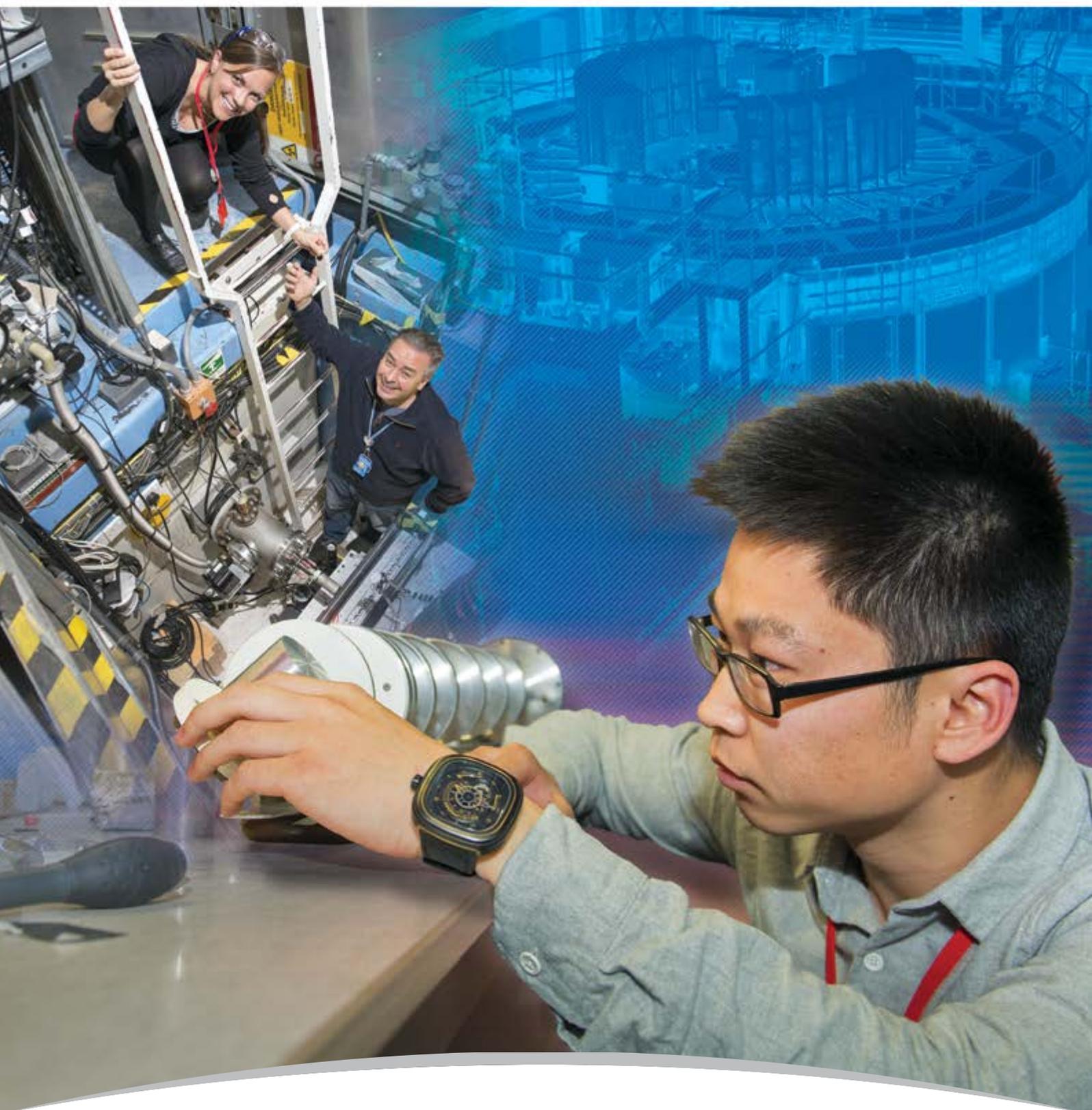


ISIS Neutron and Muon Source Annual Review 2016



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Professor Robert McGreevy, Director of ISIS, explains how ISIS operates to Mr Jiang Sunan, Chinese Embassy, during a visit to the facility.



Above: Members of the Dongguan Government visited ISIS.

Left: Dr Corrado Spinella, Director of the Department of Physics and Technology of Matter at the Consiglio Nazionale delle Ricerche (CNR) at the inauguration of the new IMAT instrument, October 2016.

Foreword

2016 has been an eventful year - for ISIS that is! In FY15/16 we delivered more protons to the targets than ever before, operated more instruments, provided more instrument days to users, who produced more publications. It's actually the first year that we have effectively exploited the investment in TS2, since the start of TS2 operation was accompanied by a reduction in ISIS operating days so our net number of instrument days didn't increase. International collaborations continue to flourish; a new agreement with India has recently been signed. This external funding, including UK Newton funding, benefits both our partners and UK users by enabling the expanded level of ISIS operation.

But these achievements are not enough – we need to continue to make the case for support for ISIS operation and development. A study of the economic impact of ISIS over the first 30 years of operation has recently been produced which provides an important part of the argument. It is very difficult to quantify the impact of more than 95% of the work carried out, which contributes to general scientific knowledge and skills. But even considering only 5% the return on investment is very healthy. In addition the UK still has a capital asset (ISIS) worth over £0.5B and, equally valuable, the skills base in both the facility itself and the user community to exploit it. Indeed, the UK has such a long tradition of operating facilities for an external user community that we tend to take this for granted.

Of course 2016 has been eventful in other ways. Fortunately (or unfortunately?), we are not very exposed to the future possible direct loss of EU funding, with the EU access programme having finished. But science, particularly in our type of work, is intrinsically international. We benefit enormously from the exchange of people and ideas, and also from the mixing of cultures. Whether inside or outside the EU we have to make sure we do not lose this.

Prof Robert McGreevy
Director, ISIS Neutron and Muon Source

Above: South West MEP for the Labour Party, Clare Moody is photographed during her visit to ISIS in February.

Above: German delegates attending a UK/ German Bilateral Information Exchange Meeting are pictured in the TS2 foyer with hosts Professor Robert McGreevy and Grahame Blair.

Below: The Indian Minister for Science and Technology and Earth Sciences, Dr Harsh Vardhan exchanges gifts with ISIS Director, Professor Robert McGreevy following a visit to ISIS.

ISIS – *past impact to future possibilities*

2016 sees the publication of the ISIS impact study, showcasing the social and economic impact of 30 years of facility operation. The report from economist company Technopolis looked at a range of metrics, from the economic benefits of applied research, to technological innovation and the wide ranging training opportunities the facility provides.

The study concluded *“ISIS has delivered a healthy return on investment of at least 214% ... supporting the understanding that publicly funded research and innovation is a key way to drive economic growth.”* It is clear that the facility, over its lifetime so far, has produced significant science achievements, generated real economic benefits, and created a wide variety of training for early-career researchers. But we can't rest on our laurels, and ISIS plans an ambitious programme of development to extend the life of the source for many years into the future. Specific instrument projects underway at present, to produce new science in key areas, are described in the Instruments and Techniques section from p28. Beyond these, plans to upgrade the first target station, replace key linear accelerator components and, ultimately, consider a complete facility upgrade, are all progressing.

Replacement of Linac tank 4

The ISIS linear accelerator (linac) consists of 4 radiofrequency (RF) accelerating tanks, accelerating hydrogen ions generated in the ion source to 37% of the speed of light before feeding them into the synchrotron for final acceleration. Tanks 1 and 4 were built at RAL in 1976, for ISIS' predecessor, Nimrod. They are now showing their age, so a project is underway to replace tank 4.

To demonstrate the principle of the new tank, a 1/6th length test piece has been fully assembled and fitted with 5 successfully aligned drift tubes. Under vacuum, this tank has provided excellent results for both its resonant frequency and field profile along its length. The final stages of preparation for full power testing with high power amplifiers, modulator room and ancillary equipment are near completion, with tests expected to get underway later in the year.



The First Target Station (TS1) upgrade project

The TS1 upgrade project is part of ISIS' commitment to ensuring the ongoing sustainability of the facility. It will:

- Secure the future of TS1 and enable it to operate for many more years
- Provide improved flexibility for future target or moderator changes
- Make current operations of the target station easier
- Provide a neutron performance increase, of up to a factor of 2, on some instruments
- Provide confidence in the ongoing operation of TS1 to enable future instrument upgrades
- Improve our knowledge and skills in target station design for future projects.

Further details of the TS1 project are given on page 36.

ISIS-II

ISIS has been studying accelerator upgrades for many years, but at the start of 2016 a new ISIS-II feasibility study was

launched in order to focus on facility upgrades in light of the advent of ESS and new forecast scenarios for neutron provision in Europe. A working group has been set up which consists of ISIS experts on accelerators, targets, neutronics, instrument science, detectors and engineering, in acknowledgement that this must be envisaged as a facility upgrade, not simply an accelerator upgrade. The working group is specifically considering possibilities for:

- A new stand-alone facility
- A facility upgrade which reuses as much existing ISIS infrastructure as possible
- Compact neutron sources.

Multiple day-one target stations, variety of repetition rates, Fixed Field Alternating Gradient (FFAG) accelerator options and muon production are all important topics of discussion. The working group is expected to produce an initial report in time for the ISIS Facility Board at the end of 2016.

Recommendations taken forward would form the basis for R&D and design studies over the next five years, leading to a full Technical Design Report. A new facility could be delivered by around 2030.

“ISIS has delivered a healthy return on investment of at least 214% ... supporting the understanding that publicly funded research and innovation is a key way to drive economic growth.”



Science *and industry*





Science at ISIS spans a wide range of scientific disciplines, from pharmacology, cultural heritage and engineering to chemistry, magnetism and bioscience. The facility is used by over 2000 scientists a year from both industry and academia. This section gives a snapshot of ISIS research from some of these areas.

Industrial science

ISIS has long-established industrial links with more than 100 companies including household names such as Rolls-Royce, Unilever, Airbus and BP. Over the past 30 years, UK and global industries have benefitted from ISIS, developing a wide range of products including catalysts, aeroplane components, shampoos and lubricants.

Companies can come in through three routes – through partnerships with academia, direct payment for beamtime, and the ISIS Collaborative R&D programme (ICRD). In the 2015/2016 year 10 companies have come in through the ICRD route, 6 through the commercial route and over 50 through the academic route.

Syngenta and Crop Protection

Farmers are facing multiple challenges when it comes to the use of pesticides to protect their crops, such as the increasing levels of resistance developing in weeds, pests and diseases. In order to design more effective formulations in the future, scientists must first determine the mechanism pesticides use to get inside by crossing a plant's defence system, a waxy cuticle.

In a project supported by Syngenta, scientists from the University of Manchester have created a model of a leaf's waxy surface, similar to those found in wheat crops. The team are using reflectometry on INTER to study how surfactants from pesticide formulations modify the wax cuticle model to cross the barrier into the leaf.

Dr Gordon Bell, a senior scientist at Syngenta said: "This research has furthered our understanding of the kinetics of plant uptake. It has shown that water can penetrate into leaf wax. This simple observation explains a lot of the basic science behind pesticide uptake into plants."

Borgwarner

Reducing emissions from commercial vehicles without compromising performance

Global efforts to reduce greenhouse gases are essential to protect our planet for future generations. While politicians set increasingly stringent targets it is up to scientists to find innovative ways to control and reduce these emissions. Borgwarner produce turbochargers for use in commercial vehicles, such as trucks and buses. To meet EU legislation Borgwarner need to redesign their turbine housing so that it can operate at higher temperatures without reducing performance. A collaboration involving scientists from Borgwarner, the University of Huddersfield and the ILL have been using Engin-X to measure stresses and strains in turbine housings to enable a better understanding of fatigue.

Heavy duty commercial turbochargers now need to withstand temperatures up to 760°C, without succumbing to fatigue. The susceptibility of components to residual stresses and strains is largely

determined in the manufacturing process. In turbochargers compressive stress within the housing can be beneficial in preventing fatigue crack propagation, while tensile stresses could potentially combine with operational stress and cause the component to fail, it is therefore important to understand how residual stresses are distributed within the turbine housing.

Katy Gannon from Borgwarner says, "The fatigue strength of the turbine housing is an important consideration when determining the lifespan of the turbocharger. Neutron diffraction is the only means to measure strain deep within the turbine housing in areas prone to fatigue. By combining measurements from Engin-X with simulation data we've shown the technique is useful for complex geometries. We are now looking at building up a complete picture of the housing in different points in its operational life."



Bioscience

Filling in the gaps: *a better understanding of dental cement durability*

Authors: AR Benetti (University of Copenhagen); J Jacobsen (University of Copenhagen and ESS AB); B Lehnhoff, NCR Momsen, DV Okhrimenko (University of Copenhagen); MTF Telling (ISIS); N Kardjilov (HZB); M Strobl (ESS AB); T Seydel (ILL); I Manke (HZB); HN Bordallo (University of Copenhagen and ESS AB).

Instrument(s): Iris; ILL; HZB

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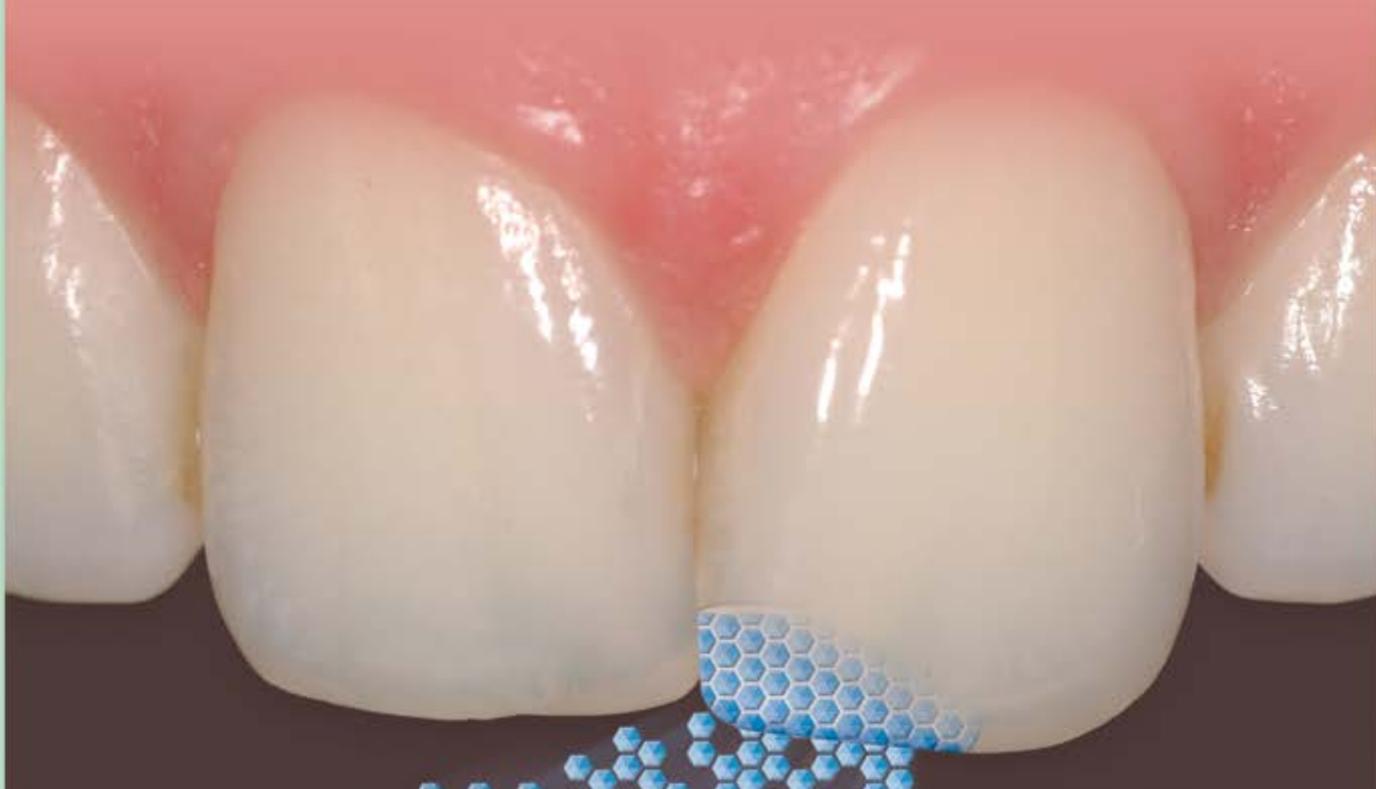
Support: Niels Bohr Institute, University of Copenhagen; ESS AB; DANSCATT.

Further reading: AR Benetti et al., Sci. Rep. 5 (2015) 8972-8979.

Glass ionomer cements offer a number of desirable properties as alternative materials to amalgams for dental restorations: the release of fluoride; a thermal expansion coefficient similar to that of teeth; chemical bonding to both enamel and dentin. Despite these advantages, and the significant developments in these materials during the past decades, their limited strength restricts clinical application. Neutrons were used to gain a better insight into the structure and hydration process of two glass ionomer cements. Neutron spectroscopy demonstrated slowing hydrogen mobility within the cements during

the first days of setting. Furthermore, neutron and X-ray imaging unveiled a complex and evolving pore structure during cement maturation in restorations placed on extracted teeth. Taken together, both hydrogen bonding and the transformation of the cements' microstructure were shown to be important contributing factors with regard to the performance of these restorative materials. We foresee application of this work to further research and advances in glass ionomer cements.

Understanding the microstructure and liquid mobility within dental cements may help future improvements.



Neutron scattering study of solution used for fish embryo cryopreservation

Authors: O Kirichek, AK Soper (ISIS); B Dzyuba (University of South Bohemia); WV Holt (University of Sheffield).

Instrument(s): Sandals

Contact: Prof Alan Soper, alan.soper@stfc.ac.uk.

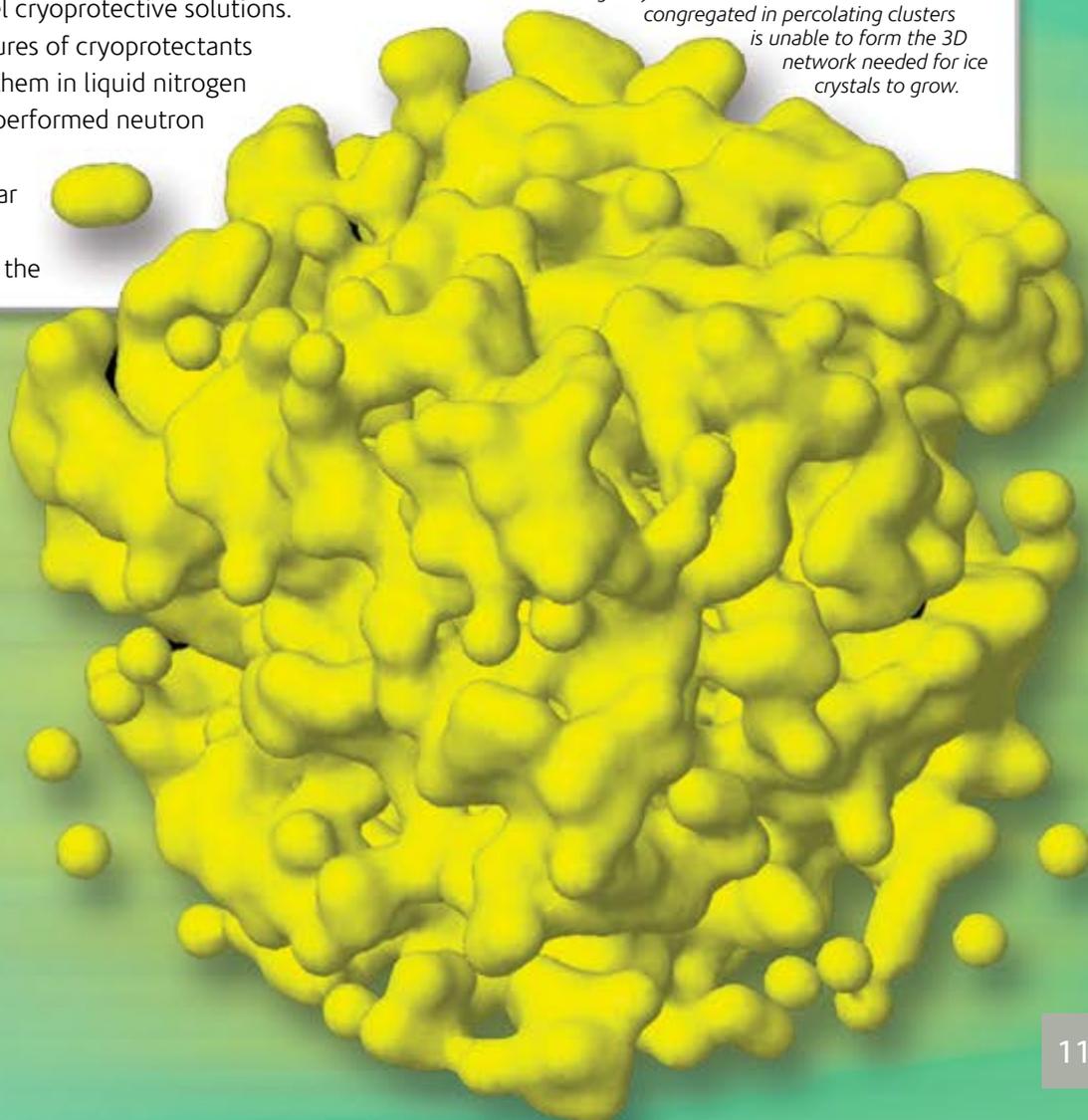
Support: Ministry of Education, Youth and Sports of the Czech Republic.

Further reading: O Kirichek et al., R. Soc. Open Sci. 3 (2016) 150655.

Development of new cryopreservation strategies has major potential in medicine and agriculture, and is critical to the conservation of endangered species that currently cannot be preserved. An essential property of any potential cryopreservative solution is its ability to prevent cell-damaging ice formation during cooling and subsequent heating. Our study focuses on the freezing behaviour of promising model cryoprotective solutions. We took three different mixtures of cryoprotectants in water and quench cooled them in liquid nitrogen to 77 K in seconds. We then performed neutron diffraction experiments using Sandals to study the molecular structure of each mixture after freezing. We found that the

water in the solution forms nano-clusters encapsulated by the surrounding matrix of cryoprotectant solute molecules. We suggest that these small volumes inhibit ice formation because water does not have space for the structural relaxation required to form ice crystals on the short timescale of the quench cooling process.

EPSR simulation box showing only water molecules. The water congregated in percolating clusters is unable to form the 3D network needed for ice crystals to grow.



Catalysis and synthesis

Lowering the barrier to polymerisation

Authors: WG Marshall (ISIS); AJ Urquhart (Technical University of Denmark); IDH Oswald (University of Strathclyde).

Instrument(s): Pearl

Contact: Dr IDH Oswald, iain.oswald@strath.ac.uk.

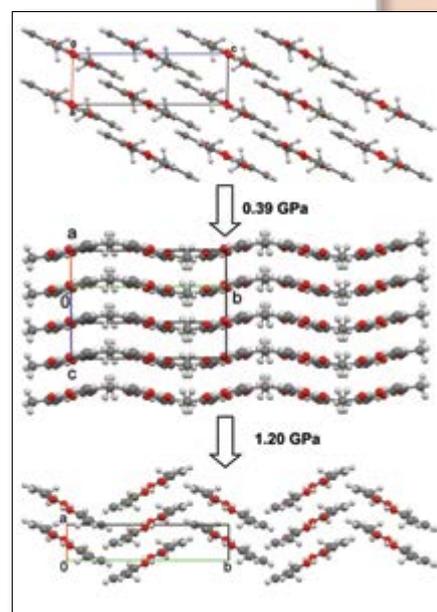
Support: Leverhulme Trust (RPG-2012-598).

Further reading: WG Marshall et al., J. Phys. Chem. B. 119 (36) (2015) 12147-12154.

Polymerisation is a significant manufacturing process that plays a vital role across many disciplines. The structure of a polymer can drastically change the macroscopic properties of the polymer, either via the percentage of crystalline versus amorphous polymer present or via a change in the structure of the polymer backbone. In this paper, we explored the use of pressure to initiate the polymerisation process in the solid state, rather than a more traditional solution-based polymerisation, to understand whether we can have more control over the polymer formed. By using the pressure route we found that we were able to initiate the polymerisation of methacrylic acid, but not before observing changes in the solid-state

structure into three different polymorphic forms. The solid-state transformations are key as the relative orientations of the molecules are locked in position for each polymorph and hence may produce different backbone architectures. In this case, we believe that we created a syndiotactic polymethacrylic acid polymer similar to one created through the use of 10 MRad of Co-60 γ -radiation.

Transformation of methacrylic acid on compression towards a polymer product.



The reaction of formic acid with Raney copper: a cautionary tale

Authors: SK Callear, SF Parker (ISIS); IP Silverwood, A Chutia, CRA Catlow (UCL and UK Catalysis Hub).

Instrument(s): Tosca; Sandals

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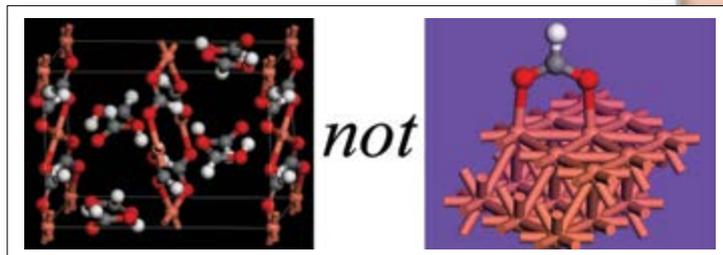
Support: EPSRC (EP/K014706/1, EP/K014668/1, EP/K014854/1, EP/K014714/1 and EP/M013219/1).

Further reading: SK Callear et al., Proceedings of the Royal Society A. 472 (2016) 20160126.

The interaction of formic acid with Raney copper proves to be complex. Previous experience and computational studies had lead us to expect that the reaction between formic acid and Raney copper – a spongy, high surface area form of copper metal – would generate a monolayer of adsorbed formate on the surface. Surprisingly, we found that the reaction goes beyond this state to produce a copper formate compound. This process occurs by direct reaction of copper and formic acid; in contrast, previous methods are by solution reaction. This is a rare example of formic acid acting as an oxidant rather than, as more commonly found, a reductant. The combination

of diffraction on Sandals, spectroscopy on Tosca and computational methods has allowed this unexpected process to be characterised.

Reaction of formic acid with Raney copper unexpectedly produces a compound (left) rather than a surface species (right).



Green chemistry: the conversion of sawdust into liquid fuels

Authors: Q Xia, Z Chen, Y Shao, X Gong, H Wang, X Liu, Y Wang (East China University of Science and Technology); SF Parker (ISIS); X Han, S Yang (University of Manchester).

Instrument(s): Tosca

Contact: Dr S Yang, sihai.yang@manchester.ac.uk

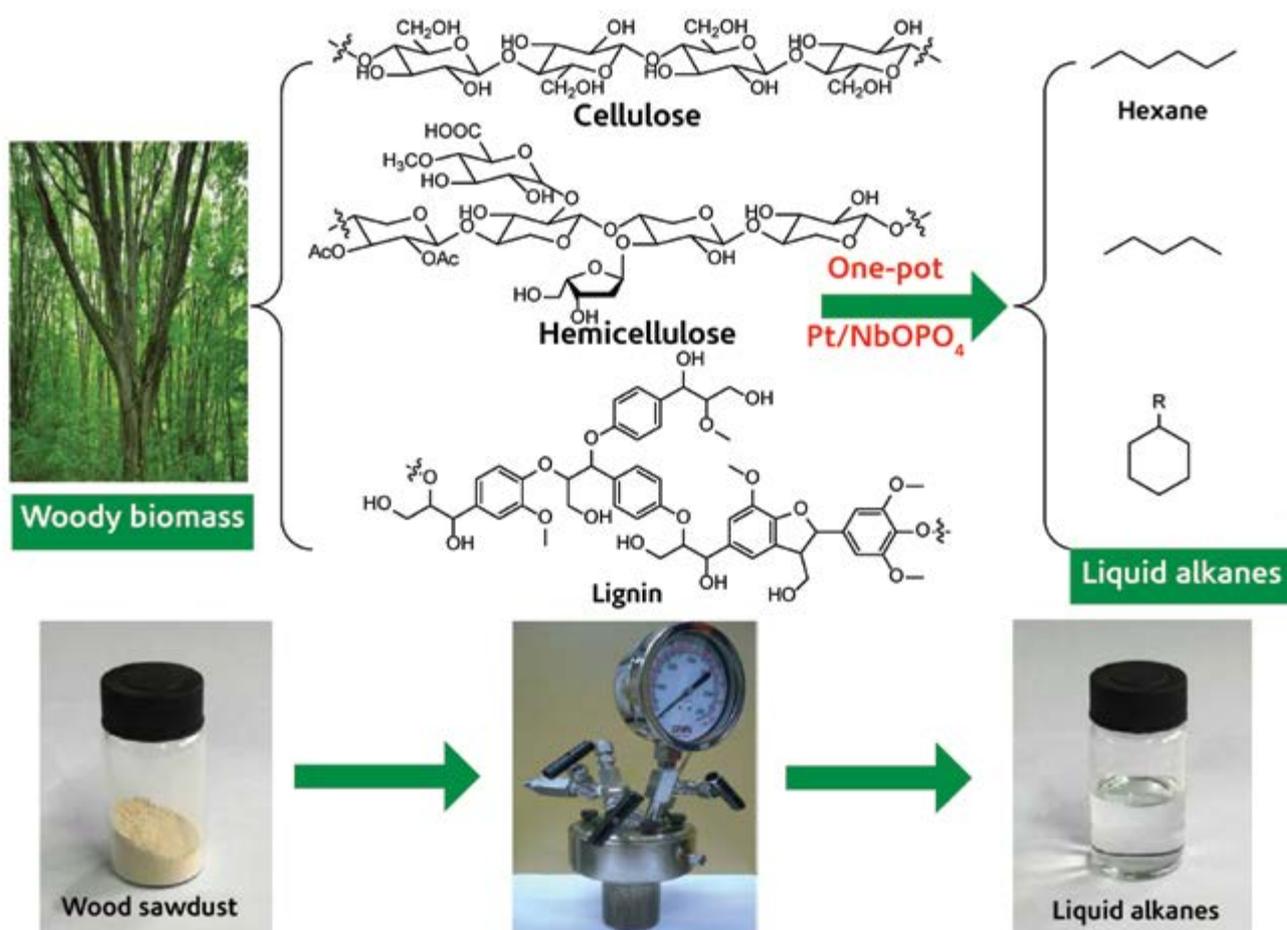
Support: National Natural Science Foundation of China; Shanghai Rising-Star Program; University of Manchester; STFC.

Further reading: Q Xia et al., Nature Communications 7 (2016) 11162.

Practicable, economic methods for the conversion of biomass into value-added chemicals are urgently needed in order to reduce our reliance on fossil fuels. Biomass typically requires complex separations into individual components in order to prepare for their further upgrading. Lignin comprises up to 30 wt% of woody sawdust but is usually discarded because it is very unreactive. A joint UK-China project has developed a new catalyst that is able to convert more than half

of the carbon present in raw wood sawdust into liquid fuels. This is done without the need for chemical pre-treatment or separations, and in an energy-efficient one-pot process. Inelastic neutron spectroscopy on Tosca combined with theoretical calculations helped to understand how the new catalyst works on a molecular level.

Schematic representation of direct hydrodeoxygenation of raw woody biomass into liquid alkanes.



Energy

Stability of double perovskite fuel cell electrodes under humid atmospheres

Authors: M Bahout, JM Hanlon, V Dorcet, S Paofai (Université de Rennes 1); SS Pramana, SJ Skinner (Imperial College London); R Smith (ISIS).

Instrument(s): Polaris

Contact: Dr M Bahout, mona.bahout@univ-rennes1.fr; Prof. SJ Skinner, s.skinner@imperial.ac.uk

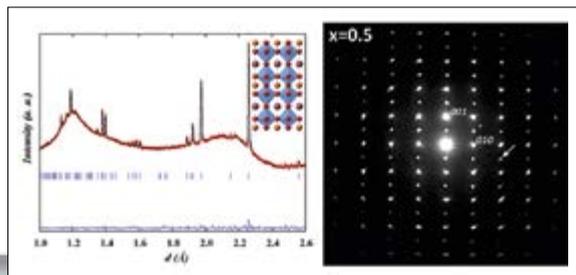
Support: ANR; King Abdullah University of Science & Technology, Saudi Arabia.

Further reading: M Bahout et al., J. Mater. Chem. A 3 (2016) 15420.

Solid oxide fuel cells provide a route to low carbon energy. The electrodes are key components of the cells and operate in a demanding high temperature environment, where temperatures exceed 600°C. Under operation these oxide electrodes, typically of the perovskite, ABO_3 (A = Lanthanide, B = Transition metal) type, must remain stable whilst continuing to conduct both electrons and ions. Efficiency and lifetime of the fuel cell therefore depend on the demonstrated stability of the functional electrode. In this *in-situ* powder diffraction study, we investigated double perovskite cathodes, $NdBaCo_{2-x}Mn_xO_{5+\delta}$ ($x = 0, 0.5$) focussing on stability and phase transitions under humid atmospheres typical of proton conducting cell operation, using D_2O to maintain a 'wet' atmosphere. The work highlights that

in these double perovskites there are competing low temperature processes (oxygen vacancy ordering and oxygen incorporation) but that the phase at elevated temperatures remains stable. No proton incorporation was identified under high steam concentrations, in contrast to what has been stated in the literature.

Electron and neutron diffraction data highlighting the oxygen vacancy order-disorder transition with crystal structure showing ion conduction channels.



Impact of nanostructuring on phase behaviour: hydrogenation kinetics of a magnesium film

Authors: LJ Bannenberg, H Schreuders, L van Eijck, JR Heringa (TU Delft); NJ Steinke, R Dalgliesh (ISIS); B Dam, FM Mulder, AA van Well (TU Delft).

Instrument(s): Offspec

Contact: LJ Bannenberg, l.j.bannenberg@tudelft.nl.

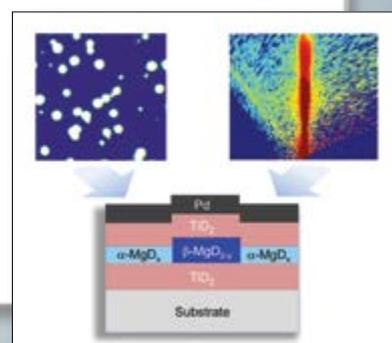
Support: Delft University of Technology.

Further reading: LJ Bannenberg et al., J. Phys. Chem. C 120 (2016) 10185.

Nanostructuring is widely applied in both battery and hydrogen materials to improve the performance of these materials as energy carriers. It changes the diffusion length as well as the thermodynamics of materials. We studied the impact of nanostructuring on the hydrogenation in a model system consisting of a thin film of magnesium sandwiched between two titanium layers and capped with palladium. While we verified optically the coexistence of the metallic α - MgD_x and the insulating β - MgD_{2-y} phase, neutron reflectometry showed significant deviations from the thermodynamic solubility limits in bulk magnesium during the phase

transformation. This suggests that the kinetics of the phase transformation in nanostructured battery and hydrogen storage systems is enhanced not only as a result of the reduced length scale but also due to the increased solubility in the parent phases.

Top-view optical-transmission of the film during hydrogenation showing the two magnesium phases, typical (off-)specular neutron reflection data, and cartoon that illustrates the hydrogenation kinetics.



Molecular lithium hydride formation in $\text{Li}_{12}\text{C}_{60}$ studied by muons

Authors: M Gaboardi, G Magnani, D Pontiroli, M Riccò (Università degli Studi di Parma, Italy); C Cavallari (Università degli Studi di Parma, Italy and ILL); S Rols (ILL).

Instrument(s): Argus; IN4C (ILL)

Contact: Dr M Gaboardi, mattia.gaboardi@stfc.ac.uk,

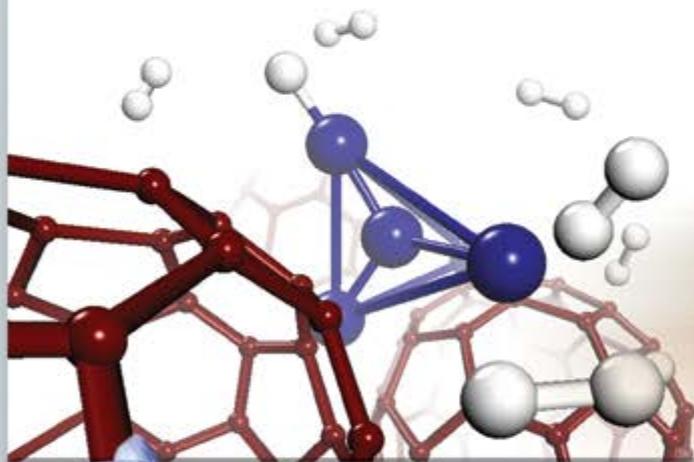
Support: EU FP7, NMI3-II (283883); Cariplo Foundation (2013-0592).

Further reading: M Gaboardi et al., Carbon 90 (2015) 130-137.

Current research on hydrogen absorbing materials may improve the future energy economy, as hydrogen is a green and abundant energy material. Fullerene C_{60} , a spherical shaped molecule entirely made of carbon, turned out to be an interesting hydrogen absorber, especially when intercalated by alkali metals, such as sodium and lithium, forming charge-transfer salts (fullerides).

Muons proved to be essential to the discovery of the key behind the hydrogenation mechanism in $\text{Li}_{12}\text{C}_{60}$ fulleride. In fact, muons easily form hydrogen-like atoms, allowing us to study individually the most stable species formed in a material. Although hydrogen is chemically absorbed on C_{60} , the intercalated lithium is able to dissociate the hydrogen molecules, forming stable Li-H covalent species. We observed this for the first time in a solid.

Hydrogen molecules (white) diffusing in $\text{Li}_{12}\text{C}_{60}$ (brown) and forming Li-H covalent bonds with Li (blue).



Heritage

Texture analysis of Napoleonic war era copper bolts

Authors: F Malamud (Centro Atómico Bariloche, Argentina); S Northover, J James (The Open University); P Northover (University of Oxford); J Kelleher (ISIS).

Instrument(s): Engin-X; Zeiss Supra FEG-SEM (The Open University)

Contact: Dr SM Northover, s.m.northover@open.ac.uk

Further reading: F Malamud et al., Appl. Phys. A 122 (2016) 276.

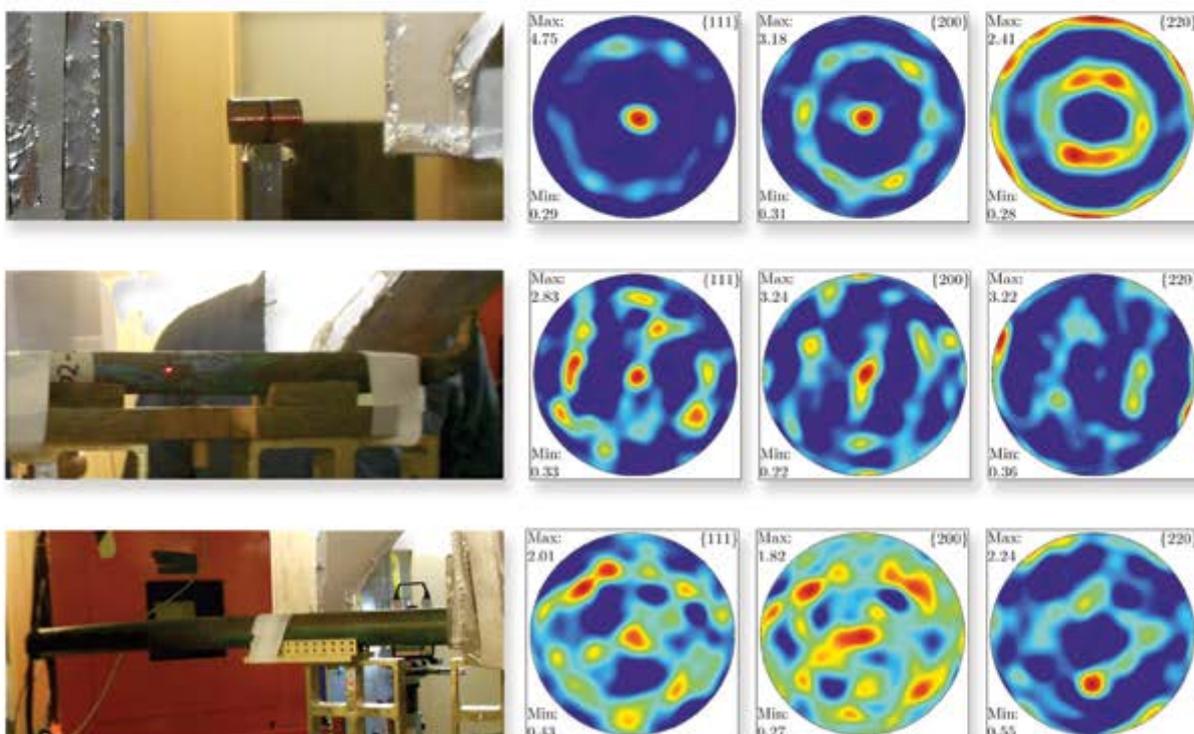
Galvanic corrosion of iron bolts in wooden warships with copper sheathing had brought the Royal Navy to crisis point by 1783, when three British inventors proposed different ways of making hardened copper bolts to replace the iron. William Forbes and John Westwood devised different systems of grooved rolls to cold roll copper to the required diameters, while William Collins' grooved rolls drew the copper through a die. The resulting bolts were identical in appearance and composition but the different processes deformed the copper in different ways, each producing an invisible 'texture' which varies across the bolt. Neutron diffraction is the only non-destructive technique to determine the texture of these bolts (which can be over 1m long) in three dimensions. We examined three bolts from

three dated shipwrecks in the English Channel and identified distinctive textures in each, one of which we could immediately associate with Collins' process. This technique can now help establish the supply chain that led to the dominance of the British navy for half a century.

Copper bolts from the wreck of HMS Pomone in situ on the seabed.



© The Maritime Archaeology Trust



Left: The three copper bolts mounted in Engin-X. Right: The corresponding measured textures.

The secrets of Damascus swords

Authors: D Edge (*The Wallace Collection*); F Grazzi (*CNR*); A Scherillo (*ISIS*); A Williams (*The Wallace Collection*).

Instrument(s): Ines

Contact: Dr A Williams, alan.williams@wallacecollection.org

Support: STFC.

Further reading: F Grazzi et al., *Microchemical Journal* 125 (2016) 273-278.

The most famous swords in medieval history were called 'Damascus' as they were traded there, but made all over India, Persia, and Central Asia. The swords were made of an incredibly hard steel that never needed sharpening, and had a pattern on their surface like "watered silk".

Non-invasive analysis by the Ines diffractometer is helping us to understand how they were made. Swords, daggers and axes from the Wallace Collection in London (the largest collection of Damascus blades in the UK) have been brought to ISIS and analysed. The blades usually have very high carbon contents (up to 1.8%) and their patterns are formed by anisotropic distribution of the iron carbide present.

Even when the passage of time and over-zealous cleaning has hidden their pattern, neutron diffraction will reveal its presence, so the museum can now restore the appearance of these objects to their former glory.

The research team studying the blades of Oriental swords. Clockwise from lower left: Francesco Grazzi (CNR), Alan Williams (Wallace Collection), David Edge (Wallace Collection) and Antonella Scherillo (ISIS).



Magnetism

Magnetism in the most unusual of the iron-based superconductors

Authors: MC Rahn (University of Oxford); RA Ewings (ISIS); SJ Sedlmaier, SJ Clarke, AT Boothroyd (University of Oxford).

Instrument(s): HRPD; Merlin; Mari

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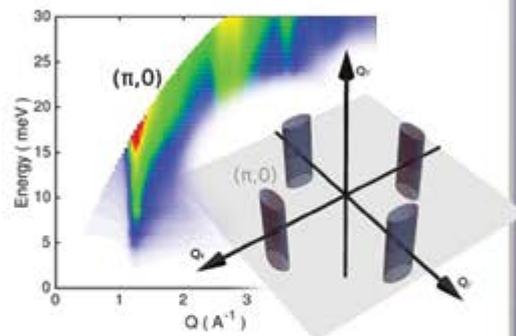
Support: EPSRC; Clarendon Fund of Oxford University.

Further reading: MC Rahn et al., Phys. Rev. B 91 (2015) 180501.

With over 230 publications, the unusual superconductor iron selenide (FeSe) received more attention in 2015 than almost any other single material. FeSe is a misfit among iron-based superconductors. Other members of the family are ordered magnets which require insertion of charged impurities to develop superconductivity, whereas FeSe remains magnetically disordered and becomes superconducting in its pure form. With a modest superconducting transition temperature of $T_c = 8$ K, FeSe does not break any records, but what stands out is the fact that T_c can be raised dramatically when pressure is applied or spacer layers are introduced. Whatever the mechanism of iron-based superconductivity, FeSe seems to sit very close to its trigger. In our study we used ISIS neutrons to excite magnetic fluctuations in FeSe.

We found that the magnetic spectrum has a particular form that is at odds with some theoretical predictions. The results provide specific information on the electronic states in FeSe that is required in models that seek to explain how iron-based superconductors work.

Magnetic fluctuations in FeSe form 'rods' in momentum (Q) space centred on $(\pi, 0)$. These rods appear as vertical streaks in a neutron spectrum from a powder.



Topological magnon bands in a Kagome lattice ferromagnet

Authors: R Chisnell (MIT and NCNR); JS Helton (NCNR); DE Freedman (MIT and Northwestern); DK Singh (University of Missouri); RI Bewley (ISIS); DG Nocera (MIT and Harvard); YS Lee (MIT and Stanford).

Instrument(s): Let; SPINS (NCNR)

Contact: YS Lee, youngsl@stanford.edu.

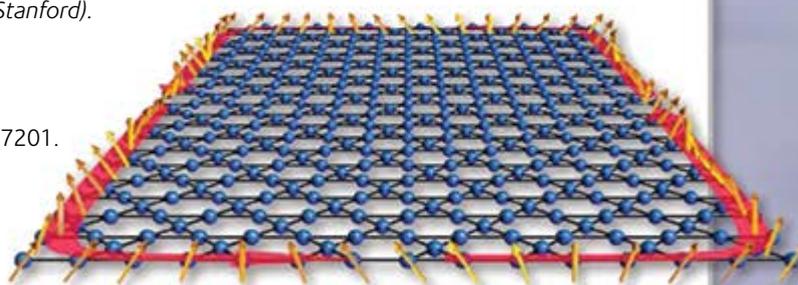
Support: DOE (DE-FG02-07ER46134); NSF (CHE 1041863).

Further reading: R Chisnell et al., Phys. Rev. Lett. 115 (2015) 147201.

Materials with topological properties have novel excitations that exist only on the edge or surface of the material, and which continue to exist even in the presence of defects. Particles in these materials can move in a single direction along the edge of the material even when they cannot move through the bulk.

These materials are of great interest for their possible applications in energy-efficient technologies, high-performance computing and data storage.

In this work, we demonstrate the existence of a new class of topological material called the topological magnon insulator, in which fluctuations of the magnetic moments (called magnons) are the topological particles that propagate along the crystal edge. We used inelastic



Schematic of the topologically protected edge mode. Magnetic fluctuations propagate in a single direction around the edge of the material and are protected from backscattering.

neutron scattering measurements of the metal-organic framework material Cu(1,3-benzenedicarboxylate). We show that the scattering results can be explained by a theory which combines the unique arrangement of magnetic moments in this material with simple interactions between nearest neighbours. This theory also predicts the topological nature and novel behaviour of the magnon particles, which have been confirmed by thermal transport measurements.

A magnetic field induces antiferromagnetism in a metal

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

Instrument(s): Let; Wish

Contact: Prof SM Hayden

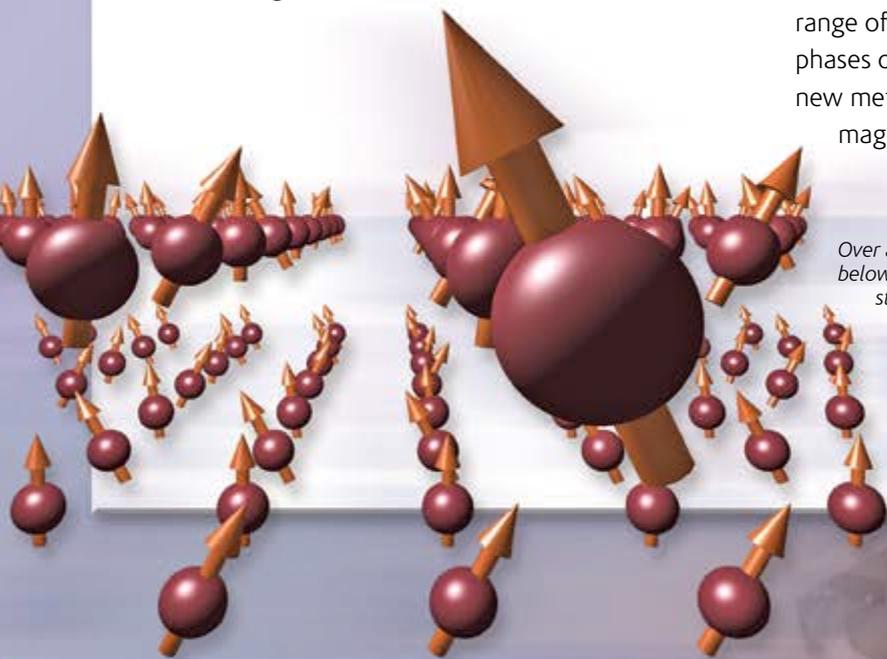
Support: EPSRC.

Further reading: C Lester et al., Nat. Mater. 14 (2015) 373-378.

Magnetic fields usually suppress antiferromagnetism by flipping magnetic moments to be parallel to the field. Here we show that a field can also stabilise antiferromagnetism in a metal where none exists in the absence of a field. We used the Let and Wish spectrometers at ISIS to study the oxide metal $\text{Sr}_3\text{Ru}_2\text{O}_7$. An 8 Tesla magnetic field induced a form of

antiferromagnetism known as a spin density wave at temperatures less than 1 K. The state of the spin density wave can be controlled by rotating the sample with respect to the magnetic field. This leads to large changes in the resistance of the metal. The results have analogies with molecular systems, where phases with broken translation symmetry (e.g. liquid crystals, ice) exist over a range of pressure (instead of field) bounded by isotropic phases of higher symmetry. The results also suggest a new method to control the resistance of a metal in a high magnetic field.

Over a narrow range in magnetic field near 8 T, and at temperatures below 1 K, an incommensurately-modulated spin density wave structure is stabilised in $\text{Sr}_3\text{Ru}_2\text{O}_7$.



Water

Revealing the nature of glass transition in amorphous solid water

Authors: CR Hill, HJ Fraser (The Open University); C Mitterdorfer, T Loerting (University of Innsbruck); TGA Youngs, DT Bowron (ISIS).

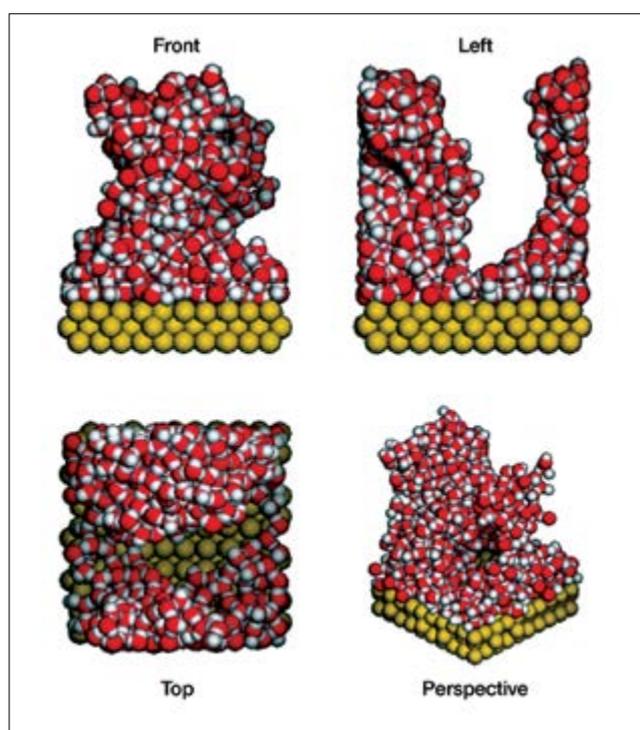
Instrument(s): Nimrod

Contact: Dr HJ Fraser, helen.fraser@open.ac.uk

Support: ESF (MicroDICE); ERC (SULIWA); Austrian Science Fund FWF (I1392); The Open University; EU LASSIE FP7 (238258); STFC (ST/M007790/1, ST/M003051/1, ST/N006488/1, ST/N005775/1 and ST/L000776/1).

Further reading: CR Hill et al., Phys. Rev. Lett. 116 (2016) 215501.

If water vapour is deposited at very low temperatures it turns into highly microporous Amorphous Solid Water (ASW) – the most abundant form of water in the universe. This ASW is disordered similar to liquid water, but with the atoms frozen in place. Using the unique simultaneous Q-range of the Nimrod instrument, we studied the atomistic and the mesoscale structural changes in the porosity of ASW when heated from 80 to 144K. Of particular debate is the nature of the 'glass transition' in ASW. The small-angle scattering reveals the onset of diffusive processes as surface and pore structures change. At 115K water molecules remain fixed, but rotate, up to 121K, where the molecules can move collapsing the porous structure. These changes are complete by 136K, well before 144K where ASW changes to cubic ice. For the first time the glass transition in water was monitored from onset to endpoint, with clear evidence for the molecular motions involved being translational rather than just reorientational.



Snapshot from a simulation where water molecules which are 'dropped' onto the model silica substrate at 20K. The ice is disordered and considerably porous and builds 'skyscrapers' or towers which result in cylindrical-like pores stretching from the bottom to the top of the ice layer.

Quantum tunneling of water in beryl

Authors: Al Kolesnikov, TR Prisk, E Mamontov, A Podlesnyak, G Ehlers, DJ Wesolowski, LM Anovitz (ORNL, USA); GF Reiter (University of Houston); N Choudhury (University of Washington); AG Seel (ISIS).

Instrument(s): Vesuvio; Sequoia; CNCS (SNS, ORNL)

Contact: Dr Al Kolesnikov, kolesnikovai@ornl.gov

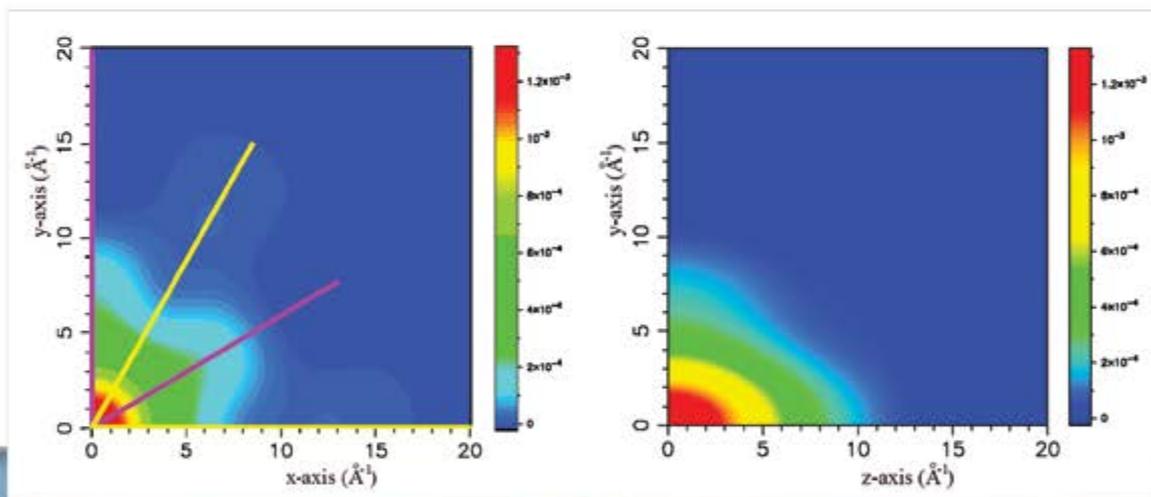
Support: Chemical Sciences, Geosciences, Biosciences and Scientific User Facilities Divisions of BES, DOE

Further reading: Al Kolesnikov et al., Phys. Rev. Lett. 116 (2016) 167802.

Water is commonly known in gas, liquid and solid states. Using neutron scattering, we discovered a new “quantum tunneling state” of the water molecule confined in 5Å channels in the mineral beryl. At low temperatures we observed a number of peaks in the inelastic neutron scattering spectra which were uniquely assigned to water quantum tunneling (quantum motion of water through the separating potential walls, which is forbidden in the classical world). The water proton momentum distribution was measured with deep inelastic neutron scattering (DINS) at ISIS. This directly revealed coherent

delocalisation of the protons (see figure). The average kinetic energy of the water protons, obtained from the DINS, is found to be ~30% less than it is in solid, liquid or vapour state of bulk water. Due to the observation of tunneling peaks and large coherent delocalisation of protons in the neutron scattering experiments, we consider that tunneling water can be called “a new state of the water molecule”.

Projection of water proton momentum distribution $n(p)$ in beryl onto the xy - and yz -planes, (a) and (b) respectively, obtained from the DINS data.



Advanced materials

Emergence of long-range order in BaTiO₃ from local symmetry-breaking distortions

Authors: MS Senn (University of Oxford); DA Keen (ISIS); TCA Lucas, JA Hriljac (University of Birmingham); AL Goodwin (University of Oxford).

Instrument(s): Gem

Contact: Dr Mark Senn, mark.senn@chem.ox.ac.uk

Support: Fellowship from the Royal Commission for the Exhibition of 1851; ERC (279705);

PhD Studentship funding from Diamond Light Source.

Further reading: MS Senn et al., Phys. Rev. Lett. 116 (2016) 207602.

Barium Titanate (BaTiO₃) is often considered the prototypical ferroelectric. In the text book picture, a spontaneous polarisation arises below the ferroelectric transition temperature from off-centre displacements of Ti atoms. This description explains the complicated phase diagram (on cooling) cubic > tetragonal > orthorhombic > rhombohedral, which is said to occur as Ti atoms displace in turn towards a corner, edge and

face of the TiO₆ octahedra. In contrast, diffuse scattering data provide evidence for an order-disorder picture, in which locally Ti atoms are always displaced towards the face of the octahedra, with long range correlations of this disorder giving rise to the observed transitions. However, the presence of these off-centre distortions across all crystallographic phases has never been fully demonstrated. Using total scattering data collected on

Switching the interpenetration of confined asymmetric polymer brushes

Authors: SB Abbott (University of Bristol); WM de Vos (University of Twente); LLE Mears (University of Bristol); M Skoda, R Dalgliesh (ISIS); S Edmondson (University of Manchester); RM Richardson (University of Bristol); SW Prescott (UNSW).

Instrument(s): Inter

Contact: Dr WM de Vos, w.m.devos@utwente.nl

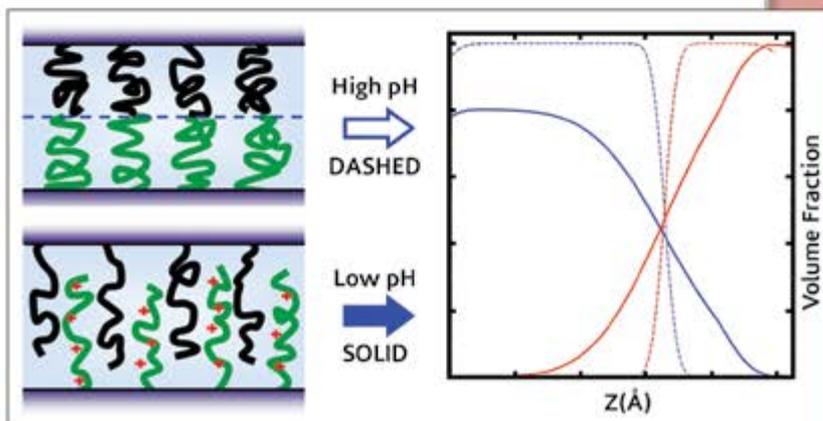
Support: EPSRC (EP/H0148611).

Further reading: SB Abbott et al., Macromolecules 49 (2016) 4349-4357.

The friction between two surfaces can be reduced by orders of magnitude by coating them with either charged or uncharged polymer brushes, a result of the very low interpenetration between confined brushes. Here we use theoretical calculations, alongside a unique combination of neutron reflectivity and a surface force type apparatus, to demonstrate a confined brush system with pH-switchable interpenetration. Polymer brushes with an asymmetric charge on each surface – one neutral and the other weakly charged – are shown to have very rich interpenetration behaviour. At a pH where the weak polyelectrolyte brush is charged, a very high degree of interpenetration is observed as interpenetration allows a dilution of charged groups. However, when the brush becomes uncharged by a switch in pH, a very low

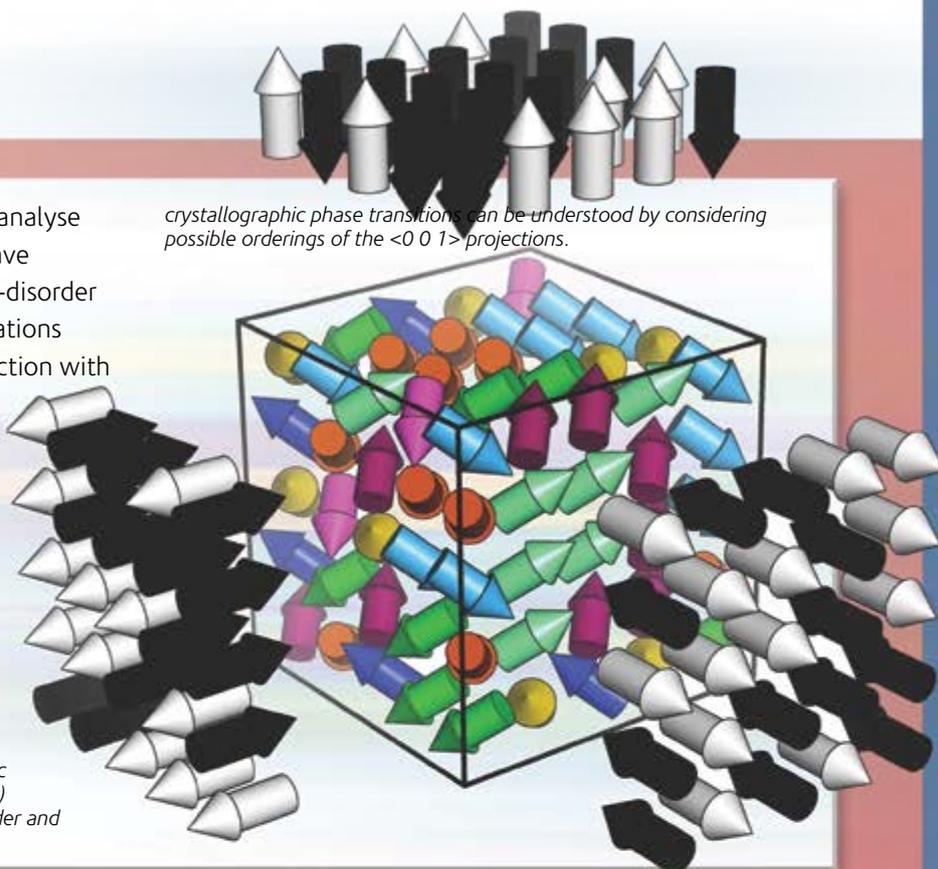
degree of interpenetration is found. These results may lead directly to the design and operation of polymer brushes with pH controllable friction properties.

The interpenetration between two polymer brushes - one neutral and the other weakly charged - can be controlled by a simple change in pH, as depicted.



Gem and a symmetry-motivated approach to analyse the resulting pair distribution functions, we have provided unambiguous evidence for the order-disorder model. Furthermore, our experimental observations allow us to propose a model which, in conjunction with Monte Carlo simulation, reproduces the observed crystallographic phase diagram, thus reconciling the order-disorder and displacive (soft-mode) model in BaTiO_3 . Our results have implications for a large number of other ferroelectrics.

crystallographic phase transitions can be understood by considering possible orderings of the $\langle 001 \rangle$ projections.



A portion of the Monte Carlo simulated model of the cubic phase of BaTiO_3 showing $\langle 001 \rangle$ projections (black/white) of $\langle 111 \rangle$ Ti displacements (colour). The correlated disorder and

Neutrons show the wrinkles in polymer-graphene oxide nanocomposites

Authors: MP Weir, N Clarke, AJ Parnell, RC Savage (University of Sheffield); DW Johnson, SC Boothroyd, RL Thompson, KS Coleman (Durham University); SR Parnell (TU Delft); SM King, SE Rogers (ISIS).

Instrument(s): Sans2d; ID02 (ESRF); BT5 (NCNR)

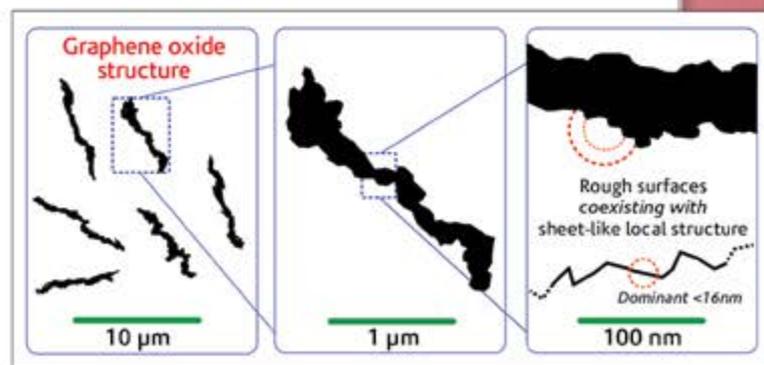
Contact: Dr MP Weir, Weir.MP@gmail.com

Support: EPSRC (EP/K016784/1).

Further reading: MP Weir et al., Chemistry of Materials 28 (6) (2016) 1698-1704. MP Weir et al., ACS Macro Letters 5 (4) (2016) 430-434.

Graphene and related materials are superb candidates to combine with polymers to produce nanocomposites, with strength, electrical conductivity and other properties that far exceed the performance of the pure polymer. However, to make good nanocomposites we must understand the structure of the graphene and polymers when they are mixed. In this study, neutron scattering data from the Sans2d instrument at ISIS helped to show that sheets of graphene oxide in our nanocomposites were extensively wrinkled and folded. A wrinkled piece of graphene is unlikely to be stiff when it is put under strain, and is thus unlikely to add strength to a (relatively) soft polymer. Furthermore, the presence of the graphene oxide sheets distorted the polymer molecules themselves from their normal shape and size. Sans2d showed that polymer chains in the nanocomposites were less

entangled with their neighbours, affecting the plateau modulus (a particular measure of the polymer network's strength), even with as little as 0.5% graphene oxide present.



Schematic diagram describing the structures present on a wide range of length scales in polymer-graphene nanocomposites

Advanced materials

Anomalous depletion of pore-confined CO₂ upon cooling below the bulk triple point

Authors: KL Stefanopoulos, FK Katsaros, TA Steriotis, AA Sapalidis (INN, NCSR "Demokritos", Greece); M Thommes (Quantachrome Instruments, USA); DT Bowron, TGA Youngs (ISIS).

Instrument(s): Nimrod

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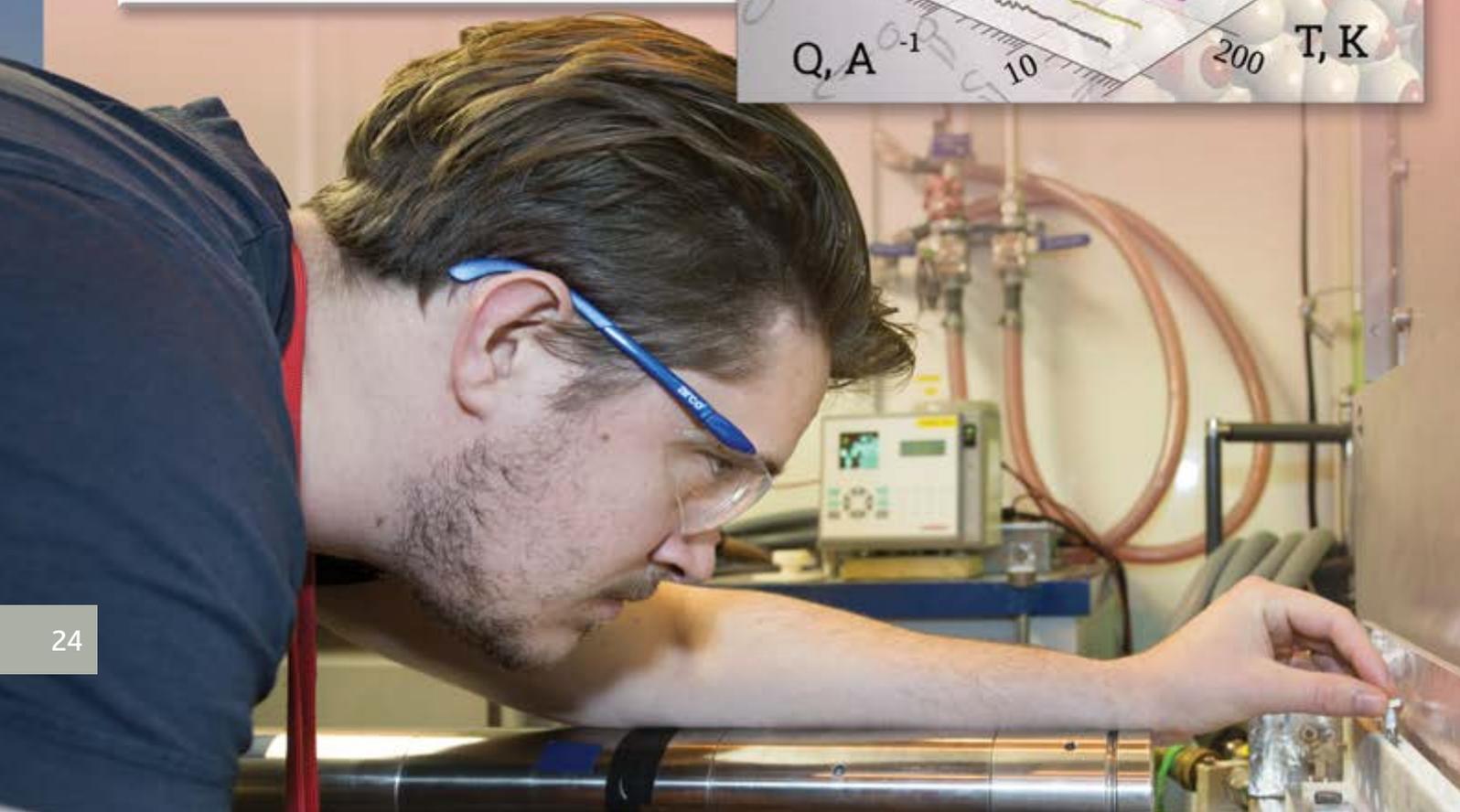
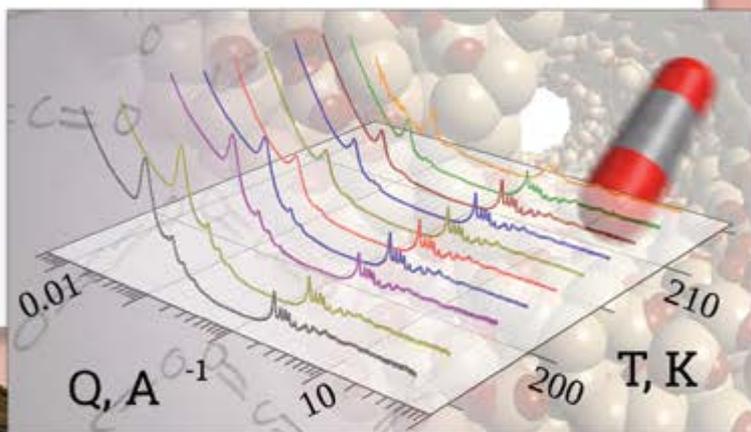
Support: EU FP7, NMI3-II (283883).

Further reading: KL Stefanopoulos et al., Phys. Rev. Lett. 116 (2016) 025502.

In most cases, the behaviour of matter confined in very small pores (width < 50 nm) is quite different from the bulk. Such differences are very important for several processes such as gas and liquid separations, drug release, oil extraction, catalysis, etc. Much like salty and pure water, wetting liquids that are confined in such small capillaries boil at higher and freeze at lower temperatures compared to the bulk. Actually, the common understanding of this phenomenon dictates that the smaller the pore, the larger the boiling point elevation and the freezing point depression. Recent neutron scattering experiments on liquid CO₂ confined in silica pores of around 7 nm revealed that, at least in some cases, freezing may not follow this rule. As a matter of fact, in the case studied, rather than freezing

in the pores, the liquid escaped from the confined space altogether and froze on the outside of the material, leaving the pores empty.

Neutron scattering spectra of porous silica soaked in liquid CO₂ at 216 K (orange curve). As temperature decreases, CO₂ is solidified externally ($Q > 1 \text{ \AA}^{-1}$), while the porous network signal ($0.01 \text{ \AA}^{-1} < Q < 1 \text{ \AA}^{-1}$) increases revealing the pore emptying process.



Magnetism in expanded metals may not be as ordered as thought

Authors: AG Seel (University of Oxford, ISIS); PJ Baker, SP Cottrell (ISIS); CA Howard, NT Skipper (UCL); PP Edwards (Oxford)

Instrument(s): Emu

Contact: Dr AG Seel, andrew.seel@chem.ox.ac.uk

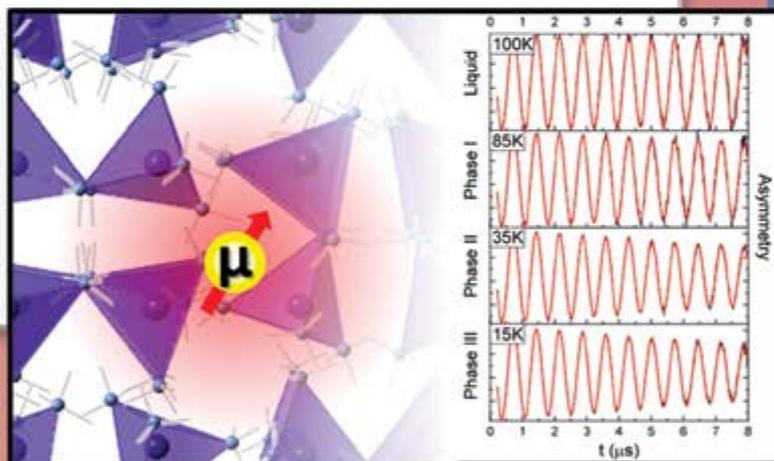
Support: University funding.

Further reading: AG Seel et al., J. Phys. Chem. Lett. 6 (19) (2015) 3966-3970.

Alkali and other electropositive metals are extremely soluble in anhydrous ammonia, leading to a series of liquid expanded metals. These lustrous golden liquids demonstrate conductivities higher than liquid mercury, tuneable through their metal content. Even at their concentration limit, however, the electron densities of these metals are low. $\text{Li}(\text{NH}_3)_4$ is particularly interesting, as upon cooling it forms a highly crystalline metal with a melting point of only 88 K. Three crystalline phases exist below this temperature, each exhibiting different conductivities and magnetic character. Historically, $\text{Li}(\text{NH}_3)_4$ has been considered both metallic and antiferromagnetically ordered below 25 K, but the difficulty in handling these systems and their thermal history complicates investigation of their weak magnetic nature. With the help of the muon and

sample environment groups at ISIS we have been able to determine that this is not the case, bringing magnetic data into alignment with neutron diffraction. Metal-ammonia systems enable us to tune electron densities over a vast range, and muon spin relaxation will aid us in understanding their interactions and correlations.

Zero field and transverse field muon spin relaxation measurements enable us to probe the magnetic state of low electron density metals.



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.

Instruments *and techniques*

IMAT

IMAT is a multi-functional neutron imaging and materials science instrument with options for radiography, tomography, and energy-selective imaging analysis on the one hand, and neutron diffraction applications on the other. IMAT will be available for a diverse range of science areas, ranging from Engineering to Earth Science, Archaeology to Soft Matter and Biomaterials, wherever non-destructive and in-situ testing is required. After significant installation progress this year, IMAT has entered a 'hot' commissioning phase including evaluation of the beam flux and assessment of the performance of the imaging cameras. Demonstration experiments have been completed which show the ability of the instrument to produce images of ancient artefacts non-destructively.

Graduate Engineer Jon Elmer working on the final commissioning of the IMAT robot

IMAT Camera Positioning System Robot

The IMAT camera positioning system robot is an example of how an industrial product can be used in a scientific environment. It is a new concept for neutron data collection on an engineering instrument. The 6 axis ABB precision robot arm and Gudel translation rail is able to provide flexibility in a confined area.

The CPS robot can pick up multiple cameras from the storage shelf and move them into the neutron beam. The camera is then held in the beam for up to 24 hours whilst data is collected. The holding stability of the robot arm is very important and extensive testing has been carried out to prove that any movement is less than the size of one detector pixel.

This project has benefitted from the input of ISIS Design Division mechatronic graduate engineers. Their work has included designing solutions for automatic tool (camera) changing with the vast array of camera electrical connections and programming of robot move trajectories.



Larmor



The Larmor project team

Larmor has now entered routine operation for SANS and polarised SANS. Almost all of the sample environment equipment available on LOQ and SANS2d has been tested and is available for use. Polarisation analysis has been tested and will be routinely available from autumn 2016. A significant number of the components required for the spin echo SANS (SESANS) configuration have now been tested on the beamline by TU Delft and installation is expected to be completed in time for the first run cycle of 2017. SESANS will therefore become available for proposals in the April 2017 proposal round.

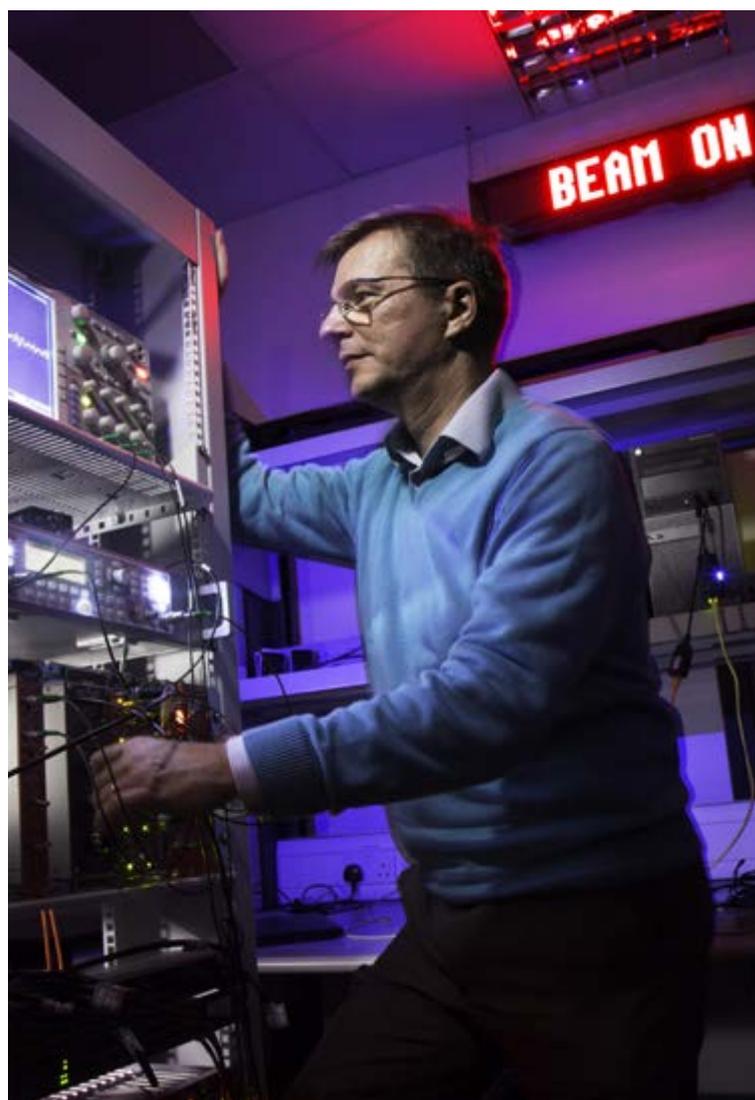
ZOOM



The ZOOM build is progressing rapidly – 4 October 2016.

The build of the small-angle neutron scattering (SANS) beamline Zoom is progressing well with commissioning commencing in early 2017. Along with standard SANS, phase one of this project will provide optional polarisation of the incoming beam through a transmission supermirror and a Drabkin spin flipper. Phase 2 will be the development of a set of neutron optics which will allow the beam to be focussed. Focusing the neutron beam at the detector will increase the accessible Q-range, allowing the study of new science with longer characteristic length scales.

Chiplr



Chris Frost (ISIS) preparing for an experiment on the new ChiPlr instrument.

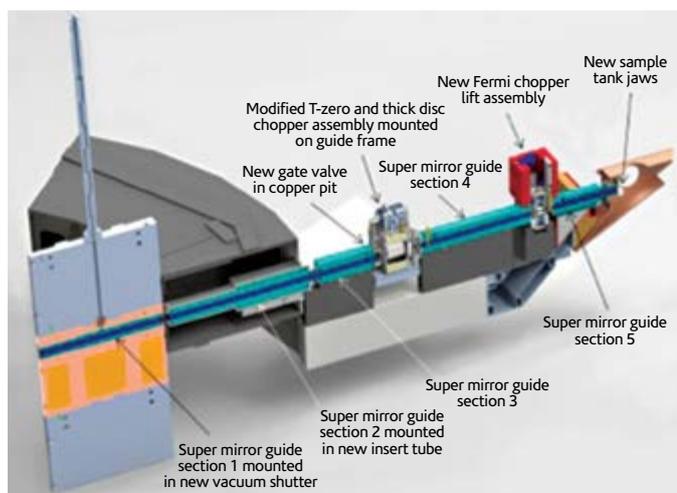
Changing a '1' to a '0' in a binary bit in one of the 250,000 binary numbers stored in a random access memory is exactly the kind of problem that naturally occurring atmospheric neutrons create in electronic and avionic systems. In June 2016 this was being achieved several times a minute on ChiPlr, showing that the intensity of its fast neutron spectrum had not just met but exceeded the design specification. About one hour on ChiPlr is now equivalent to many hundreds of years in the real environment, enabling the instrument to provide extensive accelerated testing of electronic devices.

The test of these SRAM memories was part of the ongoing commissioning of ChiPlr's fast, mega-electron volt, neutron beam where the ChiPlr team have been focused on fully characterising the flux, size and profile of the beam, preparing for full operation.

MARI upgrade

MARI will undertake a significant upgrade in 2017 to install $m=3$ supermirror neutron guides. The instrument is now over 25 years old but its unique capability for certain science problems remains unmatched even at the new generation of spallation sources – particularly in the area of wide-angle lattice and molecular dynamics measurements on polycrystalline and amorphous materials. The upgrade will increase the thermal neutron flux by a factor of 10 and by a factor of up to 20 at lower energies, bringing the flux on MARI into line with modern direct time-of-flight spectrometers. The design of the new layout of the instrument for the guides and the shielding is completed with manufacturing beginning in September 2016. A new disk chopper will also be installed to enable data collection with simultaneous multiple incident energies using the well-established repetition rate multiplication mode.

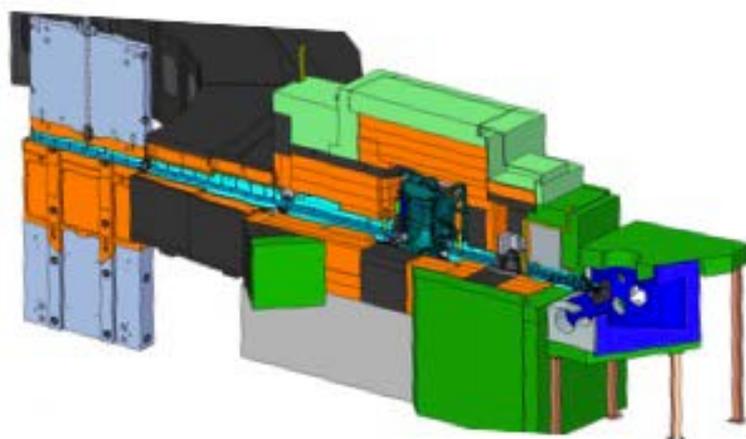
To minimise the downtime of the instrument and of ISIS TS-1 we expect to start the installation together with the new MAPS guide during the TS-1 shutdown in June 2017.



Schematic of the MARI guide upgrade project

MAPS upgrade

The project to install a neutron guide on MAPS has made good progress this year. All of the components have been delivered to ISIS; of particular note is the $m=3$ neutron guide, which was manufactured by Mirrotron. Notable features are the use of thin (3mm thick) glass substrates so that MAPS can continue to utilise high-energy neutrons without significant increase in background / spurious counts; electronic inclinometers mounted on the reverse side of the glass to allow in-situ monitoring of alignment throughout the lifetime of the guide; and a novel mechanism for clamping the guide in position with B4C bars, thus combining shielding with the alignment mechanism.



Schematic view of the MAPS guide, with new shielding elements shown in orange and the guide system shown in light blue.

Installation will take place in Summer 2017, and is expected to take until November 2017. Thereafter technical and scientific commissioning will take place and the instrument will re-enter the user programme in 2018.

TOSCA upgrade



The provision of a high- m guide on TOSCA will significantly enhance the flux available on the instrument across whole energy range and in particular between 10-50 meV by 21 times, 50-100 meV by 12 times, and 100-200 meV by 8 times. 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. Work on the installation of the new guide started at the end of May 2016, and the first stage (work near the target station) has been completed. Further guide sections will be installed in late 2016, with the final shutter section being installed in December. The instrument will return to the user programme in Spring 2017 following a commissioning phase.

Developments on LET

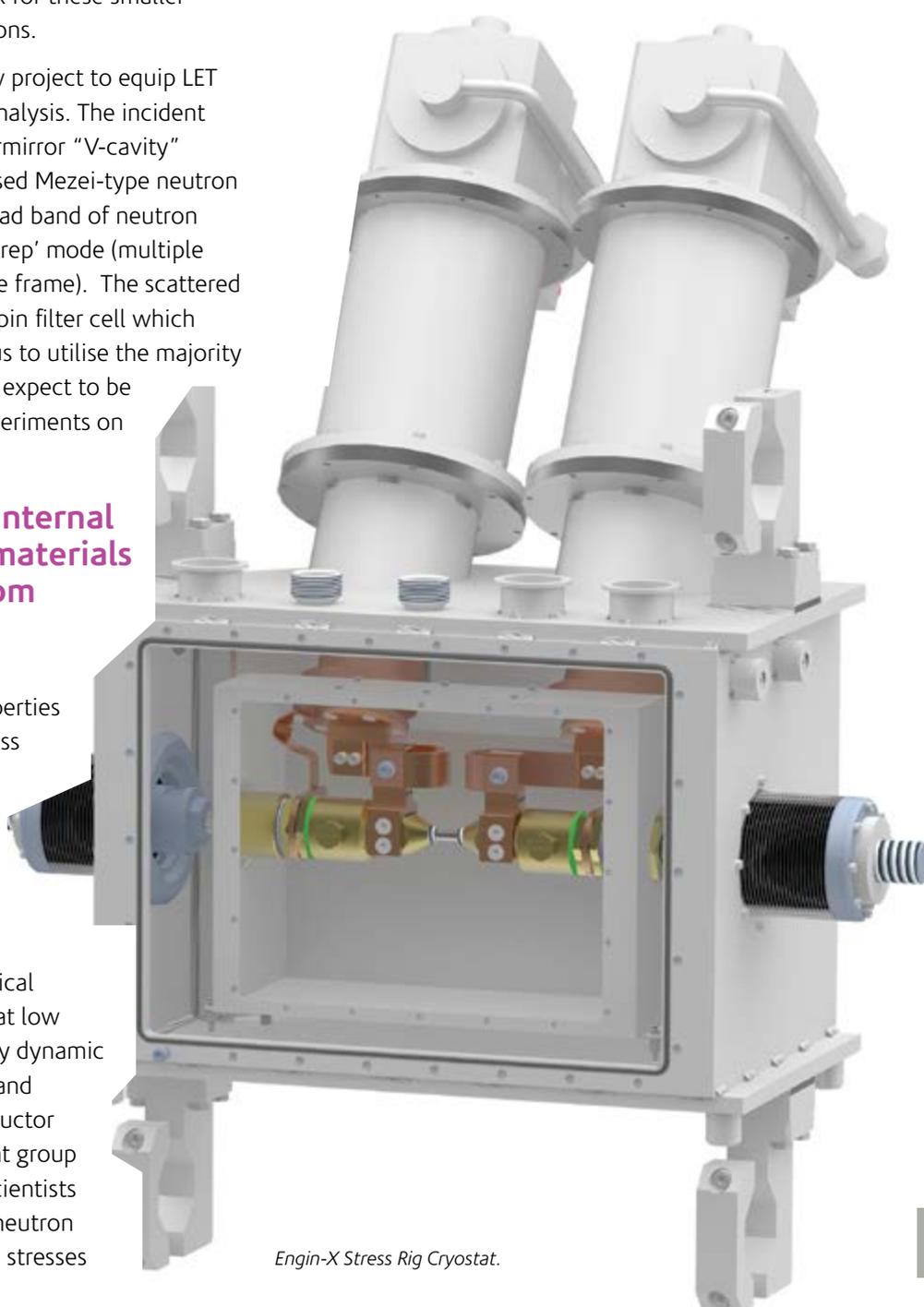
LET has been in the user programme for almost 6 years now. It was initially designed to investigate fairly large samples with a neutron beam of area 4 x 5 cm at the sample position. However, most experiments performed on LET use complicated sample environment equipment such as dilution fridges (to get to mK temperatures) and high magnetic fields. Correspondingly sample sizes are often fairly small – typically just a few grams. To boost the flux for these small samples we have replaced the last few sections of LET guide to focus the beam down to 2 x 4 cm at the sample position. Measurements have shown this gives close to a factor of 3 more flux for these smaller samples in agreement with simulations.

Recently we have also started a new project to equip LET with uniaxial neutron polarisation analysis. The incident beam will be polarised using a supermirror “V-cavity” supplied by Swiss Neutronics. A pulsed Mezei-type neutron spin-flipper will be used to flip a broad band of neutron wavelengths for operation in ‘multi-rep’ mode (multiple incident energies in a single ISIS time frame). The scattered beam will be analysed using a ^3He spin filter cell which wraps around the sample allowing us to utilise the majority of LETs large detector coverage. We expect to be performing polarisation analysis experiments on LET in the second half of 2017.

Cryostat for measuring internal stresses in engineering materials in temperature range from 6K to 300K

Internal stresses in materials have a considerable effect on material properties including strength, fracture toughness and fatigue resistance. The Engin-X beamline is an engineering science facility at ISIS optimised for the measurement of strain and stress using the atomic lattice planes as a strain gauge. Nowadays the rapidly rising interest in mechanical properties of engineering materials at low temperatures has been stimulated by dynamic development of cryogenic industry and advanced applications of superconductor technology. ISIS Sample Environment group together with Engin-X Instrument Scientists have developed a new cryostat for neutron scattering measurements of internal stresses

in engineering materials under load up to 100 kN in the temperature range from 6 K to 300 K. Complete cooling of the system starting from the room temperature down to the base temperature takes just 90 minutes. High temperature superconductor current leads integrated into the cryostat design enable measurement of internal strain in a sample by neutron diffraction simultaneously with critical current of a superconducting wire. This technique allows precise measurement of the critical mechanical stress at which superconductivity gets destroyed – vital parameter for modelling and designing of advanced MRI, NMR and other superconducting magnets.



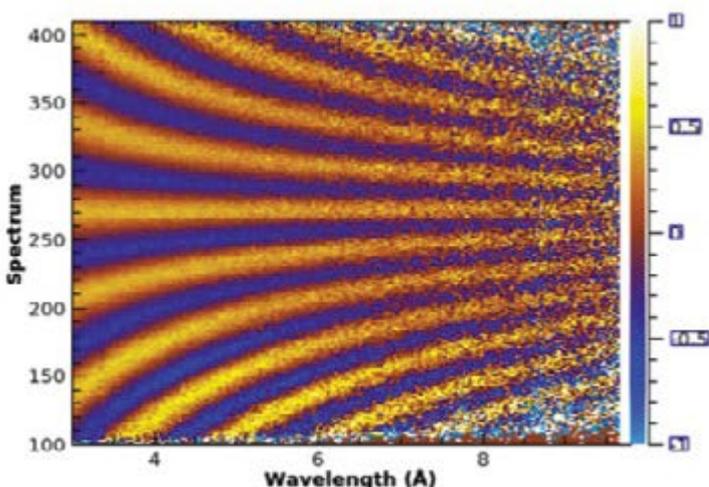
Engin-X Stress Rig Cryostat.

Developing new capabilities for polarised neutrons

Polarised neutrons expand the horizons of neutron scattering in several directions, granting access to longer time and length-scales than normally possible, as well as permitting observation of otherwise invisible cross section components. At the heart of the polarised neutrons program at ISIS is the FLYNN filling station, providing ^3He spin filters to an increasing range of neutron instruments. Following a series of improvements and upgrades, FLYNN is now operating at a typical ^3He polarisation of 75%, which translates into an excellent neutron polarisation and transmission across a broad wavelength range.

These advances in ^3He polarisation have been used in two recent experiments on LARMOR. Firstly, a team from Delft University of Technology demonstrated the possibility of simultaneously measuring conventional and spin-echo modulated SANS (SEMSANS), thereby providing structural information from nanometer to micrometer length-scales in a single shot. Another success was achieved by researchers from Indiana University, who used superconducting neutron Wollaston prisms to increase both the maximum possible beam size and length-scale probed in SEMSANS. Their work promises the possibility of kinetic SEMSANS measurements and neutron phase contrast radiography, among other applications.

With the LET time-of-flight spectrometer next in line to support polarised experiments, exciting times lie ahead for polarised neutrons at ISIS.



Polarisation fringes measured on LARMOR using a camera of 28mm x 28mm with 512 x 512 pixels. At 4 Angstroms, the period is 2.5mm. The maximum and minimum polarisation is +0.5/-0.5 and the instrument polarisation is about 0.65.

New high-pressure single-crystal infrastructure

A new alignment mechanism has been designed and commissioned for the study of high-pressure samples on the PEARL instrument. The assembly incorporates one of the existing 100Kbar Paris/Edinburgh high-pressure clamp cells used on the instrument, which typically have a mass of 50Kg. Aligning of the single-crystal samples is achieved with a vacuum rotary unit providing full 360° motor-driven axial rotation along with a +/- 10mm vertical adjustment to compensate for the compression of the sample under the extreme pressures applied. High-pressure feed pipes to the Paris/Edinburgh ram are introduced through

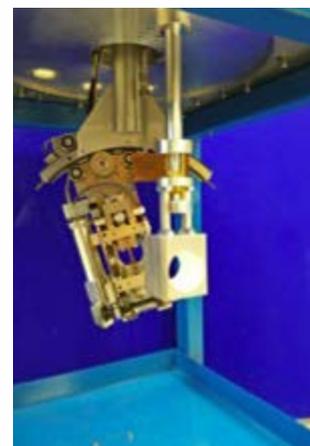


The new high-pressure assembly ready for action.

vacuum fitting at the top of the vertical adjustment mechanism. Sample loading is performed in an inverted position within the swinging trolley. The alignment mechanism will allow faster sample loading and alignment on the PEARL instrument. Typically the neutron beam height is only 2mm and the compression of the sample can shift the effective centre out of beam. Previously it has not been possible to compensate for this without breaking the vacuum and manually realigning the clamp cell.

New tensile testing stage for SXD

A new tensile testing stage assembly has been designed and commissioned for use on the SXD instrument. The assembly incorporates a small 10 KN tensile rig optimised for neutron scattering use. A small amount of heating or cooling of the sample can be achieved and the incoming neutron beam collimation reduces the beam size to match the small samples subjected to the 10 KN tensile loads. The assembly will allow real-



The tensile testing stage



Above: The team involved in ISIS muon beamline upgrade work over summer 2016.

time tensile testing to be observed in the neutron beam whilst optimising of the sample crystal structure takes place. As a fully encoded assembly, accurate orientation of the sample can be achieved with a precision which has never been possible before.

TS1 moderator upgrade

A planned upgrade to the water moderator on the first target station was successfully completed in early 2016. The upgrade means that beamlines on the south side (MAPS, SXD and VESUVIO) benefit from a factor of up to two increase in thermal neutron flux. The neutron flux and resolution profiles measured after the upgrade were in excellent agreement with simulations performed beforehand by the ISIS neutronics group, and thus provide a useful additional benchmark for the wider TS1 project. The benefits of the extra flux for the south side instruments include the ability to measure smaller samples (SXD), improve diffraction data collection done in parallel with spectroscopy experiments (VESUVIO), and improve the

speed and statistical quality of low energy excitations measurements (MAPS).

Muon Beamline Phase 2

During summer 2016, Phase 2 of the muon beamline upgrade project was installed, revamping the remaining parts of the original 1987 installation. With many pieces of equipment being made in the 1960's and having been used previously in CERN, they had a long and successful working life but it was time they were retired and new equipment brought in! Quadrupole magnets were replaced with new optimised assemblies, as were other components such as beam pipes, vacuum pumps and slits. The upgrade has led to increases in the muon flux on all the muon instruments, as well as ensuring the facility can run for many years to come.

THE SCIENCE & TECHNOLOGY FACILITIES COUNCIL
& TESSELLA
MANTID - AN OPEN SOURCE SOFTWARE FRAMEWORK FOR HIGH-PERFORMANCE
COMPUTATIONAL ANALYSIS AND VISUALISATION OF SCIENTIFIC DATA

HIGHLY COMMENDED HIGHLY COMMENDED HIGHLY COMMENDED

Software and Computing

IBEX: Instrument Control System

Development of IBEX, the new EPICS-based instrument control software, continues to progress well. EPICS is a software framework which has been used for building control systems at other 'big science' facilities around the world, including Diamond Light Source and the US Spallation Neutron Source, and will also be used at the European Spallation Source. The first iteration of IBEX was used for commissioning the new TS2 LARMOR instrument. Over the past years the development team has steadily increased the capabilities of IBEX, improving the user interface and extending support for the broad variety of measurement and control devices used on instruments at ISIS. IBEX is currently controlling user experiments on LARMOR and being used for final commissioning of the IMAT instrument. In the immediate future we have plans to use IBEX to provide control and monitoring for the Muon front-end upgrade, for commissioning of ZOOM, and for running user experiments on IRIS. Longer term, as the user programme allows, we will steadily migrate more existing instruments to IBEX. The IBEX development team is also actively collaborating with the two ESS in-kind teams, to share ideas, expertise and code, to help maximise the benefit to both ISIS and ESS.

Mantid

Mantid is the ISIS data reduction and analysis framework which is continuing to see increasing usage at ISIS and other neutron sources around the world. Development

is an ongoing process, and a variety of instruments have seen Mantid taken forward this year. For example, Mantid support has been added to handle an entirely new type of instrument at ISIS – the new neutron imaging beamline IMAT.

As a professional software project Mantid was highly commended at the BCS & Computing UK IT Industry Awards in the Project Excellence category for the best not-for-profit product November 2015. This was a crowded category and the picture above is from the event celebrating the UK IT Awards at the London's Battersea Park Events Arena.

Computing Infrastructure

As data volumes at ISIS grow, and the compute requirements to effectively analyse data increase, ISIS is working to provide a number of compute and storage resources. STFC's SCARF (Scientific Computing Application Resource for Facilities) is a 5800 core high performance computing cluster and is available for use by all ISIS users. A range of scientific software is installed on SCARF including CASTEP, Gaussian and RMCProfile as well as general tools such as Paraview, IPython and Matlab. Users can also compile their own code on SCARF. For more information and to register please see www.scarf.rl.ac.uk

The 'ISIS Compute' service allows users to remotely access high powered analysis resources and their ISIS data and software, via the NoMachine client or a web browser. The system has proved popular, so the ISIS computing group is working STFC Scientific Computing Department to extend the system and make it available to more users over the next year.

ISIS supporting the European Spallation Source

UK-ESS is the name for the UK's contribution to the European Spallation Source (ESS), a new €1.8Bn facility being built in Lund, Sweden. The UK is contributing £165M to ESS, and has trusted STFC with the task. We have established a small Project Office to manage the work. Two programme managers are being supported by an office manager, a management accountant, and a contracts expert. The main work of the programme goes on in various STFC departments and in partner organisations including UKAEA's Remote Applications in Challenging Environments (RACE) facility and the University of Huddersfield.

Part of the UK's contribution will be to build neutron instruments, drawing on the extensive experience built up at ISIS. A new ESS Instrument Design Group has been set up to carry out this work. The first of the instruments, called Loki, is a broad range, high flux SANS instrument that will be used at ESS for bioscience and materials science. Initial work is focussed around ensuring that the finished instrument and its associated beamline will fit into the complex geometry of the ESS experimental hall. Staff at ISIS are also working on development of software for ESS, and helping ESS to set up the vital support laboratories it will need. ISIS is also supporting ESS by contributing members to all of ESS's technical and collaboration Boards, the In-Kind Review Committee, the ESS Annual Review, and numerous other review bodies.



Initial Layout for the Loki Beamline to be built as part of the ESS instrument project.

The rest of the UK-ESS programme being overseen by the UK-ESS Project Office consists of projects in STFC's Technology Department and Accelerator Science and Technology Centre (ASTeC) and a single large project at RACE. The STFC-managed projects are an RF distribution system (carried out jointly with the University of Huddersfield), a set of superconducting RF cavities for the

high-beta end of the ESS linac, a set of Beam Transport modules that between them make up the bulk of the length of the linac, and detector electronics systems. The RACE project is to build the remote handling facility that will deal with radioactive components at ESS once it is running.



The ESS project team ISIS, left to right, John Webber, Philippa Kingston, Justin Greenhalgh, Louise Dixon and Deena Fernandes.

First Target Station *project*

The ISIS First Target Station has run for over 30 years without significant maintenance or development work being carried out on it. The ISIS First Target Station Project will develop and upgrade key elements of the First Target Station to enable it to run for many more years to come. This is a large project involving many years of planning; the actual work is likely to be carried out during a 1-year shutdown of TS1 around year 2020.

The project will involve complete refurbishment of the internals of the target station, including the target design itself, the target cooling systems, and the moderators and reflector and all their cooling and services systems. It doesn't include instrument developments – they will carry on in parallel as part of the ongoing ISIS instrument development programme.

Building on the work done in the definition phase, the TS1 upgrade project has now moved into its implementation phase. Work on the neutronic simulation has continued and designs have developed further. The focus of the neutronic optimisation was to try to increase efficiency wherever possible, while respecting the key requirement to maintain the performance of the existing instruments (in terms of flux or time-structure). This work culminated in the recent release and imminent sign-off of the MkVII neutronics model. This model contains a high level of engineering 'reality' including representative pipework, materials and clearance gaps.

The TS1 upgrade project is part of ISIS' commitment to ensuring the ongoing sustainability of the facility. It will:

- Secure the future of TS1 and enable it to operate for many more years
- Provide improved flexibility for future target or moderator changes
- Make operation of the target station easier, e.g. improving the time for methane moderator changes
- Provide a neutron performance increase, of up to a factor of 2, on some instruments
- Provide confidence in the ongoing operation of TS1 to enable future instrument upgrades
- Further improve our knowledge of target station design for future projects and further develop our staff in this area



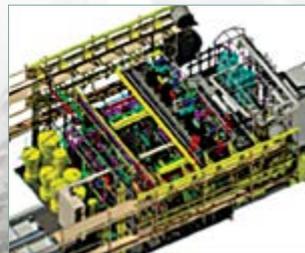
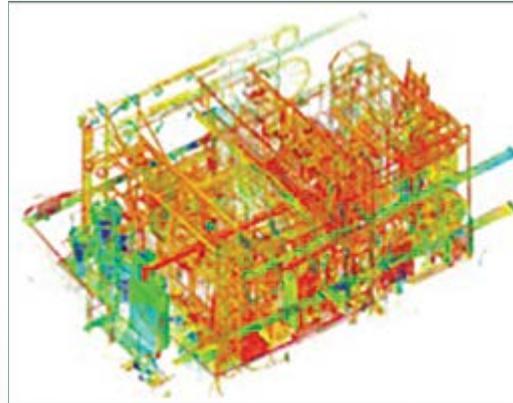
The upgrade project is about a lot more than just the target, it represents nearly a complete refurbishment of the internals of the target station, also including: target cooling systems, moderators and reflector, and all their cooling systems and services which sit behind the target station.

The TS1 project is being undertaken in order to enable TS1 to operate for many more years. It will also provide improved flexibility for future target or moderator changes, and will make operation of the target station easier. Some neutron instruments will see flux increases of perhaps up

From both a neutronics and engineering point of view, one key area is the design of the target. Above shows a comparison of ISIS Target module cross-sectional views (TS2 left, TS1 upgrade proposal centre & TS1 current, right)



to a factor of 2, whilst others will see a largely unchanged neutron performance. The project is also enabling ISIS to improve our knowledge of target station design for future projects, and to give confidence in the ongoing operation of TS1 for future instrument upgrades.



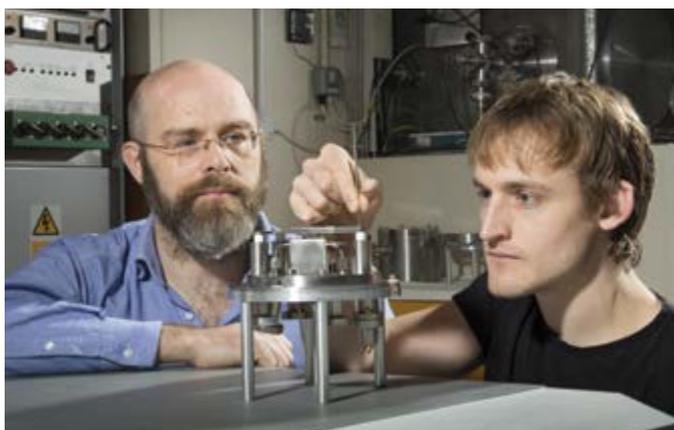
A laser scanning system mapped the pipework and components in the target services area effectively capturing millions of coordinate points which can then be compared to and used to inform the CAD models.



Accelerator and targets

Scaling-up the Ion Source

The entire ISIS facility begins with a tiny device that fits in the palm of your hand: the ion source. Inside the ion source is a plasma the size of a fingertip into which over three thousand watts of electrical power are pumped. This is a tremendously high power density which does significant damage to the internal surfaces of the ion source, limiting its lifetime to three or four weeks. The ISIS Low Energy Beams (LEB) Group have been developing a 'scaled source' which is twice as big as the operational source, meaning it should suffer less damage and last longer. It will also deliver ion beams of increased power for future projects and accelerator-based facilities.



LEB Group leader Dan Faircloth and mechanical engineer Theo Rutter assembling the scaled ion source.

New power supply for the Injection Septum Magnet

A replacement 375 kW power supply for the injection septum magnet was commissioned in January 2016. This supply is of a modular construction and includes sufficient power modules to provide redundancy. This means that in the event of a power module failure, the supply will detect and isolate the failed module from the output and adjust the remaining modules to maintain the required overall output power. The process occurs within 1 millisecond and does not cause a beam trip.

In addition to the power supplies commissioned last year for the high energy drift space, extraction septum and extracted proton beam magnets, these continual upgrades provide lasting improvements to the accelerator's availability.



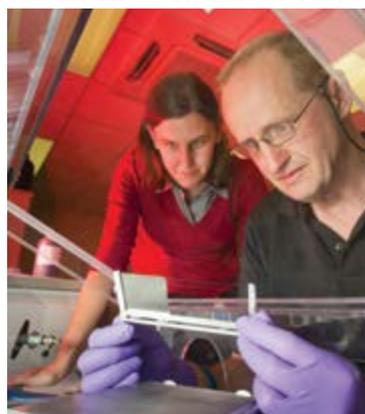
Electrical Engineering Group members Andy Black and Steve Reeves with the new injection septum power supply.

Carbon Stripping Foils – reducing downtime

The ISIS linear accelerator (Linac) accelerates a beam of H⁻ ions to an energy of 70 MeV prior to injection into the synchrotron. During injection, these ions pass through a stripping foil which removes their electrons, leaving a beam of protons. Throughout its 30 years of operation ISIS has developed aluminium oxide (Al₂O₃) stripping foils in-house for this purpose.

The manufacture and installation processes for these foils are both time consuming and radiologically dose intensive. As a result, commercially available carbon-based foils have been trialled at ISIS over the past year, following their successful operation at neutron sources in both Japan (J-PARC) and the USA (SNS).

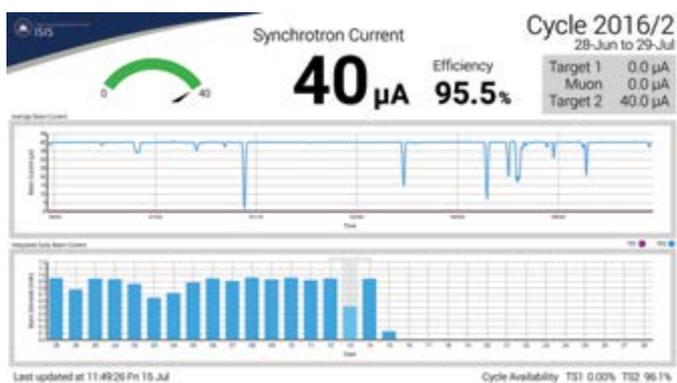
These carbon foils provide the same stripping efficiency as those currently in use and are both faster and simpler to replace, reducing both operational downtime and radiation exposure during the process. The carbon foils will also be able to handle the increases in injection energy that



are likely to arise during future upgrades to ISIS. Experience gained from initial testing of the new foils was built upon throughout the year and in May 2016 the first cycle at ISIS using only carbon foils was completed.

Mark Waite and Hayley Cavanagh using the carbon foil mounting station in the foil lab.

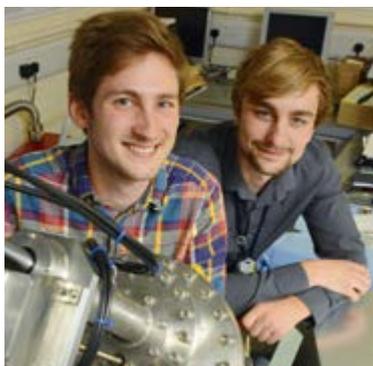
Updated ISIS status page



The new ISIS status page displaying performance statistics during cycle 2 of 2016, during which a beam of 40 μA was delivered exclusively to target station 2.

A new status page for ISIS has been developed to provide up-to-the-second information on the accelerator's performance. This allows visitors and beamline users to see how the accelerator is operating whether they are in the experimental hall, popping into the user office or grabbing a coffee in one of the café areas. The web page is compatible with modern browsers and is scalable, meaning it can be viewed on a wide range of devices from anywhere on the ISIS computer network.

A new Profile Monitor for the ISIS HEDS



ISIS diagnostics section graduates David Posthuma de Boer and Daniel Harryman with the new profile monitor.

Wire scanner profile monitors are used along the High Energy Drift Space (HEDS) to measure the shape of the H- beam once it has left the Linac. This is

achieved by moving a pair of silicon carbide wires across the beam aperture and measuring the signal generated by collisions between the beam ions and the wires. The larger the generated signal, the more intense the beam is at that location.

ISIS' current set of wire scanners are approaching the end of their lifetimes, having been in use for more than 20 years. In order to replace these monitors an updated wire scanner design has been created. The first of this new generation of monitors was constructed and tested during the year and is now ready for installation. The new design offers an increased speed of measurement along with a significant improvement in positional resolution.

Linac Tank 4 replacement progress

The ISIS Linac uses 4 radio-frequency (RF) tanks to accelerate H- ions from 35 keV to 70 MeV. Having been constructed in 1976 for ISIS' predecessor, Nimrod, tank 4 is now due to be replaced by a newly designed vessel. To demonstrate the principle of the new tank, a 1/6th length test piece has been fully assembled and fitted with 5 successfully aligned drift tubes. Under vacuum, this tank has provided excellent results for both its resonant frequency and field profile along its length. The final stages of preparation for full power testing with high power amplifiers, modulator room and ancillary equipment are near completion, with tests expected to get underway later in the year.



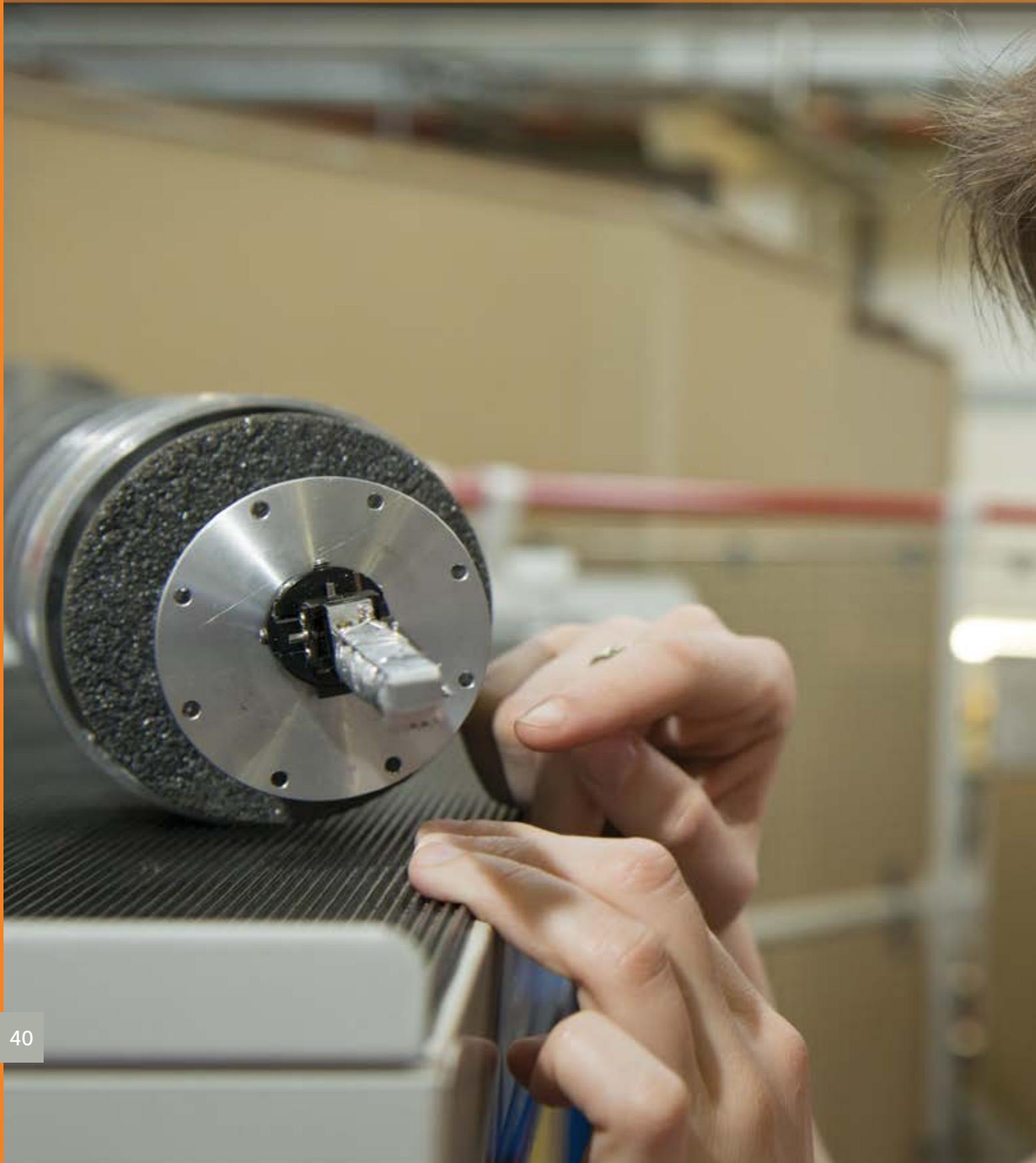
Members of the ISIS RF Group, Diagnostics Section and Design Division with the new 2 metre section of Linac tank 4.

Extracted Proton Beam (EPB) 1 upgrade work



A new horizontal dipole magnet for EPB1, installed this year as part of the continued upgrade works to the beamline.

Skills and training





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.

Inspiring the next generation of scientists and engineers



Daniel Harryman, ISIS, shows visitors a Ruben's tube, demonstrating standing waves at the Daresbury campus open day in July 2016.



ISIS ion source scientist Scott Lawrie won 'I'm a Scientist, Get Me Out of Here' after engaging in fast-paced live chats online with school students, who were full of questions about science.

2016 has seen a surge in ISIS public engagement activities, expanding into new areas of science and engineering and reaching new audiences. As well as hosting visits by over 1400 school pupils, teachers and members of the public, the past year has seen ISIS staff and students heading out to local schools and science festivals, showcasing the amazing science and engineering undertaken at the facility.

Opening its doors to the public for several large events a year, ISIS has seen hundreds of visitors flooding into the facility to hear about the vast range of science that goes on. Public access days continue to be very popular, and participation in new events such as Stargazing at RAL, the Institute of Engineering and Technology Open Day and RAL Apprentice Open Day have captured new audiences. School activities including the long-standing Particle Physics Masterclass and Education Access Days, and newer activities including Chemistry at Work and Science in Your

Future have excited hundreds of pupils from across the country about ISIS science and technology, inspiring the next generation of scientists and engineers.

This year ISIS has also embarked upon new and innovative outreach projects with new partners, including a 6-month display on neutron diffraction at the Wallace Collection National Museum in London. The exhibit is centred around research on arms and armour undertaken at facility, and hopes to reach a diverse audience in the tens of thousands. ISIS has also been the focus of a short film on accelerator science produced by The Royal Institution, as part of an STFC large public engagement grant. "Powering a Particle Accelerator" explores what it takes to keep the synchrotron running and focuses on the people that make it happen, receiving over 10,000 views in the first three months of launching.

Dr Preeti Kaur, ISIS, demonstrates a model beamline as part of the IET Open House event.



Younger visitors making planets as part of Stargazing Live.



Above: Students getting their hands dirty in the lab as part of Chemistry at Work.



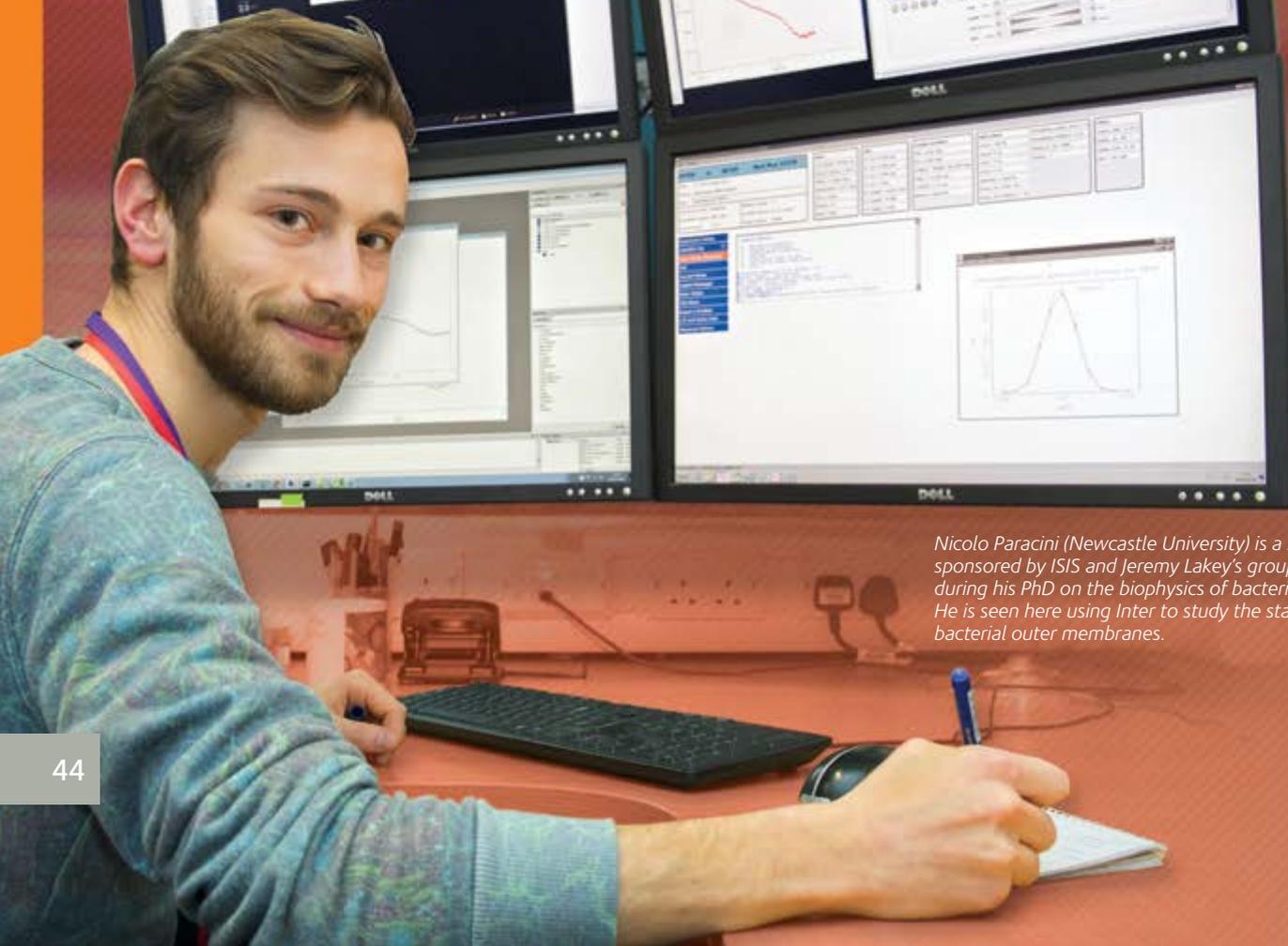
Right: Sixth form students in ISIS Target station 1 as part of the Particle Physics Masterclass

Graduates and PhD students

PhD students are a major part of the life of ISIS, with students making up around half of researchers coming to run experiments. ISIS runs dedicated courses and training days for students, in addition to the training they get during experiments. 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.



Left: Andrew McCluskey and Oliver Hammond (Bath University) at ISIS during their Nimrod studies of catalyst cerium oxide synthesis. Oliver is jointly sponsored by ISIS and Karen Edler's group at Bath University, as part of the Sustainable Chemical Technologies Centre for Doctoral Training.



Nicolò Paracini (Newcastle University) is a student jointly sponsored by ISIS and Jeremy Lakey's group at Newcastle during his PhD on the biophysics of bacterial membranes. He is seen here using Inter to study the stability of model bacterial outer membranes.



The annual UK Neutron and Muon Science and User Meeting includes a day for PhD students, and a student poster session with poster prizes. Here, Ai Woon Yee (Keele University) is describing her poster to Sean Langridge (ISIS).



ISIS and Diamond run an annual training school for around 80 students supported by EPSRC's Centres for Doctoral Training. Here, students from the latest school run in May are being shown the new Chiplr instrument by ISIS scientists Carlo Cazzaniga.



Below: PhD students at the Oxford School of Neutron Scattering in September 2015.



Right: Bo Chen and Ranggi Ramadhan (Coventry University) using Engin-x to explore microstructures in materials generated from additive manufacturing. Ranggi is a co-sponsored joint student between ISIS and Mike Fitzpatrick's group at Coventry University.



Above: Graduate electrical engineer Stephen Turner testing superconducting materials on the Engin-x instrument.

Top right: The ISIS Muon Training School is run every two years to provide PhD students and early-career researchers with a grounding in the muon technique. Here, Naëmi Leo from the Paul Scherrer Institut is working on the HIFI muon spectrometer.



Seminars 2015-16

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
Apr 2015	Panos Soutanas (University of Nottingham)	Inhibition of biofilms by ferric quinate and its mimics; mechanistic understanding and commercial exploitation
Apr 2015	Alberto De La Torre (University of Geneva)	Doping evolution of the pseudospin-1/2 antiferromagnets Sr_2IrO_4 and $Sr_3Ir_2O_7$ from ARPES
Apr 2015	Matthew Watson (University of Oxford)	The electronic structure of superconducting FeSe
May 2015	John Saunders (Royal Holloway, University of London)	Fundamental condensed matter physics with helium films: an overview
May 2015	Dominic Fortes (University College London)	Thinking "outside the pressure cell" – Applications of analogues high-pressure phases made under ambient conditions using chemical substitution
May 2015	Bartomeu Monserrat (University of Cambridge)	Minima and saddle points: the phase diagram of high pressure hydrogen
Jun 2015	Chris Stock (University of Edinburgh)	Orbital memory of spin order in MgV_2O_4
Jul 2015	Rob Atkin/ Gregory Warr (University of Newcastle, Australia)	Structure, Solutes, and Surfaces in Ionic Liquids
Jul 2015	Raghav Adharapurapu (GE Global Research)	Materials Modeling of Superalloys – An Industry Perspective
Jul 2015	Paritosh Wadekar (University of Liverpool)	Valence Fluctuations in Ultra-Thin $Ti_{1-x}O_2$ on Rutile TiO_2
Aug 2015	Luca Lutterotti (University of Trento)	The Combined Analysis with MAUD
Aug 2015	Bruno Uchoa (University of Oklahoma)	Anomalous Hall effect in graphene
Sep 2015	Anita Zeidler (University of Bath)	The pressure induced structural transformations in oxide glasses
Oct 2015	Simon Beaumont (University of Durham)	Next generation heterogeneous catalysis – insights from nanomaterials
Oct 2015	Jon Goff (Royal Holloway)	Strongly correlated thermoelectric oxides
Oct 2015	Johan Chang (University of Zürich)	Charge order and superconductivity in the cuprates
Nov 2015	Jochen Stahn (PSI)	The Selenite Neutron Guide
Nov 2015	John Mydosh (University of Leiden)	Hidden order, superconductivity and magnetism in URu_2Si_2
Dec 2015	Markus Braden (University of Cologne)	Anisotropy of magnetic correlations in FeAs based superconductors
Dec 2015	Phil King (University of St Andrews)	Hidden spin textures of centrosymmetric transition-metal dichalcogenide semiconductors and superconductors
Dec 2015	Manuel Moliner (UPV-CSIC)	Synthesis of zeolitic catalysts for $DeNO_x$ applications
Dec 2015	Silvano Tosti (ENEA)	The interaction of hydrogen with metal alloys of interest for hydrogen separation and storage
Feb 2016	Alexandros Lappas (IESL, Crete)	Frustration-Induced Nanoscale Inhomogeneity in a Triangular Spin Lattice
Mar 2016	Bruno Tomasello (ISIS)	A microscopic theory beyond the Ising model of spin ice
Mar 2016	Tim Burnett	Correlative Tomography: 3D characterization across time and length scales
Mar 2016	Ed Pickering	High-Entropy Alloys: Founding Principles and Future Prospects
Mar 2016	Alexander Belushkin (JINR)	Modeling total reflectometry experiments using a kinematic approximation in combination with the finite element method

Workshops, conferences and user groups

Organised by ISIS or with major input from ISIS in the 15/16 year.

Date	Event
Apr 2015	IOP Advanced School in Soft Condensed Matter "Solutions in the Spring"
Apr 2015	The 1st STFC-ANSYS Joint FEA workshop
May 2015	Muon Site Calculation Meeting
May 2015	Neutron and Muon Science and User Meeting 2015
Jun 2015	Theoretical and Experimental Magnetism 2015
Jun 2015	Red Kite Crystallographers Meeting
Jun 2015	ISIS Facility Access Panel
Jun 2015	Neutron Training Course
Jun 2015	ISIS User Committee
Jul 2015	EPICS Oxfordshire Workshop
Sep 2015	Muon Soft Matter Meeting
Sep 2015	Oxford School of Neutron Scattering 2015
Sep 2015	Mantid Training Courses
Oct 2015	ISIS Crystallography User Group Meeting
Oct 2015	ISIS Student Meeting
Nov 2015	Deuteration Facility Users Meeting
Nov 2015	Electronic Properties of Modern Materials
Dec 2015	ISIS Facility Access Panel
Dec 2015	ISIS User Committee
Feb 2016	High Pressure Neutron Diffraction - In Memory of Bill Marshall
Mar 2016	Muon Training Course
Mar 2016	The 2nd STFC FEA Workshop



A year around ISIS





The past year has seen another of our scientists appointed as a Fellow of the Royal Society, 25 years of the RIKEN-RAL collaboration, a new helium recovery facility opening and a host of events and visits.

A year around ISIS

Below: First year PhD students from Doctoral Training Centres attended a training school at RAL which involved visits to ISIS and the Diamond Light Source in May 2016.



Below right: A small gathering was held at ISIS on the 11th September 2015 to celebrate the signing of the RIKEN-RAL contract 25 years ago and the 20 years since the inauguration of the facility. The cake is being cut by Prof Eiko Torikai and Philip King.



Left: Congratulations to Bill David, senior scientist at ISIS, on being made a Fellow of the Royal Society! The fellowship recognises Bill's significant contributions to the development of neutron and X-ray powder diffraction, including software to accelerate the determination of crystal structures.



Above: ISIS held a meeting at Cosener's House in June 2016 for new members joining the science groups.

Left: ISIS hosted a workshop on the "Quantum Theory of Atoms in Molecules" on 24th May 2016.

Right: The team involved in the build of Target Station 2 (TS2) Phase II instrument, Larmor gathered inside the instrument to mark its handover to the user programme on 4th May 2016.

A year around ISIS



The High Pressure Neutron Diffraction meeting was held in February at Cosener's House, Abingdon in memory of Bill Marshall.



The BTM Willis Prize, awarded by the Neutron Scattering Group of the Institute of Physics (IOP) and the Royal Society of Chemistry (RSC), was presented by Dr Ian Tucker, Chair of the IOP and RSC Neutron Scattering Group, to Dr Katharina Edkins, Durham University.



Left: Italian staff at ISIS met to celebrate the 30th anniversary of the STFC-CNR agreement on 11th November 2015.

Bottom left: The Van der Graaf generator proved to be popular with visitors to ISIS during a Stargazing Live event in February 2016.



Above: Students and tutors of the 2016 ISIS Neutron Training Course. This annual event is aimed at PhD and post-doctoral researchers who have little or no experience of neutron scattering, but whose future research programme will make use of neutron techniques at ISIS.

Right: Members of the ISIS TS2 Phase II project board toured the instruments under construction to hear about the latest developments. Image shows ChipIR instrument scientist, Chris Frost (far right) briefing board members (left to right): Robert McGreevy, Kevin Jones, Sean Langridge, Adrian Hillier, Matt Fletcher, Jim Kay and Giuseppe Gorini inside the ChipIR instrument.



Cryogenics Team Leader, Richard Down and Head of ISIS Operations, Zoë Bowden celebrate the opening of the helium recovery facility at ISIS. The opening of this facility is the first stage in a cost reduction programme that will see liquid helium from the many cryogenic experiments at ISIS recycled for use elsewhere in the facility as helium gas, which could save the organisation up to £500k per annum.

Students of the Muon Spectroscopy Training School photographed on the MuSR instrument in Target Station 1 (TS1).



Facts *and figures*

In 2015-2016, 940 experiments were run and 4,096 days were delivered to the user programme across five run cycles. 462 journal papers were published based on ISIS research in the 2015 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 2015 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)	Holbrey, John (Chair)	Barlow, Dave (Chair)	Boothroyd, Andrew (Chair)	Skipper, Neal (Chair)	Paul, Don (Chair)	Holden, Tom (Chair)
Allan, David	Arai, Masa	Edler, Karen	Braden, Markus	Andreani, Carla	Alberto, Helena	Davies, Catrin
Arnold, Donna	Bingham, Paul	Hase, Thomas	Hayden, Stephen	Bresme, Fernando	Aronson, Meigan	Dye, David
Cussen, Eddie	Bychkov, Eugene	Lee, Steve	Pappas, Catia	Golunski, Stan	Carretta, Pietro	Francis, John
Fortes, Dominic	Dougan, Lorna	Martin, Simon	Ronnow, Henrik	Karlsson, Maths	Giblin, Sean	James, Jon
Knee, Chris	Ferlat, Guillaume	Nylander, Tommy	Staunton, Julie	Krzystyniak, Matthew	Luetkens, Hubertus	Lodini, Alain
Levin, Igor	Salzmann, Christophe	Prescott, Stuart	Stock, Chris	Marques, Maria Paula	McKenzie, Iain	Quinta da Fonseca, João
McLaughlin, Abbie	Jan, Swenson	Scott, David	Stockert, Oliver	Nogales Ruiz, Aurora	Watanabe, Isao	Yescas, Miguel
Skinner, Stephen	Hannon, Alex (ISIS Rep)	Titmuss, Simon	Ewings, Russell (ISIS Rep)	Sartbaeva, Asel	Wright, Joseph	Zhang, Shu Yan (ISIS Rep)
Thompson, Amber	Bowron, Daniel (Secretary)	Tucker, Ian	Stewart, Ross (Secretary)	Senesi, Roberto	Hillier, Adrian (ISIS Rep)	Kelleher, Joe (Secretary)
Vaqueiro-Rodriguez, Paz		van Well, Ad		Fernandez-Alonso, Felix (ISIS Rep)	Cottrell, Steve (Secretary)	
Vaughan, Gavin		Webster, John (ISIS Rep)		Parker, Stewart (Secretary)		
Tucker, Matt (ISIS Rep)		Skoda, Max (Secretary)				
da Silva, Ivan (Secretary)						

ISIS User Committee Membership December 2015

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.

UG1 Crystallography	Peter Slater, Birmingham University Anthony Powell, Heriot Watt University
UG2 Disordered Systems	John Holbrey, Queen's University, Belfast Beau Webber, University of Kent
UG3 Large Scale Structures	Ali Zorbakhsh, King's College Jeremy Lakey, University of Newcastle-upon-Tyne Aiden Hindmarsh, Durham University
UG4 Excitations	Jon Goff, Royal Holloway, University of London (CHAIR) Phil Salmon, University of Bath
UG5 Molecular Spectroscopy	Christoph Salzmann, University College London Roberto Senesi, Rome University
UG6 Muons	Don Paul, University of Warwick Alan Drew, Queen Mary College, London
UG7 Engineering	David Dye, Imperial College, London Michael Preuss, University of Manchester Hongbiao Dong, Leicester University

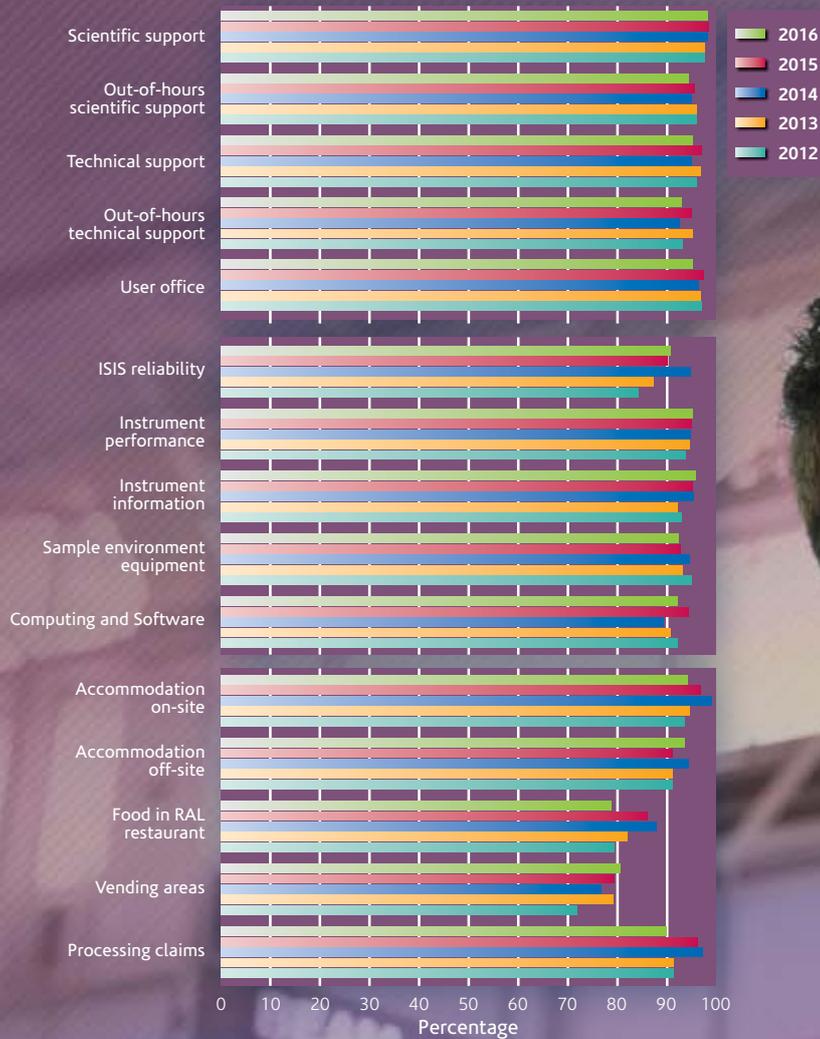
ISIS representatives

Zoe Bowden	Head, ISIS Experiment Operations Division
Debbie Greenfield	Head, ISIS Instrumentation Division
Andrew Kaye	ISIS User Programme Manager
Philip King	Head, ISIS Spectroscopy and Support Division
Sean Langridge	Head, ISIS Diffraction and Materials Division
Robert McGreevy	Director, ISIS
Steve Wakefield	ISIS Experimental Operations Division representative

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 2012- 2016



Beam statistics 2015-16

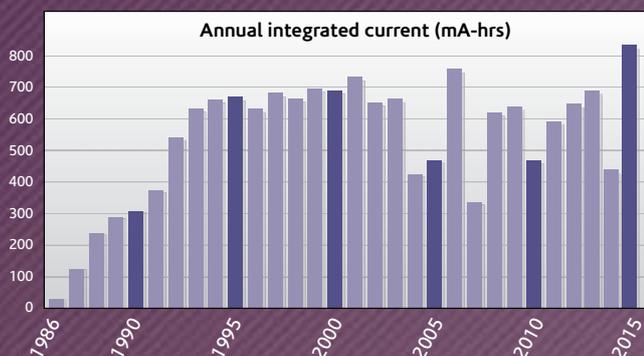
ISIS delivered 824 mA-hrs of beam over these five cycles. The accelerator delivered 174 days for the user programme; taking into account instrument down-time, plus calibration and commissioning time, the fully-scheduled instruments delivered 151 days to the user programme.

Cycle	14/3 (part)	15/1	15/2	15/3	15/4
	1 Apr – 3 May 2015	2 Jun – 24 July 2015	8 Sept – 15 Oct 2015	3 Nov – 16 Dec 2015	16 Feb – 24 Mar 2016
Beam on target (hr)	629	919	831	867	744
Total beam current delivery for both targets (µA-hr)	134,860	196,996	167,497	174,627	149,688
Combined beam current for beam on target (µA)	215	214	202	201	201
Target 1	175	174	162	161	161
Target 2	39	40	40	40	40
Averaged combined beam current per hour (µA)	201	205	189	187	183
Peak beam current over 24 hrs (µA)	216	220	209	206	201

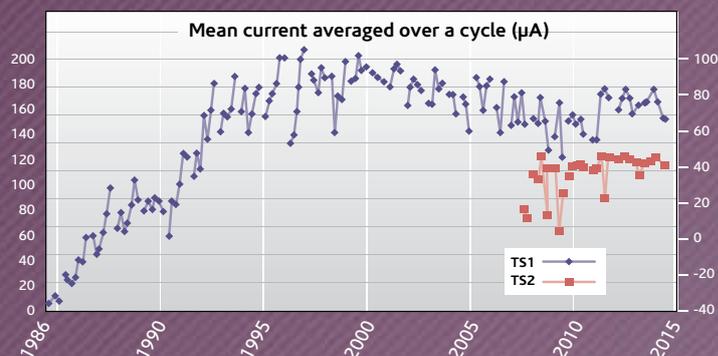
ISIS operational statistics for year 2015-2016.

Year	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015
Total scheduled user days	119	190	86	163	156	116	138	145	153	102	191
No. of scheduled instruments	22	22	22	20	27	27	27	27	27	27	28
Total time on target (days)	104	172	75	144	126	97	125	132	140	90	166
Total integrated current (mAh)	445	738	317	612	630	459	583	642	694	448	824
Average beam current (µA)	178	179	176	177	208	197	194	203	206	207	206
Peak current Averaged over 24 hrs	185	195	200	195	217	204	208	214	213	214	220
Current averaged over year (µA)	156	162	154	156	168	165	176	184	189	185	192

ISIS Performance: Year by Year for the last 12 years



ISIS annual integrated current (mAhrs).



ISIS mean current averaged over a cycle (µA).

Other statistics

In the 15/16 year, 55 days were agreed under the ICRD scheme involving 10 separate companies. Engin-x, SANS and reflectometry, HRPD, GEM, Polaris and Vesuvio were all used under the scheme.

Purchased beamtime

Where a company wishes to keep results of experiments confidential, they can elect to pay for beamtime at commercial rates. In the 15/16 year, 11.5 days of beamtime were purchased by 6 separate companies; 5 of these days came through the ICRD scheme and 6.5 days were direct purchases.

Overall industrial usage

Across the 15/1 and 15/2 proposal rounds, and including the ICRD scheme and direct (paid-for) access, over 53 separate companies were involved in ISIS experiments in 15/16. These represent a variety of industrial areas, including chemicals/plastics, healthcare, automotive, aerospace, manufacturing, energy/oil and other high-tech companies. Together with the ICRD scheme and directly paid-for time, industrial use of ISIS represents some 13.5% of the ISIS programme.

UK Research Council grants supporting ISIS proposals

In round 15/1 and 15/2 respectively, 102 and 83 separate UK Research Council grants were listed as supporting ISIS proposals within the ISIS proposal system – 142 unique RC grants across the two proposal rounds. These grants were primarily from EPSRC, with a small number from other research councils; figures do not include additional proposals with students supported by Research Councils through departmental allocations, CASE awards, etc.

Publications

462 journal publications arising from work at ISIS have been identified to date that were published in calendar year 2015, not including theses, RAL Technical Reports and other non-refereed articles. An annex provides the full publication list.

ISIS science *as it happens*

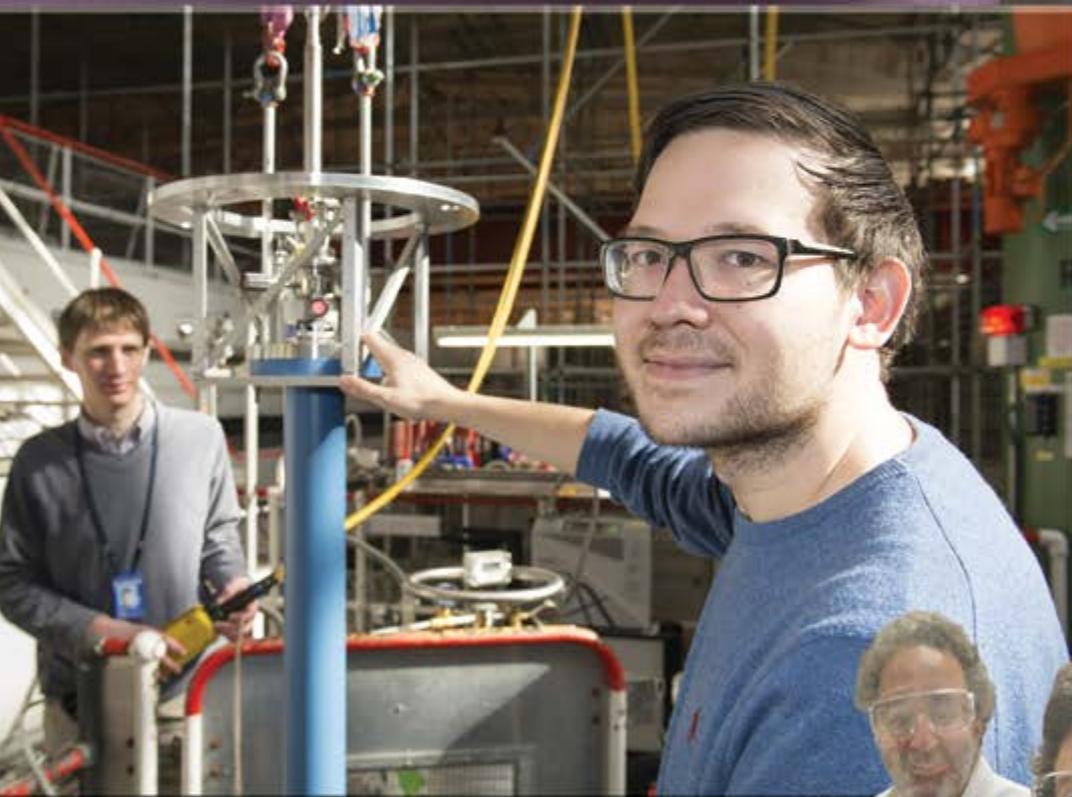
Left: Marie de la Fuente and Philipp Bender (Universidad de Cantabria) using Sans2d to study magnetic interparticle coupling and magnetisation process in $TbCu_2$ superantiferromagnets.

Below: Nicolo Paracini (Newcastle) preparing samples for Polref studies of interaction of antimicrobial agents on floating asymmetric bacterial membrane models.



Right: Dr Sabrina Gaertner, The Open University Astrochemistry Group, on NIMROD studying the properties of ice found in star and planet forming regions of space.

Below: Marein Rhan (Oxford) preparing a cryostat on MuSR for studies of magnetism in $\text{Ca}_2\text{Os}_2\text{O}_7$.



Right and below: Maria Paula Marques and Louis Batista de Caivallio from the Universidade de Coimbra, Portugal, prepare samples for a Maps experiment exploring human bone structure after burning.



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