

ISIS 2007

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2007 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.

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Foreword

As I write, ISIS is coming towards the end of a ten month shut-down. This has been a period of very intense activity – work that, perhaps, is not always externally visible, but which is vital to maintain and improve the ISIS machine and instrument performance and to enable new capability. Second Target Station work – the linking of the new extracted proton beam to the ISIS synchrotron and installation of its many beamline components, continued construction of the target itself, and provision of the first components for the seven day-one instruments – has been very significant, and we look forward to first neutron production over the next year. But in addition, replacement of the 20-year old hydrogen moderator on the first target, major refurbishment of part of the existing extracted proton beamline and replacement of synchrotron extraction kicker power supplies will ensure ISIS' continued running for many years to come.

Even as the first TS-2 instruments are being installed, the steps to provide the next set of the instrument suite have begun. This will proceed via the government Gateway process over the next year, in consultation with the user community. And we look forward to the inclusion of a final phase of instrumentation within the Large Facilities roadmap presently being constructed by STFC along with its sister research councils. Of course the first target station instrument suite is also continually being developed, with work presently at

full speed improving the guide on HRPD, upgrading POLARIS and providing a new high-field muon spectrometer.

The merging this year of CCLRC with PPARC to form the new Science and Technology Facilities Council provides new opportunities for strategic development of large facility research within and beyond the UK. We are rapidly settling into our changed environment and looking forward to progressing UK science within STFC. This year has also seen first users at DIAMOND, our sister facility on site. DIAMOND

provides complementary facilities to ISIS and adds significantly to the strengths of the Laboratory.

As we anticipate first beam following our shut-down activities, I would like to thank all those who have worked so hard to complete the very tough shut-down work programme, and look forward to welcoming our user community once again for some exciting and significant science.

Handwritten signature: A. T. J.

ISIS and DIAMOND provide complementary facilities for condensed matter, molecular and materials science at RAL. 06EC3818

1. Prof. Peter Littlewood (Cambridge University), Prof. John Seddon (Imperial College London), Prof. Steve Bramwell (University College London) and Prof. Hans Rudolf Ott (ETH Zurich, Switzerland) toured ISIS and met with instrument scientists as part of their review of ISIS internal science. They are seen here with Andrew Taylor, Robert McGreevy and Uschi Steigenberger (ISIS) by the entrance to the new Second Target Station building. 07EC4199



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2. Rt Hon Ed Vaizey, MP, seeing the ISIS Second Target Station project in February. Jonathan Carkeet, TS-2 installation task leader, is showing him round. 07EC1279

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3. Paul Williams and Ron Egginton from the Office of Science and Innovation, DTI, visiting the ISIS Second Target Station building with Andrew Taylor. 07EC3056

4



4. Prof. David Wallace, Director of the Isaac Newton Institute for Mathematical Sciences at the University of Cambridge, viewing ISIS during a visit in June. 07EC3057

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5. Professor Mianheng Jiang, Vice President, Chinese Academy of Sciences with Professor John Wood, CEO CCLRC, (left) and Andrew Taylor, during his visit in March. 07EC2095



A year around ISIS



1. Masa Arai and colleagues (J-PARC, Japan), signing a memorandum of understanding for co-operation in neutron scattering with Andrew Taylor in September. 06EC3536



2. Prof Juan Urrutia, Chairman of the Executive Committee of the ESS-Bilbao Consortium and Dr Javier Campo representing the Spanish Ministry of Science and Education at the ESS-Bilbao consortium, visited ISIS in April. 07EC2561

3. ISIS Facility Access Panels consist of members of the international community who meet following each call for proposals to review beamtime applications. Here we see three of the panels at work. 07EC2931, 07EC2941, 07EC2981



4. Particle Physics Masterclass students visited the ISIS experimental hall in March. James Treadgold (ISIS) is showing the LOQ instrument station. 07EC2117

5. The first magnet for the Second Target Station extracted proton beamline was installed in February. 07EC1486

6. Richard Heenan (ISIS) oversees delivery of the Sans2d instrument tank in March. 07EC1503



7. The HRPD instrument guide has been replaced to provide significant neutron flux increases. Here we see the guide installation team at work, mirrored in the guide face. 07EC3220

8. Ed Gerstner, Senior Editor, Nature, viewing ISIS operation with Andrew Taylor during his visit in June. 07EC3059

9. A joint meeting of the Royal Society of Chemistry Molecular Spectroscopy Group and the Infrared and Raman Discussion Group was held at RAL in August to discuss vibrational spectroscopy studies at central facilities.



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.

Environmental and Earth Sciences

Atmospheric oxidation of organic pollution in cloud droplets – a climate effect?

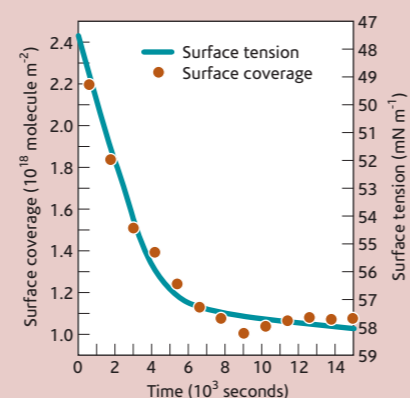
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MD King et al., J. Am. Chem. Soc. 126 (2004) 16710; New Scientist 184 (2004) 2478 p9

Atmospheric aerosol affects global climate both directly, by absorbing and scattering solar radiation, and indirectly, by influencing cloud formation and growth. Cloud droplets coated with an organic layer have different optical properties and potential to cause rain than uncoated droplets. Atmospheric oxidation of the organic layer in polluted air-masses may decrease drizzle potential and cloud albedo. We have used neutron scattering to demonstrate that the oxidation of an organic surfactant film (oleic acid) on aqueous atmospheric aerosol by atmospheric ozone will hinder cloud droplet growth. Our experiments reveal that the organic film is not destroyed by oxidation but chemically altered to give a film containing about half the original organic material and with a higher surface tension. These results are also important for the study of the stability of

organic films on Langmuir troughs towards oxygen and ozone.



Surface coverage of oleic acid (left axis, circles) and surface tension (right axis, solid line) versus time measured when a film on synthetic seawater was exposed to gas-phase ozone.

A clear view through muddy water

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HP Jarvie and SM King, Environmental Science and Technology 41 (2007) 2868.

In recent years water quality scientists have become increasingly aware of the significance of nanoparticles (defined as <100 nm in size) in the transport of pollutants and their potential impacts on the ecology and health of streams and rivers. While conventional techniques (such as microscopy) have advanced understanding, new methods are now required to characterise the structure, stability and interactions of these nanoparticles in aquatic environments. Small angle neutron scattering (SANS) on LOQ has been used to study suspensions of complex mixtures of mineral and organic particles from river water, runoff from agricultural fields and river bed sediments. The smallest nanoparticles are typically clay minerals and the SANS studies have revealed the way in which these are linked together by large organic molecules, derived from

decaying plants and micro-organisms. Preliminary results have provided new insights into these complex heterogeneous nanoparticle aggregates in river water. It seems that they have a ragged and porous 'fractal' shape, resulting in a much higher surface area than previously assumed. The larger the surface area, the greater the potential for pollutant uptake and transport.

Helen Jarvie (NERC) and Steve King (ISIS) with a river water sample. 06EC2459



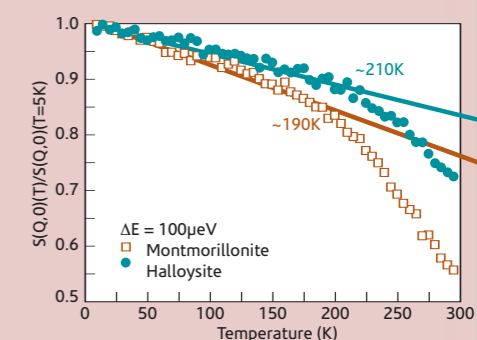
Gate-keepers holding on to the water in clay

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Even in a barren and hot desert, clays can contain a significant fraction of water that is normally unavailable to plants. This is because cations, such as sodium, act as gate-keepers regulating the reversible adsorption of water. To explore possible differences in the water dynamics related to the presence of cations in clays, and to examine the dynamics of surface water which plays a significant role in water diffusion in clay barriers, we have carried out a quasi-elastic neutron scattering study on two clays, montmorillonite and halloysite. Halloysite is unique – a clay where no cations are present in the interlayer space so that interlayer water is weakly held and can readily and irreversibly dehydrate. The quasi-elastic spectra we observed can be ascribed to different diffusion processes, with montmorillonite having four times the

diffusion coefficient compared with halloysite. Differences in the elastic incoherent scattering intensity highlight the important role that cations play in regulating water uptake in clays.



The effect of interlayer cations is shown by the lower temperature activation of the motions in the montmorillonite compared to the halloysite interlayer water.

Asphaltene aggregation in the presence of laponite clay

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J Roux et al., Langmuir 17 (2001) 5085

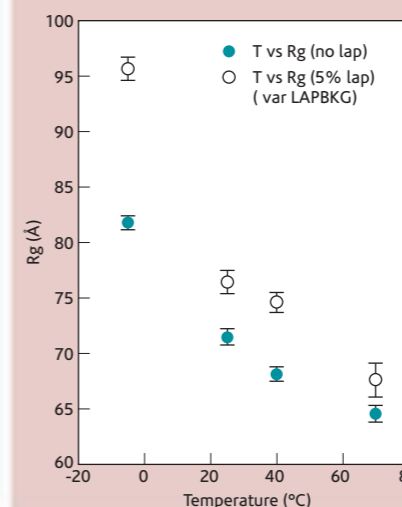
Asphaltenes are known as the 'cholesterol' of crude oil. They precipitate, adhere to surfaces and, in the worst cases, cause costly pipe blockages (see photograph). Furthermore they alter the wetting characteristics of mineral surfaces within the reservoir, hindering oil recovery efficiency.



Photograph showing a crude oil pipeline blocked by asphaltenes and waxes.

Asphaltenes are a complex mixture of different molecules with similar chemical characteristics which are insoluble in aliphatic

solvents (e.g. heptane) but soluble in aromatic ones (e.g. toluene). Even at very low concentrations in 'good' solvents, they still have a propensity to form 'nanoaggregates' whose structure and formation remain largely unknown despite much research. Small-angle neutron scattering (SANS) has been used to examine asphaltenes in deuterated toluene in the absence and presence of laponite clay, the hypothesis being that the clay surface would enhance asphaltene aggregation. This appears to be borne out by the change in the radius of gyration (Rg) of the asphaltene nanoaggregates as a function of temperature (see figure). Hopefully this observation will help provide a route for the oil industry to predict and control asphaltene precipitation and deposition in the field.



Graph of radius of gyration for asphaltene samples with (white) and without (blue) Laponite clay.

ISIS Highlights

Fundamental Magnetic Systems

Double exchange from valence fluctuations in magnetite

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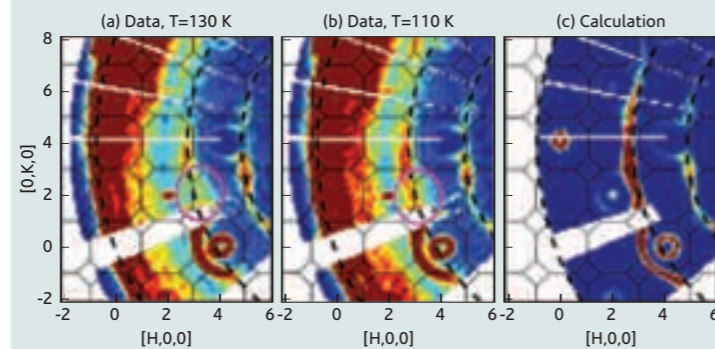
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RJ McQueeney et al, arXiv:0707.2253

Magnetite (Fe_3O_4) is one of the most ancient and technologically important magnetic materials. Beyond its magnetic properties, magnetite is also the prototypical example of a metal-insulator transition called a Verwey transition (below $T_V = 122$ K) which is argued to arise from the charge ordering of 2^+ and 3^+ iron valences. Since its discovery nearly 70 years ago, the driving forces behind the Verwey transition are still not completely understood. In the metallic phase, valence fluctuations modify the magnetic coupling between spins. The measurement of magnetic excitations with neutron scattering

provides a window to observe the complicated electronic behaviour near the transition. Using the MAPS instrument, we observe anomalous magnetic excitations whose behaviour is modified above T_V due to the occurrence additional ferromagnetic coupling, called double exchange. We find that the double exchange interaction affects only certain special modes, not all modes, indicating that valence fluctuations are constrained by intersite electronic correlations above T_V . Our results support some of the early ideas about magnetite from PW Anderson and NF Mott.



Images of magnetic excitations measured on the MAPS spectrometer above and below T_V compared to computer calculations. Note the anomalous behaviour of excitations in the circled region.

A new candidate for spin liquid physics

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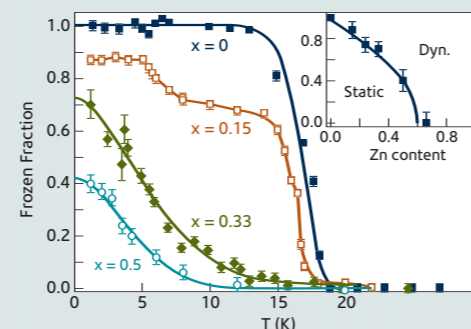
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P Mendels et al., Phys. Rev. Lett. 98 (2007) 077204

In most common magnetic ground states, the moments of atoms in crystals order because of interactions with their neighbours. However, in triangular lattices three spins can not be simultaneously anti-parallel to each other and therefore cannot satisfy antiferromagnetic interactions. In 1973, Anderson proposed that such magnetic frustration associated with large quantum fluctuations for $S = 1/2$ spins could stabilize a 'spin liquid' ground state built on the resonance of singlets between neighbouring bonds. This concept has been seminal for many theoretical investigations, including high temperature superconductors, but has not yet been realized experimentally. A new synthetic material $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$, a close relative of a mineral compound discovered in a Chilean mine in 2004 and based on spin triangles forming a Kagomé net, could well be the very first realization of this novel

state. Using the high sensitivity of muons, we demonstrated the absence of any magnetic ordering down to a 50 mK, well below the 200 K coupling energy of the spins. This makes $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$ a very promising candidate for spin liquid physics.



Phase diagram of the paratacamite family compounds $\text{Cu}_{4-x}\text{Zn}_x(\text{OH})_6\text{Cl}_2$. Magnetic order vanishes as the perfect Kagomé case ($x=1$) is approached.

Charge order to remove orbital degeneracy in triangular antiferromagnet AgNiO_2

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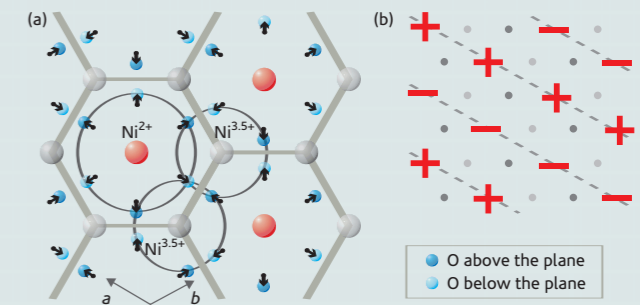
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E Wawrzyńska et al., arXiv:0705.0668v2

The layered hexagonal magnet AgNiO_2 realizes a unique example of a triangular antiferromagnet with both spin and orbital moment (Ni^{3+} with one e_g electron) and with metallic conductivity. Both the spin and orbital order are frustrated in a triangular geometry and the electronic ground state when electrons are mobile is not well understood. Using high-resolution diffraction on Osiris and HRPD we have uncovered a supercell crystal structure where expanded NiO_6 octahedra are surrounded by a honeycomb network of contracted sites (see figure). Band-structure calculations indicate

that this structural modulation is naturally explained by a spontaneous charge order on the Ni sites: expanded sites are electron rich Ni^{2+} and contracted sites are electron depleted $\text{Ni}^{3.5+}$. Our results show that in weakly-delocalized metallic systems the orbital degeneracy can be lifted by charge order as opposed to the Jahn-Teller distortions found in insulating systems. At base temperature the honeycomb sites are nonmagnetic and the expanded Ni sites order in an unusual collinear pattern of alternating stripes on a triangular lattice (see figure).

(a) Charge order on the Ni sites leads to displacements of the surrounding oxygen ions, directly observed by high-resolution diffraction measurements. (b) Magnetic order: +/- are spins in/out of plane, dots are unordered sites.



Pinch points and Kasteleyn transitions in Kagome ice

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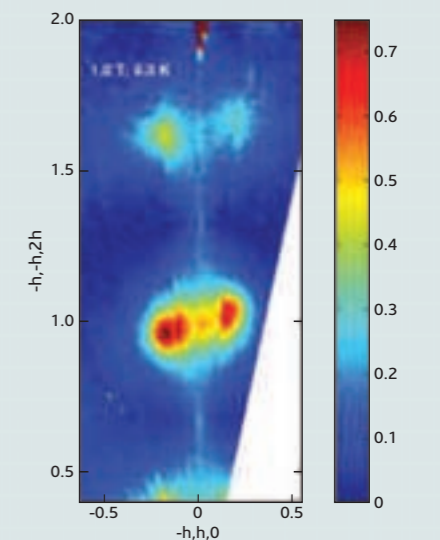
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T Fennell et al., Nature Physics 3, (2007) 566

Spin ice is an example of a system in which the geometry of the lattice produces frustration, i.e. if two neighbouring spins are mutually arranged a third neighbouring spin cannot be. This leads not to long range order as found in many magnetic systems at low temperatures, but to a multitude of degenerate states. In such a system unusual transitions are expected in which the entropy decreases to zero while the internal energy is unchanged. Such so-called 'Kasteleyn transitions' have previously been observed in lipid bilayer systems: spin ice affords the first magnetic example. $\text{Ho}_2\text{Ti}_2\text{O}_7$ is an example of a spin ice and in applied magnetic field the quasi-two dimensional version can be obtained (so-called Kagomé ice). Using PRISMA we were able to verify that the neutron scattering in the Kagomé ice phase changes as expected close to a Kasteleyn transition. Simultaneously we observed the highly anisotropic 'pinch point' scattering, seemingly indicative of simultaneous long and short range order, being sharp in one direction and diffuse in all others. In fact such features are the key signature of any type of topological constraint in a

frustrated system which can be mapped to the ice rules. These observations open the way to the observation of similar effects in other related systems, such as some hydrogen bonded networks, where it is also expected that ice rule constraints operate.



Diffuse scattering from the Kagomé ice phase of $\text{Ho}_2\text{Ti}_2\text{O}_7$, showing distinctive pinch point scattering at $x = 0, y = 0.667$ and 1.333 .

Molecular and Polymeric Materials

Designing drug nanodispersions

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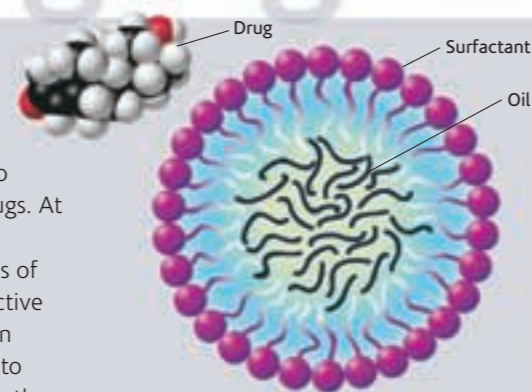
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MJ Lawrence and DJ Barlow (2006) in Encyclopedia of Pharmaceutical Technology (Third Edition), J Swarbrick (Ed), Marcel Dekker Inc.

Oil-in-water microemulsions are spontaneously formed, nanosized dispersions of oil in water stabilised by surfactant. They have recently found favour as 'solvents' in which to encapsulate poorly water-soluble drugs. At present, however, there is little understanding as to the combinations of oil and surfactant that are most effective for encapsulating drug. We have been using small angle neutron scattering to perform the first studies to determine the location of a range of steroidal drugs encapsulated within these nanodispersions, with a view to determining the oil/surfactant combinations best for drug delivery. We have used the technique of neutron contrast variation by employing deuterated and hydrogenous oils and surfactants. By fitting the neutron scattering results to models of microemulsion shape and size, the location of the drugs within the



Cartoon of an oil-in-water microemulsion with steroidal drug (testosterone) shown.

microemulsions has been deduced. At low steroid concentration, the drug is preferentially located in the surfactant shell, while at higher concentrations it enters the particle's oil core – thus demonstrating the importance of the oil in determining the level of drug encapsulation.

Interfacial structure in conjugated polymers

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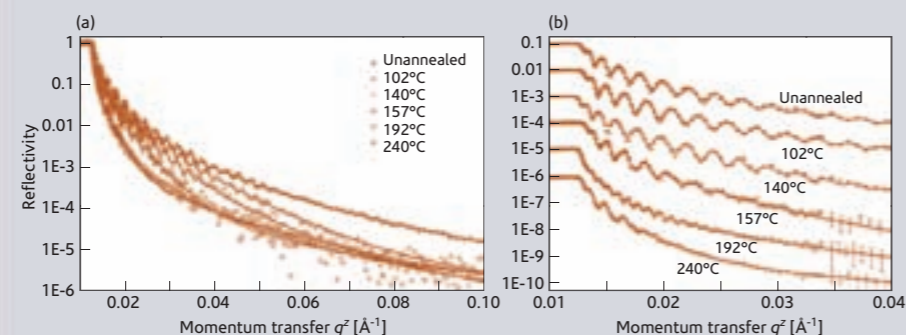
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AM Higgins et al. Macromolecules 39 (2006) 6699

We have used neutron reflectivity and nuclear reaction analysis to look at the interfacial width between two different types of conjugated polymer. The interfacial widths are far greater than observed previously at amorphous polymer interfaces. To understand these broad interfaces we have compared our results to the predictions of self consistent field theory (SCFT), for both Gaussian and semiflexible chains. We have also demonstrated the ability to control the

interfacial width in thin (~ 100 nm) bilayers, independent of the properties of the bulk of the films. This opens up the potential for fabricating LEDs that have identical charge transport properties from the electrodes to the interface, and differ only in the width of the polymer-polymer interface. We believe that this could provide a model system for studying the effect of mixing at polymer-polymer heterojunctions on device performance.



Reflectivity data and bilayer fits for annealed thick F8BT(339nm)/dF8(221nm) bilayers on silicon. (b) shows the low q_z data shifted vertically for clarity.

Dihydrogen complex or classical dihydride?

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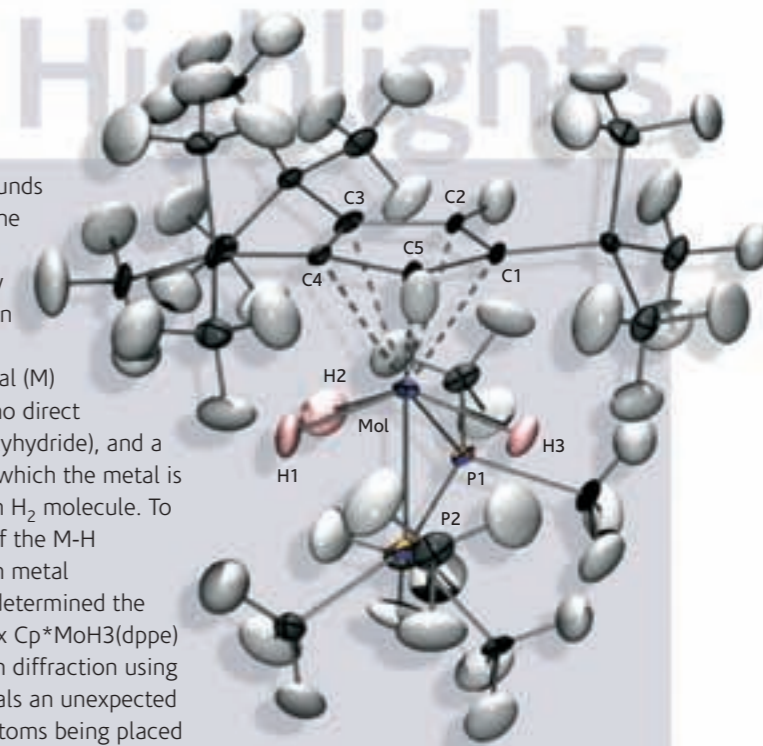
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M Baya et al., Chem. Eur. J. 13 (2007) 5347

The structure of compounds containing more than one H atom bonded to a transition metal may lay on a continuum between two extremes: separate bonds between the metal (M) and each H atom with no direct H-H bonds (classical polyhydride), and a dihydrogen complex in which the metal is covalently bonded to an H₂ molecule. To investigate the nature of the M-H interactions in transition metal polyhydrides, we have determined the structure of the complex Cp*MoH₃(dppe) by single crystal neutron diffraction using SXD. This complex reveals an unexpected geometry, with two H atoms being placed at a distance from each other that is too long for a direct H-H interaction (H₂-H₃ ~ 1.4 Å), but short compared to typical classical polyhydrides (~ 1.8 Å). Furthermore, one-electron oxidation of the metal induces a significant closing of the H-H separation. This the first structurally characterised example of two polyhydride



The neutron structure of complex Cp*MoH₃(dppe).

complexes having the same composition but differing by one electron, illustrating the effect of the metal oxidation state on the tendency of polyhydrides to undergo collapse and elimination of H₂.

Magnetic order in the quasi-one-dimensional spin-1/2 molecular chain compound copper pyrazine dinitrate

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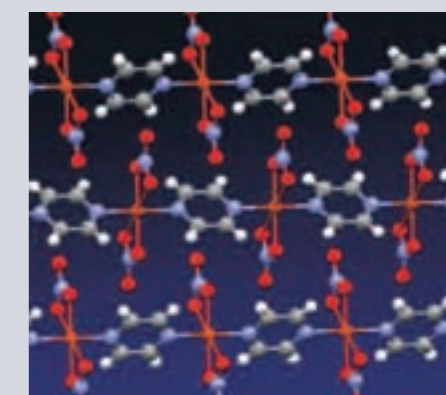
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T. Lancaster et al., Phys. Rev. B 73 (2006) 020410

Low dimensional magnetism is a fascinating experimental testing ground for fundamental many body quantum physics. The quantum magnet copper pyrazine dinitrate consists of isolated 1D chains of Cu²⁺ ions which each have spin-1/2. Long range magnetic order is not expected to occur in an ideal 1D material, and no magnetic transition had been detected in copper pyrazine dinitrate. However, measurements using muons have recently shown that a transition to magnetic order does occur below 107 mK in this material. At these very low temperatures the interchain coupling, though weak, starts to have an effect and the system 'realises' that it is really three-dimensional. Muons are very useful for detecting this effect and contrast with conventional bulk probes which are ineffective in very anisotropic systems and often miss the ordering transition.



The chain compound CuPzN consists of S=1/2 Cu²⁺ ions linked by pyz ligands. Muon measurements show that the material magnetically orders at 107 mK.

Technological Materials

Nature of the Bound States of Molecular Hydrogen in Carbon Nanohorns

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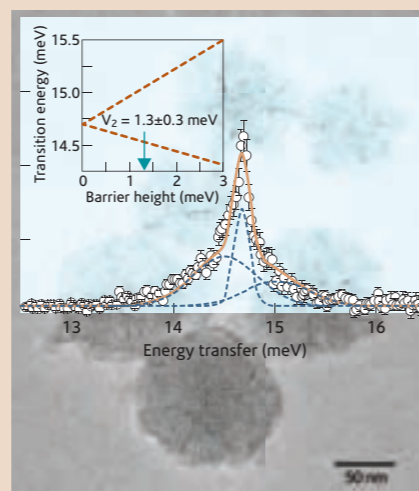
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F Fernandez-Alonso et al., Phys. Rev. Lett. 98 (2007) 215503

Hydrogen has great potential as an energy source. Unlike fossil fuels, it can be generated from renewable sources. It is also non-polluting and forms water as a harmless by-product. Yet it is so difficult to store in a safe and cost-effective manner that its use as a fuel has been very limited. Carbon nanotubes (NT) have been considered for this task but, so far, their feeble interaction with molecular hydrogen (H_2) has kept storage temperatures below a chilling $-196\text{ }^\circ\text{C}$. Carbon nanohorns (NH), however, appear to offer some hope. NHs have an average length of 2-3 nm and aggregate to form beautiful dahlia-like structures (see figure). As a result, they display huge surface areas, approaching $1500\text{ m}^2\text{g}^{-1}$ (that is, roughly the area of a football field in just a handful of this material!). High-resolution neutron spectroscopy experiments on Isis have provided quantitative insight about the adsorption of H_2 in this novel form of carbon. A high density of conical 'nanotips' leads to solid-fluid interaction energies at least four times stronger than those found

in NTs. Our results therefore suggest that NHs and related nanostructures can offer significantly better prospects as light-weight media for hydrogen storage applications.



Background: TEM image of NH aggregates. Graph: H_2 -NH neutron spectrum; its characteristic line shape provides direct access to the energetics (rotational barrier) and geometry (quantization axis) of the H_2 adsorbate.

Microscopic magnetic ordering at exchange-biased interfaces

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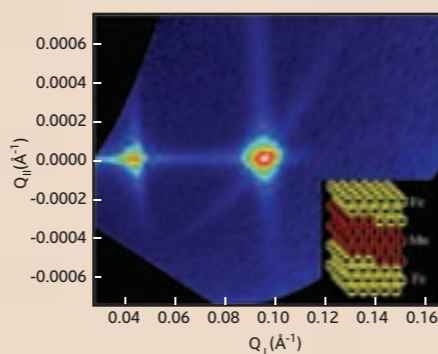
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SJ Lee et al., Phys. Rev. Lett. 99(3) (2007) 037204

There has been intense interest in the exchange-bias phenomenon in recent years due to its importance in technological applications such as read heads, sensors, and magnetic random access memory. Bias fields arise within magnetic multilayers from the interaction between ferromagnetic (FM) and antiferromagnetic (AF) components, but these fields are an order of magnitude smaller than expected using simple microscopic models. Until now it has proved impossible to determine the magnetic structures at the interfaces between the layers on the nanoscale using neutrons due to signal limitations. Using Fe/Mn multilayers we have been able to reveal the magnetic ordering at buried interfaces with atomic resolution in a simple system with uncompensated moments with all spins aligned in the AF Mn atomic layer next to the FM Fe. Our measurements show completely unexpected orthogonal magnetic

structures, which may arise from frustration of the interfacial interaction at terraces (see figure). The results readily explain why the bias fields are so small, and show that the microscopic magnetic ordering assumed in a variety of exchange-biased systems may have to be revised.



The vertical streaks in the polarised neutron reflectivity measured using CRISP show correlated magnetic roughness from terraces, explaining the magnetic ordering shown in the inset.

The effects of mechanical tensioning for controlling residual stresses in friction stir welds

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Further information:

DG Richards et al., Materials Science Forum 524-525 (2006) 71

Aluminium is very difficult to weld; that is why aircraft are traditionally riveted. Friction Stir Welding (FSW) is a new method by which panels can be joined together by passing a rotating tool down the weld-line. As the tool advances metal moves past it to form a joint without melting. It is of great interest to the aircraft industry to replace riveting both to reduce weight and remove the holes that act as stress concentrators from which cracks can form. However as with conventional welding FSW can introduce substantial residual stresses which can

have a detrimental impact on service life. We used neutron diffraction as an atomic strain gauge to see if it was possible to reduce the weld stresses by tensioning the plates as they are joined. We found that the stresses decrease linearly with the level of tension applied. In fact almost no stress was present after welding under tensile stresses 30% of the yield stress. Larger stresses were found to introduce compressive stresses into the weld region. This work is being used to optimise the weld stresses to improve performance and joint lifetimes.

Large aircraft such as the A380 superjumbo contain over 300,000 rivet holes.



Patterning of sodium ions and the control of electrons in sodium cobaltate

DJP Morris, JP Goff (University of Liverpool), DA Tennant (HMI Berlin, Germany), M Roger (CEA Saclay, France), D Prabhakaran (University of Oxford), MJ Gutmann (ISIS)

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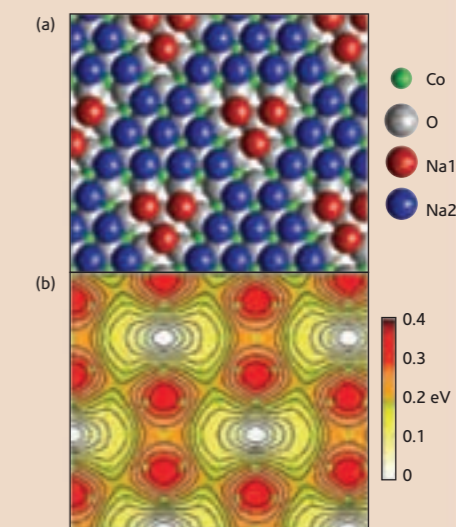
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Further information:

M Roger et al., Nature 445 (2007) 631

Na_xCoO_2 is a promising candidate for thermoelectric applications to cool electronic devices and convert wasted heat into electricity. We have used neutrons to better understand its properties. Neutron diffraction from Na_xCoO_2 reveals a kaleidoscope of sodium ordering patterns as a function of concentration. Electrostatic forces stabilize sodium vacancies into clusters (shown in red in the figure) and these order long range at simple fractional fillings. The sodium superstructures strongly affect the electronic behaviour of Na_xCoO_2 . They cause some of the charge carriers in the Co layers to be trapped, and in this way the sodium ordering can be used to control the electronic properties. The Coulomb landscape in the figure shows how the mobile charge carriers are confined to restricted regions of the plane, enhancing their interactions and explaining their anomalous properties. The vacancy clusters form cages in which sodium ions can rattle, disrupting phonon propagation

without affecting the electrical conductivity and resulting in Na_xCoO_2 's thermoelectric properties.



(a) $Na_{0.8}CoO_2$ forms an ordered array of vacancy clusters. (b) The Coulomb potential in the Co layer calculated using the superstructure from Sxd.

The Importance of Disorder

Local environment of ferric iron in a silicate glass

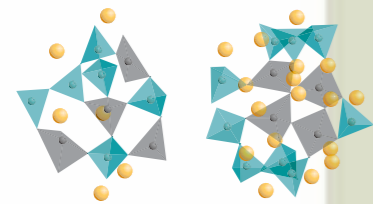
C Weigel, L Cormier, L Galoisy, G Calas (Universités Paris 6 et 7, France), B Beuneu (Laboratoire Léon Brillouin, France), DT Bowron (ISIS)

Contact details:

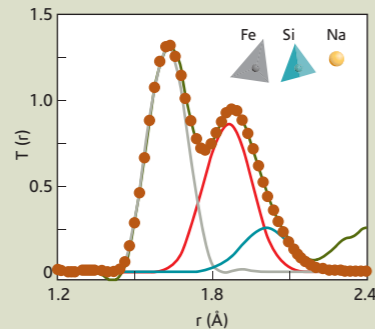
Dr L Cormier, cormier@impmc.jussieu.fr

Further information:

C Weigel et al., *App. Phys. Lett.* 89 (2006) 141911



The presence of iron in glassy materials, either as a ubiquitous impurity or as an intentional additive, affects important properties such as melt rheology, and optical and thermodynamic properties. Fe³⁺ is the most abundant valence state of iron in technological glasses, for example controlling UV-transmission in 'solar-control' soda-lime glasses for housing and automobiles. The determination of the local structure around Fe³⁺ in glasses is limited by disorder effects and by the



permanent coexistence with Fe²⁺. Neutron diffraction with iron isotopic substitution was used to determine the detailed iron environment in a Na₂O-Fe₂O₃-2SiO₂ glass. High real-space resolution neutron diffraction data obtained on SANDALS and Empirical Potential Structure Refinement (EPSR) simulations have been combined to quantify the extent of two different iron coordination environments. Tetrahedral Fe³⁺ constitutes 76% of the total Fe sites and a second contribution corresponds to 5-coordinated Fe³⁺ and Fe²⁺. These results are important for understanding the structural role and distribution of iron within the glass structure and provide a rationale for modelling redox properties in silicate melts.

Correlations between atoms in a Na₂O-Fe₂O₃-2SiO₂ glass. The two Fe-O contributions (red and blue) are also observable in EPSR simulations, with typical distinct environments for Fe³⁺O₄ tetrahedra.

Strain at a phase transition in perovskite suppressed by cation disorder

CJ Howard, Z Zhang (ANSTO, Australia), MA Carpenter (University of Cambridge), KS Knight (ISIS)

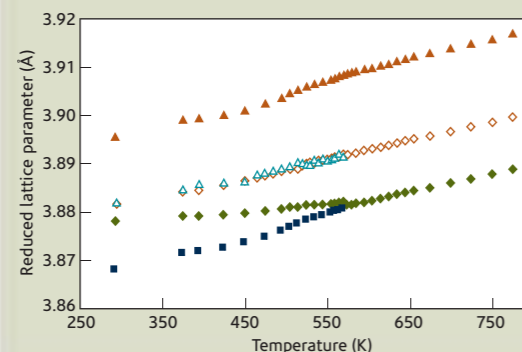
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Further information:

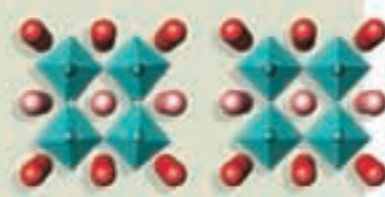
CJ Howard et al., *Phys. Rev. B* 76 (2007) 054108.

Phase transitions in perovskites and their variants, of general formula ABX₃, are important for technological applications and also of great interest in the earth sciences. Those with partial occupation of the A site, such as La_{2/3}TiO₃, have useful dielectric properties and show potential as ionic conductors too. We have prepared samples in which layers of cation A sites are alternately fully and partially occupied and, by quenching, different samples at the same composition in which the A sites are occupied at random. We have used HRPD to make precise measurements on the



Reduced lattice parameters for samples of La_{0.6}Sr_{0.1}TiO₃ with layered ordering (filled symbols) or random occupation (open symbols) on the perovskite A-site. Schematics of the ordered structures are included.

transition associated with the tilting of BX₆ octahedra. The samples with cation ordering show a tetragonal metric above the transition, and become orthorhombic as the strain associated with tilting takes effect. Those with disordered cations show a cubic metric above the transition as expected but, surprisingly, the tilting induces no measurable strain. We believe cation disorder inhibits the development of long-range strain fields, and that the frequent occurrence of near cubic metrics in perovskites can be a consequence of similar effects.



Perturbation of water structure by dissolved ions

R Mancinelli, A Botti, F Bruni, MA Ricci, (University of Rome III, Italy), AK Soper (ISIS)

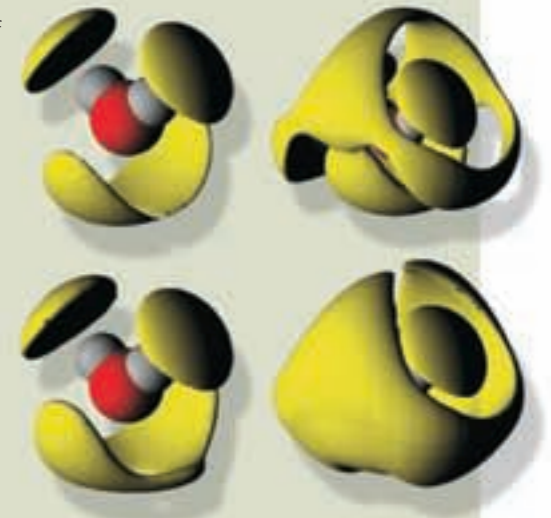
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Phys. Chem. Chem. Phys. 9(23) (2007) 2959

Most naturally occurring water has ions (charged atoms) dissolved in it. Whilst there is plenty of information available about how ions in solution strongly orientate the water molecules that hydrate them, there is surprising paucity of information – and controversy – about how water structure itself (the relative arrangement of one water molecule to another) is affected by the presence of dissolved ions. In pure water this arrangement has a 'tetrahedral' structure, giving water the characteristic of a disordered network of hydrogen bonded molecules. Using a series of neutron diffraction experiments on Sandals with hydrogen/deuterium substitution, the structure of water in a number of ionic solutions and over a range of concentrations was investigated. With increased concentration, the first shell of water molecules around a central molecule remains largely intact, but the second shell collapses inwards (see figure),



Spatial density of water (inner shell left, second shell right) around a central water molecule in pure water (top) and concentrated sodium chloride (bottom).

Spin glass order induced by dynamic frustration

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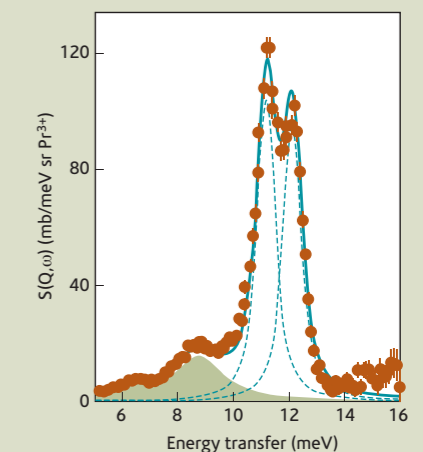
Dr EA Goremychkin, E.A.Goremychkin@rl.ac.uk

Further information:

EA Goremychkin et al., *J. Mag. Mag. Mat.* 310 (2007) 1535

Spin glasses (SG) are systems whose magnetic moments freeze at low temperature into random orientations. The presence of frustration and disorder are necessary ingredients for an SG transition. It was therefore surprising that PrAu₂Si₂ was reported to show all the characteristics of a SG, even though it is a stoichiometric compound with a well-ordered structure. To understand the origin of the SG ground state in PrAu₂Si₂, we have performed inelastic neutron scattering measurements of the crystal field (CF) excitation spectrum. These measurements classified PrAu₂Si₂ as an induced moment SG where the exchange interaction is only just above the critical value for induced moment magnetism with substantial CF linewidth at T_g which plays a central role in disrupting of induced moment formation (see figure) and resulting in the SG ground state. We suggest that PrAu₂Si₂ reveals a new way to achieving frustration in systems with neither static disorder nor geometrically

frustrated lattices, through dynamic fluctuations in proximity to a critical phase boundary.



Inelastic neutron scattering from PrAu₂Si₂ measured at 1.5 K on HET with an incident energy of 18 meV. The solid line is the result of a fit to a crystal field model, with the individual crystal field transitions displayed as dashed lines. The shaded area is the phonon scattering estimated from data taken at high scattering angle.

Technology Development for Neutron Scattering

Cryo-free low temperature sample environment based on pulse tube refrigeration

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to be published in Measurement Science and Technology

Recent rapid progress in cryo-free technology has become possible due to a new generation of commercial cryo-coolers developed during the last decade. The most successful example is the Pulse Tube Refrigerator (PTR). A unique feature of the PTR is the absence of cold moving parts. This considerably reduces the generated vibration and increases the reliability of the cold head, as expensive high-precision seals are no longer required and the cold head can be operated without service inspection. In order to introduce PTR into cryogenic sample environment for neutron scattering experiments, ISIS user support group started a project to create a cryo-free system as a substitute for the conventional ILL-type Orange cryostat which has been the cryogenic workhorse of the neutron community for many years. The cryo-free system prototype has successfully passed initial tests and we are now in the final stages of the project.



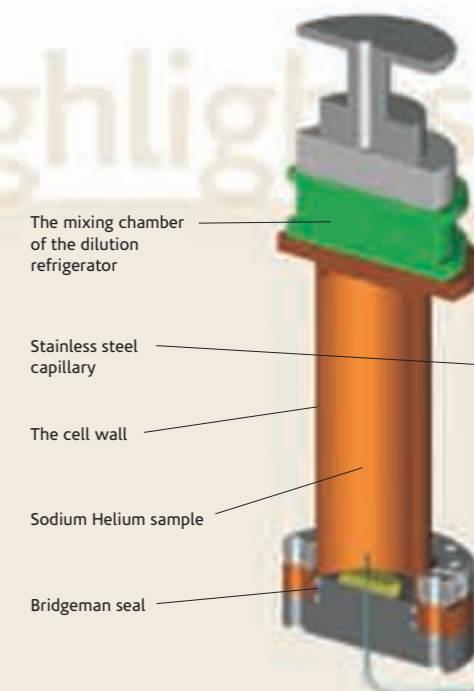
The prototype cryo-free system based on the PTR for providing cryogenic sample environment for neutron scattering experiments.

High pressure experimental apparatus for studies of superfluid flow in solid helium

MA Adams, J Mayers, R Done, M Chowdhury, RBE Down, OI Kirichek (ISIS)

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Dr Jerry Mayers, j.mayers@rl.ac.uk;
Dr O Kirichek, o.kirichek@rl.ac.uk
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MA Adams et al., Phys. Rev. Lett. 98 (2007) 085301

The study of superfluidity in liquid helium has spawned nearly 20 Nobel prizes. Its fundamental interest lies in the manifestation of quantum mechanics on macroscopic length scales – for example quantisation of angular momentum. This implies that superfluid helium contained in a torus remains stationary if the torus is rotated slowly. In 2004 it was shown that below 0.2 K, ~2% of the mass of **solid** helium contained in a torus similarly does not rotate when the torus is rotated! It has been proposed that Bose Einstein condensation (BEC), which is responsible for superfluidity, is also responsible for ‘supersolidity’. BEC in the liquid gives a sharp drop in atomic kinetic energy and spaces develop in the liquid structure. In contrast a VESUVIO experiment observed no change in the structure or kinetic energy of the crystalline solid, suggesting that BEC does not occur. This kind of experiment requires special high pressure and ultra-low temperature sample



The high pressure cell developed for neutron scattering measurements of single atom kinetic energy in solid ⁴He.

environment. ISIS user support group developed the experimental apparatus for the Vesuvio experiment, together with the experimental procedure used for growing a controlled quality solid ⁴He sample.

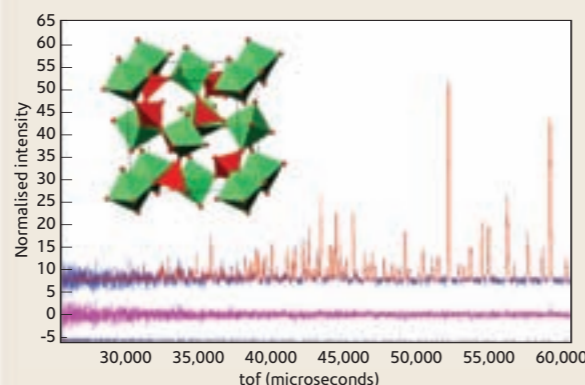
Monte-Carlo modelling of the HRPD guide using distributed computing

RM Ibberson, KS Knight, L Chapon, TAN Griffin and K Shankland (ISIS)

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<http://www.ud.com/products/gridmp.php>

Whether designing a new neutron instrument or upgrading an existing one, Monte-Carlo (MC) simulations play an increasingly important role in optimising instrument performance. The final design of the supermirror guide upgrade for the high-resolution powder diffractometer (HRPD) at ISIS, which will significantly enhance the neutron flux that is incident upon the sample, has been heavily influenced by MC simulations performed using the McStas computer program. Such

simulations are computationally demanding and by distributing sub-components of the calculation over a network of several hundred desktop personal computers, controlled by the GridMP system, simulations were able to be performed in much greater detail than ever before. In fact, not only could incident flux distributions be rapidly simulated as the design was altered, but entire diffraction patterns for well-characterised reference materials could also be rendered. The latter calculation for zirconium tungstate accrued some 230 days of CPU time in only 2.5 calendar days. Such calculations are clearly impractical for a single processor PC.



Simulated diffraction for cubic ZrW_2O_8 on HRPD using the new guide. Only a small portion of the full range (which extends to 120,000 μ s) is shown.

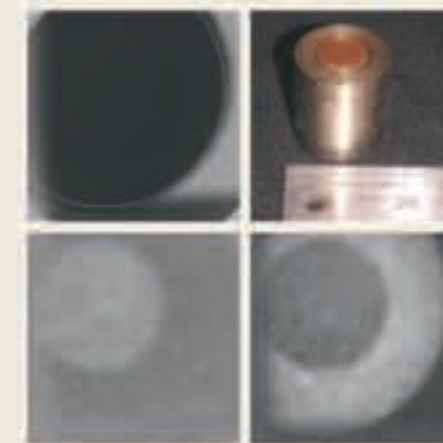
Energy-selective neutron radiography at a pulsed source

G Frei, P Vontobel, EH Lehmann (Paul Scherrer Institut, Switzerland), JR Santisteban (CNEA, Argentina), W Kockelmann (ISIS)

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W Kockelmann et al., Nucl. Instr. Meth. A 578 (2007) 421

Pioneering pulsed-source neutron radiography experiments were carried out on OSIRIS and ENGIN-X. This neutron transmission imaging technique combines the hardware used for conventional neutron radiography with the Bragg edge transmission features of time-of-flight methods. The main component of the energy-selective radiography set-up was a gated image-intensified CCD camera that viewed a neutron-sensitive scintillation screen via a mirror. Energy resolution was obtained via synchronization of the light-intensifier with the pulse structure of the neutron source. A main advantage of the imaging method at a pulsed source is that energy-selection can be achieved for a large field of view and with high wavelength resolution in terms of the band width. Contrast variation and enhancement of materials that are indistinguishable by conventional neutron or X-ray radiography can be straightforwardly achieved taking advantage of the excellent crystallographic-phase sensitivity of the method, by

collecting images below and above characteristic Bragg edges of the phases. Microstructural features such as crystallographic texture can be directly visualized with high spatial resolution, in principle even for distinct texture components.



Contrast-enhanced radiographs of a copper cylinder shrink-fitted into a ferrite cylinder, compared with a conventional radiographic image of the same object.

Instrument Developments

Development at ISIS is a continuous process, driven both in response to the changing needs of the user community and to maintain ISIS as a world-class neutron and muon source. Evolution of the existing instruments, and design and construction of new ones, open up fresh opportunities for materials investigations. Some of the major developments over the past year on ISIS instruments are described here.

Merlin

Merlin is the new high flux inelastic instrument at ISIS, designed to have 10-30 times the count rate of its predecessor HET. The instrument is now finished and we are awaiting beam to complete the technical and scientific commissioning. Merlin will work in an energy range similar to MAPS and HET (10 – 1500 meV) and has a very large position sensitive detector bank to enable studies of magnetic or lattice excitations in crystals or powders.

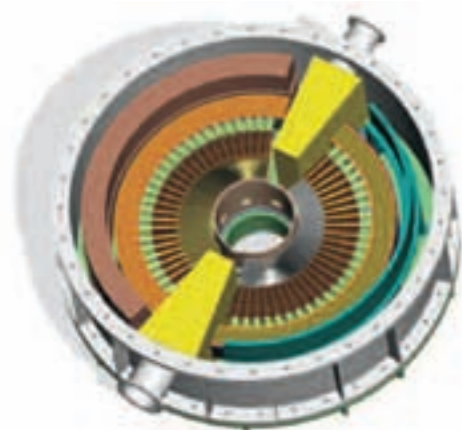


The new MERLIN instrument.

IRIS

The long shut-down has seen an extensive upgrade of IRIS detector banks. The work has included production of new photomultiplier tube manifolds for the graphite and mica analyser banks; addition of μ -metal shielding to avoid stray-field interference from cryomagnet operation on neighbouring instruments; and improved stability by use of GEM-type detector electronics and relocation to a temperature-controlled environment. Following an initial commissioning period, IRIS is expected to resume its user programme later this year.

Top view of the IRIS spectrometer showing the new graphite (left) and mica (right) detector banks.



HRPD

HRPD is presently undergoing a major upgrade with the installation of a high-reflectivity supermirror guide. Supermirror technology allows major flux increases in the key high-Q region (an order of magnitude more than the existing instrument) and, in addition, the increased radius of curvature of the new guide design will allow the transmission of shorter wavelength neutrons making it feasible to access even smaller d -spacings. The intrinsically high instrumental resolution, $\Delta d/d$ better than 10^{-3} and effectively constant across the whole diffraction pattern, is retained. The old guide has been removed and preparations are underway for installation of the supermirror replacement.

LOQ

Conversion of LOQ from VMS/CAMAC-based to PC/LabView/SECI-based control has been completed, and there is also a new XML-based format for reduced data which will be common to SANS beamlines at ILL and SAXS at

DIAMOND. The new 'SANS Xpress' access mechanism has been launched, where one day of beam per cycle is available for samples sent in by post, either to obtain desperately needed results, to complete earlier work or to try new ideas. A new Anton-Paar Rheometer for LOQ, and eventually for SANS2d and I22 at DIAMOND, is now available for users.

SURF

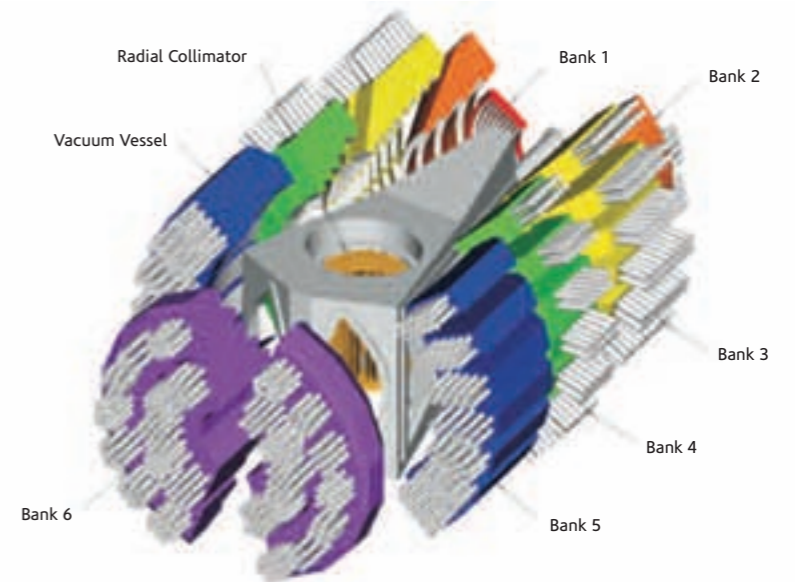
The motion control electronics on SURF have been upgraded to run with the new standard ISIS Galil control system, requiring a complete rewiring of the instrument. The data acquisition electronics have been upgraded to the new DAE-2 system, and the DEC alpha instrument control workstation has been replaced with a PC. Finally, the instrument control program and motor controls software are being upgraded to comply with the standards set for the new TS-2 instruments.

CRISP

The CRISP reflectometer has also completed its transition to the Galil controller system. The motor control software developed during this project is providing a template for the control systems for TS-2. CRISP continues to run a diverse program of science ranging from detergency to quantum effects in liquid ^3He . About 1/3 of beamtime is devoted to thin film magnetism with an increasing emphasis on off-specular scattering.

Hifi

Hifi is the new high field muon spectrometer being built with funds from the Facility Development programme. The past year has seen the ordering of the main 5 T magnet from Cryogenic Ltd, with delivery expected in March 2008. Design of the instrument detector array is also almost finalised. The geometry of the array has proved a challenge, as the magnetic field strongly affects the decay positron trajectories, but prototype detectors have just been tested, and the full array should go for



Schematic of a possible design for the upgraded POLARIS instrument.

manufacture later this year. To make way for Hifi the DEVA spectrometer has been decommissioned, so that the EC muon facility will run with just two instruments rather than three for a period of around a year. Hifi is expected to be operational from late 2008.

POLARIS

The POLARIS upgrade, funded through the STFC Facility Development programme with contributions from Swedish and Spanish partners, will see a complete rebuild of the instrument. Detector banks will be replaced by large solid angle GEM-type modules to give a significant increase in count rate; incident beam collimation will be improved; and an oscillating radial collimator will reduce background scattering when using complex sample environment equipment. Detailed design work is now in progress, and installation of the new instrument is provisionally planned for late 2009.



Schematic of the new Hifi muon spectrometer, showing the 5T superconducting magnet, instrument detector array and beamline.

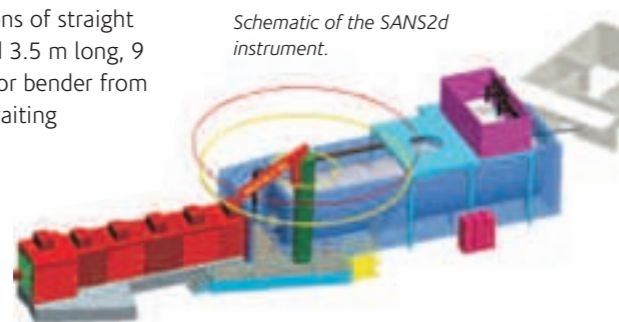
Instrument Developments

SANS2d

The 13 m long, 3.25 m diameter vacuum tank for Sans2d was the first major TS-2 beamline component to be delivered (in March 2007). Later in the year it will disappear under a very large wax shielding blockhouse. A contract has been placed for the design and installation of the rails and trolleys for the moving detectors, the beam stops and shielding baffles inside the tank. Two 1 m square multiwire detectors have been delivered from the USA and tested. The five 2 m sections of straight neutron guides and 3.5 m long, 9 channel, supermirror bender from Switzerland are awaiting installation.



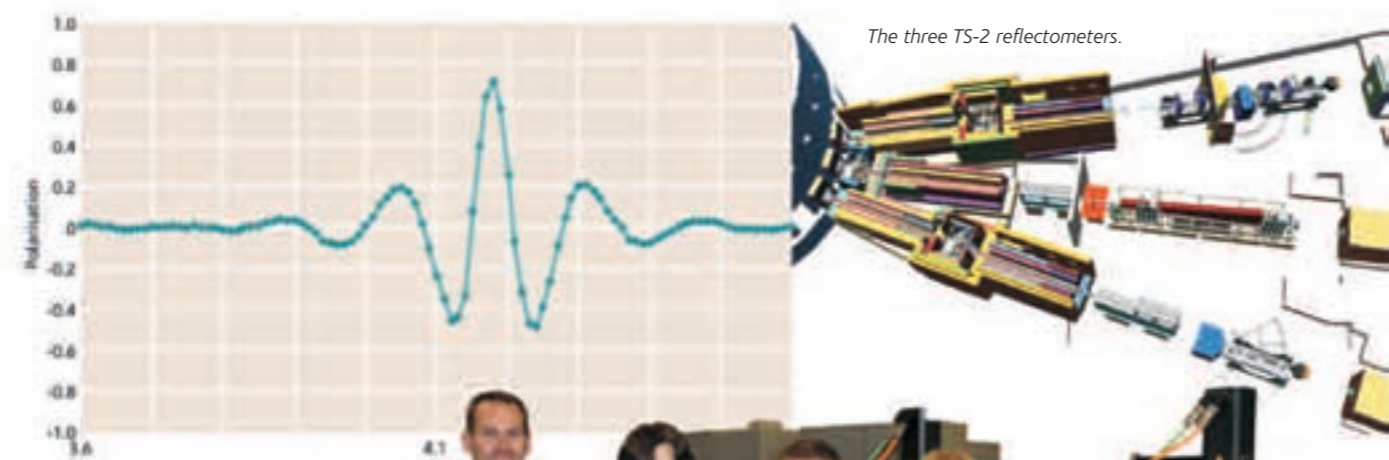
From left to right: the SANS2d vacuum tank, blockhouses in grey undercoat for the Polref, Inter and Offspec reflectometers (25th May 2007).



Schematic of the SANS2d instrument.

Polref, Inter and Offspec

Polref, Inter and Offspec are the three day-1 TS-2 reflectometers. Work has started on their respective blockhouses and should be complete by early June. Final design reviews have been held for the guide systems and work on choppers, sample positions, detector mounts and incident optics continues. We have also obtained our first spin echo data from the Offspec equipment running at Delft, Holland.



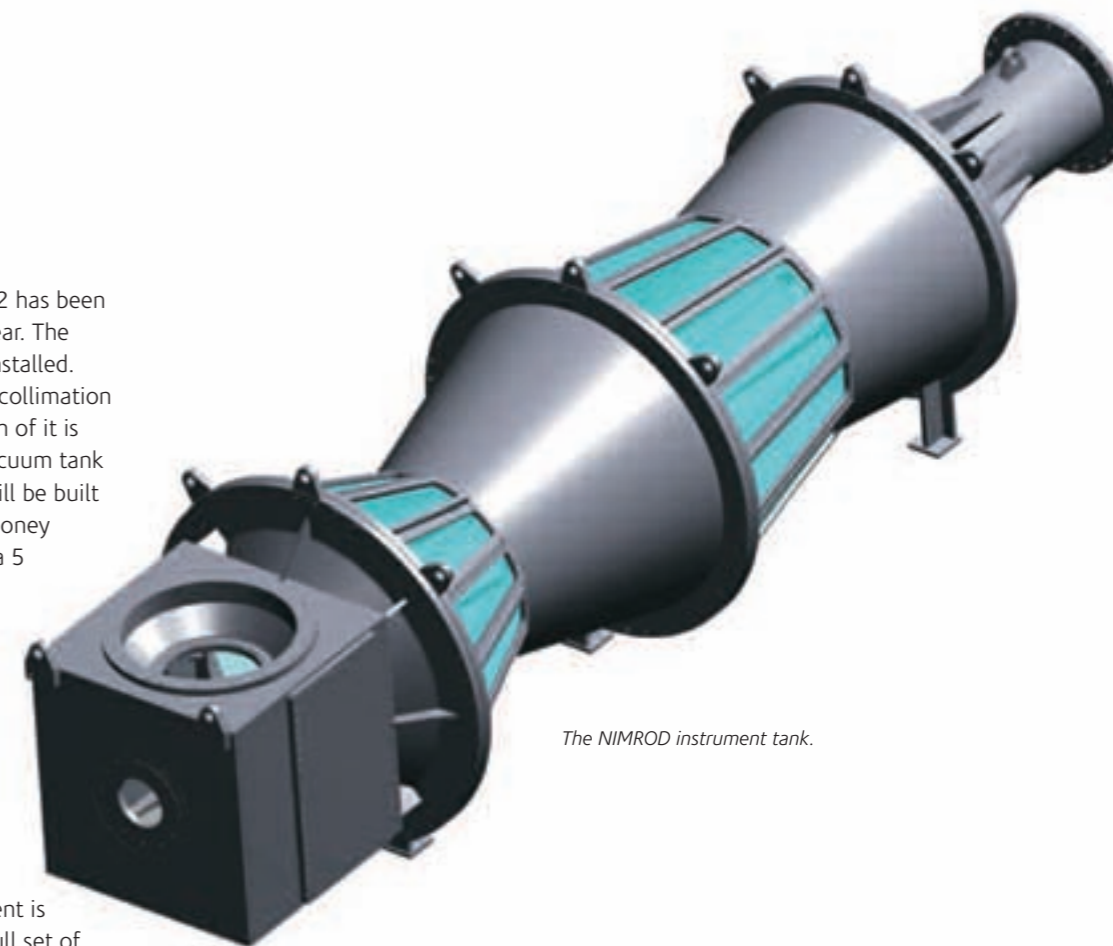
The three TS-2 reflectometers.

First spin echo signal obtained on Offspec equipment (in Delft). Picture shows Tim Charlton, Rob Dalgleish and Sean Langridge (ISIS) and Jeroen Plomp (far left) who collected the data with Prof Ad Van Well and Dr V de Haan (not pictured).



Nimrod

Progress on Nimrod for TS-2 has been substantial over the past year. The beam stop has now been installed. The incident beamline and collimation are now designed and much of it is under manufacture. The vacuum tank is now fully detailed and will be built by CNR in Italy, releasing money for the purchase of an extra 5 detector modules. The detector moulding is now in progress, following satisfactory tests of a prototype detector on Sandals. Work is in progress to finalise the detector support frame and the low angle detector bank. Much of the electronics for the instrument is under construction and a full set of detector cables will be installed ready for the complete set of detectors when they become available.



The NIMROD instrument tank.

Let

Let is low energy chopper instrument that is being built on the ISIS second target station. It is a versatile multi-chopper instrument with a wide dynamic range (incident energies in the range between 0.5 and 80 meV) and the ability to collect several incident energies simultaneously. By trading incident energy for resolution it will be able to achieve either 5 μ eV resolution (with an incident energy of 1 meV), or fluxes an order of magnitude greater than the group's other chopper instruments at low energies. With 5 choppers, a 25 m guide and a sample tank 4 m in radius and 5 m tall Let is a huge piece of engineering. It is on target to be ready for commissioning towards the end of 2008.

Wish

Wish (Wide angle In a Single Histogram) is a long-wavelength TS-2 diffractometer primarily designed for powder diffraction in magnetic and large unit cell systems. Over the last year, progresses have been made in many areas. The elliptic guide is currently being manufactured and the optic bench and supporting frame are being installed. Testing of the 8 mm ³He 1m-long detector tubes was completed in December and 750 tubes have been ordered from Reuter-Stokes. Successful testing of the curved tank windows has released the sample tank for manufacture. The contract for the oscillating radial collimator has been awarded to JJ-Xray. Delivery of disk-choppers is expected before the end of the summer, and work is also progressing on the design of ADC cards.

Fires

Fires is a proposal for a new high resolution back scattering spectrometer to replace Iris. It aims to achieve an order of magnitude higher energy resolution through having a long supermirror flight path, with a concomitant unchanged range of momentum transfers. The extension to μ eV resolution will provide new opportunities in diverse fields such as viscous liquids, biopolymers or quantum magnets and liquids. Short neutron pulses will be generated with a fast chopper, with variable pulse width to enable resolution to be traded against intensity. The secondary spectrometer will consist of huge plates covered with silicon wafers to reflect neutrons in near back scattering geometry on to position sensitive detectors. Detailed Monte Carlo simulation study is now underway.

The Second Target Station

The Second Target station project has progressed rapidly throughout the year.

1. September 2006: First stages of the target station build. Rectangular viewports have been installed to allow neutron beams to travel out to instrument positions. 06EC3076



2. January 2007: Installing instrument beam shutters into the target station. 07EC1113

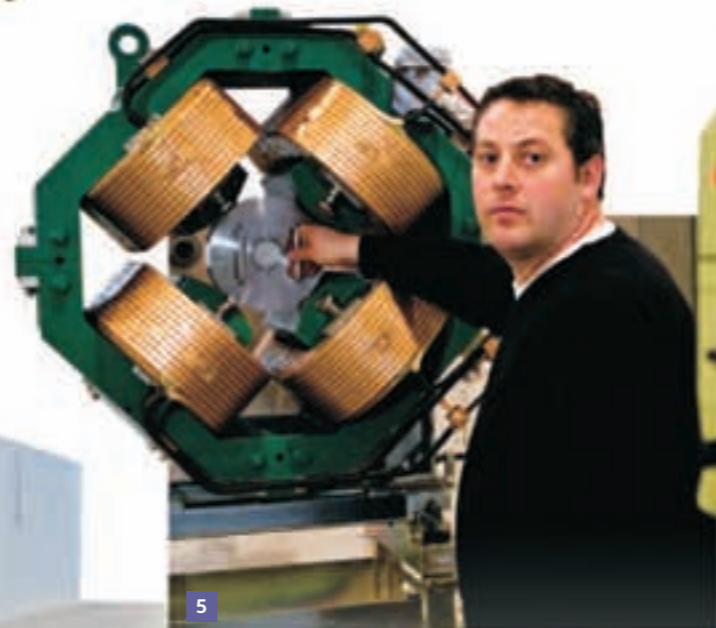


3. March 2007: Core steelwork of the target station nears completion. The final structure contains 5000 tons of steel and is 7 m high and 12 m in diameter. 07EC1672



4. Inserting locating pins into the proton beam tunnel floor to position steering and focussing magnets. 06EC3069

5. Adrian Hooper checking the alignment of a quadrupole focusing magnet before installation. 06EC3781



7. Over 100,000 electrical cable terminations are required throughout the Second Target Station Project. 07EC2038

8. Assembling the beam stop at the end of the Wish instrument. 07EC1698



6. Steel and concrete walls over 1m thick form the proton beam tunnel, through which high energy protons will be fired at the target station. 06EC3727



9. Installation of the TS-2 proton beamline extraction components in the ISIS synchrotron. 07EC3307



10. Scientists working on the development of instruments for the Second Target Station Project standing in the floor recess for the Let spectrometer. Left to Right: Laurent Chapon (Wish), Rob Bewley (Let), John Webster (Inter), Robert Dalglish (Offspec), Sean Langridge (Instrument Working Group Leader), Steve King (Sans2d) and Peter Bradley (Buildings Task Leader). 06EC3716

Accelerator and Target Developments

The 2007 long shut-down has seen large amounts of activity on the accelerators and target. Some of the major projects are described here.

TS-2 Extraction A

The TS-2 extracted proton beam has been joined to the ISIS synchrotron and extraction components installed in the accelerator.

TS-2 extraction in the ISIS synchrotron. 07EC3332



Interlock System Replacement B

Many precautions at ISIS are taken to eliminate access to hazardous areas when ISIS is operating. The personnel interlock systems across the accelerator and target have been upgraded to conform to current safety requirements.

David Rolfe, Steve Clark and Mark Arnold of the Electrical Engineering section testing the new interlock system.



Synchrotron Power Supply Replacement C

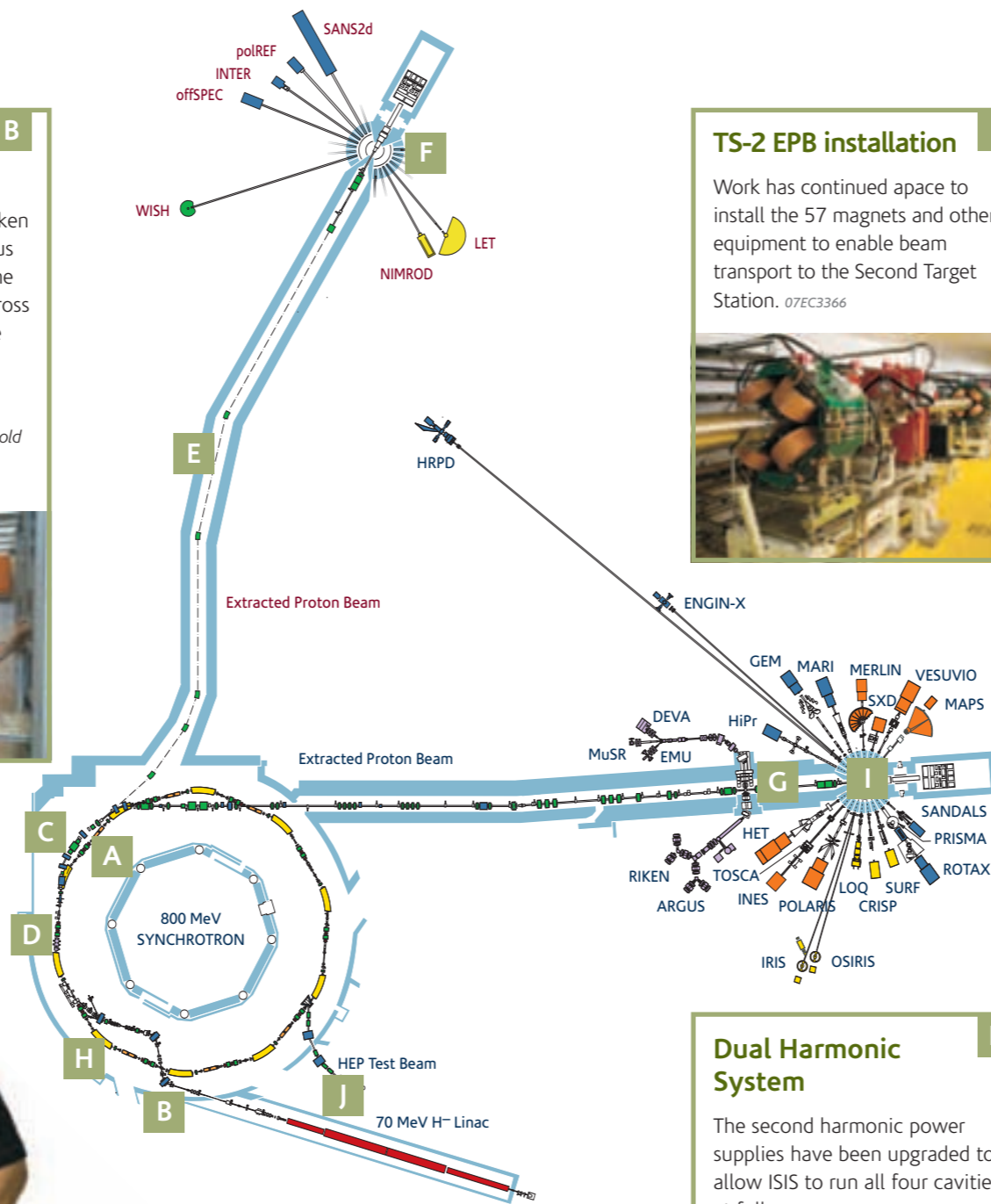
Synchrotron work has included the installation of new extraction kicker power supplies, new injection and extraction septum power supplies, and re-cabling 20 km of magnet power cables for the extracted proton beam line to TS-1.

Adrian McFarland connecting power cables to one of ISIS's upgraded synchrotron kickers. 07EC3109



Synchrotron Diagnostics D

A new 'gas ionisation' beam profile monitor has been installed. This monitor will measure the vertical profile of the proton beam over the full 10ms acceleration cycle, in real time - something that has not been possible before.



TS-2 EPB installation E

Work has continued apace to install the 57 magnets and other equipment to enable beam transport to the Second Target Station. 07EC3366



TS-2 Target Construction F

Work has continued to build the main components of the Second Target Station monolith. 07EC3341



TS-1 EPB Refurbishment G

A failed quadrupole magnet in the extracted proton beam (EPB) has made beam steering difficult and reduced muon production intensity. Three beamline quadrupole magnets have been replaced, and beam collimation and shielding improved.

Concrete shielding removal during EPB refurbishment. 07EC3348



TS-1 Hydrogen Moderator I

The H₂ moderator has been replaced after over 20 years of service, with an improved design allowing greater accessibility and connectivity. Removal of the existing moderator has been a complicated process, requiring specialist remote manipulation equipment. The H₂ moderator control system has also been completely replaced, allowing fully-automated cool-downs.

John Hogston and Mikie Ruddle, (left), adjust the new hydrogen moderator. 07EC3062



Dual Harmonic System H

The second harmonic power supplies have been upgraded to allow ISIS to run all four cavities at full power.

The Dual Harmonic Section - Clive Applebee, Neil Farthing, Derek Morton and Andy Seville. 07EC2888



MICE construction J

The Muon Ionisation and Cooling Experiment, currently being constructed next to the ISIS synchrotron, will demonstrate technology required for a neutrino factory.

Martin Hughes testing a MICE power supply.



1. Sarah Whitehead and Peter Barnes of the ISIS Diagnostics section discussing computer simulation results for the beam diagnostics used in the ISIS synchrotron.



2. Underpinning the design of new accelerators, for example for ISIS upgrades, are studies of high intensity beam loss mechanisms, with appropriate theoretical, simulation and experimental work. Robert Williamson is seen here analysing results of beam acceleration simulations.



ISIS users at work

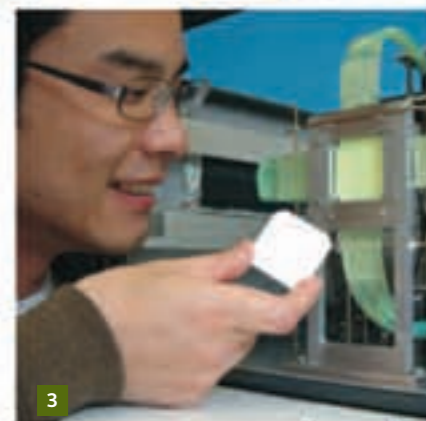
1. Xiubo Zhao and Qingshan Mu (Manchester University) using SURF to look at antibody adsorption by neutron reflection. 06EC2897



2. Marion Jasnin (IBM/LBM Grenoble, France) undertaking a scattering study of macromolecular dynamics inside E. Coli cells on IRIS. 06EC2905



3. Robert Moss and Dave Pickup (Kent University) employing GEM to determine the structure of silver doped, antibacterial, biocompatible phosphate glasses. 06EC4256



3. Tatsuya Nakamura, a visiting scientist from JAEA, examines a neutron sensitive scintillator for his 2D Wavelength Shifting Fibre detector



4. The last, original, operational GEC4000 series computer in the world is finally turned off after 28 years of service running ISIS controls by electronic engineer Steven Lochhead (who wasn't born when it was installed), watched by Controls group Leader Bob Mannix (who was, unfortunately!). 07EC1284

5. ISIS' direct drive chopper team. Left to right Peter Galsworthy, Tim Carter, Mike Brind & Adam Warne. 07EC3074



4. Valerie Linton (University of Adelaide, Australia) looking into residual stresses in full-scale, highly restrained T-butt steel welds using ENGIN-X. 06EC4285



5. Guillaume Huchet and Blair Johnston (University of Strathclyde) using SANDALS to investigate radial distribution in liquid water at room temperature. 06EC4270



A year around the Facility

ISIS Science Away Day 2007

Held at The Cosener's House in February, the away day provided an opportunity for RAL staff to present their research using neutrons, x-rays and muons in areas as disparate as solvation structure in aqueous solutions, chip irradiation, chemical applications of x-ray spectroscopy and high-field muon spectroscopy. The meeting also included a lively poster session at the end of the day to encourage cross-collaboration amongst different departments at RAL. Attendees particularly valued the opportunity for ISIS and DIAMOND staff to get together and build collaborations.



The ISIS Science Away day provided opportunities to hear about neutron, muon and x-ray studies.

ISIS Muons celebrate 20 years!

The ISIS muon source produced its first muons on 23 March 1987. The source was built by a collaboration between the UK, the European Economic Community, Germany, France, Italy and Sweden, and initially consisted of a single muon spectrometer. Further upgrade funds from the European Union in the early 1990s enabled expansion of the facility to three beamlines. To date, at least 800 different muon experiments have been performed. With the provision of a new high-field muon instrument shortly, we look forward to many more years of muon experiments at ISIS.

The ISIS Pulsed Muon Source celebrated its 20th birthday this year. Here, Adrian Hillier, Philip King, Francis Pratt, Steve Cox and James Lord of the Muon Group are cutting the cake for twenty years of muon production.



Third Empirical Potential Structure Refinement Workshop

In November, the third workshop on Empirical Potential Structure Refinement (EPSR) of liquids and disordered solids was held at RAL. The meeting was organised by Daniel Bowron and Alan Soper and celebrated ten years since the original development of EPSR. On the first day, the 25 participants enjoyed a diverse programme of presentations reporting recent scientific highlights and developments of the method. This was followed by trialling of the latest version of the analysis code by the workshop participants under tutorial supervision.

2006 Disordered Materials User Group Meeting

The 2006 ISIS Disordered Materials User Group meeting was held on the 31st October and 1st November at RAL and was attended by 29 participants. The meeting was split into two half-day sessions separated by a lively user group dinner. The first session consisted primarily of activity reports from the facility, whilst the second provided a valuable opportunity for both the younger and more established members of the community to give short presentations on their recent scientific projects.



Participants at the Disordered Materials Group User Meeting.



After a competitive proposal process, ISIS was awarded a display at this year's Royal Society Exhibition. ISIS staff Mark Telling, Dan Fairclough, Chris Frost, Ben Pine, Rowan White and Alan Soper (l to r) helped to explain what ISIS does to the many hundreds of visitors over the exhibition's four days of opening.

Current Challenges in Liquid and Glass Science

This workshop, sponsored by the IOP Liquids and Complex Fluids Group, ISIS Disordered Materials Group, Centre for Materials Science and the Centre for Molecular Structure and Dynamics, focused on present challenges facing the Disordered Materials community. It was also an excellent opportunity to celebrate the considerable contribution that Spencer Howells has made to ISIS science. International speakers from a broad range of disciplines, including computer simulation, experimental studies of materials under extreme conditions and data interpretation, were present, and two poster sessions accommodated contributions that due to time limitations could not be allocated an oral presentation.

Vibrational Spectroscopy at Central Facilities

A joint meeting of the Royal Society of Chemistry Molecular Spectroscopy Group and the Infrared and Raman Discussion Group was held at RAL in August with 37 attendees, half of which were from industry. The talks showed the range of activities in vibrational spectroscopy at CCLRC, including gas phase infrared atmospheric studies, surface science using synchrotron radiation, time resolved Raman studies, neutron scattering and theoretical work. There was a look-forward at how vibrational spectroscopy will develop as Diamond and 4GLS come on-line. The contributed talks are available as a RAL report (RAL-TR-2006-028).

Theoretical and Experimental Magnetism Meeting

The Theoretical and Experimental Magnetism Meeting was held at The Cosener's House in Abingdon in August, organised by the Centre for Materials Physics and Chemistry of CCLRC and by the Magnetism Group of the Institute of Physics, and attracted 87 participants from seven different countries. The meeting presented an excellent opportunity to interact with leading experts from all over the world on topics of current interest in magnetism, and there were 27 oral and 12 poster presentations.

The Disordered Materials community met in January to consider challenges and opportunities in the field.



A year around the Facility

Neutron Training Course

The Neutron Training Course was held again in December 2006 and was, as usual, heavily oversubscribed and very successful. The students benefited from a combination of lectures on key aspects of the neutron technique and practical work on ISIS instruments. We plan to hold the next Training Course in February 2008, with more information available on the ISIS website when the details have been confirmed (www.isis.rl.ac.uk/trainingcourse)

Workshop in Computational Methods for the Exploitation of Vibrational Spectra

This course showed how computational methods can be used for the exploitation of vibrational spectra. ISIS staff Barbara Montanari, Stewart Parker, Timmy Ramirez-Cuesta, Keith Refson and John Tomkinson helped the 29 participants learn more about state-of-the-art software (Gaussian03, DMOL3, CASTEP). For each method the areas of application, its limitations and how to recognise and overcome them were shown. Participants came from a wide range of backgrounds and experience, and over half were from outside the neutron community. This was the second such Workshop we have run and there is still clearly a considerable demand for such training so we propose to run it again in autumn 2008.

Students at the week-long neutron training course held in December.



Attendees at the Computations Methods for the Exploitation of Vibrational Spectra Workshop.

Workshop on the Future Development of European Muon Sources

A workshop on the Future Developments of European Muon Sources took place at Cosener's House, Abingdon in November. The Workshop was funded as a foresight study through the EC Neutron and Muon Integrated Infrastructure Initiative (NMI3) and attracted 36 participants from 9 countries. It brought together European users of the μ SR technique to discuss future possibilities for the development of muon sources within Europe. The workshop enabled consideration of current European sources (ISIS, UK and PSI, Switzerland) and their future development plans; developments in the muon technique and their implications for future sources; the extent to which new neutron sources in Europe might be used for muon production; and the further development of a science case to support new muon source initiatives. A report is available from www.isis.rl.ac.uk/muons.

ISIS People

Each year sees the comings and goings of ISIS staff. Peter Bradley retired from his job at ISIS TS-2 and is now a retained consultant. Other people to retire are Richard Lloyd, Dennis Hylton and Darren Todd, and Tim Broome retired as head of the Target Division. Katie Hopgood moved from ISIS to take up the position of PA in HR/Admin and Finance. Paula Woods left the ISIS User Office after many years and is now working in the Administration Services Group.

Mike Johnson also retired as Head of the Technology Department at RAL this year. Mike has had a thirty-year association with neutrons, joining the Neutron Beam Research Unit at RAL in 1975, progressing through to ISIS Instrumentation Division Head and then continuing to support neutron instrumentation development in the Technology Department. A symposium to mark his retirement, 'From Neutrons to Nanotechnology' was held in March.

Instrument Scientists to join ISIS include Chris Stock on Let and Silvia Imberti on Sandals and Nimrod. The Accelerator Division has welcomed John Govans, Adrian Hooper, Mark Dyer, Weihe Li, Stephen Clark, Terence Jeffcock, Andrew McMenemy and Simon Aldworth. The Target Division were joined by Rajesh Gupta, Detlev Riedel, Richard Bennett, Yanling Ma, Tomilayo Odupitan Gareth Powell, Philip Wise, Daniel Brioti, Richard Rawcliffe, Ian Davies, Brian Ford and Neil Parsley. Diffraction were joined by Gareth Howells and Tom Griffin. Adam Warne and Steve Roberts joined the User Support Group.

Congratulations to Jeff Penfold who has been awarded the 2007 Halg Prize of the European Neutron Scattering Association in recognition of his ground breaking work in neutron reflectivity. Bill David has received the 2006 Award of the European Society for Applied Physical Chemistry for structural studies of molecular materials using powder diffraction techniques. Richard Nelmes has been awarded the Institute of Physics' Duddell Medal for his work in high pressure structural science. Felix Fernandez-Alonso and Steve Bennington were appointed Visiting Professors at University College London, and Sean Langridge was promoted to Individual Merit Band 2.

Tim Broome admires the target station model presented to him on his retirement. 07EC2751



Building Task Leader Peter Bradley retired from the Second Target Station project having played a key role in the realisation of the project infrastructure. 06EC3224

Mike Johnson at the symposium to mark his retirement, with friends from the neutron community Phil Withers and Carla Andreani during their talks. 07EC2149, 2156, 2161



Publications

Publications relate to all work carried out at ISIS. Listed here are 363 publications resulting from work at the facility that have been published since ISIS 2006.

For many articles, a Digital Object Identifier (DOI) is now given. For more information on DOIs, and on how to resolve them to locate the relevant article, please see www.doi.org.

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Acta Mater (submitted 2007)

DS Sivia

On the kinematic approximation to specular reflectivity data

Philosophical Magazine **87** (10) 1575-1580 (2007)
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Oxford University Press, Second Edition

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Fatigue degradation and martensitic transformation of austenitic stainless steel AISI 321: new results and prospects
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Methane hydrate formation and decomposition: structural studies via neutron diffraction and Empirical Potential Structure Refinement
 J Chem Phys (accepted 2006)

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 Biomembranes **1768** (5) 1036-1049 (2007)

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 Acta Mater (accepted 2007)

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 Adv Mater **18** 3169-3173 (2006) [doi:10.1002/adma.200601636]

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Large impact of particle size on insertion reactions, a case for anatase Li_xTiO₂
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Nitric acid dihydrate at ambient and high pressure: An experimental and computational study
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Proc. Tenth European Particle Accelerator Conference (EPAC'06), Edinburgh, 26-30 Jun 2006

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*International Conference on Neutron Scattering (ICNS 2006), Sydney, Australia, Physica B **385-386** 1164-*

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 Nuclear Instruments and Methods in Physics Research A **571** 622-635 (2007)

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Determination of stress field in textured duplex steel using TOF neutron diffraction method
 Acta Mater (submitted 2007)

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Quantitative estimation of the second order plastic incompatibility stresses in textured duplex steel
 Mater Sci Forum **524-525** 841-846 (2006)

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 Langmuir **22** (13) 5825-5832 (2006) [doi:10.1021/la053316z]

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Crystal structure of Ln_{1/3}NbO₃ (Ln = Nd, Pr) and phase transition in Nd_{1/3}NbO₃
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Structures and phase diagram for the system CaTiO₃-La_{2/3}TiO₃
 J Solid State Chem **180** 1083-1092 (2007) [doi:10.1016/j.jssc.2007.01.005]

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DNA immobilization using biocompatible diblock phosphorylcholine copolymers
Proc. 11th European Conference on Applications of Surface and Interface Analysis, Vienna, Austria, 25-30 Sep 2005

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High-resolution roton spectra around the superfluid transition temperature in liquid ⁴He
 Physica B (submitted 2007)

ISIS Seminars 2006 - 2007

Listed here are the seminars given at ISIS during the year by international speakers.

18 April 2006
Fu-Chun Zhang (Hong Kong University)
Rotational symmetry breaking in sodium doped cuprates

25 April 2006
Rajan Mittal (Bhabha Atomic Research Centre, India)
Modeling of anomalous thermodynamic properties using lattice dynamics and inelastic neutron scattering

16 May 2006
Daniel Cabra (University of Strasbourg, France)
The influence of phonons on low dimensional magnetic systems

30 May 2006
Prof. Richard Saykally (University of California, USA)
Water music: some new notes in a favourite composition

13 June 2006
David Logan (University of Oxford)
Transport and optical properties of heavy electron materials: theory and experiment

20 June 2006
Milan K Sanyal (Saha Institute, Kolkata, India)
Two-dimensional magnetic ordering in gadolinium based organic multilayer structures

27 June 2006
Sylvia McLain (ISIS Facility and Oxford University)
Insights into the structure of neurotransmitters and other biological molecules in solution using neutron diffraction

4 July 2006
Bill Buyers (National Research Council, Canada)
Hidden order in the heavy fermion superconductor URu₂Si₂

11 July 2006
Sean Giblin (ISIS)
Local matrix-cluster interactions in La_{1-x}Sr_xCoO₃

18 July 2006
Theresa Head-Gordon (University of California and LBNL, USA)
Thermodynamic, dielectric and structural consequences of chain networks for liquid water

25 July 2006
Günther Rupprechter (Vienna University of Technology, Austria)
Vibrational spectroscopy of molecules on catalyst surfaces

5 September 2006
Aldo Boccaccini (Imperial College)
Bioactive materials for tissue engineering

14 September 2006
John W Freeland (Argonne National laboratory, USA)
Creating magnetic order at interfaces between dissimilar complex oxides

19 September 2006
Alain Yaouanc (CEA Grenoble, France)
Spin correlations and dynamics in geometrically frustrated magnetic materials

3 October 2006
Karl Sandeman (University of Cambridge)
Metamagnetism and the magnetocaloric effect in CoMnSi and related materials

16 October 2006
John Saunders (Royal Holloway, University of London)
Quantum phase transitions and quantum criticality in helium films

31 October 2006
Maxim Mostovoy (University of Groningen, The Netherlands)
Magnetic frustration and ferroelectricity

7 November 2006
Craig Brown (University of Indiana and NIST, USA)
Applying neutron scattering to the understanding of potential hydrogen storage materials

15 November 2006
Jane Francis (University of Leeds)
Fossil forests in Antarctica: signals from the past forecast climates of the future

29 November 2006
Dirk Holland-Moritz (DLR Koeln, Germany)
Neutron scattering experiments on undercooled metallic melts

12 December 2006
Antonios N Andriotis (Institute of Electronic Structure and Laser, Crete)
Tailoring the induced magnetism of carbon-based and the non-traditional inorganic materials

8 January 2007
V.G. Storchak (Kurchatov Institute, Russia)
Spintronics via μ SR: Magnetic Polarons in Magnetic Semiconductors

16 January 2007
Ross McKenzie (University of Queensland, Australia)

Interplay of unconventional superconductivity and frustrated antiferromagnetism

23 January 2007
George E Froudakis (Heraklion, Crete)
Designing Nanoporous Materials for Hydrogen Storage

30 January 2007
Andrew F Ho (Imperial College)
Strong correlation physics in ultra cold atom traps

6 February 2007
Chris Stock (ISIS)
Disordered spin ground state in a S=1 triangular lattice

13 February 2007
Andrew Parry (Imperial College)
Wetting transitions: past, present and future

20 February 2007
Jerry Mayers (ISIS)
Temperature dependence of the kinetic energy and spatial order through the supersolid transition in ⁴He

27 February 2007
Paul Goddard (University of Oxford)
The Fermi Surface of AuZn: towards an understanding of the shape memory effect

1 March 2007
Alan Drew (University of Fribourg, Switzerland)
Spin injection and transport in a metal-organic spin valve

6 March 2007
Malte Grosche (Royal Holloway, University of London)
Exploring the edge of magnetism in NbFe₂

13 March 2007
Peter Kopietz (University of Frankfurt, Germany)
Spin-wave interactions in quantum antiferromagnets and Bose-Einstein condensation of magnons

20 March 2007
José C Gómez-Sal (University of Cantabria, Spain)
Complementarity of neutron and μ SR techniques for the study of inhomogeneities in strongly correlated systems: The CeNi_{1-x}Cu_x case

29 March 2007
Hinrich Grothe (Vienna University of Technology, Austria)
Metastable nitric acid hydrates – possible constituents of polar stratospheric clouds?



1. Elisabetha Gliozzo (University of Siena, Italy) with one of her Roman army bronze artefacts from North Africa which she was investigating using INES. 06EC4291



2. Samuele Sanna (University of Cagliari, Italy) and Francesco Coneri (University of Parma, Italy) using MUSR to examine the effect of structural disorder on the CuO₂ layer of cuprates. 06EC2921



4. Katarzyna Morawa (Reading University) and Dario Stacchiola (MPI Berlin, Germany) studying the role of carbon species on the acetylene cyclomerization on supported Pd catalysts with TOSCA. 06EC4299



3. Tom Fennell (University College London) during his time at ISIS using PRISMA to observe the Kasteleyn transition in the spin ice HO₂Ti₂O₇. 06EC4306



5. Robert Van Langh (Riks Museum, Amsterdam), Dirk Visser (ISIS/NWO), and Wandalin Van Den Abeele (Riks Museum, Amsterdam) using ENGIN-X to investigate Renaissance bronze casts. 06EC4266

ISIS in facts and figures

FAP 1	FAP 2	FAP 3	FAP 4	FAP 5	FAP 6	FAP 7
Diffraction	Liquids	Large Scale Structures	Excitations	Molecular Spectroscopy	Muons	Engineering
J Evans <i>(Chair)</i>	D Holland <i>(Chair)</i>	J Lawrence <i>(Chair)</i>	D Paul <i>(Chair)</i>	G Reiter <i>(Chair)</i>	J Davies <i>(Chair)</i>	S Hainsworth <i>(Chair)</i>
R Angel	S Billinge	I Gentle	S Bramwell	C Andreani	N Clayden	R Burguete
S Clarke	L Cormier	J Goff	J Chalker	P Fairclough	G Gehring	M Daymond
L Falvello	M Gonzalez	P Griffiths	R Coldea	R Ford	S Kilcoyne	M Hutchings
D Gregory	C Hardacre	J Lu	R De Renzi	HG Gomez	T Matsuzaki	N O'Dowd
W Harrison	T Kanaya	J Petkov	B Fak	M Hayward	R Moessner	M Preuss
P Hatton	P McMillan	P Steadman	A Huxley	M Johnson	M Ricco	R Tomlinson
N Hyatt	MA Ricci	R Thompson	S Itoh	D Lennon	R Scheuermann	C Truman
T Koetzle	M Wilson	A Zurbakhsh	D McMorrow		P Wood	
J Rodriguez-Carvajal						
P Schofield						
P Woodward						
R Ibberson	D Bowron	J Webster	T Perring	J Mayers	S Cottrell	E Oliver
S Hull	A Hannon	S Langridge	S Bennington	J Tomkinson	A Hillier	

ISIS Facility Access Panel Membership for the June 2007 meetings. The FAPs meet normally meet twice per year to review all proposals submitted to the facility based on scientific merit and timeliness. This year, due to the ISIS shutdown, there was no December 2006 meeting – business was resumed as normal in 2007. ISIS attendees act as Secretary and give technical advice, but are not involved in the experiment review process.

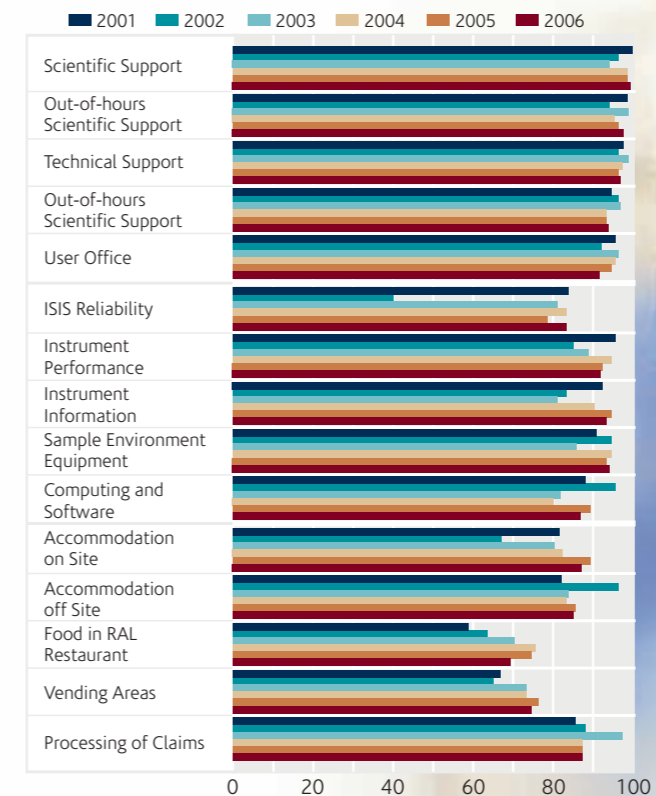
Chairman	S Kilcoyne	University of Salford
IUG1 Crystallography	D Gregory	University of Glasgow
	P Lightfoot	University of St Andrews
IUG2 Liquids & Amorphous	D Holland	University of Warwick
	B Webber	University of Kent
IUG3 Large Scale Structures	R Thomas	University of Oxford
	A Zurbakhsh	Queen Mary College, London
IUG4 Excitations	A Boothroyd	University of Oxford
	P Mitchell	University of Manchester
IUG5 Molecular Spectroscopy	K Ross	University of Salford
	P Mitchell	University of Reading
IUG6 Muons	T Lancaster	University of Oxford
	S Kilcoyne	University of Leeds
IUG7 Engineering	G Swallowe	Loughborough University
	M Fitzpatrick	Open University

A D Taylor	Director ISIS
U Steigenberger	ISS Division Head
R Browning	ISIS User Programme Manager
R L McGreevy	IDM Division Head
Z A Bowden	ISIS User Support Group Leader

ISIS User Committee Membership for June 2007. The IUC exists to represent the user community on all aspects of facility operation.

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.



ISIS user survey results 2001 – 2006.

Rob Richardson
(Bristol University)
during his time at
ISIS using LOQ to
investigate the
translational order
parameter of liquid
crystal 8CB.



Alberto Fraile
(University of Zaragoza, Spain)
studying spin
dynamics in a
ferromagnetic
semiconductor on
HET. 06EC4280



Maria Antometta Ricci *(Università Roma Tre, Italy)* exploring the structure of water confined in Xerogel pores using SANDALS. 06EC4300



Beam Statistics 2006 - 2007

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 749 mA.hrs of user proton beam to the muon and neutron targets.

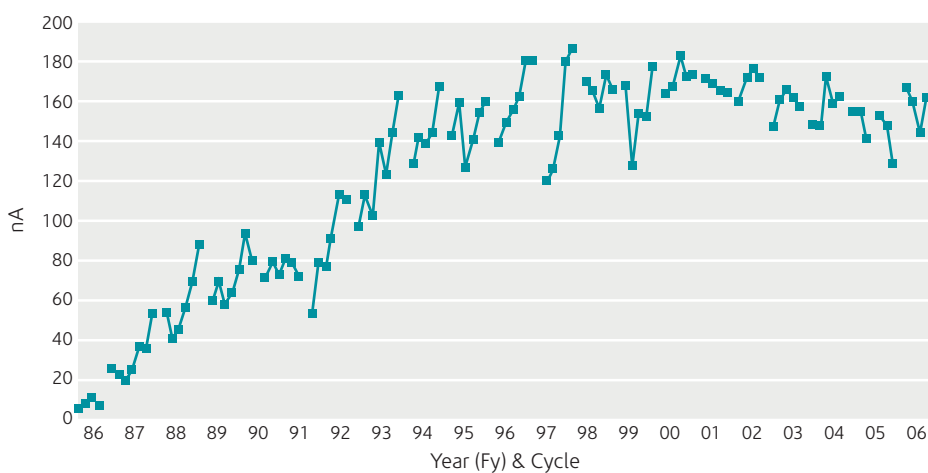
The tables below give beam statistics for the individual cycles in the year 2005-2006, together with year-on-year statistics for ISIS performance.

Cycle	06/1	06/2	06/3	06/4	06/5
	7 Feb - 23 March	4 April - 11 May	20 June - 3 August	8 Sept - 8 Oct	7 Nov - 13 Dec
Beam on target (hrs)	997	814	877	679	806
Total beam current (mA.hr)	1179	145	156	120	147
Average beam current for beam on target (μ A)	180	179	178	177	182

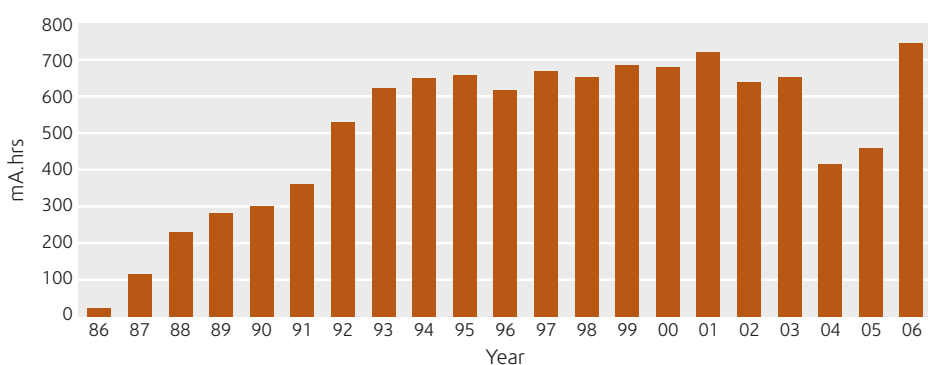
ISIS operational statistics for year 2006 - 2007.

Year	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006
Total scheduled user time (days)	168	175	168	168	168	160	172	106	134	196
Total time on target (days)	153	160	153	154	158	148	154	96	107	174
Total integrated current (mA.hrs)	672	656	687	687	725	630	656	409	459	749
Average current on target (μ A)	183	171	187	186	192	178	177	177	178	179

Year-on-year ISIS performance summary for the past 10 years.



Average ISIS average beam current per cycle.



The ISIS integrated beam current over the last twenty years.