ISIS 2009

The ISIS Neutron and Muon Source Annual Report

Science & Technology Facilities Council

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ISIS 2009 was produced for the ISIS Neutron and Muon Source,
STFC Rutherford Appleton Laboratory,
Harwell Science and Innovation Campus,
Didcot, Oxfordshire, OX11 0QX, UK

ISIS Director, Dr Andrew Taylor
01235 446681

ISIS User Office
01235 445592

ISIS Facility Web pages
http://www.isis.stfc.ac.uk

***ISIS 2009* production team:**
Philip King, Bryan Jones, Alex Hannon, David Clements

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Ampersand Design Ltd, Ardington (01235 861444)

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ISIS 2009

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2009 details the work of the facility over the past year, including accounts of science highlights and descriptions of major instrument and accelerator developments, together with progress on the Second Target Station Project and the facility's publications for the year.

Contents

▶ *Professor John Beddington, CMG FRS, Government Chief Scientific Adviser and Head of the Government Office for Science, visited the ISIS Second Target Station in November with STFC Chief Executive Prof Keith Mason (left).* ***09EC4671***

▼ *David Willetts MP, Shadow Minister for Universities and Skills, visiting ISIS in February with his son Matthew and STFC Chief Executive Prof Keith Mason.* ***09EC1060***

◀ *Dr Arden Bement, Director, National Science Foundation, Arlington, USA, with Dr Andrew Taylor at the ISIS Second Target Station during his visit in June.* ***09EC2196***

▼ *HRH Prince Andrew the Duke of York visited ISIS in April. Here he is being introduced to the facility by Director Dr Andrew Taylor.* ***09EC1664***

▲ *Dr Frances Saunders, Chief Executive, Defence Science & Technology Laboratory (left), visited ISIS in June with Prof Keith Mason, Dr Liz Towns-Andrews and Dr Andrew Taylor (STFC).* ***09EC2110***

ISIS is, and is destined the world's

Foreword

The thrill of delivering first neutrons to the Second Target Station last year has been more than matched by the scientific commissioning and early operation of its instrument suite.

The first seven instruments have been completed – on time, on budget, and to specification – and have demonstrated performance capabilities that are exceeding the expectation of the instrument scientists themselves!

This is a tremendous achievement. My thanks go to all who have contributed to the success of the TS-2 project: ISIS staff, the user community, external contractors and companies. And we must not forget those who have kept ISIS operating at the top of its game delivering a world-leading programme while all this was happening. Tremendous indeed!

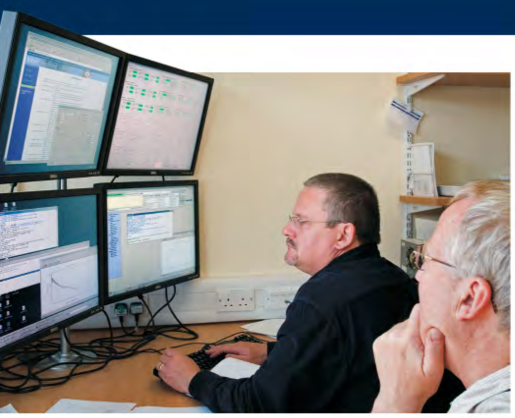
Whilst we rightly focus on the success of the Second Target Station, the main scientific delivery from ISIS still rests with the efficient and effective operation of the existing target. This target station, with its fully developed instrument suite, highly sophisticated sample environment equipment and dedicated user support teams, has set the standard to which the new sources being developed elsewhere aspire. In addition, the Second Target Station instrument suite represents innovation not yet being contemplated anywhere in the world. Taken as an entity, ISIS is, and is destined to remain for some considerable time, the world's premier pulsed neutron facility.

As we introduce new instruments, we also say 'goodbye' to old friends – the HET spectrometer, a flagship ISIS instrument for 24 years, finally closed as the new chopper machine Merlin (with a performance some 30 times greater) came online. And Prisma, the pioneering single crystal spectrometer developed through our Italian collaborations, also saw its last experiment.

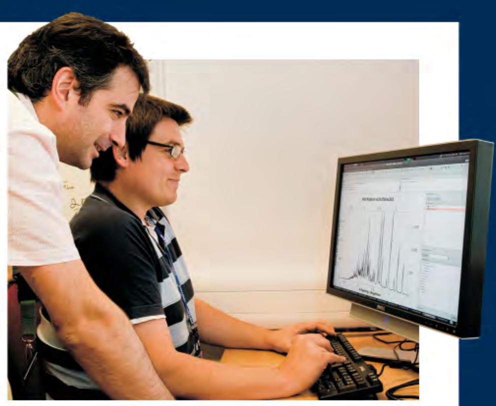
Beyond ISIS itself we can look forward to developments on the wider Harwell campus that will further feed ISIS science. The Research Complex at Harwell opens its doors at the end of the year to foster experimental programmes in support of ISIS, Diamond and the Laser Facilities at RAL, and to attract new science capabilities and develop new partnerships.

The ISIS user programme is fully aligned with the developing STFC strategy and delivers 'impact' in all senses of the word: impact through the science programme, through innovation, inspiration, the nurturing of skills, attracting inward investment to the Harwell Campus and underpinning economic well-being by addressing key science-led government challenges.

These are difficult times for the economy and we recognise that pragmatic short term budget savings needed to be made. Nevertheless we are confident that a proper evaluation of STFC's priorities will soon restore the ISIS user programme to an appropriate level of operation.



▲ *John Webster and Jeff Penfold (ISIS) studying data from the Inter reflectometer during the first experiment on the Second Target Station.* ***09EC2086***



▲ *Laurent Chapon and Pascal Manuel (ISIS) pleased with first data from Wish.* ***09EC2794***

to remain for some considerable time, premier pulsed neutron facility.

A year around ISIS

▲ Danish Science and Technology Institute members visiting ISIS in June: Inge Maerkedahl (Director General) Johnny Mogensen (Head of Division), Morten Scharff (Special Advisor) and John Renner Hansen (Neils Bohr Institute, University of Copenhagen). **09EC2306**

Secondary school teachers attending the ‘Living in a Materials World’ teacher weekend in June learning about ISIS with Chris Frost and Martyn Bull (ISIS). **09EC2472**

▲ Dr Anantha Dasannacharya visiting ISIS in September.

▶ Dr Brian Bowsher, Managing Director, National Physical Laboratory, touring the Second Target Station in June. **09EC2604**

▼ Tony Moore and Jim Brassington from BNS Nuclear Services, formally ALSTEC, hand over the Second Target Station building to ISIS director Dr Andrew Taylor in April. Also present were ISIS staff Harry Jones and Zoe Bowden, and BNS site representative Fred Guttridge. **09EC1592**

▲ In March, Professor Luciano Maiani, President of the National Research Council of Italy, inaugurated the Nimrod instrument on the Second Target Station. He is seen here with Prof Carla Andreani (University of Rome Tor Vergata) viewing archaeological artefacts being studied on Engin-X. **09EC1122**

◀ Oxford University Heads of Department were shown around the Second Target Station in December by STFC Chief Executive Prof Keith Mason. **08EC4851**

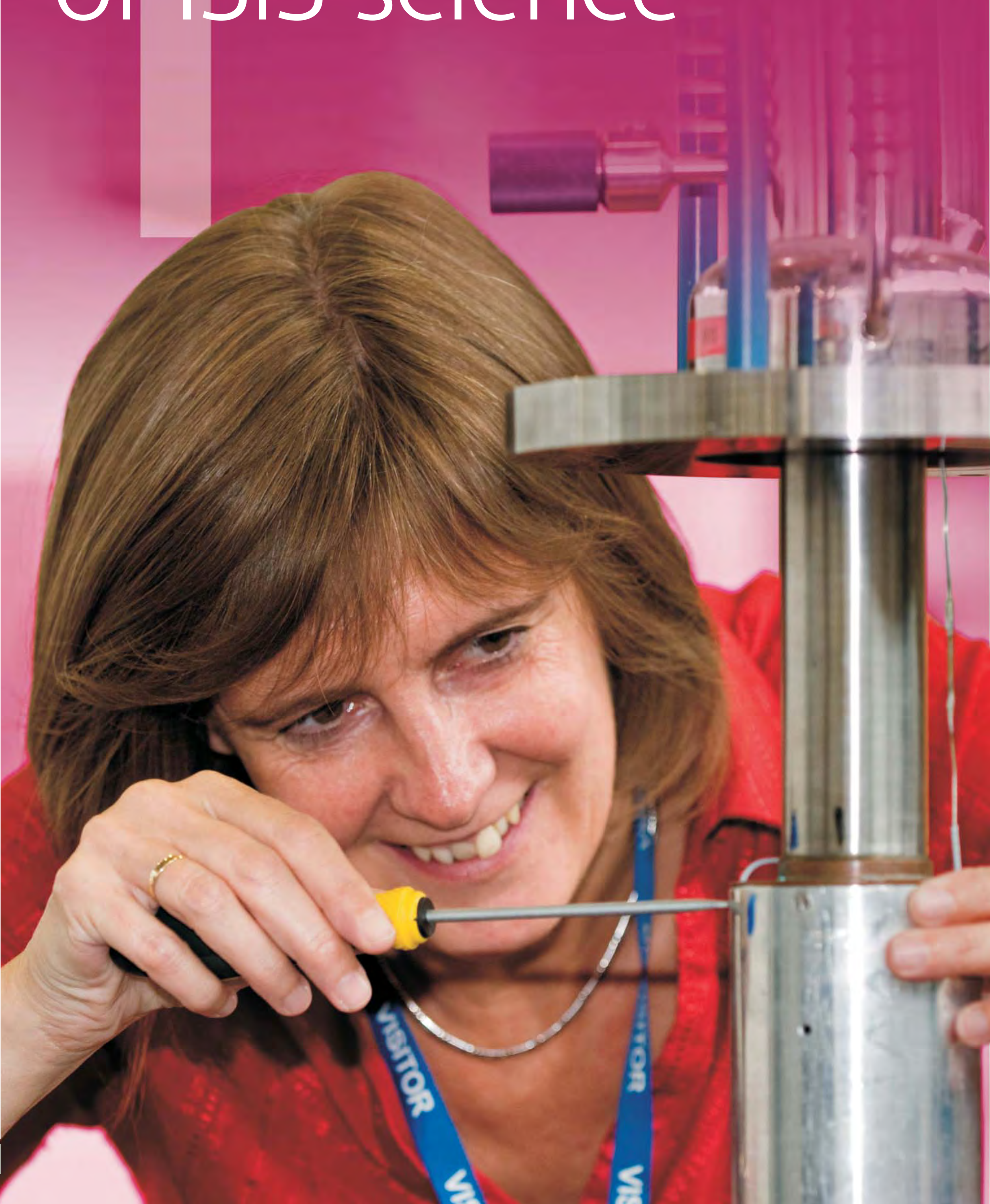
▼ Prof Steven Cowley (Director, UKAEA Culham, left) and Mr Martin Cox (Assistant Director, Operations, UKAEA Culham) viewing TS-2 instruments in July. **09EC2914**

▲ March saw students attending the Particle Physics Masterclass visiting ISIS and learning about TS-2. **09EC1236**

▼ The ISIS Second Target Station was one of the first facility projects to receive European construction funding. The EU project team members visited ISIS for their final meeting in March. **09EC1590**

▲ Prof Michael Steiner, CEO, Hahn-Meitner Institute, Germany (left) and his appointed successor Prof Anke Pyzalla (second from right) visiting ISIS in November with Robert McGreevy, Andrew Taylor and Uschi Steigenberger (ISIS). **08EC4552**

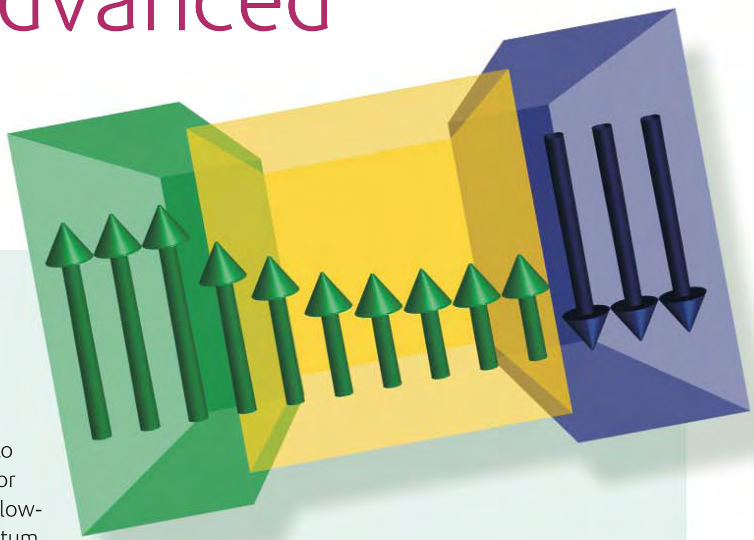
1 Highlights of ISIS science



Section 1
Highlights of ISIS science

The advanced facilities provided by ISIS enable world-class research to be performed by scientists from around the world together with facility staff. Academic and industrial applications of the intense neutron and muon beams encompass a very broad range of science areas. Presented in the following pages are brief summaries of recent science highlights.

Materials for advanced electronics



Organic spin valves open up to neutrons

AJ Drew (Queen Mary University of London), **L Schulz** (University of Fribourg), **S Langridge** (ISIS)

Contact:

Dr Alan Drew, A.J.Drew@qmul.ac.uk

Further reading:

AJ Drew et al., Nature Materials 8 (2009) 109

Electronic devices that utilise atomic-level spins – as opposed to charge – hold unique prospects for future technology. They promise low-power logic, possibly at the quantum level, and the combination on the same chip of communication, logic and memory elements. When such spintronic devices include use of organic materials, which have low manufacturing costs and are mechanically flexible, there is considerable further potential for extending the scope that these devices have. This may lead to an entirely new generation of spin-enabled electronics. However, the mechanisms behind spin injection and transport in organic materials are not well known, as there is a severe lack of suitable experimental techniques. Using spin polarised neutron reflectivity, we have imaged the injected spin polarisation and its transport away from a buried interface within a fully functional and realistic device. The results highlight the unique potential of the technique to reveal the mechanisms that limit the spin coherence within devices, especially in those involving organic materials. Specifically, it can enable bulk and interface-related spin decoherence phenomena to be differentiated.

A spintronic device of the sort already used in hard drive read heads and magnetic memory: the spin valve. A spin polarised current is injected from a magnetic layer (green) into a non-magnetic spacer layer (yellow), where the spin polarisation is reduced as the current flows until it finally reaches a second magnetic layer (blue). Current flow depends on the spin alignment through the device.

Nanoscale spin-spirals to aid magnetic switching

J Witt, A Aziz, M Blamire (Cambridge University), **R Fan, C Kinane, T Charlton, S Langridge** (ISIS)

Contact:

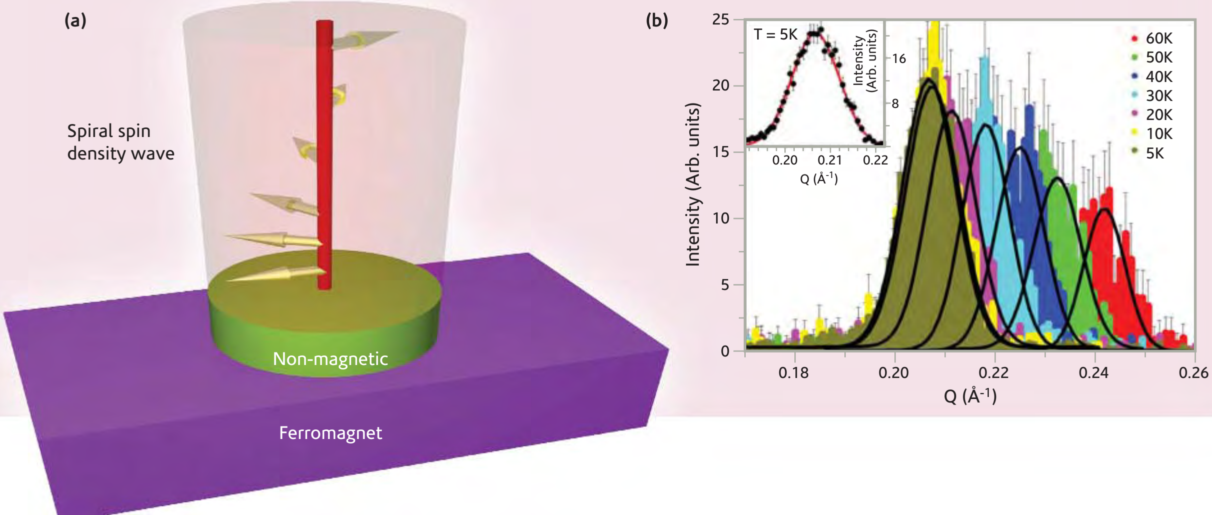
James Witt, jdsw2@cam.ac.uk

Further reading:

O Wessely et al., Phys Rev B 79 (2009) 104433

Spintronics, technologies based on the use of the electron spin as opposed to conventional charge-based electronics, has seen enormous recent development. In the mid-nineties it was proposed that a spin-polarised current of electrons would be able to rotate its magnetisation, removing the need for applied magnetic fields. This has been demonstrated – however, the primary hurdle for making use of these devices is the prohibitively high switching current densities required. An alternative is to use a spin-spiral material, such as holmium. Holmium is ferromagnetic, but the moments rotate from one plane to the next in a spiral fashion. In devices, the entire spin-spiral can be employed in the switching, thereby lowering the necessary current densities. Using polarised neutron reflectometry we have been able to study the temperature and layer thickness dependence of the spin-spiral in films only 25 atomic layers thick. Such information is essential to produce optimised spin-spiral devices.

(a) A schematic of a Ho based spin-spiral device.
(b) Temperature dependence of the magnetic Bragg peak from a 50 nm Ho epitaxial film.



Nanoscale properties of organic solar cell polymers

A Urbina, J Padilla (University of Cartagena, Spain), F Batallán, C Díaz-Paniagua (ICMM-CSIC, Spain), V García Sakai (ISIS)

Contact:

Dr A Urbina, antonio.urbina@upct.es

Further reading:

A Urbina et al., Phys Rev B 78 (2008) 045420

Conjugated polymers have been intensively studied since it was demonstrated that they could behave as semiconductors. The ability to use these polymers to produce organic light emitting diodes (OLEDs) and solar cells (OSCs) has created great expectations. Our neutron diffraction and quasielastic scattering experiments performed on the Osiris spectrometer are the initial stage of a program intended to investigate the structure and dynamics of the most widely used conjugated polymers – the poly-3-alkyl-thiophenes. The added functional groups along the conducting backbone provide solubility, improving the ability to process the polymers. Nevertheless, their structure has to be controlled and their dynamics understood in order to avoid hindering the charge carrier motion that provides the basis for their usefulness in devices. We have demonstrated the coexistence of amorphous and crystalline phases, determined their melting and crystallisation temperatures and provided evidence of a low temperature glass transition. This information, characterisation of the structure and dynamics at the nanoscale, is crucial to achieve the production of higher performance organic solar cells.

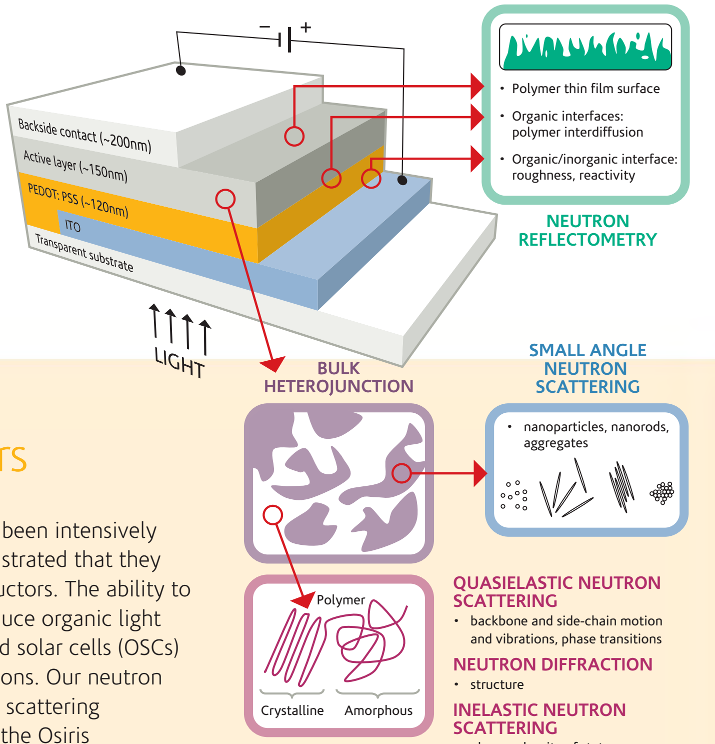


Diagram of an organic solar cell showing where neutron scattering experiments can improve our understanding of the device structure.

Muons probe charge transport in organic semiconductors

AJ Drew (University of Fribourg, Switzerland), FL Pratt (ISIS), NA Morley (University of Sheffield), P Desai (Queen Mary, University of London), R Scheuermann (PSI, Switzerland)

Contact:

Dr AJ Drew, a.j.drew@qmul.ac.uk

Dr FL Pratt francis.pratt@stfc.ac.uk

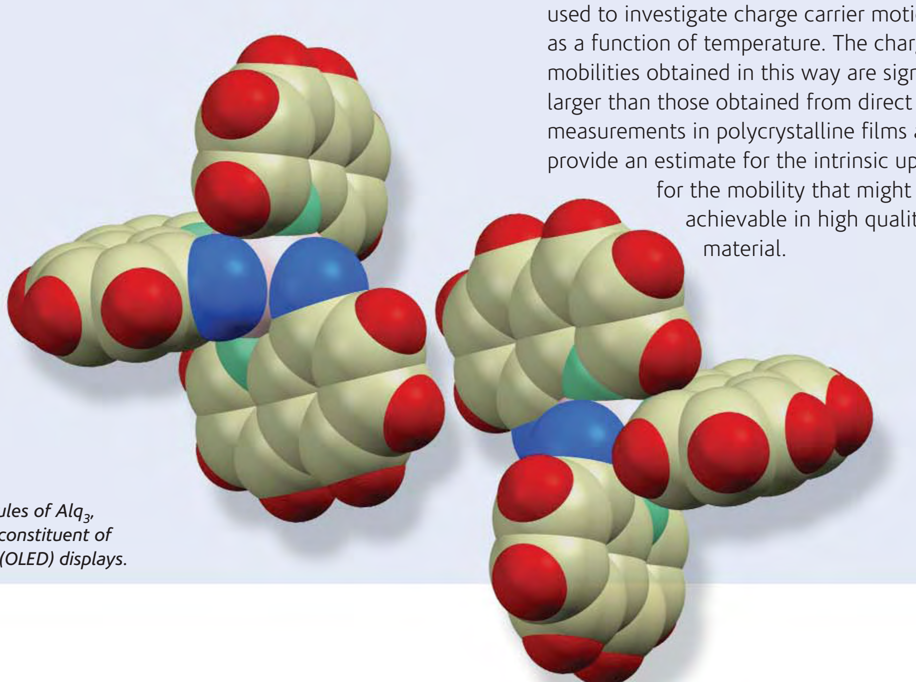
Further reading:

AJ Drew, FL Pratt et al, Phys Rev Lett 100 (2008) 116601

Electronic devices based on organic semiconductors such as Alq_3 (tris[8-hydroxy-quinoline] aluminium) are revolutionising electroluminescent displays and large-area electronics. These organics are economically favourable, can be easily processed in large areas, have tuneable electronic properties, and are simple to grow into high quality thin films.

Even though charge transport in such organic conductors is fundamental to their operation, many of its mechanisms are still only poorly understood. Progress in this area may be pivotal to utilising these materials to their fullest extent.

Implanted muons provide a powerful local probe for studying the dynamics of mobile spins. Muon spin relaxation studies at ISIS have been used to investigate charge carrier motion in Alq_3 as a function of temperature. The charge mobilities obtained in this way are significantly larger than those obtained from direct transport measurements in polycrystalline films and thus provide an estimate for the intrinsic upper limit for the mobility that might be achievable in high quality bulk material.



The propeller-shaped molecules of Alq_3, which are used as an active constituent of organic light emitting diode (OLED) displays.

Competing interactions: studies of frustration

The trigonal bipyramid: a new building block for making frustrated magnets

P Manuel, LC Chapon (ISIS), PG Radaelli (Oxford University), JF Mitchell, H Zheng (Argonne National Laboratory, USA)

Contact:

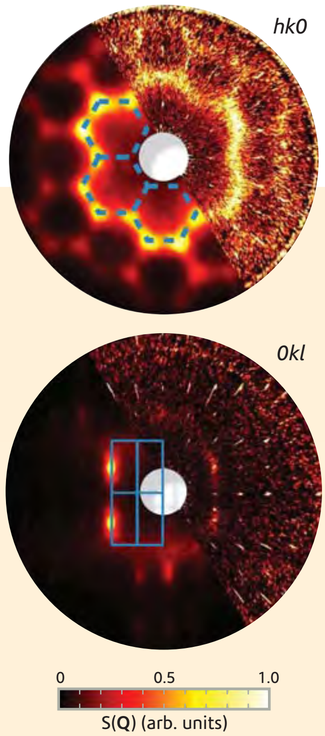
Dr P Manuel, Pascal.Manuel@stfc.ac.uk

LC Chapon, Laurent.Chapon@stfc.ac.uk

Further reading:

P Manuel, LC Chapon et al., Phys Rev Lett 103 (2009) 037202

From compasses to iPods, magnets are the basis of many technological applications. Our understanding of magnetism is based around the idea of atomic-level spins and the interactions between them. Positive interactions result in a ferromagnet with all spins aligned, whereas negative interactions (antiferromagnetic, AF) between spins give rise to more complicated magnets. AF spins located on a two dimensional (2-D) square produce an arrangement with alternating spins. However, it's not possible for AF spins on the vertices of triangles to align themselves so that all of their interactions with their neighbours are satisfied. In this case the system is said to be 'frustrated'. An example of a frustrated 2-D magnet, named after a Japanese weaving technique, is the kagome lattice. In real systems, 2-D kagome layers (KL) are coupled together through other layers that tend to break the frustration. It is generally thought that the best way to keep the KL frustrated is to decouple the layers to reduce these interlayer interactions.



Magnetic diffuse maps, data and simulation, from $YBaCo_4O_7$ in two scattering planes.

Using a combination of neutron scattering and computer simulations on a kagome like system $YBaCo_4O_7$, we show that in fact, strong coupling between the KL can help to keep them frustrated. Our model also introduces a new magnetic entity, a trigonal bipyramid, where the sum of the basal spins is opposite to the sum of the apex spins.

An outsider's view: **a novel muon study of frustration**

SR Giblin, JDM Champion (ISIS), HD Zhou and CR Wiebe (Florida State University, USA), JS Gardner (NIST, USA), I Terry (Durham University), S Calder, T Fennell, ST Bramwell (University College London)

Contact:

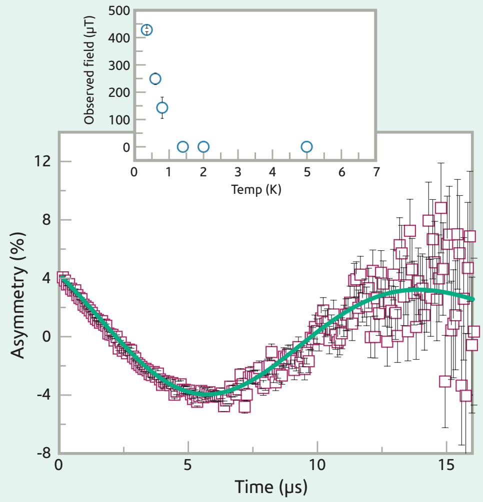
Dr Sean Giblin, sean.giblin@stfc.ac.uk

Further reading:

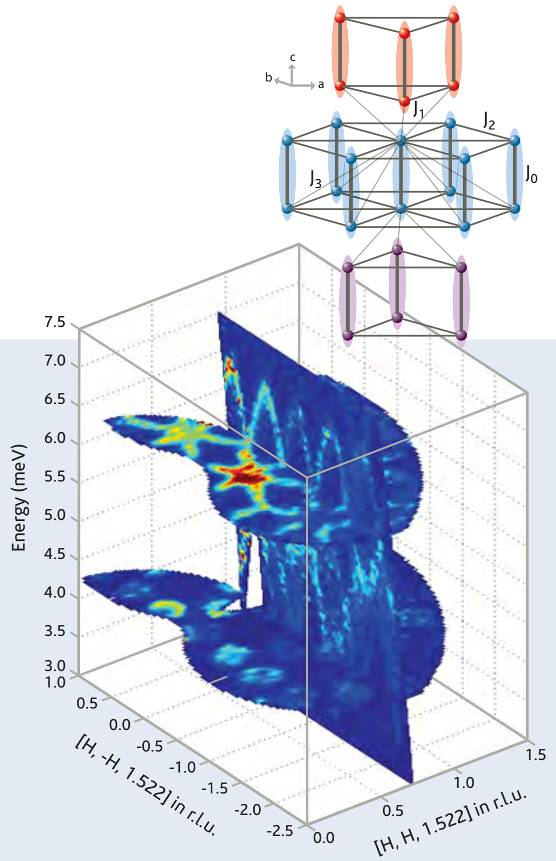
SR Giblin et al., Phys Rev Let 101 (2008) 237201

Frustration occurs when it is not possible to satisfy all interactions between atoms. As described in the article above, a magnetic atom might want its spin direction to be misaligned with that of a neighbouring atom (if the interactions are antiferromagnetic). But for some arrangements of atoms, misalignment with one neighbour prevents misalignment with another – producing frustration. Frustration plays an important role in a diverse range of physics, from magnetism to protein folding. Pyrochlores – magnetic materials with atoms arranged in a way that leads to frustration – are fascinating as by changing one atom the frustration behaviour changes, culminating in properties such as a 'spin liquid', 'spin glass' or 'spin ice'.

The frustration in pyrochlore $Tb_2Sn_2O_7$ has previously led some to believe it exhibits a novel state of magnetism in which the magnetisation direction reverses multiple times a second. This is not how a permanent magnet normally behaves. We tested the behaviour using muons implanted into silver in front of the sample (rather than into the sample itself). If the sample behaved like a permanent magnet, its field lines would penetrate the silver and be detectable by the muons. This is indeed what is revealed – so that $Tb_2Sn_2O_7$ does in fact behave like a permanent magnet below its transition temperature of 0.87K.



An oscillatory signal in the muon data is a clear indication of static internal magnetic fields in $Tb_2Sn_2O_7$. The inset shows the temperature depence of the internal field below the transition.



Merlin's magic reveals quantum magnet behaviour

DL Quintero-Castro, B Lake, EM Wheeler, ATMN Islam (Helmholtz Zentrum Berlin, Germany), **T Guidi** (ISIS)

Contact:

DL Quintero-Castro,
diana.quintero_castro@helmholtz-berlin.de

Further reading:

DL Quintero-Castro et al., arXiv:0909.3941v2, accepted for Phys Rev B

A dimerised quantum antiferromagnet is a system in which quantum atomic spins are strongly coupled into pairs or dimers with only weak interactions between the dimers. The lowest energy state of such a system is a spin singlet (S=0), and this is separated from the S=1 excited state by an energy gap. Because these dimers have integer spins, they have been observed to form an unusual quantum state at very low temperatures, called a Bose-Einstein Condensate, in which all the particles are identical and in the lowest energy state of the system.

We investigated the magnetic properties of a recently discovered dimerised antiferromagnet, $Sr_3Cr_2O_8$. The magnetic chromium ions are arranged on frustrated triangular bilayers and the dominant intra-bilayer interaction couples them into dimers. A structural distortion removes the frustration giving rise to spatially anisotropic inter-dimer interactions and resulting in three twinned domains. The magnetic behaviour can be studied in detail using single crystal samples and a neutron spectrometer such as Merlin. The data confirm the structural distortion and enable the magnetic interactions to be characterised in detail.

Neutron scattering data from Merlin from $Sr_3Cr_2O_8$ in the low temperature phase showing three dispersive magnon modes.

Fundamental magnetic **properties of spin-chain systems**

DT Adroja (ISIS), **S Rayaprol** (UGC-DAE CSR, India), **AD Hillier, M Telling** (ISIS), **EV Sampathkumaran** (TIFR, India)

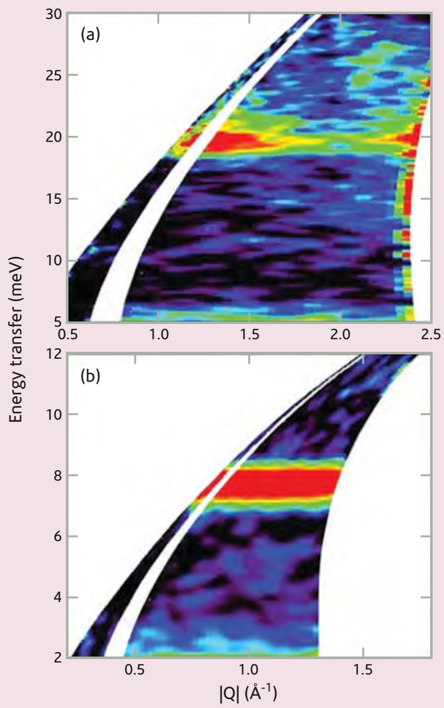
Contact:

Dr DT Adroja,
Devashibhai.adroja@stfc.ac.uk

Further reading:

DT Adroja at el, to be submitted to Phys Rev B

The spin-chain systems with general formula A'_3ABO_6 have been attracting considerable attention in recent years as they offer the possibility of probing several phenomena in a single family of materials: geometrical frustration, the behaviour of linear (Ising) chains of magnetic spins, and ferroelectricity (spontaneous electric polarisation of a crystal). Among these compounds, Sr_3NiRhO_6 and Sr_3NiPtO_6 exhibit interesting properties, having magnetic (Ni^{2+}, Rh^{4+}) and nonmagnetic (Pt^{4+}) ions. Sr_3NiRhO_6 shows a complex magnetic ground state below 40K, while Sr_3NiPtO_6 remains paramagnetic (spin-liquid-like) down to mK temperatures. The crystal structure has Ni and Rh (or Pt) ions surrounded by six oxygens, forming distorted trigonal-prisms and octahedra respectively, that are connected to form 1D-chains. Inelastic neutron scattering on HET has provided direct information on the nature of the magnetic ground state. Data from Sr_3NiRhO_6 indicate the importance of intersite interactions, whereas that from Sr_3NiPtO_6 may suggest a single ion type of response.



Inelastic neutron scattering data from Sr_3NiRhO_6 and Sr_3NiPtO_6 at 5K.

Structural investigations of technologically-relevant materials

Sorting out the structure of **multiferroic $BiFeO_3$**

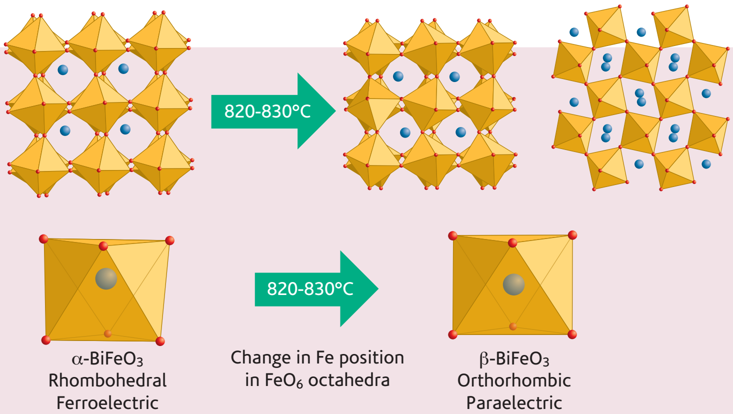
DC Arnold, FD Morrison, P Lightfoot (University of St Andrews), KS Knight (ISIS)

Contact:

Prof Phil Lightfoot, pl@st-andrews.ac.uk

Further reading:

DC Arnold et al, Phys Rev Lett 102 (2009) 027602



Schematic representation of the α- and β-phases of $BiFeO_3$ showing the change in structural symmetry from rhombohedral to orthorhombic at the ferroelectric-paraelectric phase transition.

Multiferroics are technologically-important materials which simultaneously exhibit electric order (alignment of electric dipoles in an electric field) and magnetic order (alignment of magnetic spins in a magnetic field). This makes them potentially useful in devices such as random access memories, sensors and actuators. $BiFeO_3$ is the most widely studied multiferroic as both the magnetic and electric ordering occur at room temperature. The room temperature structure of $BiFeO_3$ (α-phase) has been well established as rhombohedral. However the transition away from electric ordering at high temperatures (ferroelectric, α, to paraelectric, β, transition around 820-830°C) is coupled with a change in structural symmetry. The exact nature of the β-phase has been a subject of much dispute with many different symmetries reported. We used high resolution neutron diffraction to investigate the β-phase with the aim of resolving these discrepancies. We were able to clearly demonstrate that this phase is orthorhombic, ruling out some of the previously suggested models, and subsequently present the first full crystallographic model.

Dopant atoms strain **perovskites**

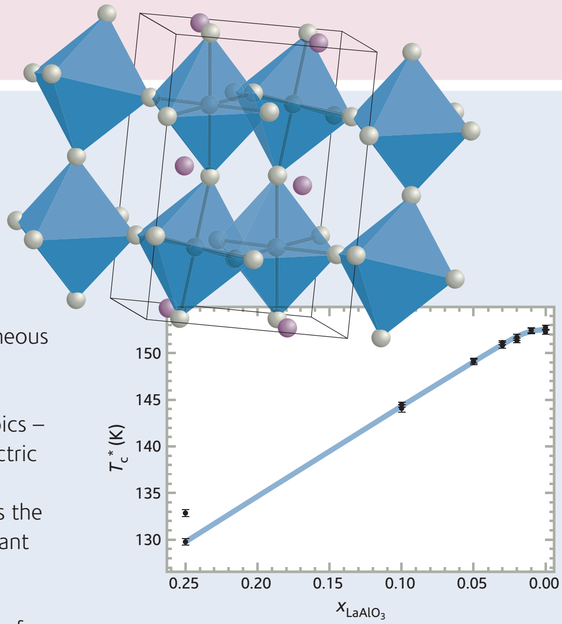
MA Carpenter, CJ Howard, REA McKnight (Cambridge University), BJ Kennedy, Q Zhou (Sydney University), KS Knight (ISIS)

Contact:

Prof MA Carpenter, mc43@esc.cam.ac.uk

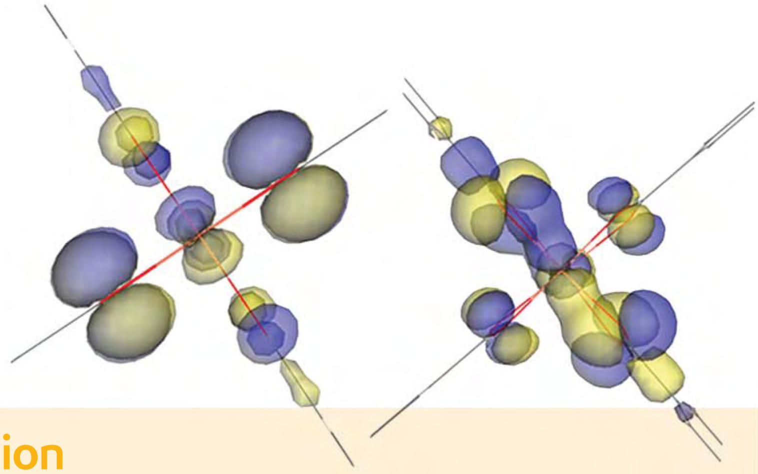
Further reading:

MA Carpenter et al., Phys Rev B 80 (2009) 214101



Temperature of the monoclinic to orthorhombic transition as a function of La dopant content in $(Pr,La)AlO_3$. This is temperature-independent to about 1.6% La. Inset: structure of $PrAlO_3$.

A variety of interesting and potentially useful materials are produced when a perovskite crystal structure is distorted by the presence of dopant atoms. Examples include ferroelectrics, which show a spontaneous electric polarisation (analogous to ferromagnetism), ferroelastics (which show spontaneous strain) or materials – multiferroics – which show a combination of magnetic, electric or elastic behaviour. Of importance for the properties and behaviour of such materials is the size of the strain field around individual dopant atoms. One method of measuring this is to determine the extent to which a material's transition temperature remains independent of dopant concentration for a suitable phase transition. In principle the transition temperature will not change from that of the pure phase until the strain fields around individual impurity atoms start to overlap. We have used HRPD to make precise measurements of the monoclinic to orthorhombic transition occurring in La-doped $PrAlO_3$ at about 150 K. We find this temperature is unchanged to a La dopant level of about 1.6%, and infer strain fields of order 1.6-1.8 pm diameter. This appears to be a characteristic length scale for strain relaxation around impurities in oxide perovskites.



Negative thermal expansion in porous frameworks

VK Peterson, GJ Kearley (ANSTO, Australia), **Y Wu** (Sydney University, Australia), **AJ Ramirez-Cuesta** (ISIS), **CJ Kepert** (Sydney University, Australia)

Contact:

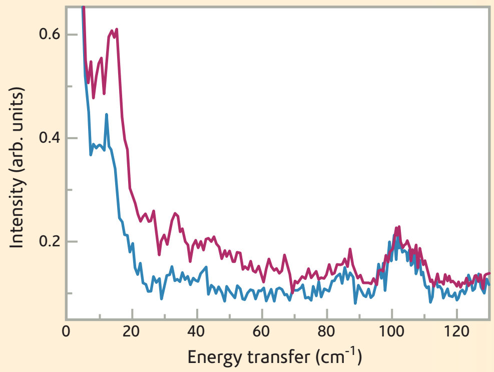
Dr Vanessa Peterson, Vanessa.Peterson@ansto.gov.au

Further reading:

VK Peterson et al., submitted.

Negative thermal expansion (NTE), or contraction upon heating, is of fundamental scientific interest and may find applications in precision engineering. Understanding the mechanisms for NTE may allow tuning of the behaviour by modification of the atomic-level structures through which it is produced. A principal cause of NTE is transverse atomic and molecular vibrations – vibrations that are at right angles to the atomic or molecular bonds. Such vibrations are often low in energy, making them difficult to model and therefore identify. However, the Tosca spectrometer can now be run with its chopper stopped during the one pulse in five that goes to the ISIS Second Target Station, enabling collection of the lower energy region of the vibrational spectrum.

NTE is being noted increasingly in metal-organic framework materials, which have been studied principally for applications such as gas storage. Using Tosca we have found a unique and relatively complex mechanism for NTE in one such framework, Cu_3(1,3,5-benzenetricarboxylate)$_2$. We find NTE arises from relief of geometric frustration through motions of its dicopper benzoate unit, which distorts from square-prismatic towards the antiprismatic configuration on heating.



Spectra (Tosca) at 100 K (red) and 20 K (blue) for Cu_3(1,3,5-benzenetricarboxylate)$_2$. Low energy features arise from the dicopper benzoate unit (inset along Cu-Cu) which changes from square-prismatic (left) to distorted (right).

Two parts order, one part disorder: **negative thermal expansion in $Ni(CN)_2$**

AL Goodwin, MT Dove (Cambridge University), **SJ Hibble, AM Chippindale, AH Pohl** (Reading University), **AC Hannon** (ISIS)

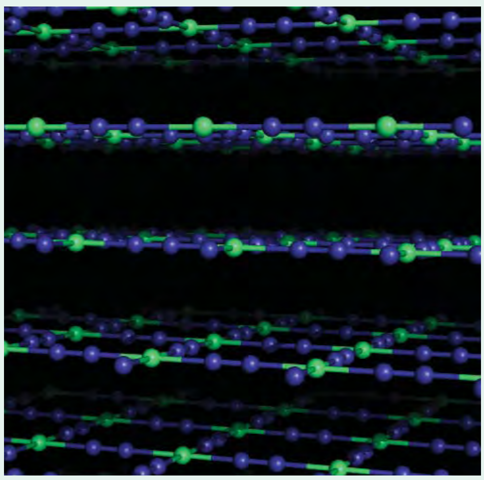
Contact:

Dr AL Goodwin, alg44@cam.ac.uk

Further reading:

AL Goodwin et al. Phys. Rev. B (submitted)

Materials with low-dimensional structures (e.g. 2-D or layered materials such as graphene, high-temperature superconductors) are important precisely because low dimensionality often leads to unusual and useful physical properties. Nickel cyanide, $Ni(CN)_2$, is a material with a layer-like structure that shows the unusual phenomenon of negative thermal expansion. This means that the dimensions of its square-grid-like layers decrease with increasing temperature, in contrast to most materials which expand as the temperature is raised. A combination of neutron scattering and X-ray diffraction has been used to show that the crystal structure of this material actually exhibits long-range structural order in only two dimensions, with no true periodicity perpendicular to its grid-like layers. This lack of periodicity reflects the weakness of the interactions between layers. Because of this, the square-grid layers can vibrate very easily and essentially independently of one another, and this in turn gives rise to its negative thermal expansion behaviour.



Disordered stacking arrangement in $Ni(CN)_2$. Weak interactions between square-grid layers allow large amplitude vibrations that cause the layer dimensions to shrink with increasing temperature.

Applications of complex molecules

Nano-structures in surfactant mixtures revealed

J Penfold (ISIS, Oxford University), **I Tucker** (Unilever), **RK Thomas**, **R Bradbury** (Oxford University), **I Grillo** (ILL)

Contact:

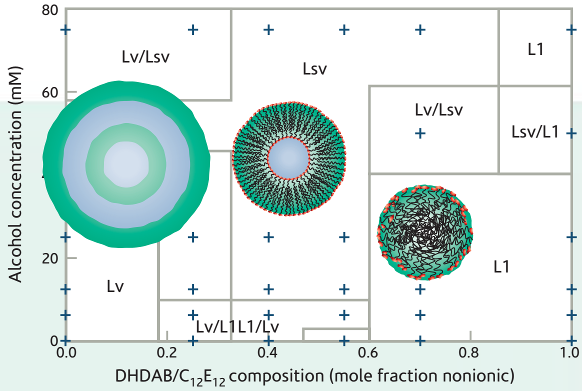
Prof J Penfold,
Jeff.Penfold@stfc.ac.uk

Further reading:

J Penfold et al., Langmuir 24 (2008) 12209;
I Tucker et al, Langmuir 25 (2009) 7674

In many commonplace surfactant-based formulations (comprising ionic/nonionic surfactant mixtures) the addition of cosurfactants such as straight-chain alkanols and more complex alcohol structures (such as perfumes) can have an impact upon the structure and stability of the solution. Recently we have used Small Angle Neutron Scattering (SANS) to study the impact of a range of straight-chain alkanols on the phase behaviour and microstructure of a di-alkyl chain cationic (DHDAB) and non-ionic ($C_{12}E_{12}$) surfactant mixture.

In the absence of alcohol the DHDAB/$C_{12}E_{12}$ mixture exhibits a rich structural evolution with composition – from small globular micelles for $C_{12}E_{12}$-rich compositions to large polydisperse bilamellar or multilamellar vesicles for DHDAB-rich compositions. The addition of the larger alkanols (dodecanol and hexadecanol) results in micelles and vesicles coexisting, and to vesicles occurring at solution compositions progressively less rich in DHDAB.



The effects of octanol addition to DHDAB/$C_{12}E_{12}$ surfactant mixtures, showing the different nano-structures formed.

Most notable, however, is the observation that the smaller alkanols (octanol and decanol) produce a transition from large polydisperse bilamellar or multilamellar vesicles to very small monodisperse unilamellar vesicles, or nano-vesicles.

These results highlight the importance of SANS in elucidating these remarkable nano-structures. These structures offer great potential for the formulation of systems in which it is important to maintain a high degree of fluidity and transport.

Exploring **protein-resistant surfaces**

MWA Skoda, **JRP Webster** (ISIS), **F Schreiber** (Tübingen University, Germany), **RMJ Jacobs** (Oxford University), **M Wolff** (ILL, France), **R Dahint**, **D Schwendel**, **M Grunze** (Heidelberg University, Germany)

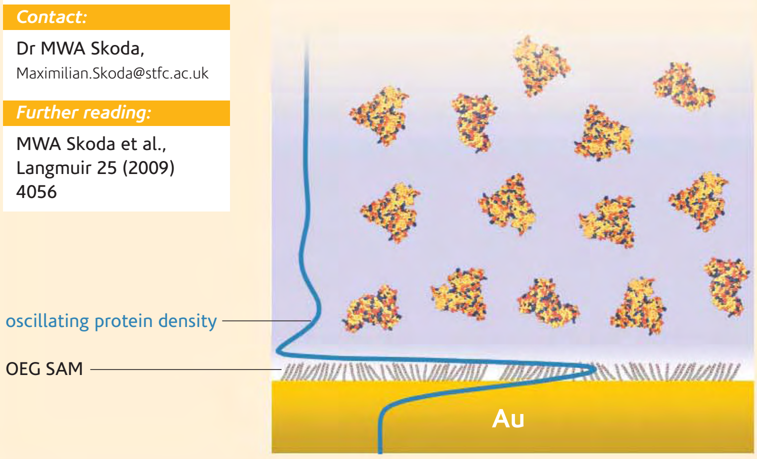
Contact:

Dr MWA Skoda,
Maximilian.Skoda@stfc.ac.uk

Further reading:

MWA Skoda et al., Langmuir 25 (2009) 4056

The study of interfaces in the fields of bio- and nanoscience, especially of interfaces between artificial and biological materials, is of tremendous importance. Oligo(ethylene glycol) (OEG) and poly(ethylene glycol) (PEG) monolayers have biotechnological applications such as biosensing, bio-compatibility (e.g. of implants) and in supporting model membranes. It has been found that these monolayers are resistant to irreversible protein adsorption, although the underlying physicochemical mechanisms for this are still under discussion. We have studied the protein density profile at the solid/liquid interface in order to obtain information about the interactions between OEG layers and proteins. Neutron reflection results reveal an oscillatory density profile for the protein solution immediately above the OEG layer. This indicates that the proteins reach the proximity of the OEG layer, but are prevented from adsorbing irreversibly, by, for instance, a strongly bound water layer. The net effect of salt was also studied and appears to be small, although charges may play a more subtle role in the complex balance of forces within this intricate system.



Protein density profile obtained from data fitting (blue line) of an OEG self-assembled monolayer (SAM) in contact with a 15 wt % bovine serum albumin protein/D_2O solution at 25 °C. The cartoon shows a snapshot of the corresponding protein layering at the interface.

Dynamics of **nanoparticles for drug delivery**

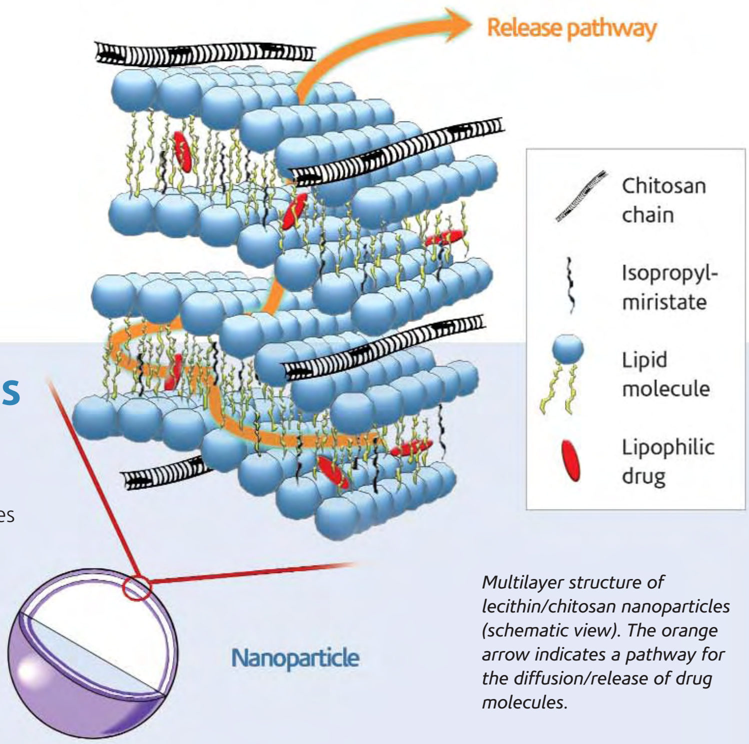
Y Gerelli, MT Di Bari, A Deriu, F Cavatorta (Università di Parma, Dipartimento di Fisica, and CNR, Italy), S Barbieri, F Sonvico (Università di Parma, Dipartimento Farmaceutico, Italy), V García-Sakai (ISIS)

Contact:

Prof A Deriu, Antonio.Deriu@fis.unipr.it

Further reading:

MT Di Bari et al., Chem Phys (2008) 239



Multilayer structure of lecithin/chitosan nanoparticles (schematic view). The orange arrow indicates a pathway for the diffusion/release of drug molecules.

Nano- and micro-particles that are composed of saccharide (sugar-like) and lipid (molecules such as fats and oils) components can be produced for potential applications as highly-biocompatible drug carriers. A detailed understanding of particle-solvent interactions is of key importance in order to tailor their characteristics for delivering drugs with specific chemical properties. For example, lecithin (a commercial mixture of different lipids) and chitosan (a positively charged polysaccharide) can be used to produce nanoparticles able to encapsulate lipophilic (fat-soluble) drugs with lower water solubility.

Using the Iris spectrometer we have investigated the local dynamics of lecithin/chitosan nanoparticles, and the effect of isopropylmiristate (IPM), a lipophilic additive commonly used to improve drug loading efficiency. The data indicate that IPM, which is fluid at room temperature, increases the mobility of the lipids with respect to pure lipid/saccharide nanoparticles by about three times. This microscopic scenario is reflected in the macroscopic kinetics of drug release: the amount of released drug in the presence of IPM is about 3 times higher than that of the same nanoparticles without IPM.

Water diffusion in **drug delivery microgels**

SV Ghugare, E Chiessi, G Paradossi (Università di Roma Tor Vergata, Italy), MTF Telling (ISIS)

Contact:

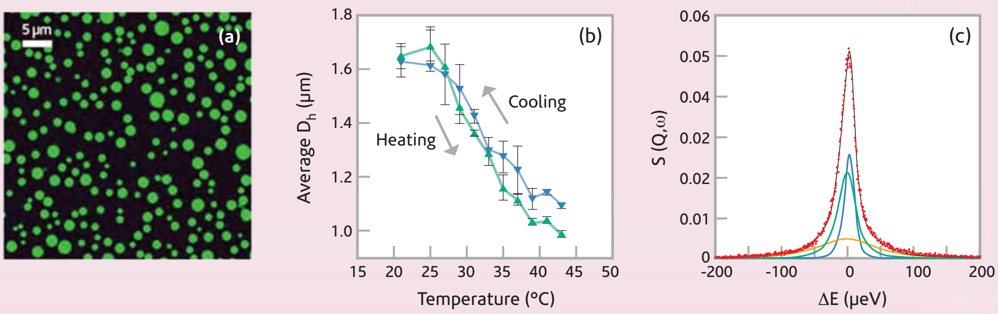
Prof G Paradossi, paradossi@stc.uniroma2.it

Further reading:

SV Ghugare et al., Biomacromolecules 10 (2009) 1589

Polymeric microgels consist of nanometer-sized spheres. The spaces inside the spheres can be filled with a pharmacologically-active material – a drug – suspended in water. Such microgels are biocompatible, and so they have promising applications as injectable drug-delivery systems. Pharmacological activity, however, is only preserved if the drug is embedded in the proper environment. The behaviour of the water and the design of the microsphere are key to providing such an environment. PVA/p(MA-co-NiPAAm) porous microgels are good candidates for controlled drug delivery since the microspheres' volume depends upon temperature – so body temperature can be used as a trigger for drug delivery. Furthermore, the drug release properties are strongly dependent upon the diffusive behaviour of the water. It is therefore necessary to characterise how water diffuses within the microgel spheres using quasi-elastic neutron scattering (QENS) in order to evaluate the diffusion characteristics of the drug itself. QENS has allowed quantitative water diffusion rates to be determined above, and below, the volume phase transition in one particular thermo-responsive microgel.

(a) Confocal micrograph of microgels, (b) Microsphere diameter vs. temperature, (c) QENS experiment on hydrated microgels at room temperature: red dots, experimental data; black line, total fit; blue line, polymer elastic contribution; green line, bound water; orange line, free water.



Superconductivity and magnetism

Symmetry breaking in superconductor $LaNiC_2$

AD Hillier, J Quintanilla (ISIS), R Cywinski (University of Huddersfield)

Contact:

Dr Adrian Hillier, adrian.hillier@stfc.ac.uk

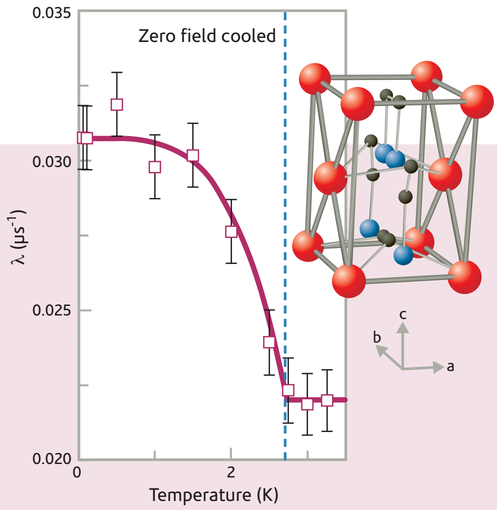
Dr Jorge Quintanilla, jorge.quintanilla@stfc.ac.uk

Further reading:

AD Hillier et al., Phys Rev Lett 102 (2009) 117007

A 'symmetry' is a property of a system which means that the system behaves in the same way even though it has undergone a change. For example, a square looks the same when it has been turned through 90°. The concept of symmetry is very important in physics, as is the idea of symmetry breaking, in which a system no longer obeys a particular symmetry. Superconductivity provides a paradigm for symmetry breaking, and in some superconductors a variety of symmetries can be broken. For example, in cuprate high-temperature superconductors, which have a layered structure with planes made of square CuO_2 'plaquettes', the 90° rotation symmetry of the plaquettes is broken on entering the superconducting state. An even more exotic possibility is failure of time-reversal symmetry in the superconducting state. This can be detected through an increase in the muon spin relaxation rate produced by the spontaneous onset of magnetic fields below T_c (such as in Sr_2RuO_4).

Non-centrosymmetric superconductors – materials whose crystal structure has no central symmetry point – are particularly interesting as the way the electrons in the material pair up in the superconducting state can take unusual forms. One example of a non-centrosymmetric superconductor is $LaNiC_2$ (critical temperature T_c=2.7K). We have shown that the muon spin relaxation rate in zero applied field increases as the material is cooled through the transition. This is the first direct proof of broken time-reversal symmetry in any non-centrosymmetric superconductor.



Crystal structure of $LaNiC_2$ and temperature dependence of its electronic relaxation rate, λ, showing magnetic fields appearing at the superconducting critical temperature (dashed line).

The unusual **properties of $SrFeO_2$**

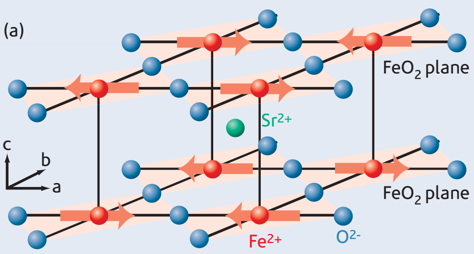
K Tomiyasu (Tohoku University, Japan), H Kageyama, Y Tsujimoto, T Watanabe, K Yoshimura (Kyoto University, Japan), JW Taylor (ISIS), A Llobet, F Trouw (LANSCE, USA), K Kakurai (JAEA, Japan), K Yamada (Tohoku University, Japan)

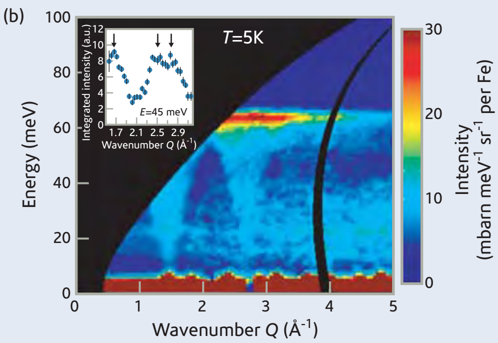
Contact:

Dr K Tomiyasu, tomiyasu@m.tains.tohoku.ac.jp

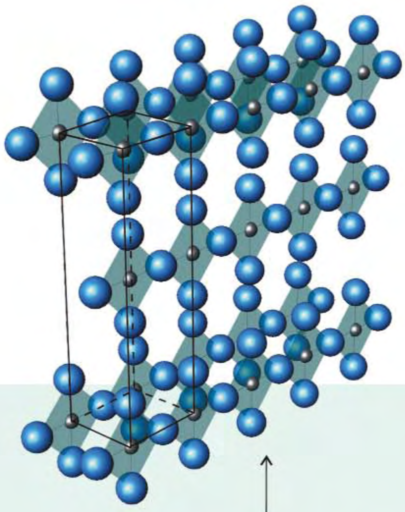
Recently, a new iron-based infinite-layer antiferromagnetic insulator $SrFeO_2$ (spin S=2) was produced. The FeO_4 square-planar arrangement in this material is very rare, because almost all iron compounds have been known to adopt three-dimensional local environments such as FeO_4 tetrahedron and FeO_6 octahedron. This unprecedented arrangement gives rise to several unexpected structural and physical properties, including a high antiferromagnetic transition temperature (473 K), stability of the novel structure and a pressure-induced transition into an intermediate spin state (S=1) accompanied by an insulator-to-metal transition.

To better understand this behaviour, we studied the magnetic excitations by inelastic neutron scattering. The results demonstrate that out-of-plane interactions are comparable to the in-plane interactions, in contrast to the cuprate (high temperature superconductor) layered compounds which have the same structure. It is therefore considered that this strong out-of-plane bonding together with in-plane bonding, explains the high transition temperature, structural stability, and intermediate spin state.





(a) Crystal and magnetic structure of $SrFeO_2$. (b) Inelastic neutron scattering intensity distribution in (Q,E) space measured at 5 K.



Bonding and magnetism in cuprates

A Walters (UCL and ISIS), TG Perring (ISIS and UCL), IA Zaliznyak (Brookhaven National Laboratory, USA)

Contact:

Toby Perring, toby.perring@stfc.ac.uk

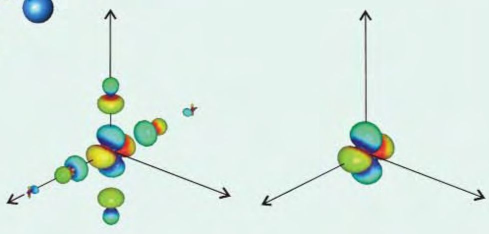
Igor Zaliznyak, zaliznyak@bnl.gov

Further reading:

AC Walters et al., Nature Physics (2009) doi 10.1038/nphys1405

The most sensitive tests of models for the magnetic interactions in materials come from detailed measurements of the magnetic fluctuations. Inelastic neutron scattering directly yields such data. The information can be separated into two parts: one part based on the spin density, and another which contains information on the spin-spin interactions.

The two components have been unambiguously separated in the one-dimensional cuprate chains in Sr_2CuO_3. The strength of the magnetic interactions in the cuprates arises from the strong mixing (hybridisation) of the copper electron orbitals with those of the oxygen atoms which lie on the line joining adjacent copper sites. Strong copper-oxygen hybridisation will alter the spin density from its normally assumed form in cuprates. This effect has generally been ignored in the analysis of high temperature cuprate superconductors – yet this experiment showed that it fully accounts for a threefold discrepancy in intensity between theory and experiment in a simple cuprate where the theory should otherwise be exact.



Copper ions (centres of the square plaquettes) form isolated chains in Sr_2CuO_3. The plots show calculated spin density isosurface (left) and that for an isolated Cu d-orbital.

Iron pnictide superconductors: **the impact of ISIS**

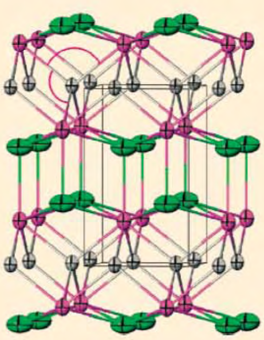
Further reading:

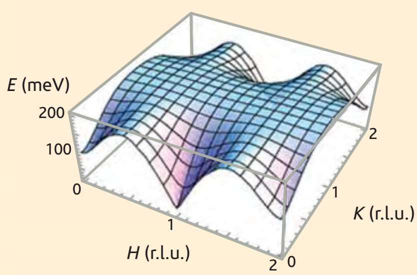
A Christianson et al., Nature 456 (2008) 930; RA Ewings et al., Phys Rev B 78 (2008) 220501(R); J Zhao et al., Nature Physics 5 (2009) 555; S Diallo et al., Phys Rev Lett 102 (2009) 187206; AJ Drew et al., Nature Materials 8 (2009) 310; MJ Pitcher et al., Chem Comm. 2008 5918; DR Parker et al., Chem Comm (2009) 2189

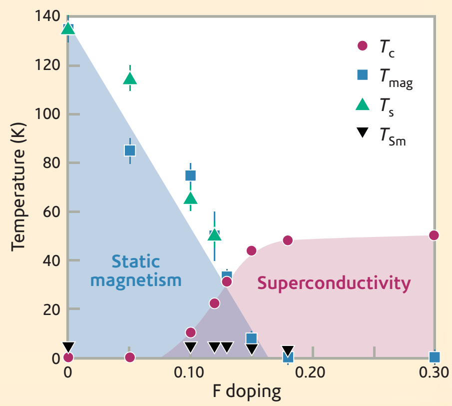
The recent discovery of superconductivity in several iron- and arsenic-based compounds with critical temperatures (T_C) as high as 55K has caused great excitement because they are the first non-copper-based high-T_C superconductors. Just like the cuprate superconductors, they are formed by doping a layered parent material, and there is strong evidence that magnetism has a central role in the mechanism responsible for the superconductivity. There are, however, many differences, and researchers are using a gamut of experimental probes to unravel the origins of the superconductivity in these materials.

Experiments performed at ISIS are making a significant impact. Muon measurements from $SmFeAsO_{1-x}F_x$ showed enhanced magnetic fluctuations near the superconducting transition, and have revealed a region of coexisting superconductivity and iron magnetism. The existence of a magnetic resonance that appears only in the superconducting phase of $Ba_{0.6}K_{0.4}Fe_2As_2$, one of another family of iron pnictides, and which is strongly reminiscent of the cuprate superconductors, was discovered on Merlin. The bandwidth of the spin fluctuations of parent materials $BaFe_2As_2$ and $CaFe_2As_2$ have been measured on Merlin and Maps, revealing excitations that extend to almost 200 meV. Such measurements help in enabling a detailed model of the magnetic behaviour to be produced. Finally, examples of structural studies are those on the oxygen-free iron pnictides LiFeAs and NaFeAs, which show superconductivity without doping.

Structure of LiFeAs (Pitcher et al); spin waves in $CaFe_2As_2$ from magnetic exchange parameters measured on Merlin (Zhao et al); phase diagram of $SmFeAsO_{1-x}F_x$ (Drew et al).







A variety of technologies – man-made and natural!

Catalysts revealed

P Albers (AQura, Germany), **SF Parker, DT Bowron, S Imberti, AK Soper, K Refson** (ISIS)

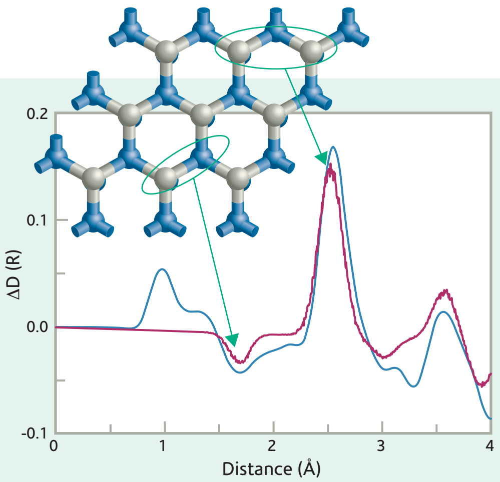
Contact:

Dr SF Parker,
stewart.parker@stfc.ac.uk

Further reading:

SF Parker et al, Angew Chemie, submitted.

Heterogeneous catalysis (catalysis where the catalyst is in a different phase from the reactants – e.g. a solid catalyst and gaseous reactants) is a key economic driver in advanced nations. It is integral to processes that range from crude oil refining to fine chemical and pharmaceutical production. Knowledge of the adsorbed species on the surface of a heterogeneous catalyst is an essential component in understanding and optimising a catalyst's performance. Real catalysts are generally nanocrystalline and there are no experimental methods available for structure determination of hydrogenous adsorbed species on such materials. We have used neutron diffraction to show that it is possible to obtain structural information for adsorbed hydrogenous species on real catalysts as opposed to idealised systems under ultra-high vacuum. Bond distances are directly obtainable from the experimental data and the method works at room temperature in the presence of 1 bar of reactive gas. The method is completely general: it is applicable to any heterogeneous catalyst whether amorphous or nanocrystalline, a metal or an oxide.



Determination using Sandals of the surface structure of hydrogen adsorbed on Raney nickel, a commonly used hydrogenation catalyst. The arrows highlight the Ni–H distance of 1.68 Å and the H·····H distance of 2.54 Å in both the experimental data (blue) and an ab initio calculation (red).

Spinning a story:
silk at the molecular level

C Dicko, I Diddens (Oxford University), **AE Terry, MTF Telling** (ISIS), **F Vollrath** (Oxford University)

Contact:

Dr Cedric Dicko,
Cedric.dicko@zoo.ox.ac.uk

Further reading:

C Dicko et al., Biomacromolecules 9 (2008) 216

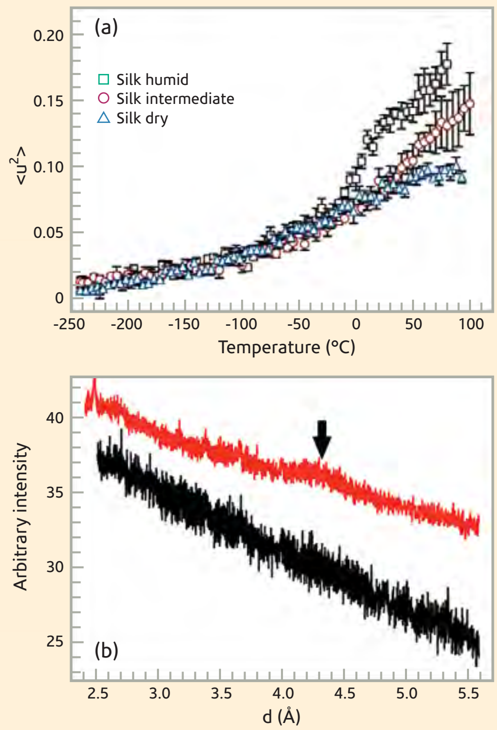
Spiders and insects have achieved what many industries and labs yearn to accomplish: the controlled assembly in water of large proteins into high performance fibres, all at ambient temperature and pressure.

The formation of silk fibres by both spiders and silkworms is characterised by a conversion of disordered proteins to sheet structures (known as β-sheets), followed by assembly into fibres.

It has been hypothesised that the interplay of water and silk proteins' structural flexibility is key to this transition. To test this hypothesis, we have used quasi-elastic neutron scattering to investigate the effect of hydration on silk protein dynamics.

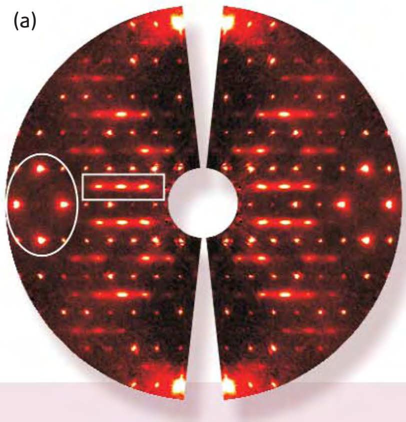
During the experiment we monitored simultaneously the evolution of structure β-sheet crystallinity) and polymer chain dynamics with increasing temperatures. We found that low and high hydration levels prevent structural conversion, whereas intermediate water content promotes β-sheet conversion.

The results suggest that a clever control of local fluctuation may be the key to enabling and/or inhibiting silk protein conversion and consequently their assembly into fibres.

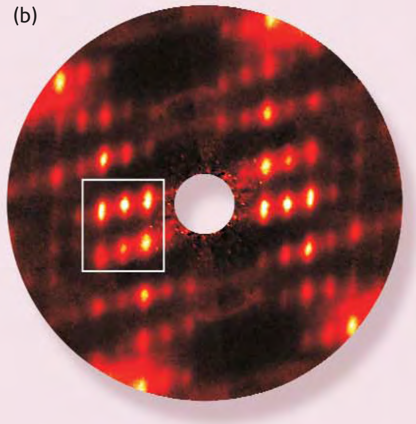


(a) Effect of increased hydration on the bulk motion (mean square displacement) of silk proteins films. (b) Neutron diffraction spectrum taken before (black) and after (red) conformational change. The Bragg reflection at 4.3 Å is evidence of regular spacing between the strands of the protein sheet structures.

(a)



(b)



How do **molecular crystals** form?

DJ Goossens (Australian National University), **MJ Gutmann** (ISIS)

Contact:

DJ Goossens, goossens@rsc.anu.edu.au

Further reading:

DJ Goossens and MJ Gutmann, Phys Rev Lett 102 (2009) 015505

How does the ordering in a crystal arise from the interactions present? Solving the structure shows what the structure is, but not how it arises. Such information is crucial in trying to predict crystal structure from the chemistry of the molecule, a long-held aim in pharmaceutical research. The influence of a molecule on the positions of its neighbours results in broad scattering features in a neutron diffraction pattern known as diffuse scattering. By modelling this scattering it is possible to determine the key molecular interactions and cooperative molecular motions and how these lead to the ordering of the molecules. We used diffuse scattering measured on SXD to examine the intermolecular interactions in deuterated *para*-terphenyl, $C_{18}D_{14}$ (D means the hydrogen has been replaced by its heavier isotope, deuterium). It was found that intramolecular and intermolecular interactions, and the molecules themselves, can be thought of as acting as nanoscale mechanical linkages.

Maps of diffuse scattering in the (a) hk0 and (b) $h\frac{1}{2}l$ planes of para-terphenyl. Key features that relate to the molecular ordering have been highlighted.

This work shows that we can use the analysis of diffuse scattering to build up a picture of how molecular interactions lead to molecular ordering.

Driving future accelerators: **first beam for the FETS project at ISIS**

M Bates, MA Clarke-Gaythor, DC Faircloth, DJS Findlay, T Knott, SR Lawrie, AP Letchford, M Perkins, P Romano, M Westall, M Whitehead, P Wise, T Wood (ISIS), **FJ Bermejo** (Bilbao, Spain), **J Lucas** (Elytt Energy, Madrid, Spain), **J Alonso, R Enparantza** (Fundación Tekniker, Elbr, Spain), **SMH Al Sari, S Jolly, A Kurup, DA Lee, P Savage** (Imperial London), **J Pasternak, JK Pozimski** (Imperial College London, ISIS), **C Gabor, C Plostinar** (ASTeC), **JJ Back** (Warwick University)

Contact:

Dr Dan Faircloth, dan.faircloth@stfc.ac.uk

Further reading:

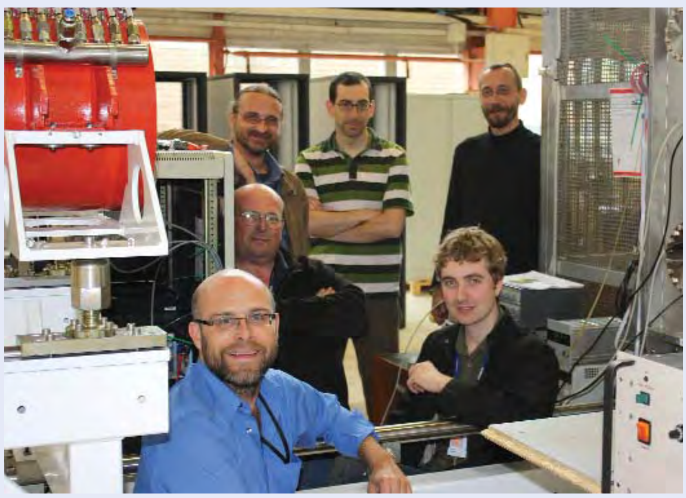
DC Faircloth et al., Proceedings of PAC09 Vancouver, April 2009

In April 2009 the Front End Test Stand (FETS) came to life when the ion source produced its first beam. FETS is being developed as a new high power injector for the particle accelerators of the future. It will produce a perfectly chopped 50 Hz ,60 mA, H^- beam at 3 MeV with a 10% duty factor. Its applications are many and include ISIS upgrades, a neutrino factory and nuclear waste transmutation.

FETS is a collaboration between STFC, Imperial College, Warwick University, The University of the Basque Country and Tekniker. It consists of a high current H^- ion source, a three-solenoid magnetic Low Energy Beam Transport (LEBT), a 324 MHz, 3 MeV, 4-vane Radio Frequency Quadrupole (RFQ), a very fast beam chopper and a comprehensive suite of diagnostics.

The ion source and laser diagnostics have been commissioned, and the LEBT will now be installed, followed by the RFQ and chopper.

Members of the FETS collaboration after the first beam was produced.



ISIS users at work

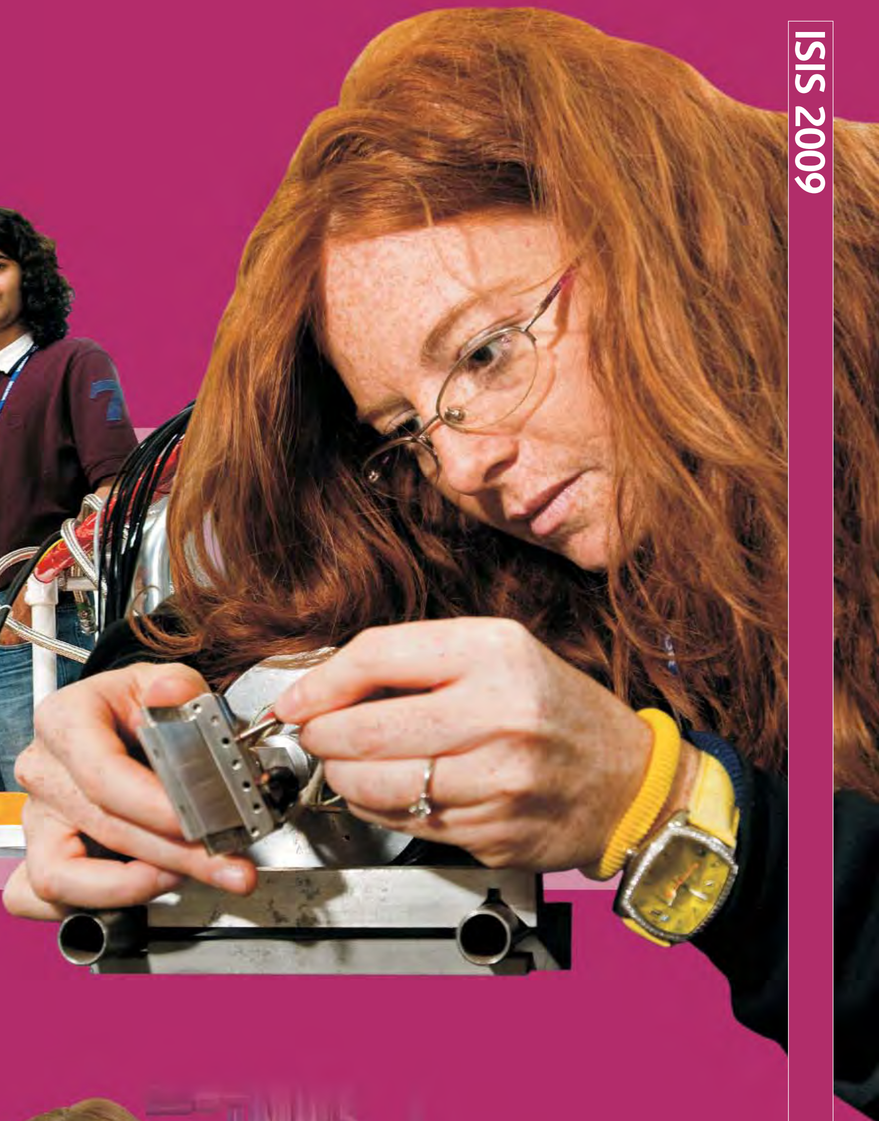
▲ Craig Brown (NIST, USA) preparing to study hydrogen interactions in metal-organic framework structures on Tosca. **09EC2738**

▲ Helena Alberto and Joao Pedro Duarte (Coimbra University, Portugal) preparing the EMU muon spectrometer to investigate phthalocyanine organic semiconductors. **09EC2746**

▼ Nikolay Vasiler (Lancaster University) at ISIS during his neutron reflectometry studies of a ^{3}He layer adsorbed on to liquid ^{4}He on Crisp. **09EC2732**

▲ Xiubo Zhao, Donghui Jia and Fang Pan (Manchester University) looking at their Surf data during studies of the effect of hydrophobic chain length on the interfacial structure of peptide surfactants. **09EC2736**

▶ Lorna Dougan (Leeds University) loading her sample for Sandals studies of hydrogen bonding in glycerol at low temperatures. **09EC2771**



▲ *Fsolt Gercis, Alex Barcza, Karl Sandeman and Rantej Bali (Imperial College London and University of Cambridge) using Gem to study giant magnetostriction in CoMnSi.* **09EC2739**

▶ *Alessia Giuliani (Università degli Studi Roma Tre, Italy) using Sandals for structural characterisation of water confined in an MCM silica matrix.* **09EC2758**

◀ *Sue Kilcoyne (Salford University) loading a sample on MuSR for studies of moment stability and spin fluctuations in ferromagnetic Au_4V.* **09EC2774**

◀ *Stefan Knupfer (Heriot Watt University) preparing his sample for residual stress characterisation of laser-formed aluminium plates on Engin-X.* **09EC2780**

▲ *Neil Hamilton, Andrew McFarlane and Ian Silverwood (Glasgow University) using MAPS to investigate reactions relevant to Fischer-Tropsch catalysis used for hydrocarbon production.* **09EC2742**

Developments and events

Section 2
Developments and events

Development at ISIS is a continuous process, driven in response to the changing needs of the user community and to maintain ISIS as a world-class neutron and muon source. Evolution of existing instruments and construction of new ones, together with advances in neutron and muon techniques, provide fresh opportunities for materials investigations.

The past year has seen first experiments on Second Target Station instruments, a very significant project achievement. Other technique and instrument developments to enable new science are also described, together with developments of the accelerator and target systems.

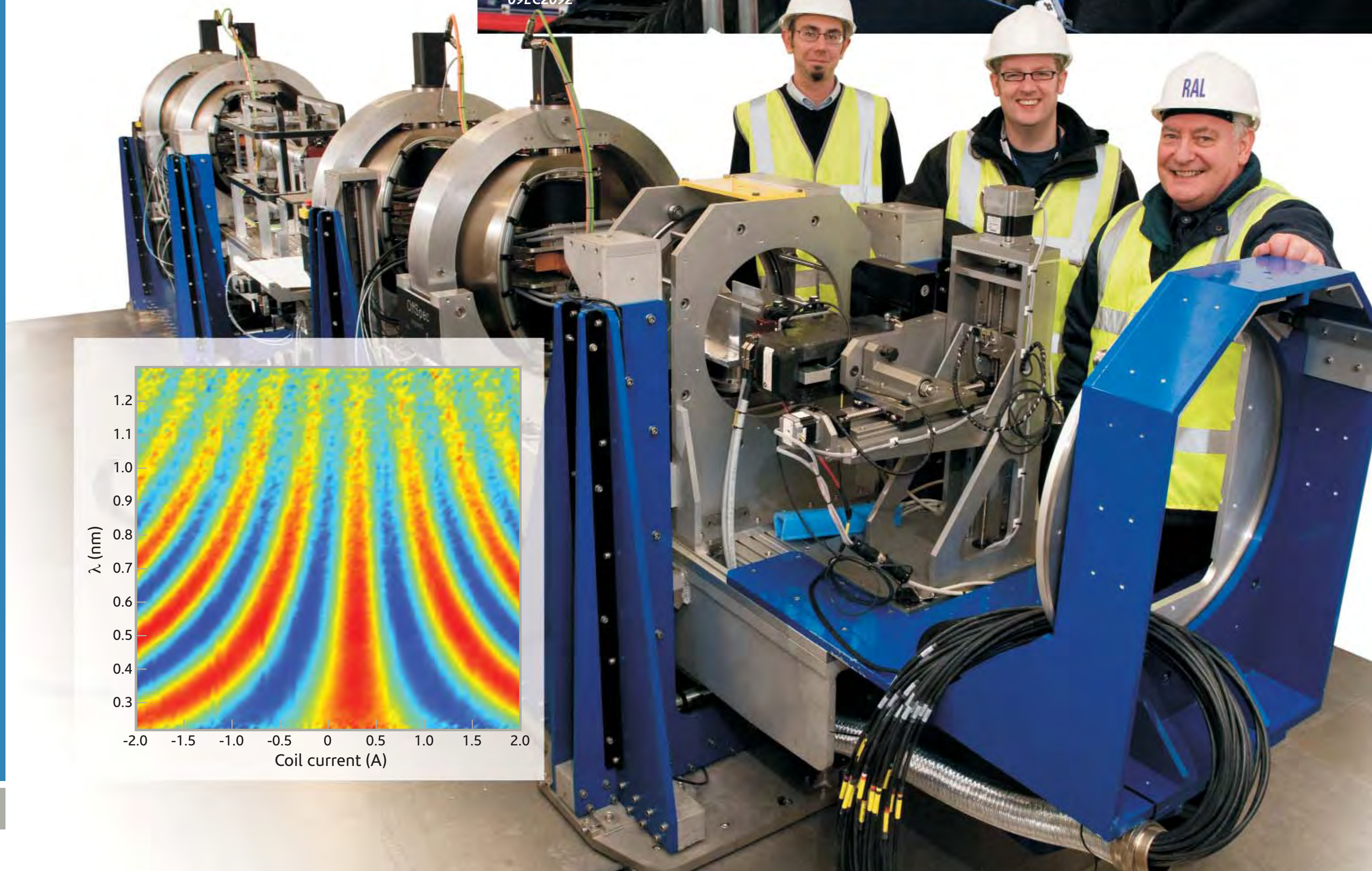
Also highlighted are some of the many training and education activities run by ISIS over the past year – from courses and workshops for the user community to projects run with schools and professional development of facility staff.

Second Target Station instruments shine!

This year has seen first science being done on Second Target Station instruments. And the instruments are more than living up to expectations!

Inter science: **the first Second Target Station experiment**

Bob Thomas (Oxford University) using the Inter reflectometer during the first experiment on the Second Target Station. ***09EC2092***

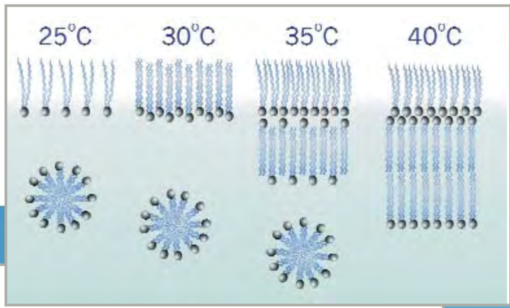


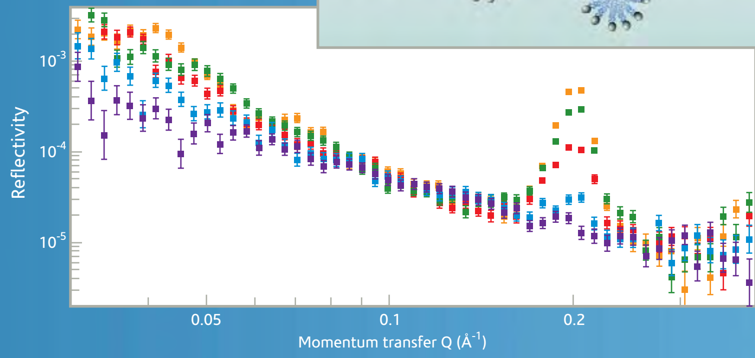
▼ *Nick Webb, Rob Dalgliesh and Richard Coleman (ISIS) with Offspec.* ***08EC4980*** *Inset: Offspec spin-echo data from a grating sample.*

On 26 May 2009 Inter opened its doors to the first TS-2 users: Jeff Penfold (ISIS) and Robert Thomas (Oxford).

Surfactant and polymer-surfactant mixtures can spontaneously form multilayer structures at interfaces. Such systems are relevant to areas such as soft lubrication, encapsulation, surface delivery and retention, and in understanding bio-lubrication (for example, lung surfactants).

This experiment used the power of Inter to explore the kinetics of formation and dissolution of such multilayer structures. A specially designed trough allowed the disassembly of the surface structure to be followed as it progressed in real time.





Inter enabled measurements to be made at time intervals as short as two minutes (with sub-minute measurements predicted for the future).

These results demonstrate the ability to follow the kinetics of such processes and open up an exciting new area of science that has been hitherto inaccessible.

Inter reflectivity data from a 2 mM sodium dodecyl benzene sulfonate (anionic surfactant) solution in 2 mM $CaCl_2$. The characteristic Bragg scattering associated with surface multilayers can be seen, together with its decrease in visibility as the surface structure disassembles towards a surface monolayer.

Inset: spontaneous formation at an interface of a multilayer structure by a polymer-surfactant mixture.

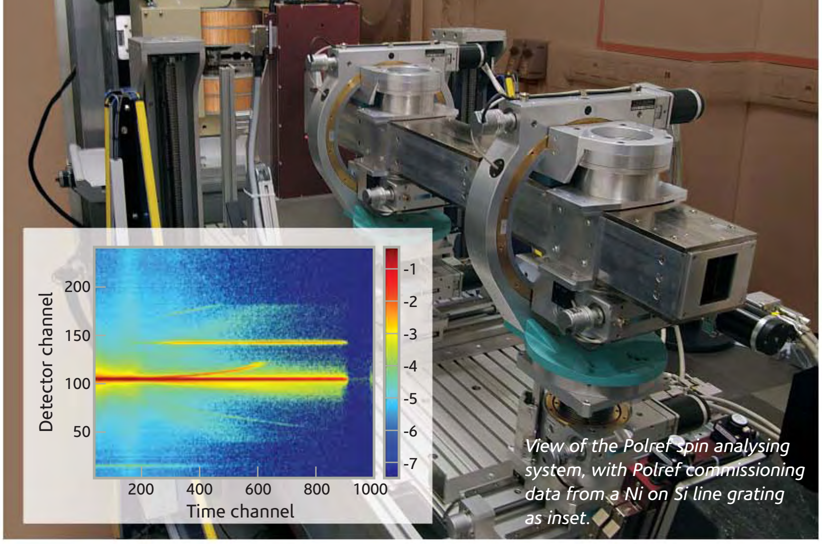
Courtesy Jennie Tucker of J T Designs

Offspec

Offspec has successfully demonstrated several of its modes of operation including spin-echo small angle neutron scattering and spin-echo resolved grazing incidence scattering. The complex series of spin manipulation (precession) devices which have been developed at TU Delft are working well and have allowed Offspec to access length scales that were previously unobtainable in traditional reflectometry. Commissioning of the remaining modes is making strong progress alongside the start of the user programme.

Polref

Polref is now into its commissioning programme. The reflectometer incorporates a polariser guide field and spin analyser for magnetic studies. This will be complemented by the imminent arrival of a three dimensional 2 T vector cryomagnet.

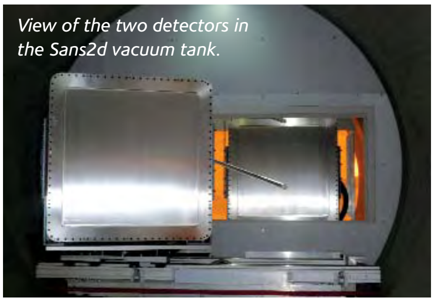


View of the Polref spin analysing system, with Polref commissioning data from a Ni on Si line grating as inset.

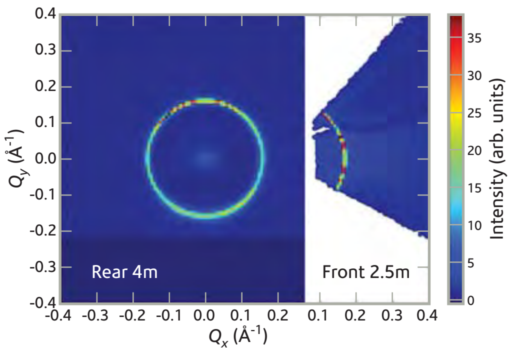
Second Target Station instruments shine!

Sans2d

First neutrons were delivered to the Sans2d sample position at the end of March and then on 30 May, to the main detectors in the 13m long, 3.25m diameter vacuum tank. Results are very encouraging and suggest that the increase in flux over the existing Loq instrument is as expected. As a first user experiment, Prof Rob Richardson (Bristol) has studied the temperature dependence of liquid crystalline polymer Bragg peaks. The data demonstrate the extremely wide simultaneous Q range available on Sans2d with the two 1m square detectors.



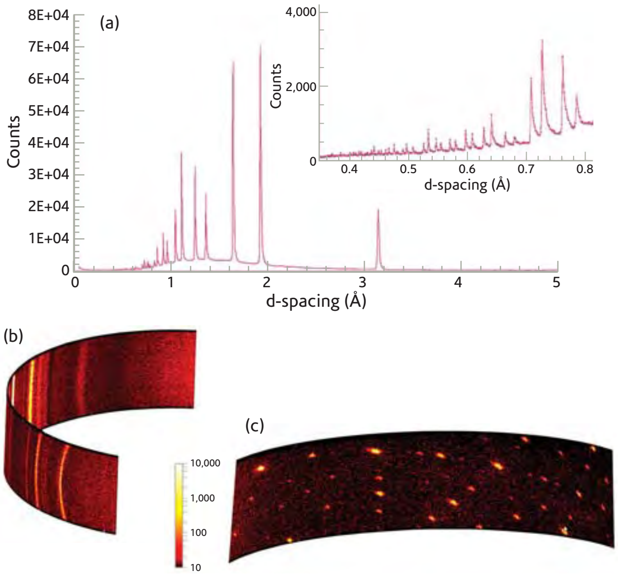
View of the two detectors in the Sans2d vacuum tank.



Initial Sans2d data from a liquid crystalline polymer.

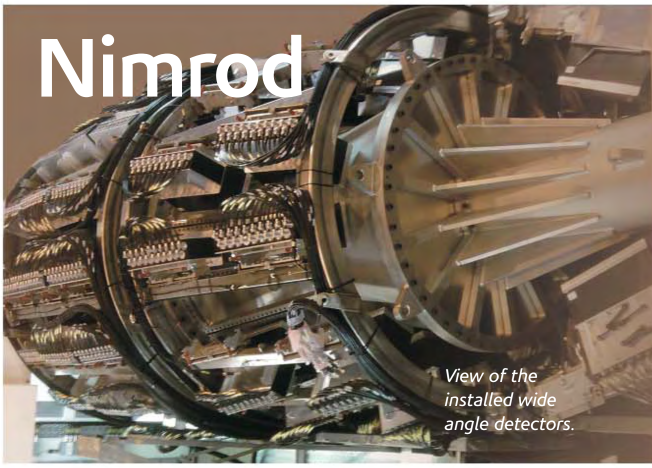
Wish

The Wish instrument opened its shutter for the first time at the end of March, and has run with a liquid methane moderator in the following cycles. Wish has been producing high-quality data from the start, with the doubly-focusing elliptical guide generating the expected high count rate. The detector array on one side of the instrument is fully operational, with the 100,000 pixels, each with 5,000 time bins, generating 1.6 Gb of data per run. Calibration of the detector linear positions is currently underway and is the final milestone before the user program starts. A 14 T magnet has been delivered and is soon to be tested on the instrument.

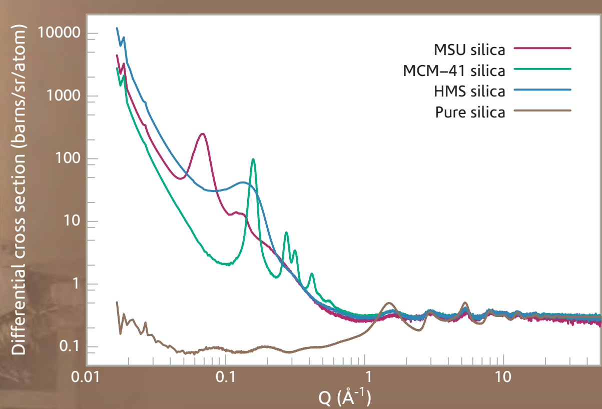


a) First diffraction pattern obtained on Wish, from a Si sample with the liquid methane moderator. b) Debye-Scherrer cones on the cylindrical detector array. c) First experiment with a single crystal of $BaMnF_4$ (sample courtesy of Dr. Bombardi, Diamond Light Source).

Nimrod



View of the installed wide angle detectors.



LET

LET is a chopper spectrometer with π steradians of detector coverage that is almost gap-free by virtue of using the world's first 4 m long position-sensitive detectors. A complex chopper system involving 7 disks ensures the maximum flux with a clean beam and full control of the energy resolution. LET opened its shutter for neutrons for the first time on the 5 August. Initial measurements show a neutron flux which is close to that predicted by simulations. Results from the detectors are excellent with a 20 mm position resolution. Over the coming months the remaining chopper housings will be put in place and more detectors added.

John Hogg (ALSTEC) working inside the LET vacuum tank. The frames that can be seen on the back will support a wall of 4 m long detectors.
08EC4125

The Nimrod diffractometer has begun commissioning. Eighteen ZnS scintillator neutron detectors are currently installed at scattering angles 5°-40°, and a low angle bank of 756 detectors cover the angle range 0.5°-2°. Initial results are extremely encouraging, with data being observed which arguably gives Nimrod the widest Q range accessible in a single experiment of any diffractometer in the world.

◀ *Normalised diffraction data measured on Nimrod for several amorphous silicas with a range of pore sizes, compared to pure silica glass. The very large rise in scattering of the porous silicas at low Q compared to pure silica is caused by their different pore structures combined with surface scattering effects at the lowest Q values.*

New science from instrument and technique advances

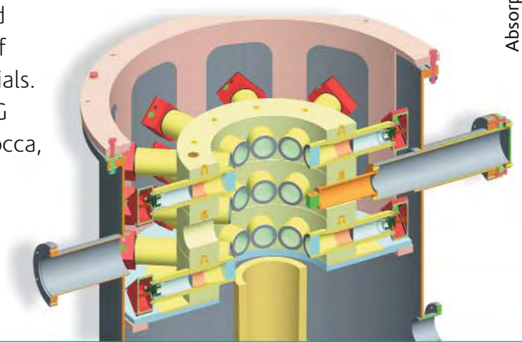
As well as larger instrument developments, advances in techniques or in other experimental equipment also enable new science to be done using neutrons and muons at ISIS.

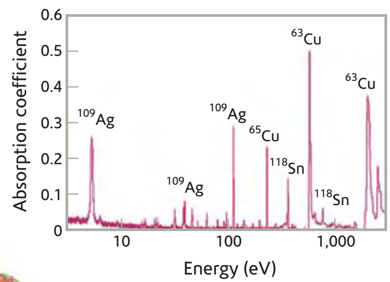
Making supercritical CO_2 thicker

A new Thar pressure cell has been used to great effect on Loq. The improved efficiency of the cell has allowed Eastoe et al., (Bristol), to study designer, low-cost hydrocarbon surfactants as fluid modifiers for supercritical carbon dioxide (sc-CO_2). Small angle neutron scattering has shown these surfactants form hydrated reverse micelles in sc-CO_2 which could be used to unlock the full potential of CO_2 as a green solvent (MJ Hollanby et al., Angew Chem Int Ed 48 (2009) 4993).

Spectroscopic neutron analysis facility for archaeological objects

A new facility based on neutron resonance capture analysis (NRCA) and neutron resonance transmission (NRT) has been installed at ISIS. This is part of the EU Ancient Charm project, which aims to develop science research techniques for cultural heritage objects. NRCA and NRT use epithermal neutrons for non-destructive bulk analysis and for mapping of elements in archaeological objects. The equipment can potentially be used also for cross section measurements of reference materials and nuclear materials. This work is a collaboration between G Gorini and E Perelli Cippo (Milano-Bicocca, Italy), P Schillebeeckx (IRMM Geel, Belgium), and W Kockelmann and E Schooneveld (ISIS).

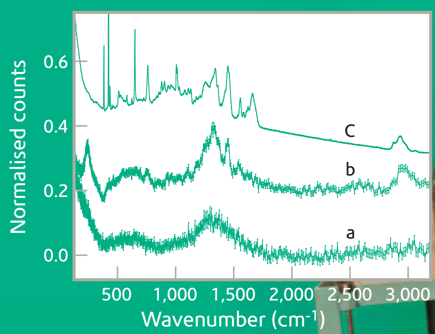


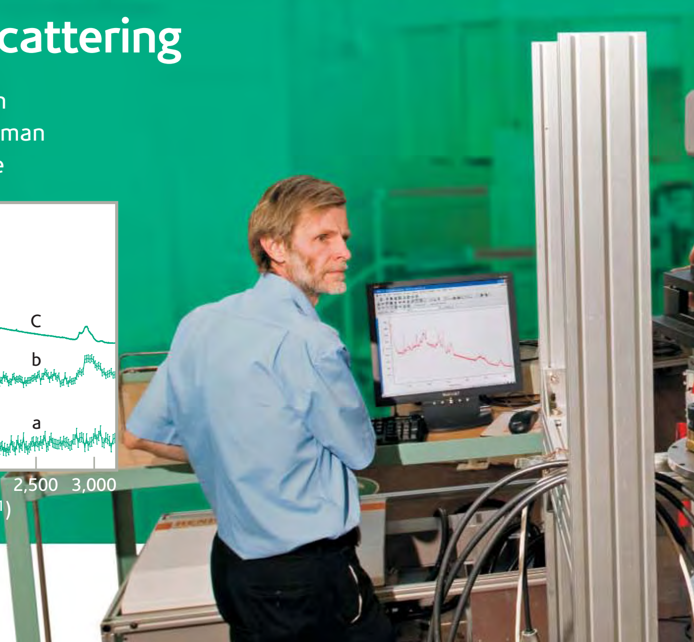


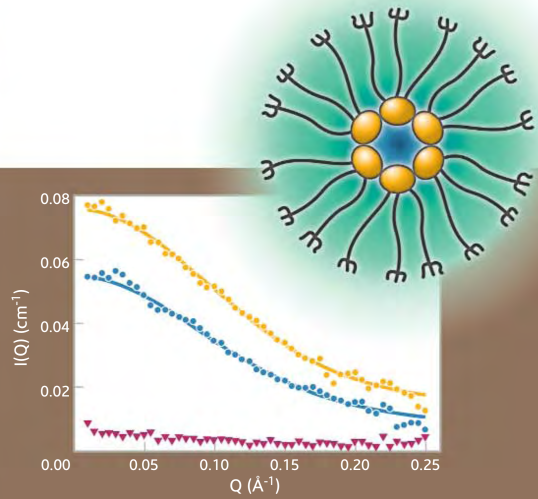
Schematic of the neutron resonance capture and transmission detectors for the INES instrument. The graph above shows a neutron resonance transmission pattern measured on a copper alloy standard.

Simultaneous neutron and Raman scattering

ISIS now has the capability to make simultaneous neutron and Raman scattering measurements at temperatures between 1.5 and 450 K. Raman measurements with a resolution of 1-4 cm^{-1} can be made over a wide wavelength range (100-3200 cm^{-1}) at the same time as a variety of neutron scattering measurements. The new equipment has been used for inelastic neutron scattering and neutron diffraction in conjunction with Raman for studies of the globular protein lysozyme (MA Adams et al, Applied Spectroscopy 63 (2009) 727).



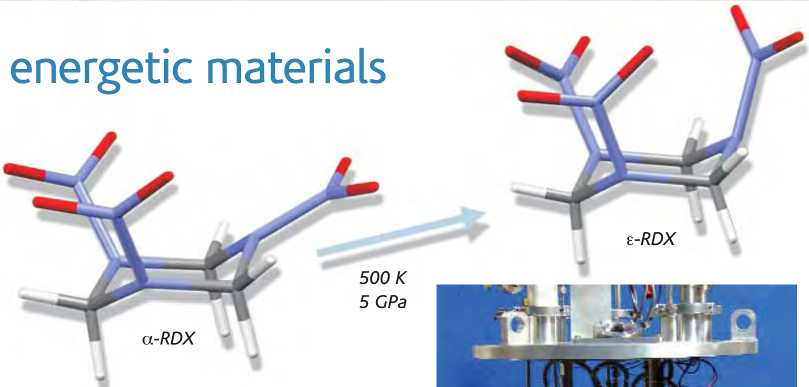


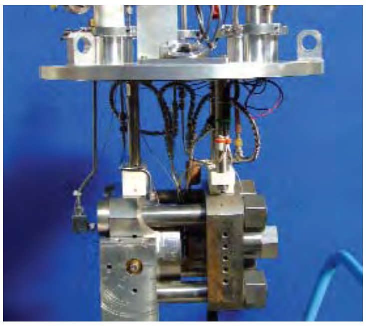


◀ Sarah Rogers (ISIS) preparing the new Loq pressure cell. **08EC2300**
The graph shows small angle scattering profiles of dry (blue circles) and hydrated micelles (yellow circles) stabilised in sc-CO_2 by the surfactant TC14. The scattering obtained (triangles) when using the surfactant AOT_4 is also shown for comparison. The inset shows a schematic representation of a hydrated reverse micelle in sc-CO_2.

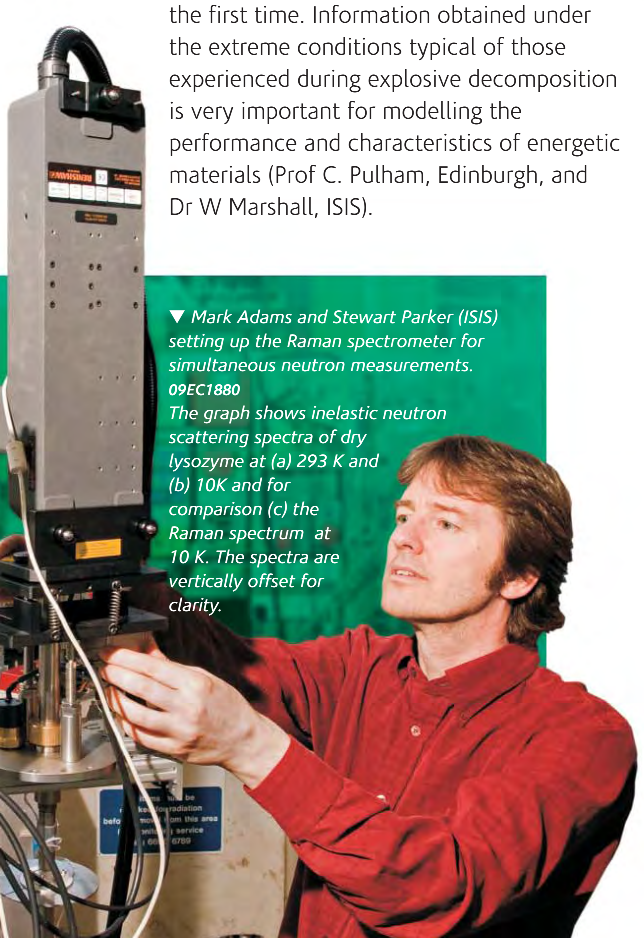
Putting the squeeze on energetic materials

The recent development of a compact variable temperature insert for the Paris-Edinburgh pressure cell has allowed study of the high-pressure, high-temperature structural behaviour of the widely used explosive RDX. The structures of three forms of this material have been characterised for the first time. Information obtained under the extreme conditions typical of those experienced during explosive decomposition is very important for modelling the performance and characteristics of energetic materials (Prof C. Pulham, Edinburgh, and Dr W Marshall, ISIS).





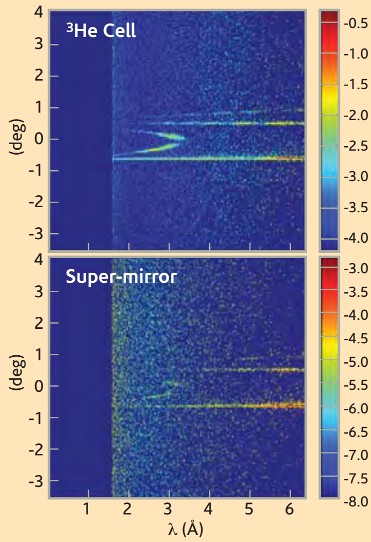
▶ *The Paris-Edinburgh pressure cell equipped with the compact variable-temperature insert. The cell allowed observation of the molecular conformation change when the alpha-form of RDX is transformed into the epsilon-form at high pressure (5 GPa) and temperature (500 K).*



▼ *Mark Adams and Stewart Parker (ISIS) setting up the Raman spectrometer for simultaneous neutron measurements.* **09EC1880**
The graph shows inelastic neutron scattering spectra of dry lysozyme at (a) 293 K and (b) 10K and for comparison (c) the Raman spectrum at 10 K. The spectra are vertically offset for clarity.

New ^{3}He analyser

▶ *A polarised ^{3}He cell has been developed at ISIS for neutron spin flipping and analysis. The ^{3}He analyser produces a better signal-to-noise ratio compared with a supermirror analyser for off-specular reflectivity data. Here we see a comparison between polarised neutron scattering data taken on Crisp with the ^{3}He cell and with a supermirror analyser from a 2.5μm pitch Ni grating.*



New science from instrument and technique advances

Detectors, computing and electronics for instrument developments

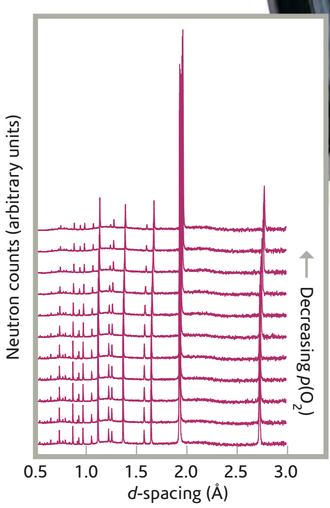
New instrument developments provide a variety of challenges for the ISIS Detector, Computing and Electronics groups.

For example, the new TS-2 reflectometers have complex motion control environments and require many motors to be moved precisely and in harmony for optimal experimental conditions. Control software has had to be developed, using the National Instruments LabVIEW package.

▲ *Freddie Akeroyd (ISIS) developing data acquisition software for ISIS instruments.* ***08EC4166***

A flow-through quartz cell with gas flow control system

A flow-through quartz gas cell, together with its complementary flow control and monitoring system, has been developed by ISIS in collaboration with Chalmers University of Technology, Sweden. This equipment allows neutron powder diffraction data to be collected on samples at temperatures up to around 1300 K when exposed to mixtures of O_2, Ar, CO_2 and CO. For example, the cell has been used to probe the crystal structure of $CeO_{2-\delta}$, which has applications in solid oxide fuel cells, as a function of oxygen partial pressure.



The flow through quartz gas cell, together with the evolution of the neutron powder diffraction pattern of $CeO_{2-\delta}$ measured at 1273K on decreasing oxygen partial pressure (S Hull et al., J Sol Stat Chem (2009)).

Hifi magnet installed

Hifi is a new high-field muon spectrometer in commissioning at ISIS. This year has seen completion of all major project elements, including delivery of the main 5T magnet (seen here being installed). First experiments are scheduled for the end of 2009. ***09EC2912***

X-ray diffraction for disordered materials

The ISIS Disordered Materials Group are now running a laboratory X-ray diffractometer, optimised for structural studies of liquids, glasses and disordered crystals. The aim is to provide X-ray diffraction data which will complement the data obtained

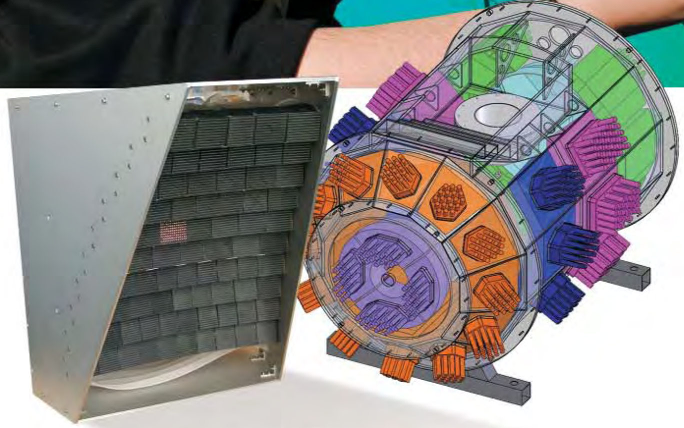
The Wish instrument has been a different sort of challenge. Its 389,125 pixels were too numerous for a single data acquisition crate and so a system for parallel access to acquisition crates was developed. The data volumes and memory requirements involved were also reaching the limits for 32bit operating systems, so a 64bit version of the acquisition software has been developed.

◀ *The first operational detector panel for the Wish instrument after testing, with members of the ISIS detector group involved in its production: Nigel Rhodes, Davide Raspino, Erik Schooneveld and Matt North.* ***08EC4976***

Kathryn Baker (ISIS) working on experiment control software for Inter. ***08EC4175***

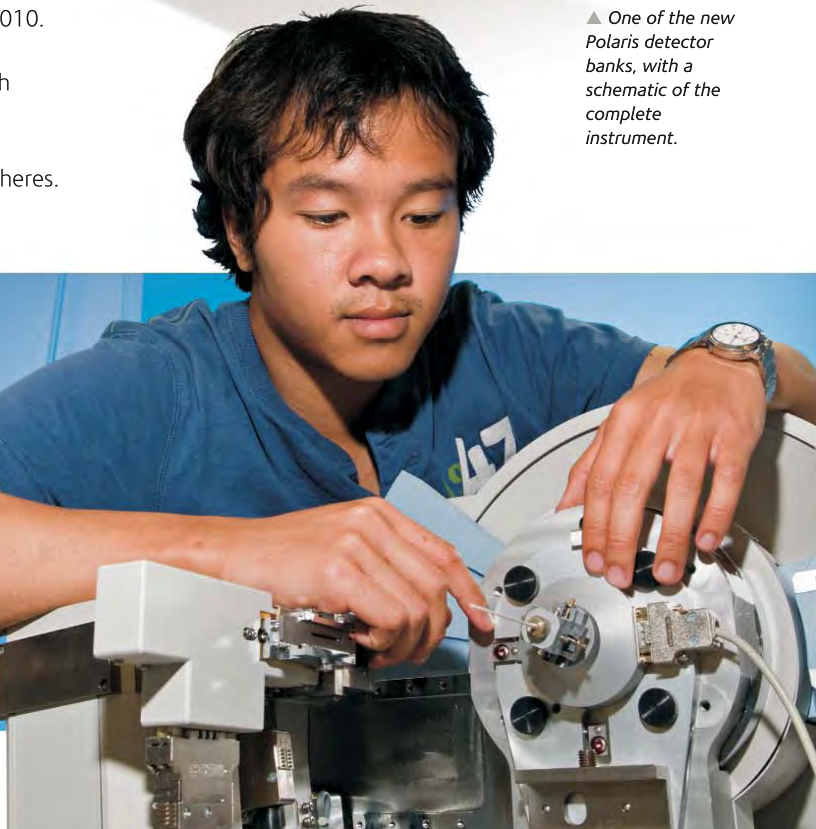
Polaris upgrade

A major upgrade programme for the Polaris diffractometer is currently in progress. This project, funded by STFC with contributions from Spanish and Swedish partners, will provide increases in count rate of between 4x and 20x (depending on the scattering angle), coupled with significant improvements to the instrumental resolution at backscattering angles. Installation of the new instrument is planned for 2010. New sample environment equipment is also being developed, with funding from the Swedish research council, including in-situ cells for studies of electrochemical processes and time-resolved investigations of samples under controlled atmospheres.



▲ *One of the new Polaris detector banks, with a schematic of the complete instrument.*

on the group's neutron diffractometers, Gem, Nimrod and Sandals, by virtue of the different contrasts for the two radiations. Currently the diffractometer is nearing the end of a period of scientific commissioning, after which it will be available for approved disordered materials experiments by ISIS users.



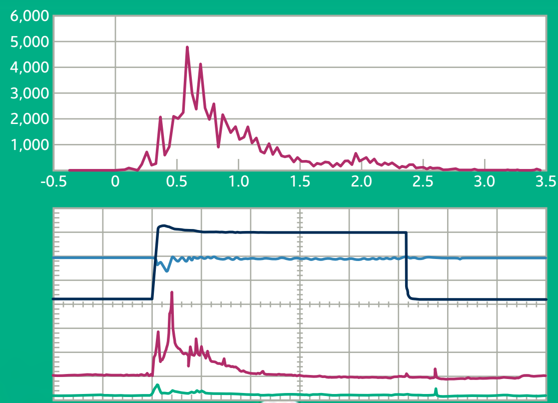
▶ *Nattapol Laorodphan (Warwick University) preparing the new X-ray diffractometer.* ***09EC2792***

Accelerator and Target developments

Higher beam currents at ISIS!

Sustained beam currents of 230 μA have been produced during ISIS run cycles this year, meaning that ISIS can deliver the same number of protons to TS-1 whilst also supplying TS-2. The secret is reducing beam loss in the synchrotron.

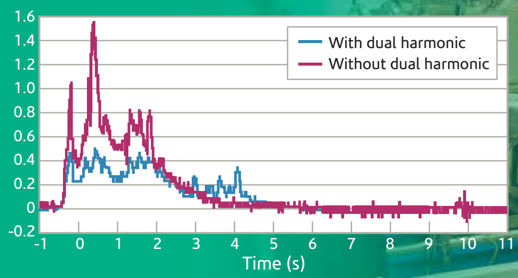
▶ *The performance of the ISIS accelerators is limited by the amount of beam that is lost during the acceleration cycle. Simulation studies (top) can be compared with measured (bottom) beam loss in the synchrotron to better understand the causes of beam loss.*



▲ *The three beamline choppers for Wish ready for installation, with team Mike Brind, Paul Chorley, Erik Johnson, Peter Galsworthy and Adam Davis (ISIS).* ***09EC1003***

▼ *The Second Target Station target, reflector and moderator assembly being prepared.* ***08EC3270***

▶ *Robin Burridge (ISIS) inspecting a newly-installed cabinet of radiation monitors for TS-1's services area. The monitor heads are positioned around the services trolley to detect any changes in background levels and to highlight any fluctuations within the $D_2$0 water cooling circuits during operation.* ***09EC2045***



▲ *The ISIS synchrotron dual harmonic system – which consists of four new accelerating cavities inserted into the accelerator – enables beam intensity to be increased by reducing proton beam loss. The figure shows beam loss with and without the dual harmonic system in operation.*

A dual harmonic accelerating cavity in the ISIS synchrotron. ***09EC1467***

Steve West (ISIS) inspecting the new synchrotron main magnet power supply chokes during installation in May. ***09EC2456***

◀ *Final preparations being made on the new tungsten neutron target and reflector assembly prior to its first operational run in May. This work was undertaken within the remote handling cell via two pairs of master/slave manipulator arms positioned either side of the target and moderator assembly.* ***09EC2037***

▲ *Mike Ruddle (ISIS) in front of new buffer tanks for the first target station cryogenic moderators. Each has a capacity of 2000 l. Five are used to hold methane following the daily transfer, with the sixth for any gas vented from the hydrogen system.* ***09EC2030***

▲ *ISIS Duty Officer Tom Noone keeping a watchful eye on accelerator parameters.* ***08EC4205***

▶ *Dan Faircloth (ISIS) inspects ISIS ion sources. An ion source typically lasts 20 to 30 days before needing to be replaced, and a collection of ten sources, which are made at ISIS, is kept ready to be used.* ***08EC4248***

A year around ISIS

A farewell to old friends!

As new TS-1 and TS-2 instruments come on-line, ISIS bids farewell to instruments that are being replaced by the next generation of spectrometers and diffractometers. This year saw final beam on HET and Prisma after many years of sterling service.

▼ *(left to right) Pascal Manuel (ISIS), Carla Andreani (University of Rome Tor Vergata, Italy), Uschi Steigenberger, Martyn Bull and Steve Payne (ISIS) celebrate Prisma's successes following the final experiment on the instrument.* **08EC5089**

▶ *Professor Keith McEwen and Dr Helen Walker (University College London) and Devashibhai Adroja (ISIS) explored the crystal field levels in the rare earth tetraborides during the final experiment on HET in October.* **08EC4348**

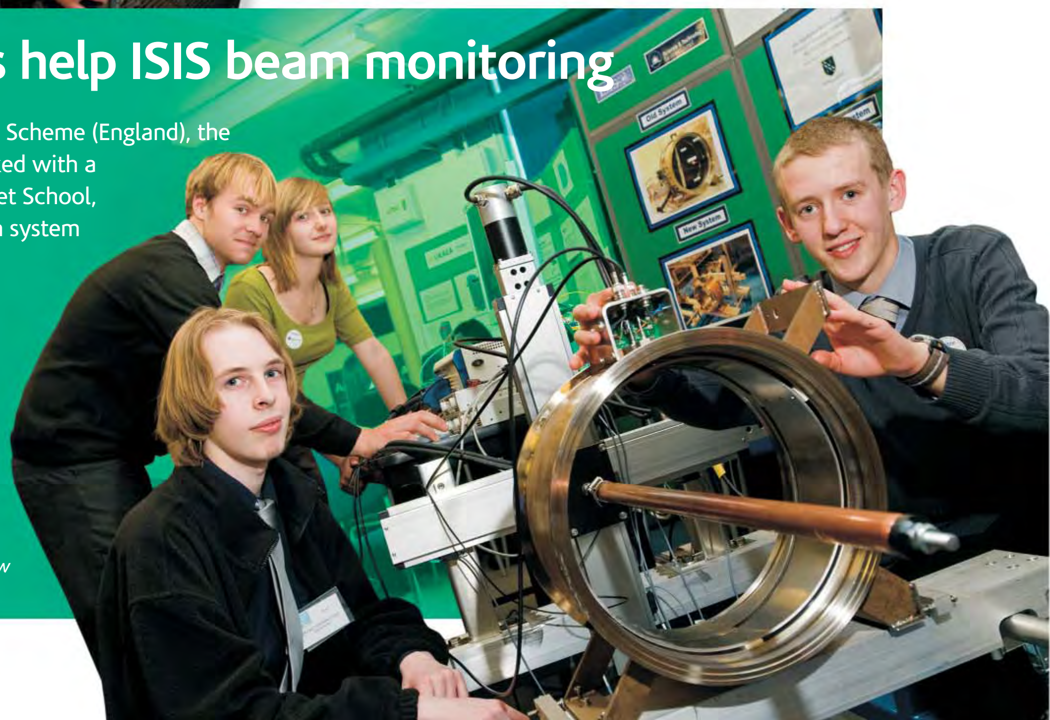
ISIS neutron training course

The annual ISIS neutron training course took place in February. This course is designed to provide practical experience of setting up and running neutron scattering experiments on a wide variety of instruments at ISIS for researchers new to neutron techniques. This year 24 participants came from UK universities – mainly postgraduate students and some post-docs. After an initial day of talks, the participants conducted real neutron experiments and then learnt data analysis techniques. Judging from the course feedback, the training was well-appreciated by all the participants – although many of them felt that the course was too short! You can never get enough of a good thing.

▲ *Aziz Daoud-Aladine (left) supervises Philip Merchant (UCL) loading a single crystal sample on SXD. (left to right) Chris Lester (Bristol), Dan Porter (Royal Holloway), Pabitra Biswas (Warwick) and Dean Whittaker (Bath) look on.* **09EC2222**

Young engineers help ISIS beam monitoring

As part of the Engineering Education Scheme (England), the accelerator diagnostics section worked with a team of A-Level students from Kennet School, Thatcham, to build a new calibration system for the ISIS split electrode position monitors. The new system uses stepper motors to move a copper pipe carrying a signal around the monitor. It has significantly decreased the time it takes to calibrate a monitor as historically this has been done manually without the aid of motors.



▶ *Students from Kennet School with the new split electrode position monitors.* **09EC1932**

▲ Keith Refson (CSED, STFC) demonstrating software during the computational methods workshop. **08EC4543**

Workshop in computational methods for the exploitation of vibrational spectra

This workshop was run at RAL by ISIS in November 2008 and attended by 29 participants. Its aims were to show how computational methods can be used for the exploitation of vibrational spectra in studies of molecular motions and dynamics. The course was largely practical and involved exploring the applications of state-of-the-art software (Gaussian03, DMOL3, CASTEP). Half of the participants were not regular neutron users, and interest in the workshop was high.

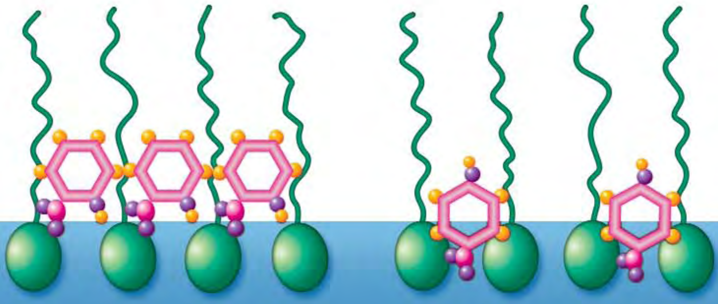
▲ *ISIS staff were involved in an exhibition at the Royal Society on 'Accelerators everywhere, from the big bang to curing cancer'. From left to right: Riccardo Bartolini (Diamond and JAI), Phil Burrows (JAI), Rolf-Dieter Heuer (Director General of CERN), Emmanuel Tsesmelis (CERN), Suzie Sheehy (JAI) and John Thomason (ISIS).*

Delegates at the joint Daresbury Laboratory and Rutherford Appleton Laboratory Accelerator workshop held at RAL in January. **09EC1954**

▲ *The 3rd Empirical Potential Structure Refinement Workshop was organised by the ISIS Disordered Materials Group at RAL and Cosener's House in April.* **09EC2601**

▼ *ISIS held an open morning in August to enable staff and contractors to bring friends and family to see the new Second Target Station building and to learn about the facility. Here, Chris Frost (ISIS) is wowing visitors with science demonstrations.* **08EC3812**

A year around ISIS



Oxford Isotope Facility

The Oxford Isotope Facility is funded by STFC and is based in the Physical and Theoretical Chemistry Laboratory in Oxford. It aims to provide deuterium labelled materials for the UK neutron scattering community for experiments at ISIS, ILL and elsewhere.

Contrast manipulation, by H/D isotopic substitution, is the main feature that makes neutron scattering an attractive and unique tool for the study of soft matter. Recent examples include a detailed study of the effects of hydroxybenzoate on the self assembly of surfactant CTAB. Deuterium labelling enabled the locations of the hydroxybenzoate at the surfactant interface to be deduced.

The Oxford Isotope Facility provides small molecule deuteration, materials such as fatty acids, alcohols, bromoalkanes, and a wide range of surfactants. Further details can be obtained from Jeff Penfold at ISIS (jeff.penold@stfc.ac.uk) or Bob Thomas at Oxford (robert.thomas@chem.ox.ac.uk).

▲ *Studies of the role of hydroxybenzoate in surfactant self assembly. Neutron scattering with deuterium labelling by the Oxford Isotope Facility has shown that the ortho form of hydroxybenzoate is partially located in the hydrophobic region of the surfactant interface (left), whereas the para hydroxybenzoate is in the hydrated head group region (right). J Penfold et al., Langmuir 20 (2004) 8054.*

▲ *'Other People's Business' events are a good way for STFC staff to learn about what goes on in other parts of the organisation. Here, John Thomason (left) is showing a group around the ISIS synchrotron.* **09EC1026**

ISIS in the media

ISIS has made the news in a number of ways this year! This includes a variety of specialised press – for example, Plant Engineer magazine featured an article on the 'extreme plant' operated routinely by ISIS; ISIS Engineers Hanna Fikremarium, Chris Benson and Sean Higgins featured in Professional Engineering, published by the Institute of Mechanical Engineering; and the ISIS timing and control systems were featured in Pinpoint, the magazine for the Location and Timing Knowledge Transfer Network. Facility Director Andrew Taylor has featured in a Public Life article in the Daily Telegraph, and been interviewed about the Second Target Station project on Radio 4's 'Today' programme. 'Metro' newspaper described ISIS as a '21st Century Wonderland' in their feature article in May!

▼ *Dr Martyn Bull, Head of ISIS Communications, being interviewed by science journalists visiting ISIS in July.* **09EC2503**

ISIS People

Congratulations are due to a variety of ISIS staff this year. Tim Broome, who played a key part in the development of ISIS, was awarded an MBE for services to science in the Queen's New Year's Honours. Tim has recently been pivotal in delivering the ISIS Second Target Station Project. Speaking about the award, Andrew Taylor, ISIS Director said: 'Tim brought a unique blend of physics understanding, engineering sense and operational practicality to this role. This is a fitting honour for an excellent scientist.'

Tim Broome after receiving his MBE from the Queen.

Laurent Chapon has been appointed Visiting Professor at the CRISMAT Laboratory (Crystallography and Materials Science) in Caen, France, and is also now ISIS Crystallography Group Leader. Sean Langridge (Large Scale Structures Group Leader) has been appointed Visiting Professor of Physics at Durham University, and Mike Johnson has been appointed as an Honorary Fellow at the University of Edinburgh.

Several ISIS engineers have been awarded Chartered status this year: Hanna Fikremariam, Jim Nightingale, John Teah and Steph Tomlinson.

Dr Dennis Mather, Managing Director, Australian Institute for Nuclear Science and Engineering (AINSE) presented an AINSE Gold Medal Award for Excellence in Research to ISIS user Paul Saines at the TS-2 Wish instrument in June. ***09EC2300***

Workshop on neutron reflection methods for the study of biomolecular systems

Neutron scattering measurements in soft condensed matter systems benefit greatly by the substitution of deuterium for hydrogen to vary the contrast between samples and their surroundings. With the increasing complexity of biomolecular systems under study the direct deuteration of biomolecules, such as large proteins or many phospholipids, is far more complex than that for synthetic soft matter materials. A workshop to discuss methods of contrast variation based upon buried magnetic reference layers was held at the Cosener's House in January, attended by 36 participants from 8 countries. Presentations included examples of the method and systems which would benefit from the method's development.

Attendees at the workshop on studying biomolecular systems using neutron reflection. ***09EC1203***

Neutron and Muon Users Meeting

The Neutron and Muon Users Meeting was held at RAL in April. The meeting aims to present the latest news and information on ISIS and the ILL and enable discussion amongst facility users. Here we see some of the 120 attendees, with Robert McGreevy (ISIS) presenting facility news.

ISIS Users at work

▲ Jim Holdaway, Matthew Wasbrough, Rob Barker (Bath University) and Luke Clifton (ISIS) during their Surf studies of the formation of ion channels in phospholipid bilayers by puroindoline-a. **09EC2754**

▲ Fabrizia Foglia (Kings College London) using the ISIS sample preparation laboratories during her SANS studies of mixed phospholipid : sterol vesicles and their interaction with amphotericin. **09EC2719**

▶ Marnix Wagemaker and Deepak Singh (University of Delft, The Netherlands) using Polaris to study particle and temperature dependent solubility limits in $LiFePO_4$ for battery electrode applications. **09EC2757**

▼ Dominic Fortes (University College London) preparing his meridianite ($MgSO_4.11D_2O$) sample to study the effects of pressure on Pearl. **09EC2723**

▲ Roger Cowley (Oxford University), Stephen Hayden, Neil Heading (Bristol University) and Chris Stock (ISIS) using Mari to study high energy excitations in La_2CuO_4. **09EC2760**

ISIS Facility Access Panels (FAPs)

There are seven ISIS FAPs covering the variety of science areas studied by neutrons and muons. Each FAP consists of experts in their subject from the international research community. The FAPs meet twice per year, roughly six weeks after the two ISIS proposal deadlines. They judge all proposals received based on their scientific merit and timeliness.

▼ *The Large Scale Structures FAP at work.* **08EC5162**

▲ *Chris Hardacre (Belfast), Gabriel Cuello, Miguel Gonzalez (ILL, France), Maria Antonietta Ricci (Roma Tre, Italy) and Simon Billinge (Colombia, USA) looking at Disordered Materials proposals.* **08EC5149**

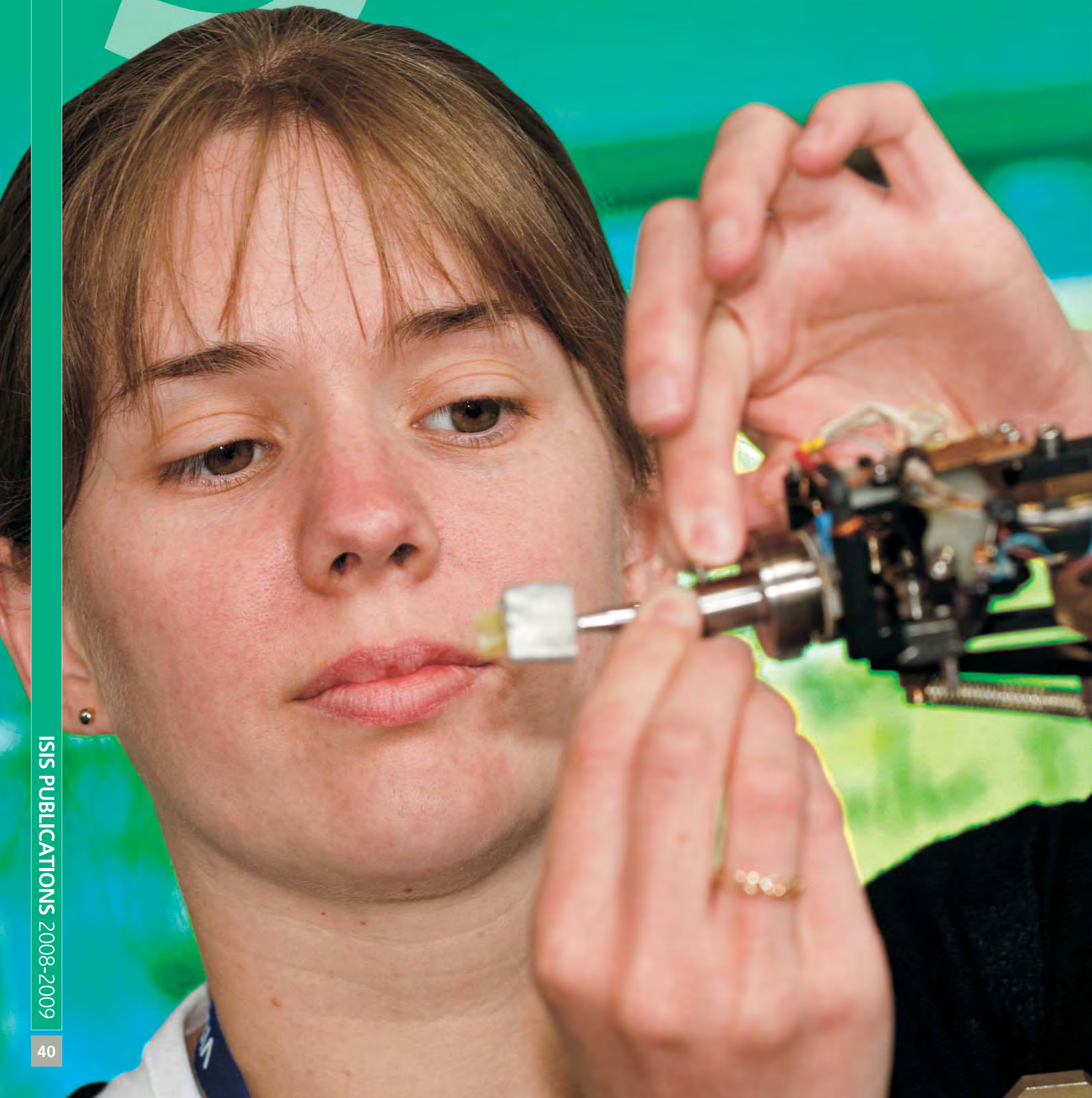
▼ *The Molecular Spectroscopy FAP reviewing proposals.* **09EC2667**

▲ *Shu Yan Zhang, Anna Paradowska (ISIS), Howard Stone (Cambridge) and Michael Hutchings (Open University) during Engineering FAP discussions.* **09EC2691**

◀ *Brian Rainford (Southampton) during Excitations FAP discussions with Andrew Huxley (Edinburgh and St. Andrew's) and Andrew Boothroyd (Oxford).* **09EC2683**

▲ *Wilson Crichton (ESRF, France) with members of the Crystallography FAP.* **09EC2652**

3 ISIS Publications 2008-2009



Section 3

ISIS Publications 2008-2009

Publications relate to all work carried out at ISIS. Listed here are 403 publications resulting from work carried out at the facility that have been reported since the 2008 Report.

ISIS Publications 2008-2009

2008

D T Adroja, A D Hillier, J G Park, W Kockelmann, K A McEwen, B D Rainford et al
Muon spin relaxation study of non-Fermi-liquid behavior near the ferromagnetic quantum critical point in $CePd_{0.15}Rh_{0.85}$
Physical Review B **78** 172505 (2008)

R Ahmed, H Yu, V Stoica, L Edwards and J R Santisteband
Neutron diffraction residual strain measurements in post-treated thermal spray cermet coatings
Materials Science and Engineering A **498** 191 (2008)

P W Albers, M Lopez and S F Parker
Characterisation of carbon supported platinum-ruthenium fuel cell catalysts
Surface Science **602** 3611 (2008)

C Andreani, A Pietropaolo, A Salsano, G G M Tardocchi, A Paccagnella, S Gerardin et al
Facility for fast neutron irradiation tests of electronics at the ISIS spallation neutron source
Applied Physics Letters **92** 114101 (2008)

R Arletti, L Cartechini, R Rinaldi, S Giovannini, W Kockelmann and A Cardarelli
Texture analysis of bronze age axes by neutron diffraction
Applied Physics A **90** 9 (2008)

A K Azad, C Savaniu, S W Tao, S Duval, P Holtappels, R M Ibberson and J T S Irvine
Structural origins of the differing grain conductivity values in $BaZr_{0.9}Y_{0.1}O_{2.95}$ and indication of novel approach to counter defect association
Journal of Materials Chemistry **18** 3414 (2008)

D Barilaro, V Crupi, S Interdonato, F Longo, G Maisano, D Majolino et al
Archaeometric investigation of red-figure pottery fragments from Gioiosa Guardia (Messina, Sicily) by INAA, FT-IR and TOF-ND techniques
Nuovo Cimento Della Societa Italiana Di Fisica C **31** 371 (2008)

S J Barnes, A Steuwer, S Mahawish, R Johnson and P J Withers
Residual strains and microstructure development in single and sequential double sided friction stir welds in RQT-701 steel
Materials Science and Engineering A **492** 44 (2008)

L F Barquín, A Arbe, F J Bermejo, J Campo, G J Cuello, J L G Munoz et al
20 Agnos de investigacion con tecnicas de neutrones en Espana
Revista Espanola de Fisica **22** 21 (2008)

L Bartoli, M Celli, F Grazzi, S Imberti, S Siano and M Zoppi
Neutron diffraction in archaeometry: the Italian neutron experimental station at ISIS
Metallurgica Italaliana **9** 33 (2008)

E D Bauer, C Wang, V R Fanelli, J M Lawrence, E A Goremychkin, N R de Souza et al
Simplifying strong electronic correlations in uranium: localised uranium heavy-Fermion UM_2Zn_{20} (M=Co, Rh) compounds
Physical Review B **78** 115120 (2008)

M Bernabei, A Botti, F Bruni, M A Ricci and A K Soper
Percolation and three-dimensional structure of supercritical water
Physical Review E **78** 21505 (2008)

G Beutier, A Bombardi, C Vecchini, P G Radaelli, S Park, S W Cheong and L C Chapon
Commensurate phase of multiferroic $HoMn_2O_5$ studied by X-ray magnetic scattering
Physical Review B **77** 172408 (2008)

S L Birch and S P Stoneham
10Hz Pulsed Power Converters for the ISIS Second Target Station (TS-2)
Proceedings of 11th European Particle Accelerator Conference (EPAC08), Genoa, Italy (2008)

L Bizo, M Allix, H Niu, M J Rosseinsky
Magnetism and phase formation in the candidate dilute magnetic semiconductor system $In_{2-x}Cr_xO_3$: bulk materials are dilute paramagnets
Advanced Functional Materials **18** 777 (2008)

H N Bordallo, L P Aldridge, G J Churchman, W P Gates, M T F Telling, K Keifer et al
Quasi-elastic neutron scattering studies on clay interlayer-space highlighting the effect of the cation in confined water dynamics
Journal of Physical Chemistry **112** 36 13982 (2008)

A Botti, F Bruni, R Mancinelli, M A Ricci, F L Celso, R Triolo and et al.
Study of percolation and clustering in supercritical water-CO_2 mixtures
Journal of Chemical Physics **128** 164504 (2008)

G R Broder, R T Ranasinghe, J K She, S Banu, S W Birtwell, G Cavalli et al
Diffractive micro bar codes for encoding of biomolecules in multiplexed assays
Analytical Chemistry **80** 1902 (2008)

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Physical Review B **77** 014427 (2008)

A P L Brun, S A Holt, D S Shah, C F Majkrzak and J H Lakey
Monitoring the assembly of antibody-binding membrane protein arrays using polarised neutron reflection
European Biophysics Journal **37** 639 (2008)

F Buchter, Z A odziana, P Mauron, A Remhof, O Friedrichs, A Borgschulte
Dynamical properties and temperature induced molecular disordering of $LiBH_4$ and $LiBD_4$
Physical Review B **78** 94302 (2008)

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Neutron Diffraction and Ab initio Studies of Te Site Preference in $Mo_3Sb_{7-x}Te_x$
Chemistry of Materials **20** 6556 (2008)

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Dynamic origin of the morphotropic phase boundary: soft modes and phase instability in $0.68Pb(Mg_{1/3}Nb_{2/3}O_3)$-$0.32PbTiO_3$
Physical Review B **78** 104103 (2008)

L Capogna, A Martinelli, M G Francesconi, P G Radaelli, J R Carvajal, O Cabeza et al
Crystal and magnetic structures of $(La_{0.70}Ca_{0.30})(CryMn_{1-y})O_3$: a neutron powder diffraction study
Physical Review B **77** 104438 (2008)

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Biophysical Chemistry **134** 34 (2008)

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Neutron-induced soft errors in advanced Flash memories
IEEE International Electron Devices Meeting, San Francisco, 2008, Technical Digest 357 (2008)

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International Journal of Solids and Structures **45** 2056 (2008)

C Chen, P Depa, J K Maranas and V G Sakai
Comparison of explicit atom, united atom and coarse-grained simulations of poly(methyl methacrylate)
Journal of Chemical Physics **128** 124906 (2008)

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Dynamic crossover phenomenon in confined supercooled water and its relation to the existence of a liquid-liquid critical point in water
Proceedings of 5th International Workshop on Complex Systems, AIP Conference Proceedings **982** 39 (2008)

S Chi, D T Adroja, T Guidi, R Bewley, S Li, J Zhao et al
Crystalline electric field as a probe for long-range antiferromagnetic order and superconducting state of $CeFeAsO_{1-x}F_x$
Physical Review Letters **101** 217002 (2008)

A D Christianson, E A Goremychkin, R Osborn, S Rosenkranz, M D Lumsden, C D Malliakas et al
Unconventional superconductivity in $Ba_{0.6}K_{0.4}Fe_2As_2$ from inelastic neutron scattering
Nature **456** 930 (2008)

A D Christianson, M D Lumsden, O Delaire, M B Stone, D L Abernathy, M A McGuire et al
Phonon density of states of $LaFeAsO_{1-x}F_x$
Physical Review Letters **101** 157004 (2008)

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Nuclear Instruments and Methods A **589** 296 (2008)

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Measurement Science and Technology **19** 047001 (2008)

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Measurement Science & Technology **19** 034027 (2008)

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Interfacial structure of wild-type and mutant forms of puroindoline-b bound to DPPG monolayers
Journal Of Physical Chemistry B **112** 15907 (2008)

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Journal of Physics-Condensed Matter **20** 445225 (2008)

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Journal of Strain Analysis for Engineering Design **44** 55 (2008)

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A high temperature cell for simultaneous electrical resistance and neutron diffraction measurements
Review of Scientific Instruments **79** 095104 (2008)

R A Ewings, T G Perring, R I Bewley, T Guidi, M J Pitcher, D R Parker et al
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Physical Review B **78** 220501 (2008)

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Inorganica Chimica Acta **361** 487 (2008)

D C Faircloth, S Lawrie, A P Letchford, C Gabor, P Wise, M Whitehead et al
Commissioning the front end test stand high performance H^- ion source at RAL
AIP Conference Proceedings **1097** 243 (2008)

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Spin dynamics in liquid and rotationally disordered solid oxygen
Physical Review B **78** 104303 (2008)

G Festa, W Kockelmann and A Kirfel
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Archeometriai Muhely / Archaeometry Workshop 1 **61** (2008)

F Fillaux, A Cousson, J F R Archilla and J Tomkinson
A neutron scattering study of strong-symmetric hydrogen bonds in potassium and cesium hydrogen bistrifluoroacetates: determination of the crystal structures and of the single-well potentials for protons
Journal of Chemical Physics **128** 204502 (2008)

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The macroscopic quantum behavior of protons in the $KHCO_3$ crystal: theory and experiments
Progress in Theoretical Chemistry and Physics **18** 319 (2008)

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Journal of Physics Conference Series **108** 12006 (2008)

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Structure of SP-B/DPPC mixed films studied by neutron reflectometry
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V Garcia Sakai, J K Maranas, I Peral and J R D Copley
Dynamics of PEO in blends with PMMA: study of the effects of blend composition via quasi-elastic neutron scattering
Macromolecules **41** 3701 (2008)

S R Giblin, J D M Champion, H D Zhou, C R Wiebe, J S Gardner, I Terry, S Calder, T Fennell and S T Bramwell
Static Magnetic Order in $Tb_2Sn_2O_7$ revealed by muon spin relaxation with exterior muon implantation
Physical Review Letters **101** 23 (2008)

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Biomacromolecules **9** 1170 (2008)

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Ceramics International **34** 679 (2008)

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Journal of Physics-Condensed Matter **20** 104249 (2008)

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PLoS One **3** e2500 (2008)

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Structural analysis of $xCsCl_{1-x}Ga_2S_3$ glasses
Journal of Non-Crystalline Solids **354** 134 (2008)

M J Hollamby, R Tabor, K J Mutch, K Trickett, J Eastoe, R K Heenan and I Grillo
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Langmuir **24** 12235 (2008)

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Journal of Applied Physics **104** 013922 (2008)

S Jahn, J Ollivier and F Demmel
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Solid State Ionics **179** 1957 (2008)

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EMBO Reports **9** 543 (2008)

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In vivo measurement of internal and global macromolecular motions in Escherichia Coli
Biophysical Journal **95** 857 (2008)

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High-pressure polymorphism in L-serine monohydrate: identification of driving forces in high pressure phase transitions and possible implications for pressure-induced protein denaturation
Crystal Engineering Communications **10** 1758 (2008)

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Advances in Fracture and Damage Mechanics VII **385-387** 517 (2008)

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Journal of Chemical Physics **28** 195106 (2008)

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Journal of Applied Physics **103** 07B513 (2008)

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Physica B **403** 1973 (2008)

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Physical Review B **78** 012502 (2008)

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A Wills, T Perring, S Raymond, B Fak, J Henry and M T F Telling

Inelastic neutron scattering studies of the quantum frustrated magnet clinoatacamite, gamma-$Cu_2(OD)_3Cl$, a proposed valence bond solid (VBS)

Journal of Physics: Conference Series **145** 12056 (2009)

K Winkel, D T Bowron, T Loerting, E Mayer and J L Finney

Relaxation effects in low density amorphous ice: two distinct structural states observed by neutron diffraction

Journal of Chemical Physics **130** 64502 (2009)

P Wise, M Bates, D Faircloth, S Lawrie, A Letchford, M Perkins, M Whitehead, T Wood, J Pozimski, P Savage and C Gabor

Mechanical engineering for the front end test stand

Proceedings of the Particle Accelerator Conference, Vancouver, Canada (2009)

F Xiao, F M Woodward, C P Landee, M M Turnbull, C Mielke, N Harrison, T Lancaster, S J Blundell, P J Baker, P Babkevich and F L Pratt

Two-dimensional XY behavior observed in quasi-two-dimensional quantum Heisenberg antiferromagnets

Physical Review B **79** 134412 (2009)

A Zarbakhsh, J R P Webster and J Eames

Structural studies of surfactants at the oil-water interface by neutron reflectometery

Langmuir **25** 3953 (2009)

F Zhang, M W A Skoda, R M J Jacobs, D G Dressen, R A Martin, C M Martin et al.

Gold nanoparticles decorated with oligo(ethylene glycol) thiols: enhanced hofmeister effects in colloid-protein mixtures

Journal Of Physical Chemistry C **113** 4839 (2009)

S Y Zhang, E Godfrey, W Kockelmann, A Paradowska, M J Bull, A M Korsunsky et al.

High-tech composites to ancient metals

Materials Today **12** 78 (2009)

Z Zhang, C J Howard, B J Kennedy, M Matsuda and M Miyake

Crystal structures and phase transition in $(Sr_{0.8}Ce_{0.2})(Mn_{1-y}Co_y)O_3$ (y = 0 and 0.2): the influence of Jahn-Teller distortion

Journal of Physics-Condensed Matter **21** 124218 (2009)

X B Zhao, F Pan, S Perumal, H Xu, J R Lu and J R P Webster

Interfacial assembly of cationic peptide surfactants

Soft Matter **5** 1630 (2009)

J Zhao, D T Adroja, D X Yao, R Bewley, S Li, X F Wang and et al.

Spin waves and magnetic exchange interactions in $CaFe_2As_2$

Nature Physics **5** 555 (2009)

ISIS Seminars 2008-2009

8 April 2008
Richard Palmer (Birmingham)
Organising atoms, clusters and proteins on surfaces

15 April 2008
Debdulal Roy (National Physical Laboratory)
Raman spectroscopy with nanometer-scale spatial resolution

22 April 2008
Maciek Krzystyniak (ISIS)
Zeno effect for Compton scattering from protons in condensed media

6 May 2008
Amir Murani (ILL)
Magnetic neutron scattering at epithermal neutron energies

13 May 2008
Laura Bartoli (ISIS and CNR, Italy)
Exploiting the technology of the present to unveil the technology of the past

21 May 2008
Mark Dadmun (Tennessee and Oak Ridge National Laboratory, USA)
Using reflectivity and SANS to probe the dynamics, thermodynamics, and structure of natural and synthetic polymers

27 May 2008
Oscar Moze (Universita di Modena e Reggio Emilia, Italy)
From single molecule magnetism to long range ferromagnetism in a giant spin molecular magnet

3 June 2008
Laurent Chapon (ISIS)
Multiferroicity in RMn_2O_5 (R = rare earth, Bi) systems probed by neutron and X-ray scattering

10 June 2008
Stephen Dugdale (Bristol)
Probing the Fermi surface with positrons

11 June 2008
Nicole Helbig (European Theoretical Spectroscopy Facility), N Lathiotakis (NHRF, Greece)
First order reduced density matrix functional theory: predicting electronic correlation

17 June 2008
Scott Kroeker (Cambridge)
Phase separation in model nuclear waste glasses: high-temperature NMR studies

24 June 2008
Tatiana Guidi (ISIS)
Quantum effects in the spin dynamics of molecular nanomagnets probed by inelastic neutron scattering

1 July 2008
François Fillaux (CNRS, France)
Macroscopic quantum entanglement of protons in the crystal Of $KHCO_3$: neutron scattering studies and theory

9 July 2008
Andreas Michels (Saarland, Germany)
Magnetic interactions in nanocrystalline bulk ferromagnets: a neutron-scattering study

15 July 2008
Boyan Bonev (Nottingham)
Membrane-disrupting antibiotics and toxins: mechanisms and targets

29 July 2008
Sarah Rogers (ISIS)
Nanoparticles and Small-Angle Scattering

2 September 2008
Kui Ming Chui (Image Enhancement Technology Ltd)
A de-convolution technique used for non-destructive testing in X-ray and computed tomography

16 September 2008
Shu Yan Zhang (ISIS)
Stress analysis of engineering components using X-rays and neutrons

23 September 2008
John Thomason (ISIS)
Accelerator upgrades to ISIS: TS-2 and beyond…

30 September 2008
Claudio Castelnovo (Oxford)
Magnetic monopoles in spin ice

7 October 2008
Francisco-José Pérez-Reche (Cambridge)
Criticality in martensites

14 October 2008
Dimitri Argyriou (HMI, Berlin, Germany)
Strong spin-lattice coupling in layered FeAs compounds

28 October 2008
Markus Eisenbach (ORNL, USA)
Non collinear magnetism in alloys

4 November 2008
Iain McKenzie (ISIS)
μSR Spectroscopy of spin labels in soft matter

11 November 2008
Valentina Venuti (Messina, Italy)
Non-invasive analysis of ancient potteries from Sicily (Southern Italy) using neutrons and synchrotron radiation

18 November 2008
Ali Alavi (Cambridge)
Electron correlation from path resummations

▼ *Fernando Rey, Susana Valencia, and Jose Jorda-Moret (ITQ, CSIC, Spain) during their experiment using HRPD to study of the structural deformation of ITQ-12 zeolite upon ethene adsorption.*
09EC2767

25 November 2008
Andrew Boothroyd (Oxford)
Spin excitations in the pnictides

2 December 2008
Don Fleming (TRIUMF, Canada)
Novel isotope effects in chemical reactivity: recent μSR studies of the Mu+H_2*(ν=1) reaction and of heavy hydrogen, the ^{4}Heμ + H_2 reaction

13 January 2009
Elmar Fuchs (Wetsus, The Netherlands)
More experiments with the floating water bridge

15 January 2009
Nic Shannon (Bristol)
Fun with frustrated magnets

20 January 2009
CF Majkrzak (NIST, USA)
Advancing the sensitivity of neutron reflectometry to nanoscale structure

27 January 2009
Cameron Neylon (ISIS)
Open access, open data, open research? The challenges and benefits of enabling public access to publicly funded research

3 February 2009
Christy Kinane (ISIS)
Off-specular soft X-ray magnetic scattering from magnetic nanostructures

10 February 2009
Ross Stewart (ISIS)
β-Manganese

17 February 2009
Rafa Roldán (Paris-Sud, France)
Interplay of metamagnetic and structural transitions in $Ca_{2-x}Sr_xRuO_4$

24 February 2009
Dario Arena (Brookhaven National Laboratory, USA)
Element- and layer-resolved magnetization dynamics at picosecond timescales

26 February 2009
Luis Fernández Barquín (Cantabria, Spain)
Surface and interparticle interactions in the magnetic and electronic properties of nanosized 3d and 4f compounds

3 March 2009
Sam Carr (Birmingham)
Strong correlation effects in single wall carbon nanotubes

10 March 2009
Chris Howard (Newcastle, Australia)
Structures and phase transitions in perovskites – sorting out the subtleties

16 March 2009
Sotiris Xantheas (Pacific Northwest National Laboratory, USA)
Development of a new interaction potential for water from first principles and simulation of clusters, liquid water and ice

24 March 2009
Kai Bongs (Birmingham)
Quantum gases: quantum simulation of condensed matter and applications in space

▼ *Stuart Calder and Bob Aldus (University College London) searching for magnetic monopoles in spin ice using Musr.* **09EC2744**

▼ *Mark Styles (Melbourne University, Australia) during an in situ study of ordered Ti_3C_2(Al) and Ti_3C_2(Si) on Polaris.* **09EC2730**

ISIS in facts and figures

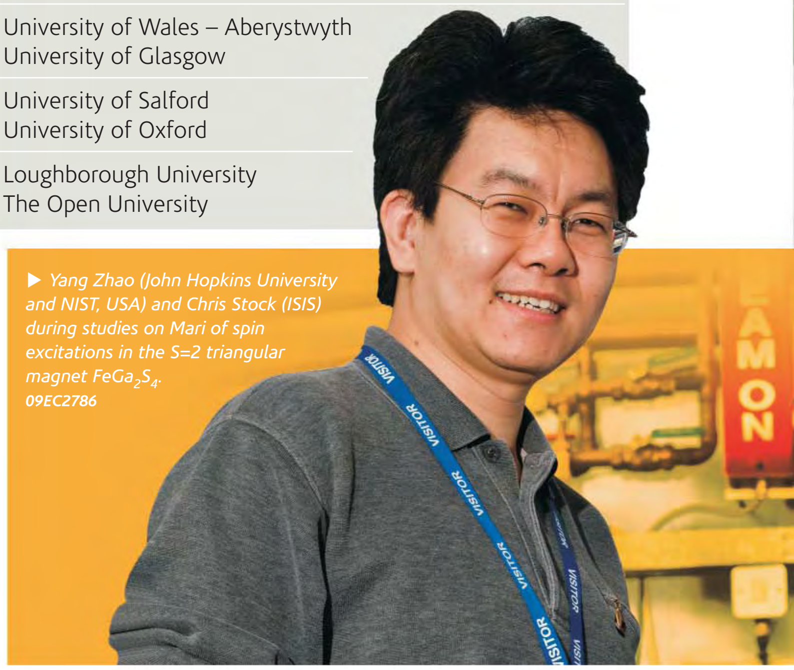
FAP 1 Diffraction	FAP 2 Liquids	FAP 3 Large Scale Structures	FAP 4 Excitations	FAP 5 Molecular Spectroscopy	FAP 6 Muons	FAP 7 Engineering
L Favello *(Chair)*	D Holland *(Chair)*	A Zarbakhsh *(Chair)*	D McMorrow *(Chair)*	J Bermejo *(Chair)*	S Kilcoyne *(Chair)*	J Bouchard *(Chair)*
A Bombardi	M Celli	S Clarke	A Boothroyd	F Bresme	A Drew	M Hutchings
J Claridge	G Cuello	I Gentle	J Chalker	D Colognesi	R Macrae	N O'Dowd
W Crichton	M Gonzalez	J Goff	R De Renzi	P Fairclough	R Moessner	M Preuss
J Evans	F Meersman	J Lakey	B Gaulin	M Jones	R Osborn	D Rugg
B Kennedy	J Tse	J Lu	A Huxley	MP Marques	R Scheuermann	A Steuwer
S Parsons	M Wilson	J Petkov	B Lake	I Silverwood	J Titman	H Stone
T Proffen	R Winter	P Steadman	O Petrenko	G Walker	I Watanabe	J Yates
P Schofield		R Thompson	D Reznik		P Wood	
P Slater						
A Wills						
C Neylon						
M Tucker	*D Bowron*	*J Webster*	*C Stock*	*J Mayers*	*S Cottrell*	*SY Zhang*
L Chapon	*A Hannon*	*S Langridge*	*T Perring*	*J Tomkinson*	*A Hillier*	*A Paradowska*

ISIS Facility Access Panel membership for the June 2009 meetings. The FAPs normally meet twice per year to review all proposals submitted to the facility based on scientific merit and timeliness. ISIS attendees act as secretary and give technical advice, but are not involved in the experiment review process.

	Chair	D Lennon	University of Glasgow
IUG1	**Crystallography**	D Gregory P Lightfood	University of Glasgow University of St Andrews
IUG2	**Liquids & Amorphous**	D Holland B Webber	University of Warwick University of Kent
IUG3	**Large Scale Structures**	A Zarbaksh	Queen Mary College, London
IUG4	**Excitations**	A Boothroyd P Mitchell	University of Oxford University of Manchester
IUG5	**Molecular Spectroscopy**	F Kargl D Lennon	University of Wales – Aberystwyth University of Glasgow
IUG6	**Muons**	S Kilcoyne T Lancaster	University of Salford University of Oxford
IUG7	**Engineering**	G Swallowe M Fitzpatrick	Loughborough University The Open University

A D Taylor	Director ISIS
U Steigenberger	ISS Division Head
Z A Bowden	IEO Division Head
D Greenfield	II Division Head
R L McGreevy	IDM Division Head
R Browning	ISIS User Programme Manager

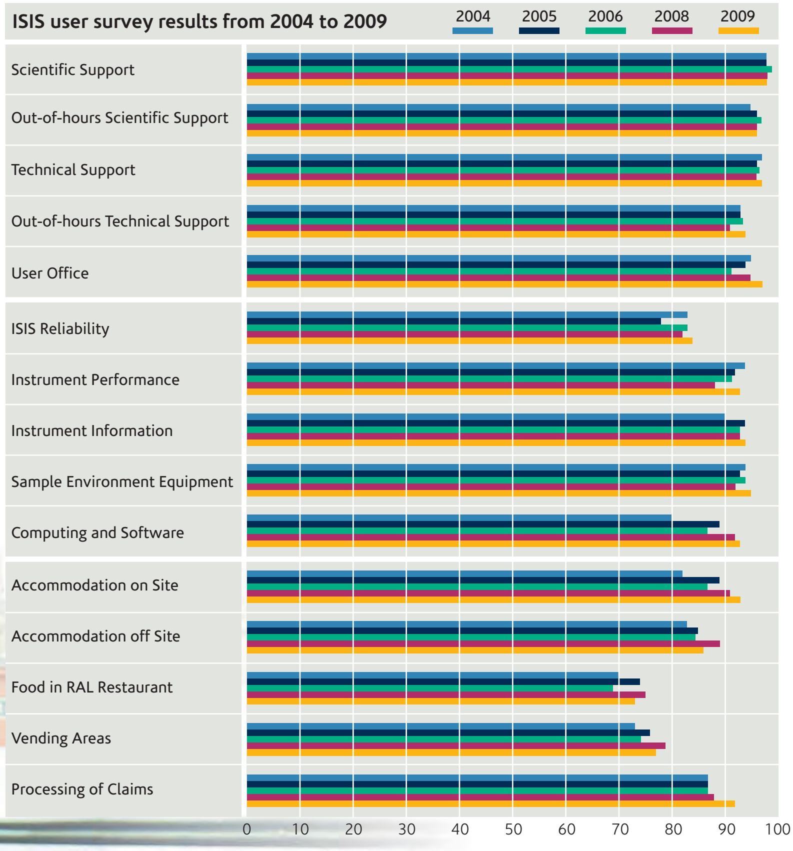
ISIS User Committee Membership for June 2009. The IUC exists to represent the user community on all aspects of facility operation.



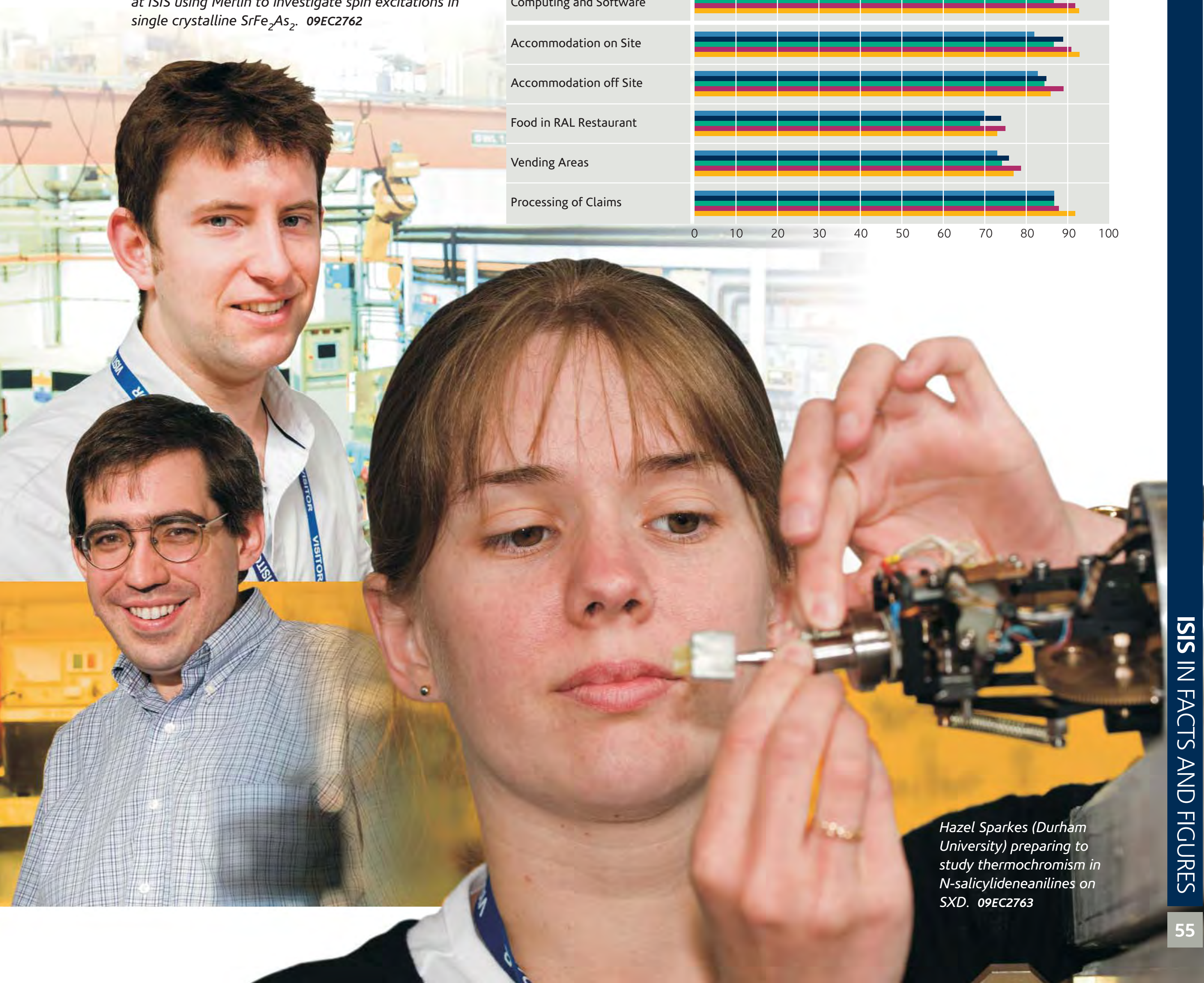
▶ Yang Zhao (John Hopkins University and NIST, USA) and Chris Stock (ISIS) during studies on Mari of spin excitations in the S=2 triangular magnet $FeGa_2S_4$.
09EC2786

User Satisfaction

All users visiting the facility are invited to complete a satisfaction survey which addresses the quality of the scientific, technical and User Office support, the ISIS, Instrument and Support Equipment performance and reliability, and the quality of the accommodation and restaurant facilities. The feedback obtained in this way helps to ensure a high quality service is maintained and improved where necessary.



▼ *Jack Gillet (Cambridge University) during his time at ISIS using Merlin to investigate spin excitations in single crystalline $SrFe_2As_2$.* ***09EC2762***



Hazel Sparkes (Durham University) preparing to study thermochromism in N-salicylideneanilines on SXD. ***09EC2763***

Beam Statistics 2008-2009

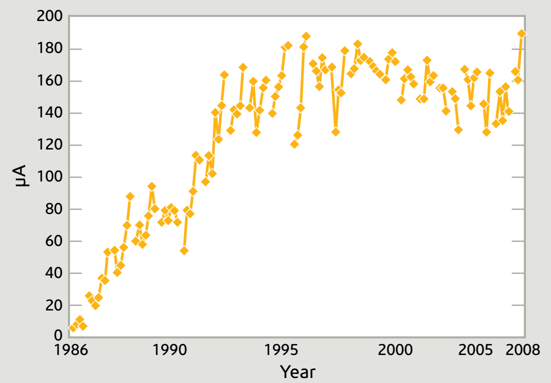
ISIS continues to be the world's most successful pulsed spallation neutron source. For the period of this report and during scheduled operating cycles, ISIS delivered a total of 612 mA.hrs of user proton beam to the muon and neutron targets.

Following first neutron production on the ISIS Second Target Station on Sunday 3 August 2008, regular proton beam transport to TS-2 started in September. Routine switching from 50 Hz operation of TS-1 to 40/10 Hz joint operation between the two target stations was achieved in November 2008.

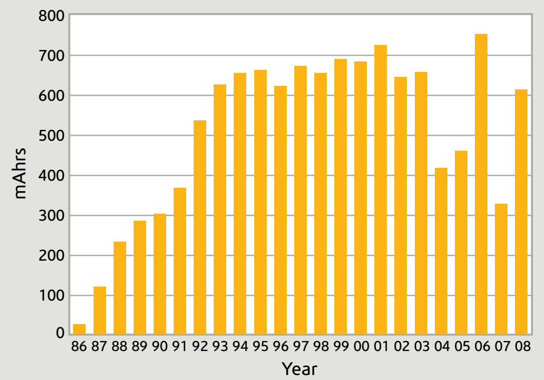
The tables below give beam statistics for the individual cycles in the year 2008-2009, together with year-on-year statistics for ISIS performance.

Cycle	08/1	08/2	08/3	08/4	08/5
	8 April-19 June	4 July-25 July	9 Sept-17 Oct	12 Nov-19 Dec	10 Feb-25 Mar
Beam on Target 1 (hr)	822	437	744	713	759
Total Beam Current (μA-hr)	147332	72638	118030	125739	136734
Average Beam Current for beam on Target 1 (μA)	179.1	173.8	185.1	176.3	180.2

ISIS operational statistics for year 2008-2009.



ISIS mean current averaged over a cycle.



The ISIS integrated beam current over the last twenty years.

▼ *Jan Swenson (Chalmers University, Sweden) preparing his IRIS sample for studies of water dynamics in porous PTFE membranes for water purification.* ***09EC2726***

▼ *Francesco Civita and Francesco Grazzi (Stibbert Museum, Italy) studying Japanese sword fragments.* ***08EC5232***

ISIS
Science and Technology Facilities Council, Rutherford Appleton Laboratory,
Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0QX, UK
T: +44 (0)1235 445592 F: +44 (0)1235 445103 E: isisuo@stfc.ac.uk

www.stfc.ac.uk

Head office: Polaris House, North Star Avenue, Swindon SN2 1SZ, United Kingdom.
Establishments at: Rutherford Appleton Laboratory, Oxfordshire; Daresbury Laboratory, Cheshire;
UK Astronomy Technology Centre, Edinburgh; Chilbolton Observatory, Hampshire; Isaac Newton Group,
La Palma; Joint Astronomy Centre, Hawaii.

Science & Technology Facilities Council