before and so we are now busy commissioning all aspects of the instrument. As the commissioning progresses our first testing of an electronic device is not too far away.



The Chiplr blockhouse and sample table.

Larmor



Larmor is a multi-purpose instrument for small angle neutron scattering (SANS) using the Larmor precession of polarised neutrons. Commissioning of the instrument has been going well, with performance in line with expectations. The first user experiments have been carried out by a group from the Technical University of Eindhoven and the Technical University of Delft, and proposals are currently being accepted for SANS and Polarised experiments. The Spin-Echo SANS system will be commissioned by our collaborators from TU-Delft in Spring 2016. Following the installation of the SESANS system attention will move to the installation of a small, high-angle detector bank that will enable SANS and limited diffraction measurements to be carried out simultaneously.

Zoom

Zoom, a new flexible small angle neutron scattering (SANS) instrument with optional polarised neutrons, is rapidly nearing its open shutter date in 2016. Much is now installed including the control cabin, counting house, and detector vacuum tank with its internal rails and motion system. Final design work will be completed shortly, ready for commissioning towards the end of that year. The SANS team are delighted to welcome two new instrument scientists for Zoom, Dr Diego Alba Venero and Dr James Douth who will bring expertise in hard condensed matter and soft matter plus food science, respectively.

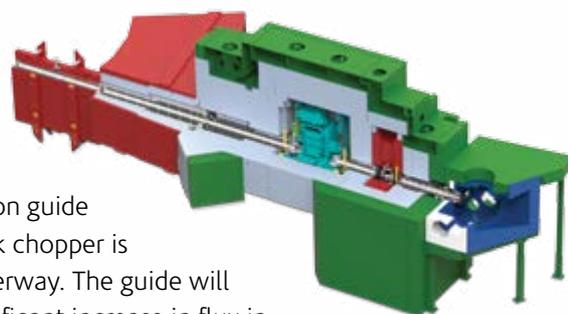
Zoom under construction.



Other instrument developments

A new guide for Maps...

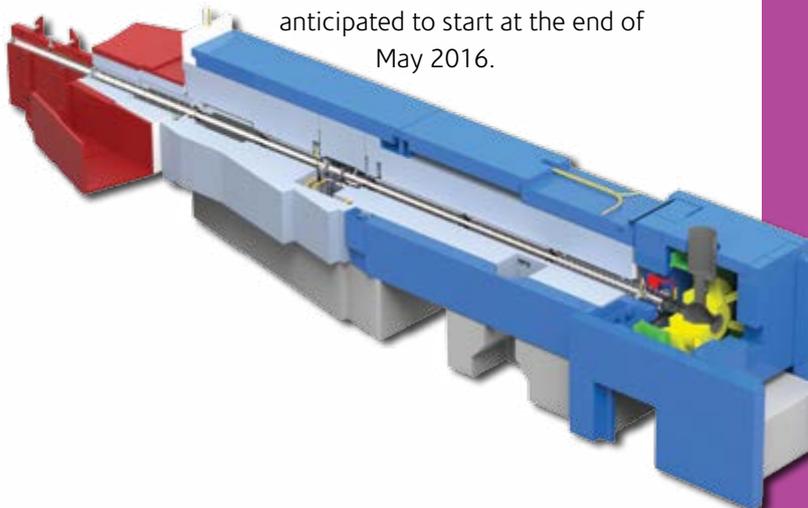
The project to upgrade Maps with the addition of an $m=3$ neutron guide and a new disk chopper is now well underway. The guide will provide a significant increase in flux in the thermal regime, with gain factors of around eight at 25meV to two at 100meV. The disk chopper will reduce the background arising from later neutron pulses passing through the chopper, and will also allow Maps to exploit the multi-repetition method that is already used successfully on Let and Merlin. Delivery of all of the remaining components is scheduled to take place by December 2015, with installation planned to take place as soon as possible thereafter.



...and for Tosca

The project to enhance the available flux on Tosca through provision of a new, high- m guide is also progressing very well. Extensive Monte-Carlo simulations show that the guide should increase the flux to the instrument across whole energy range and in particular between 10-50 meV by a factor of around 20. Such an increase in incident flux implies an order-of-magnitude reduction in counting times, access to smaller specimens, and it means that parametric studies would become routine.

Final delivery of components is expected at the end of March 2016, with work on the installation of the new guide anticipated to start at the end of May 2016.



Let detectors complete



A 'panoramic' view from the sample position of the Let detectors, covering 140° horizontally and $\pm 30^\circ$ vertically.

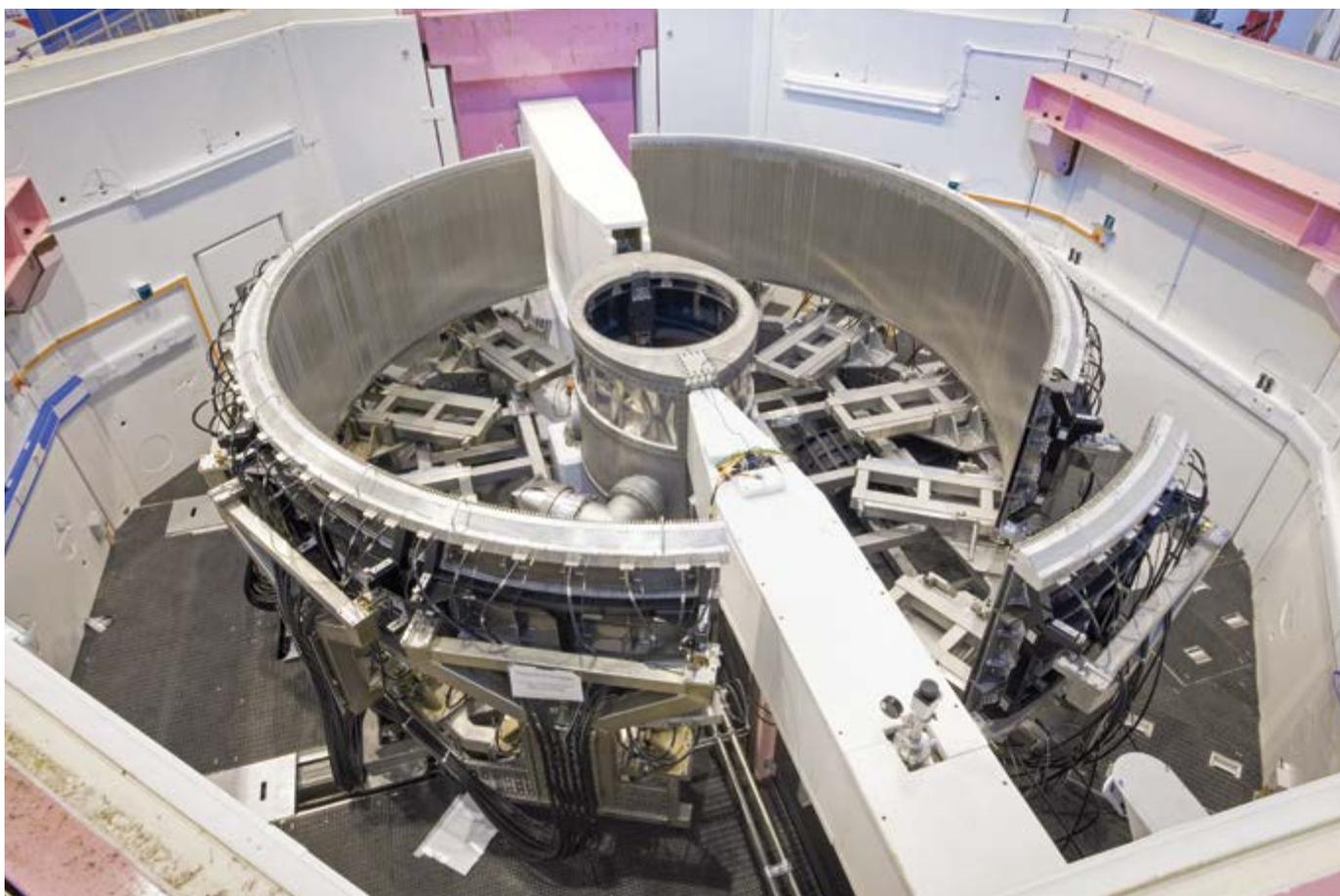
Let's detectors, at 4m long, are the longest ^3He position sensitive neutron detectors in the world. Technical problems have delayed full installation of the entire detector array, but this was completed recently to give a massive π steradians and providing almost gap-free coverage. The tubes have a position resolution of around

25 mm along their length leading to over 100,000 pixels in the full array! We have also just installed a radial collimator on Let. This will almost eliminate scattering from most sample environment equipment so as to reduce the background of any measurements, particularly quasi-elastic studies.

Wish detectors

Following the completion of the second side of the instrument last year, Wish is now operating with its full complement of detectors (1520 pixelated 8 mm diameter ^3He tubes). This has enabled a factor 2 increase in the count rate for powder experiments and a greater q-coverage in single crystal mode. During the long shutdown, two shielded argon tanks have been installed between the primary vacuum tank and the detectors to reduce the already very low background even further (factor 4 in the low angle bank) as well as slightly improve the flux.

The Wish detector array.



Muon beamline upgrade

The first stage of the muon beam upgrade (replacing the two quadrupoles nearest the production target with a new triplet) is complete, and the beam tuning has been optimised for this layout. As well as securing the future of the muon beamlines into the foreseeable future, this



The muon beamline upgrade team.

has also led to an improvement in muon rates of about a factor of 2. Stage 2 of the muon beamline upgrade, to replace the remaining components common to the three beams, is planned for next year.

Elemental analysis using negative muons

Using negative muons as a tool for elemental analysis is possible at ISIS. Indeed, element analysis on a layered sample has shown that depth-dependent studies are possible and that measurements deep within a sample are feasible. Moreover, this technique is sensitive to all elements and is completely non-destructive. The bronze standards used for test measurements have shown the sensitivity of the technique, even whilst only a single X-ray detector is available. This technique has the potential to be

used in a wide range of applications, including engineering samples, archeological artifacts, bio-systems and battery materials. A series of experiments has started on Roman coins, with ones on biomaterials in the pipeline.

Mantid

The ISIS data reduction and analysis framework, Mantid, continues to grow and develop. As well as its use across the ISIS instrument suite, Mantid has also been adopted by the Spallation Neutron Source in the US and, most recently, by the European Spallation Source currently being built in Lund, Sweden. In addition, other neutron facilities in Europe such as the ILL in Grenoble and SINQ at the Paul Scherrer Institute in Switzerland are also using the framework. The picture below shows the Mantid Steering Committee meeting at the Cosener's House in January.



Dr Chu Chuan Dong, right, and James Crosland (ISIS) working in the ISIS Deuteration Laboratory.



Accelerator and targets

The ISIS long shutdown – from August 2014 to March 2015 – saw a huge amount of work undertaken to refurbish and upgrade parts of the ISIS accelerator and target systems. Some examples of this work are given here.

Upgrade of Extracted Proton Beam (EPB) magnets

The largest task undertaken on the accelerator during the long shutdown was the upgrade of parts of the first target station EPB. This involved the replacement of six quadrupole focusing magnets in the area around the intermediate muon target, requiring removal of a lot of shielding. Radiation damaged magnets (some of which came from ISIS's predecessor NIMROD – so were decades old) were replaced with new, more reliable ones. In addition, the layout of the magnets has been designed to allow ISIS to continue operations in the event that any one of them suffers a failure.

Geoff Matthews, Barry Wilkes, John Carter and Roy Symes (ISIS) fitting one of the new focusing magnets into the extracted proton beamline.



TS2 target reflector upgrade

The long shutdown also saw replacement of the beryllium reflector on the ISIS Second Target Station. The new reflector was designed with two main changes in mind: to give the new Chiplr instrument the view of the ISIS target that it requires, and to widen Larmor's view of its moderator. The new reflector was also designed with greater flexibility for upgrades to the reflector and



moderators in the future. A specially built rig enabled the new reflector to be assembled, pre-aligned and the cooling system flow tested offline, key to the successful installation which has to be done in a remote handling cell.

The TS2 reflector assembly.

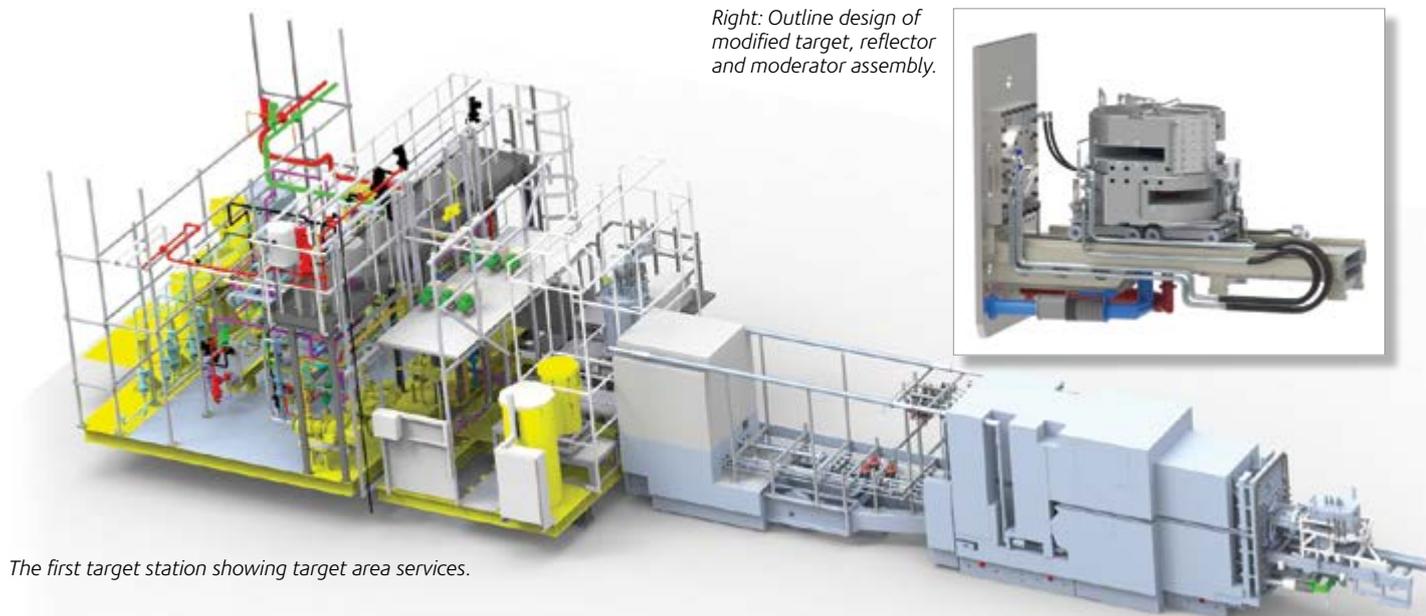
Main Control Room Refurbishment

A major task during the long shutdown was the complete refurbishment of the ISIS Main Control Room (MCR). Whilst state-of-the-art when ISIS began operations in 1984, and despite multiple improvements since then, by 2014 it was showing its age and a full redesign was necessary. Once the long shutdown began, the old MCR was completely taken out and new custom-made desks, beam controls and arrays of monitors were installed and fine-tuned.



Neal Grafton and the crew at work in the new look MCR.

First Target Station Project



Right: Outline design of modified target, reflector and moderator assembly.

The first target station showing target area services.

The ISIS first target station – TS1 – has been operating since ISIS started up in 1984. Over these 30 years there has been no significant work carried out to maintain or develop its internals – the moderators, reflector and target infrastructure, including cryogenic and cooling circuits, etc.

Around three years ago, ISIS began a project to upgrade TS1, to ensure that it is fit for operations for many years more. This has meant firstly making sure we know exactly what is in the target station! We have updated 30-year-old engineering drawings and simulated the neutron production using computer codes to check that this agrees with what we see on the instruments. This first part of the project has been very successful, with a large amount of working having been done to understand exactly how the target station is working.

A second part of the project has then been to redesign elements of the target station assembly, plus associated services, to improve operations, build in greater flexibility to make future changes, and improve the neutron output.

During this process, several engineering reviews, and reviews of the neutronics calculations, have been made by internal and external panels of experts. These have shown that the project has been progressing well. The plan is now to refine the new target, moderator and reflector design

over coming months, and then to produce detailed plans for implementing the upgrade. The actual installation is likely to take around a year and will happen in 2019 or 2020 - ensuring many more years of neutrons from the ISIS first target station.

RF upgrade during the long shutdown

A new High Power Drive (HPD) amplifier for the synchrotron accelerating cavities, designed to use a more stable and sustainable tetrode, has been built and tested.



Members of the RF group's synchrotron section with the new high power drive system.

The HPD can drive both the fundamental and second harmonic RF cavities in the accelerator. Currently these are driven by two tetrodes, which can struggle to reliably provide the required power for operating at high beam intensities. As well as being more economic and able to provide higher powers more consistently, the new HPD modular design allows for significantly faster maintenance or replacement in the event of a failure.

Make way for a MEBT...

The entire pre-injector ion source area was reconfigured and extended during the long shutdown, to make enough space for a Medium Energy Beam Transport (MEBT) line to be installed between the Radio Frequency Quadrupole (RFQ) and Tank 1 of the Linac. The MEBT line will consist of several quadrupole magnets and re-bunching cavities, and installation is planned for 2018. The MEBT will reduce the 30% loss in beam current caused by the mismatch between the RFQ and Tank 1. By adding a chopper to the MEBT there is also the potential to reduce activation in the synchrotron caused by trapping losses, significantly improving ISIS operations by allowing quicker access.



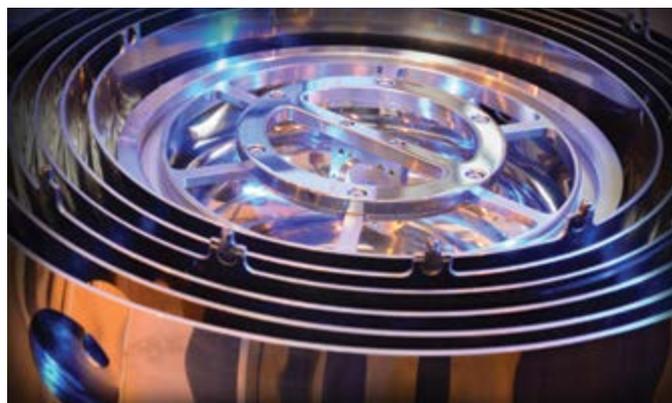
Members of the Low Energy Beams Group in the enlarged and reconfigured pre-injector area.

ISIS Linac tank replacement project

The ISIS linear accelerator (Linac) is composed of four separate tanks that accelerate H^- ions from an energy of 35keV to 70MeV before injection into the synchrotron. Linac tank 4 was made in the 1970s and is now showing signs of wear and tear. To keep ISIS operational, a new 12m Linac tank will be made and installed during the next long shut down. A 2m long test tank, which consists of the first 5 drift tubes, has been created to demonstrate the principle of the new tank. Once all the testing criteria have been met the manufacture of the full size replacement tank will be undertaken.

Siemens ONIAC – a novel compact accelerator for industry

Siemens are using the unique specialist skills and facilities available at ISIS to develop a new proof-of-concept particle accelerator. The ONIAC is a DC electrostatic tandem accelerator in which the high voltage generator and accelerating structure are integrated in one assembly. It includes a group of nested hemisphere shells that resemble an onion (hence the name ONIon ACcelerator). The ONIAC represents a paradigm shift in compact accelerators with an extremely small ($2 \times 2 \text{ m}^2$) footprint and a variable energy range of 1-20 MeV. Designed at Siemens AG, it offers energy efficiency, robustness, reliability and a low total cost, making particle accelerators more accessible for industry. The Siemens ONIAC has the potential to reduce the cost of on-site radio-isotope production and has applications as diverse as cargo scanning and water treatment.



The inner shells of the ONIAC, whose 'onion like' appearance give the accelerator its name. Photo courtesy of Siemens, www.siemens.com.



Oliver Newell (ISIS) installing one of the drift tubes in the test tank for the ISIS Linac tank 4 replacement programme.

*James Wilgeroth,
Emily McDougall
(Cella Energy)
during their ISIS
experiment.*



*Below: Amaia Uriz, Jose Ramon Isasi, Raquel
Barbosa, Cecile Dreiss, Gustavo Gonzalez
(University of Navarra and Kings College
London) using Loq to study micellar
aggregates of direct and reverse
Tetronics for enhanced drug
solubilisation.*



Right: Martin Mansson (KTH Royal Institute of Technology, Stockholm) and Hiroshi Nozaki (Toyota Central R & D Labs, Japan) using EMU to explore Li diffusion in battery electrode material $\text{Li}(\text{FeMn})\text{PO}_4$.

Above: Giogia Albani (Univita Milano Bicocca) using INES to test a new neutron detector based on gas electron multiplication

Left: Arpita Mitra (Leeds) mounting samples for polarised neutron reflectivity measurements of spin pumping in an organic semiconductor.

Working *with industry*





The capabilities of ISIS enable key insights into industrial research problems for a wide range of companies across the industrial spectrum, from SMEs to multinational corporations. The unique properties of neutrons have been successfully applied to the chemicals and plastics industry, healthcare, aerospace, transport, large and small scale manufacturing, automotive and the energy industrial sector.

Working with industry

There are a range of mechanisms available for industry to access the scientific expertise and instrumentation at ISIS – through partnerships with academia, by direct payment for beamtime, or through the ISIS Collaborative R&D programme (ICRD).

The ICRD scheme was set up in 2011 to widen the use of ISIS by industry and increase the economic benefit to the UK. The scheme has been highly successful with an increase in both the diversity and number of companies now directly involved with this programme. In 2015 a total of 31 companies accessed ISIS through the ICRD scheme. Many more were involved in ISIS experiments through collaborations with university partners.

Case Study Assessing the safety of our nuclear reactors

EDF Energy owns and operates 8 of the 9 remaining civil nuclear stations in the UK – generating around one sixth of the UK's electricity. As its Advanced Gas Cooled Reactors (AGRs) come to the end of their life, degradation of critical systems and components could affect reliability and even become life limiting. Whilst plant lifetime is predicted and assessed through modelling, the key to actual lifetime is real plant condition as measured through inspection.

On behalf of EDF Energy, Dr Hedieh Jazaeri from the Open University has been using the Sand2d small angle neutron scattering instrument to identify and measure actual creep damage in pressurised steel components used in AGRs. Without the need for sample preparation, this technique has provided a volumetric measure of cavitation damage ranging from a few nm up to about 400 nm.

"This research could help in safety assessments of nuclear reactor components, as neutron scattering allows you to identify and quantify creep damage in the early stages," says Dr Jazaeri.



EDF's Advanced Gas Reactor at Hartlepool.

Courtesy of EDF Energy

Case Study Challenging knee implants

It is estimated that 90,000 knee replacement procedures were carried out in 2014 in the UK and 720,000 in the US^{1,2,3}. Some predictions anticipate that by 2030 this figure will grow to 3.48 million for the US alone⁴. Therefore it is of great importance that the production of such implants is optimised to meet demand and create a sustainable manufacturing process.

DePuy, a Manufacturer of Cobalt Chrome (ASTM F75) femoral knee implants, currently experience scrap as a result of out-of-tolerance parts. Femoral implants are "C"-shaped and the dimension across the open end of the "C", the Anterior-Posterior (A-P) feature, can vary, requiring high levels of control and dimensional inspection.

The A-P dimension is considered critical in order to ensure optimum fit to the patient's bone and parts which fall out of specification are rejected. Femoral implants pass through a large number of manufacturing process steps before distortion is identified, resulting in a significant environmental and business cost.

Redistributed or induced residual stress is the cause of such distortion. Residual stress states are influenced by various manufacturing process and in order to investigate the effect of each process, a reliable stress determination method is required. Therefore, Brian Conroy, a DePuy



SIGMA® Total Knee System.

Courtesy of DePuy Synthes

sponsored PhD student from the University of Limerick, has conducted experimentation on an ISIS instrument, Engin-x. The purpose of experimentation is in order to non-destructively determine residual stress within femoral components. The components will subsequently be destructively tested and comparisons made between results. Neutron diffraction measurements will help validate destructive residual stress determination techniques, which can subsequently be applied to investigate various manufacturing processes.

Cobalt chrome is an extremely difficult alloy for neutron experimentation as it absorbs a large portion of the beam and also causes a large amount of incoherent scattering which result in background noise. As a result, experimentation capabilities are limited and measurement times are much longer than those for materials such as steels. Experimentation conducted was the first known application of neutron diffraction to ASTM F75.

¹ Office for National Statistics: <http://www.ons.gov.uk/ons/guide-method/compendiums/compendium-of-uk-statistics/population-and-migration/index.html>.

² OECD (2013) http://dx.doi.org/10.1787/health_glance-2013-38-en

³ US Census Bureau (2015) <http://www.census.gov/popclock/>.

⁴ Kurtz, S. et al., (2007) *Journal of Bone & Joint Surgery* 89, 780-785.

Case Study

Fuelling efficiency with Infineum

Formed through a joint venture between ExxonMobil and Shell, Infineum is one of the world's leading formulators, manufacturers and marketers of fuel and lubricant additives. Their work is driven by reducing emissions into the environment, improving engine performance and responsible, more efficient use of chemicals.

The additives in fuel and lubricant prevent damage to the engine through lubrication, prevention of mechanical and corrosive wear (which manifests via acid corrosion in the engine) and conferring beneficial properties such as improved fuel economy. Challenges presented by changes to engine designs and the use of biofuel, formed from various plant structures, create opportunities for further research.

Infineum's Lead Scientist Prof Peter Dowding and his team have been using ISIS instrument, LOQ to understand at the atomic scale how calcium carbonate particles in their additives form. The locality of Infineum's headquarters enables the team to prepare samples and measure them on LOQ in real time. These results filter into different preparation methods of surfactant additives, enabling

Infineum to formulate additives more effectively and ensure a globally-consistent product.

"Neutrons give us the ability to switch on and off parts of the system, so if I'm interested in the surfactant layer I can look at that specifically, and that can be key," says Prof Dowding.

"Our work at ISIS allows us to not only use the products we make more efficiently but to improve fuel economy in the future, as we can look at which molecules influence friction at the molecular level."

Emma Packard and Peter Dowding (Infineum) load samples on Loq.



Skills and training

A photograph of a control room. A prominent red sign with the words "BEAM ON" in black capital letters is mounted on a wooden wall. Above the sign is a computer monitor displaying a grayscale image. To the right, a person's shoulder and arm are visible, holding a purple folder. In the foreground, a red metal panel with a yellow warning label and a silver connector is visible. The background shows a control panel with several green indicator lights.

BEAM ON



Training forms a major part of the ISIS programme, and happens in a wide variety of ways. ISIS has programmes and events aimed at school students including work experience, regularly takes apprentices, sandwich students and graduates, and has a wide variety of training activities for PhD students, post-docs and scientists in the ISIS user community. A selection of examples can be seen within this section.

Luiza Rosa de Araujo (Durham) using Polaris to explore time dependent order-disorder phenomena in the $Zr_xSn_{1-x}Mo_2O_8$ negative thermal expansion material.

Inspiring the next generation of scientists

Open days at ISIS

On 11 July, Harwell Campus opened its doors so that members of the public could see behind the scenes at ISIS, Diamond, the Central Laser Facility and other departments on site. In total 16,000 people visited, of which around 4,300 came to ISIS. Demonstrations in ISIS included the opportunity to make slime, see vibrations in a wall of flames, make crystal molecules out of jelly babies, grow crystal gardens and see the amazing Dr Frost's liquid nitrogen show. A schools' day earlier in the week saw 240 secondary school pupils tour ISIS and learn about ISIS science through hands-on activities and demonstrations.



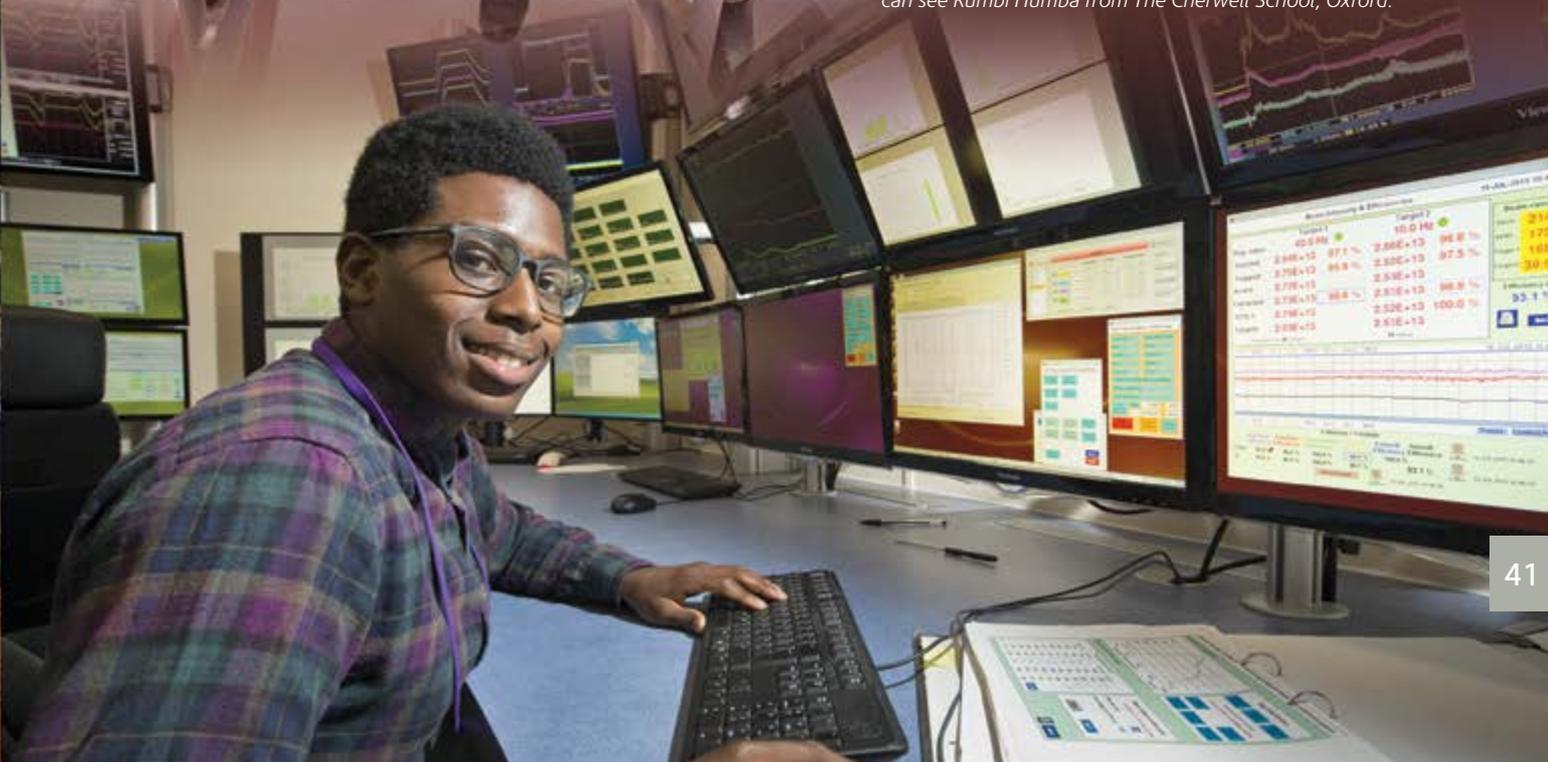
Schools at ISIS

ISIS hosts sixth form students every year (below) who come to RAL as part of the Particle Physics Masterclass. Around 400 students tour ISIS over a 4 day period.



Top and above: Forty secondary school students experienced a Chemistry at Work event at ISIS in January. Chemistry at Work is a scheme organised by the Royal Society of Chemistry aimed at connecting school students with real-world chemistry. The students were able to experience a variety of demonstrations and participate in chemistry activities and experiments.

Below: ISIS regularly takes work experience students during summer months. The students are often at the end of their GCSE exams, and come to ISIS as part of STFC's work experience programme. Here we can see Rumbi Humba from The Cherwell School, Oxford.



Graduates and PhD students

PhD students receive hundreds of days of on-the-job training every year when they come to run experiments at the facility, but in addition ISIS runs courses dedicated to helping students learn about neutron scattering and muon spectroscopy. ISIS also recruits people who have just finished their degrees as part of STFC's graduate training programme, and has around ten university students on sandwich placements as part of their degree courses for a year. ISIS is also heavily involved in STFC's apprentice training programme.

Below: ISIS runs a 5-day muon training school every two years to introduce students to the technique and applications of muon spectroscopy. Here we see two students using the HiFi muon spectrometer.



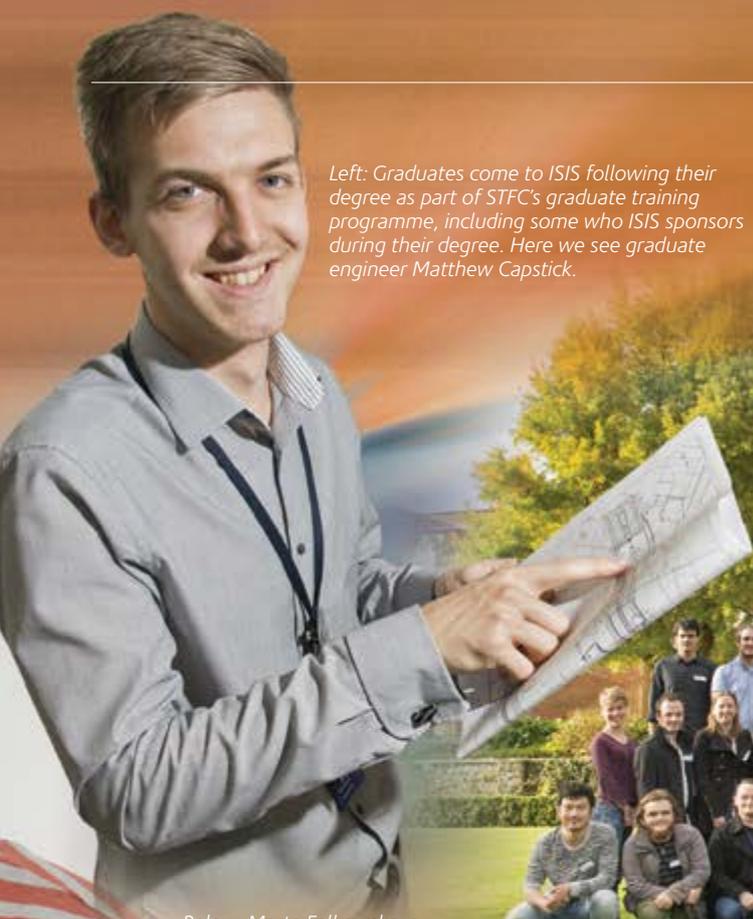
Left: ISIS takes around 10 sandwich students each year. The students spend a year at ISIS as part of their university course, working in areas from computing to communications, detectors to data analysis. Here we see Sean Ashiru, who worked in the ISIS business systems group.

Above and below: The ISIS practical neutron training course for PhD students ran for 10 days in June. It includes lectures on all aspects of neutron scattering, plus hands-on time running experiments on the instruments.



Left: Graduates come to ISIS following their degree as part of STFC's graduate training programme, including some who ISIS sponsors during their degree. Here we see graduate engineer Matthew Capstick.

Below: ISIS staff co-supervise a large number of PhD students in partnership with university colleagues. A student day was held in October to help students get to know each other and for them to discuss their science projects. This year also saw the first call for ISIS Facility Development Studentships, with 14 studentship projects being selected.



Below: Marta Falkowska, a PhD student from Queens University, Belfast, preparing samples for Nimrod studies of catalytic alkyne hydrogenation. Marta is co-supervised by Chris Hardacre at Belfast and Daniel Bowron at ISIS.



Left and below: The EPSRC funded a new group of Centres for Doctoral Training (CDTs) in 2014 with the aim of providing training and research opportunities for scientists and engineers. A school designed to introduce CDT students to X-rays, neutrons and muons was organised by Diamond and ISIS in March. The school was attended by 92 CDT students, mainly in their first year of their doctoral work, from 18 separate CDTs ranging in subject area from engineering, materials characterisation and condensed matter physics to chemical biology, regenerative medicine and sustainable chemical technologies.



Conferences and workshops

ISIS staff are involved in organising a very wide variety of conferences, meetings and workshops each year. A few examples are given here.

Below: The Molecular Spectroscopy User Meeting was held in January and attracted around 80 participants.



Above and below: The UK Neutron and Muon Science and User Meeting (NMSUM) was held over three days in May and attracted 230 users of ISIS and ILL. The first day saw around 55 PhD students learning about ISIS science and discussing their work. This was followed by a day organised around five science themes, followed by updates from facilities and UK research councils.



Above: A meeting to discuss Future Muon Sources and their uses was held in Huddersfield in January, co-organised by the ISIS muon group.

The UK pledged construction funds for the European Spallation Source last year, and these will be managed through the UK ESS project office being set up by STFC. A meeting was held in December at RAL for UK universities and industry to discuss the UK's involvement in the ESS, with around 130 people attending.



Right: The 8th ESS In-Kind Contributions (IKON) meeting was held at Milton Hill House near the Rutherford Appleton Laboratory in February – the first time that the meeting had been held outside Sweden. The meeting discussed progress with the ESS technical design, focusing on neutron instrumentation and technology as well as science.



Roger Eriksson, ESS

Below: To mark 25 years of operation of the Sandals disordered materials and liquids instrument at ISIS, a science meeting was held at The Cosener's House in January, followed by a workshop on Empirical Potential Structure Refinement.



Above: As part of marking the ISIS-India agreement which was signed in January, ISIS held a science meeting including a talk by distinguished scientist Prof CNR Rao.

Below: The Theoretical and Experimental Magnetism Meeting was held in July at the Cosener's House with 80 participants discussing the latest developments in the field.



Seminars

ISIS seminars continue to attract a wide variety of national and international speakers. Many are organised jointly with Diamond, and some are focused on particular themes such as a series on strongly correlated electron systems.

Date	Speaker/Affiliation	Title
April 14	Alston Misquitta (Queen Mary University of London)	Do we really understand intermolecular interactions? An overview and recent surprises
April 14	Frank Kruger (ISIS / Oxford)	Spirals near Ferromagnetic Quantum Criticality
April 14	Bob Newport (University of Kent)	Glass: a look inside
May 14	Gabriel Bernardo (University of Minho)	Structure-Property Relationships in Functional Polymer Systems
June 14	Stefan Klotz (Université Pierre & Marie Curie, Paris)	Decker versus Brown: The NaCl and Pb pressure scales
June 14	Dave Allen, Claire Wilson, Mark Warren (Diamond Light Source)	High-pressure single-crystal diffraction studies on beamline I19 at Diamond Light Source
Aug 14	Andrew Boothroyd (Oxford)	Magnetic phenomena in correlated 5d and Dirac systems
Sept 14	Jeroen van den Brink (IFW Dresden)	Resonant Inelastic X-ray Scattering on high T_c cuprates and magnetic iridates
Sept 14	Paul McClarty (ISIS)	Fluctuation-induced phases in the rare earth pyrochlores
Sept 14	Malcolm Guthrie (ESS)	Micro-diffraction on the SNAP diffractometer at the SNS
Oct 14	Alex Bogdanov (IFW Dresden)	Theory of chiral skyrmions in noncentrosymmetric ferromagnets
Oct 14	Claudio Castelnovo (Cambridge)	Dynamics of fractionalised excitations in spin ice materials
Oct 14	Daniel Roach (University of Salford)	Obtaining dispersion curves from powders: the interpretation of polycrystalline coherent inelastic neutron scattering (poly-CINS)
Nov 14	Steve Simon (Oxford)	Topological matter and why you should be interested
Nov 14	Thorsten Schmitt (PSI)	Probing high-energy spin fluctuations in iron pnictide superconductors and the metal-insulator transitions in rare-earth nickelates by soft X-ray RIXS
Nov 14	Leo Bañuelos (ISIS)	Nanoscale confinement and surface effects in electrical energy storage systems
Dec 14	Roser Valenti (Frankfurt)	Fe-based superconductors: An overview
Dec 14	Chris Lester (Bristol)	Antiferromagnetic order and quantum criticality in $\text{Sr}_3\text{Ru}_2\text{O}_7$
Dec 14	Mark Dean (Brookhaven Nat Lab, USA)	Magnetic Excitations in Hole-Doped Cuprates and their Evolution with Doping and Dimensionality
Jan 15	I15 Team (Diamond)	The I15 Extreme Conditions Beamline at Diamond
Feb 15	Elizabeth Blackburn (Birmingham University)	How are electrons ordered in the underdoped high- T_c cuprates?
Feb 15	Branton Campbell (Brigham Young University, Utah and Durham University, UK)	The symmetry-mode description of distorted crystals
Feb 15	Frederic Mila (EPFL Lausanne)	Frustrated Magnets in High Magnetic Fields and the Mystery of $\text{SrCu}_2(\text{BO}_3)_2$
Mar 15	Luigi Amico (University of Catania and the Centre for Quantum Technologies in Singapore)	Local response of topological order to an external perturbation
Mar 15	Giniyat Khaliullin (Max Planck Institute Stuttgart)	Magnetism and Doping Effects in Spin-Orbit Coupled Mott Insulators



Other events

ISIS staff are involved in organising a wide range of meetings and events. Some examples from the past year are given below.

Date	Event
April 2014	Neutron and Muon User Meeting (NMUM)
May 2014	Muon Training Course
June 2014	Muon site calculation session at International Muon Conference 2014
July 2014	Theoretical and Experimental Magnetism Meeting
Sept 2014	Neutron Characterisation Meeting
Sept 2014	EU Muon Joint Research Activity Meeting
Sept 2014	DENIM 2014 - Engineering workshop in the field of neutron scattering instruments
Oct 2014	8th International Sample Environment Workshop
Oct 2014	Horace Workshop – visualisation and analysis of large datasets from time-of-flight neutron inelastic scattering spectrometers
Oct 2014	ISIS Student Meeting
Oct 2014	Careers in Polymer Science: Beyond Academia
Oct 2014	2nd UK-US CCP-SAS (Collaborative Computational Project for Small Angle Scattering) Project Workshop
Nov 2014	Crystallography User Group Meeting
Nov 2014	Particle Accelerator Open Day
Nov 2014	An Introduction to Neutron Techniques in Catalysis
Dec 2014	ISIS Facility Access Panels
Dec 2014	Institute of Physics BRSG Christmas meeting - Magnetic Resonance and Muons - A Complementary View of Materials
Jan 2015	SANDALS 25th Anniversary
Jan 2015	EPSR Workshop
Jan 2015	Future Muon Sources, Huddersfield
Jan 2015	Molecular Spectroscopy Science Meeting – MSSM2015
Feb 2015	IKON8, ESS In-kind contributions meeting
Feb 2015	1st International Sample Environment Technical Training School

A year around ISIS





*This year has seen
ISIS marking 30 years
of neutron production,
the signing of further
international agreements,
and prizes for
ISIS scientists!*

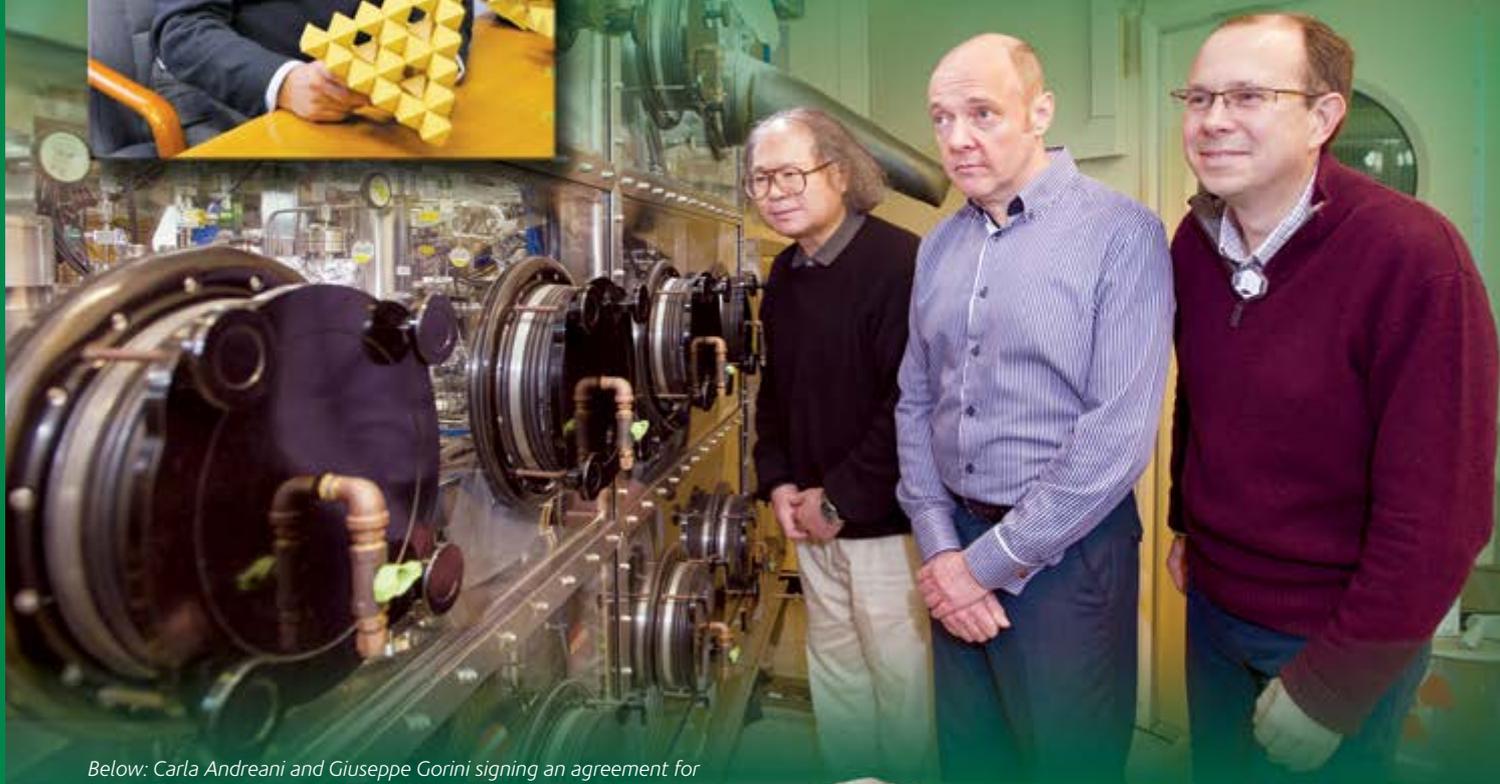
David Tam (Rice University, Texas) uses Merlin to explore high energy nematic spin correlations in BaFe_2As_2 .

A year around ISIS



Left: Senior ISIS Scientist Prof Bill David has been awarded the Royal Society of Chemistry John B Goodenough Award for 2015. Bill's work focuses on chemical storage, primarily of ammonia and hydrogen, both with potential uses in sustainable energy generation. The Award recognises an exceptional and sustained contribution in the area of materials chemistry.

Below: The RIKEN-RAL Muon Facility at ISIS has, since it began operations 20 years ago, had a programme of research in muon catalysed fusion. This programme has produced notable results in this area, but, with RIKEN muon research turning to other areas, a new home was needed for the tritium handling system which was a key piece of equipment for these studies. RIKEN, ISIS and the UK Atomic Energy Authority teamed up to provide a new use for the system in the Material Research Facility currently being established at Culham, and the equipment was moved there in March.



Below: Carla Andreani and Giuseppe Gorini signing an agreement for joint collaboration between ISIS and CNR (Italy) with ISIS Director Robert McGreevy in April.





Above: ISIS periodically asks external panels to review its instruments, to ensure the facility is continuing to have the best instrumentation possible. Here we see Neil Skipper (UCL, panel Chair), Bernhard Frick (ILL), Heloisa Bordallo (Copenhagen) and Craig Brown (NIST) with members of the Molecular Spectroscopy Group during a review of the Iris and Osiris instruments in November.

Below: The BTM Willis Prize, awarded by the IoP and RSC Neutron Scattering Group (NSG) for outstanding work in neutron science, was presented this year to Aleksandra Dabkowska (left) by NSG secretary Katherine Thompson at the Neutron and Muon Science and User Meeting in May. Aleksandra won the award for her studies of drug and gene delivery systems.



Right: Thirty years of neutron production at ISIS was marked by an event for staff, including cake cutting! ISIS Director Robert McGreevy is seen here about to remove part of the ISIS synchrotron!

A year around ISIS



Left: Bryan Jones of the ISIS Synchrotron Group undertook a six-month secondment to CERN working with the PS Booster Operations Group. The Booster is a 50–1400 MeV ring similar to the ISIS synchrotron except that it consists of four vertically stacked rings rather than one. The placement built upon existing collaboration between ISIS and CERN on H^- ion injection. The picture shows Bryan (right) at the injection point of the CERN PS Booster with Klaus Hanke, the PS Booster Operations Section Leader.

Right: Representatives from the China Steel Research Institute visited ISIS in May. They are seen here with Prof Hongbiao Dong (Leicester University, second from left), ISIS Director Robert McGreevy and engineering instrument scientist Shu Yan Zhang.

Below: Engineers from the European Spallation Source visited ISIS in October to meet with ISIS staff and discuss construction of instruments at the ESS.





Above and right: The ISIS Facility Access Panels (FAPs) meet twice per year, in June and December, to review all the proposals which come into the facility. There are seven FAPs covering the range of ISIS science.



Facts *and figures*



In 2014-2015 530 experiments were run and 1854 days were delivered to the user programme. This was across three run cycles, a smaller number than usual as the facility had a planned maintenance shutdown from September 2014 to February 2015. 456 journal papers were published based on ISIS research in the 2014 year.

Facility Access Panels *membership*

ISIS Facility Access Panels (FAPs) meet twice a year to review all proposals submitted to the facility based on scientific merit. The membership for the December 2014 FAP meetings is shown here.

FAP 1	FAP 2	FAP 3	FAP 4	FAP 5	FAP 6	FAP 7
Diffraction	Disordered	Large scale structures	Excitations	Spectroscopy	Muons	Engineering
Claridge, John (Chair)	Hardacre, Chris (Chair)	Barlow, Dave (Chair)	Boothroyd, Andrew (Chair)	Skipper, Neal (Chair)	Paul, Don (Chair)	Bouchard, John (Chair)
Allan, David	Arai, Masa	Bouwman, Wim	Braden, Markus	Andreani, Carla	Alberto, Helena	Davies, Catrin
Arnold, Donna	Bingham, Paul	Edler, Karen	Hayden, Stephen	Bresme, Fernando	Aronson, Meigan	Dye, David
Cussen, Eddie	Bychkov, Eugene	Hase, Thomas	Pappas, Catia	Golunski, Stan	Dilger, Herbert	Francis, John
Hofmann, Michael	Cabrillo, Carlos	Lee, Steve	Ronnow, Henrik	Karlsson, Maths	Giblin, Sean	Holden, Tom
Knee, Chris	Ferlat, Guillaume	Martin, Simon	Shannon, Nic	Krzystyniak, Matthew	Morley, Nicola	Lodini, Alain
Levin, Igor	Holbrey, John	Nylander, Tommy	Stock, Chris	Marques, Maria Paula	Suter, Andreas	Quinta da Fonseca, João
McLaughlin, Abbie	Monaco, Giulio	Prescott, Stuart	Stockert, Oliver	Nogales Ruiz, Aurora	Watanabe, Isao	Stone, Howard
Skinner, Stephen	Hannon, Alex (ISIS Rep)	Scott, David	Ewings, Russell (ISIS Rep)	Sartbaeva, Asel	Hillier, Adrian (ISIS Rep)	Yescas, Miguel
Thompson, Amber	Bowron, Daniel (Secretary)	Titmuss, Simon	Stewart, Ross (Secretary)	Senesi, Roberto	Cottrell, Steve (Secretary)	Zhang, Shu Yan (ISIS Rep)
Vaqueiro-Rodriguez, Paz		Tucker, Ian		Fernandez-Alonso, Felix (ISIS Rep)		Kelleher, Joe (Secretary)
Wood, Ian		Webster, John (ISIS Rep)		Parker, Stewart (Secretary)		
Tucker, Matt (ISIS Rep)		Skoda, Max (Secretary)				
Sparkes, Hazel (Secretary)						

ISIS User Committee Membership December 2013

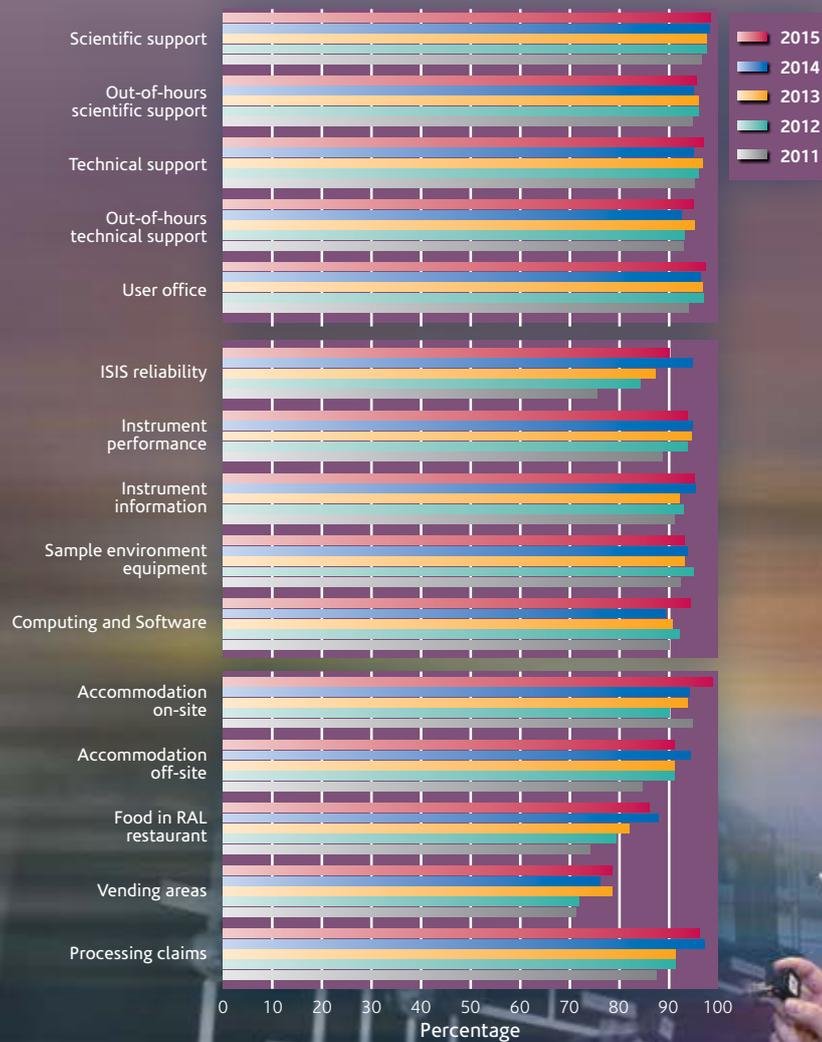
The ISIS User Committee (IUC) represents the user community on all aspects of facility operations. Minutes of IUC meetings are available on the ISIS website.

IUG1 Crystallography	Peter Slater, Birmingham University Anthony Powell, Heriot Watt University
IUG2 Disordered Systems	John Holbrey, Queen's University, Belfast Beau Webber, University of Kent
IUG3 Large Scale Structures	Ali Zarbakhsh, King's College Jeremy Lakey, University of Newcastle upon Tyne
IUG4 Excitations	Jon Goff, Royal Holloway, University of London (CHAIR) Phil Salmon, University of Bath
IUG5 Molecular Spectroscopy	Christoph Salzmann, University College London Silvia McLain, University of Oxford
IUG6 Muons	Don Paul, University of Warwick Alan Drew, Queen Mary College, London
IUG7 Engineering	David Dye, Imperial College, London Michael Preuss, University of Manchester Hongbiao Dong, Leicester

User satisfaction

All users visiting the facility are asked to complete a satisfaction survey which addresses scientific, technical and administrative aspects of their experience in using ISIS. This feedback helps to ensure a high quality service is maintained and improved where possible.

ISIS user satisfaction 2011- 2015



Sabrine Gaertner, Olivia Auriacombe (Open University) using Nimrod to study structural changes in amorphous solid water on heating.



Beam statistics 2014-15

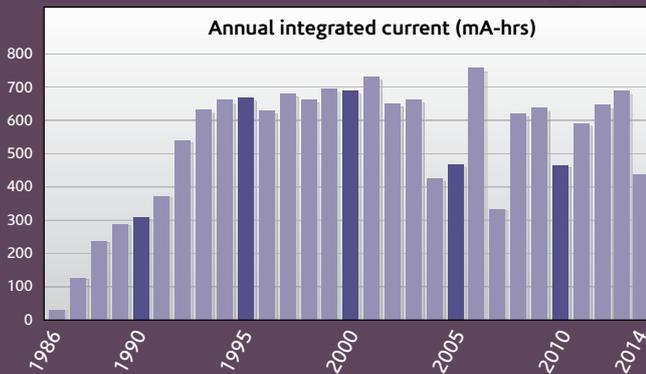
ISIS ran for three cycles in the 14/15 year, and had a planned six-month shutdown in the middle of the year for extended work on the first target station proton beam, reflector on the second target station, muon beamline upgrade and other work. Over the three operational cycles, ISIS delivered 448 mA-hrs of beam to the neutron and muon targets.

Cycle	14/1	14/2	14/3 (part)
	6 May – 27 Jun 2014	15 Jul – 28 Aug 2014	17 Mar – 31 Mar 2015
Beam on target (hr)	1068	777	323
Total beam current delivery for both targets (mA-hr)	222	160	66
Averaged combined beam current per hour (μA)	188	187	184
Peak beam current over 24 hrs (μA)	211	214	214

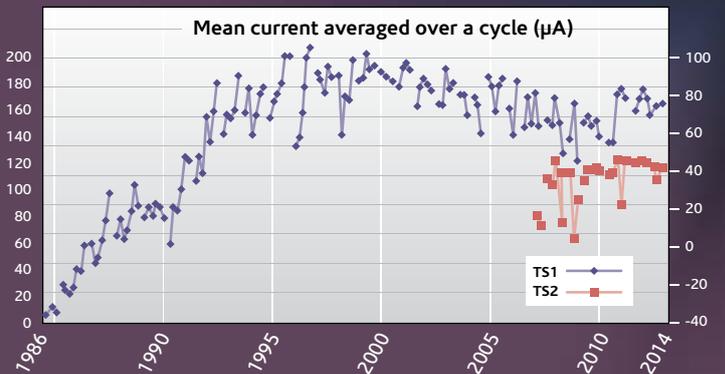
ISIS operational statistics for year 2014-2015.

Year	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014
Total integrated current (mA-hr)	409	445	738	317	612	630	459	583	642	694	448
Average beam current (μA)	177	178	179	176	177	208	197	194	203	206	207

Year-on-year ISIS performance summary for the past 10 years. 2004, 2007, 2010 and 2014 were years which included a long shut-down.



ISIS annual integrated current (mAHrs).



ISIS mean current averaged over a cycle (μA).



Joel Barker (Warwick) preparing a centre stick for studies of superconductivity in Ti_xV_{1-x} alloys on Musr.

Other Statistics

The 14/15 year included a long shutdown from September 2014 to February 2015 to allow significant work to be done within the facility. Hence the number of reported experiments and days delivered to the use programme is less than in other years.

In the 2014-2015 year:

- 530 experiments were run.
- 1854 days were delivered to the user programme.
- 1716 visits to the facility were made by 1071 individual users, 479 (45%) of which were students.
- Over 39 separate companies were involved in ISIS experiments, from large multi-nationals to small hi-tech start-ups.
- Over 77 individual Research Council grants supported ISIS proposals submitted this year.
- 456 journal publications came out in 2014 based on ISIS research (see end of this review).

ISIS science *as it happens*



Above left: *Xiaozhi Zhan (Institute of High Energy Physics, China) using polarised neutrons on Polref to study thin film magnetic structures.*

Above right: *Giovanni Rossi (Glasgow) studying iron-based Fischer-Tropsch catalysts on Maps.*

Below: *Laura Stimpson (Kent) during her HRPD structural studies of multiferroic materials.*

Right: Peter Newton, Razan Aboljadayel, David Love (Cambridge) determining the induced magnetism in graphene by high-angle polarised neutron reflectivity on Polref.

Right: Edmund Cussen (Strathclyde) observing valence bond glass formation in $Ba_{2-x}Sr_xLuMoO_6$

Below: PRick Mengyan (Texas Tech University) using Wish to investigate the low temperature magnetic structure in vanadium dioxide compounds.



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