ISIS 2006
The ISIS Facility Annual Report

Council for the Central Laboratory of the Research Councils

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ISIS 2006

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2006 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

Prof. Randall Richards (EPSRC Director of Research and Innovation) and Jane Nicholson (EPSRC Physics Programme Manager) discussing neutron reflectometry studies of surfaces and interfaces with Sean Langridge and Stephen Holt (ISIS) during their visit in January. 06EC1066

ISIS has an ongoing partnership with the Japanese RIKEN Institute for both muon and neutron studies, including operation of the successful RIKEN-RAL pulsed muon facility. Dr. Toichi Sakata, RIKEN Executive Director, visited ISIS in January with Prof. Koji Kaya, Director of the Wako RIKEN Institute. Dr Sakata is pictured here with Prof. John Wood, CCLRC Chief Executive. 06EC1083

A delegation from the Chinese Institute of High Energy Physics, Beijing, visited ISIS in September. Shouxiang Fang, Senior Supervisor of the Beijing Spallation Neutron Source Accelerators, is seen here touring the ISIS synchrotron. 05EC3535

Dr Robert Kirby-Harris, Chief Executive, the Institute of Physics and Mark Turner of the Shareholder Executive being shown ISIS by facility Director Andrew Taylor. 06EC2946

Members of the Institute of Physics International Review of UK Physics and Astronomy Research panel visited ISIS in November. Toby Perring (ISIS) is showing a MAPS sample to Prof. Daan Frenkel (University of Amsterdam, the Netherlands), Prof Massimo Inguscio (University of Florence, Italy), Prof. Mildred Dresselhaus (MIT, USA) and Prof. Sir Anthony Leggett (University of Illinois, USA). 05EC4031

Foreword

The depth, breadth and range of applications of science performed at ISIS is truly impressive. The versatility of neutron and muon techniques allows hydrogen storage materials with potential fuel-cell applications to be studied alongside the behaviour of confined water with implications for biophysical and geological systems. Exploration of the structure and function of naturally-occurring surfactants runs in parallel with alloy ageing studies relevant to current and future nuclear reactors. In depth, fundamental investigations of magnetism coincide with studies of mechanisms to improve new, 'green' solvents. These are just a few of the examples described within this report and represent a small fraction of the work of the facility over the past year.

And the variety of ISIS science will continue to grow. The Second Target Station Project will provide a new suite of ISIS instruments giving a step-change in the facility's potential. This year has seen the completion of the target station building itself and the first components for the proton beamline and target station arriving on site. Preparations are being made for the installation of the seven day-1 instruments which will open up further science areas for neutron studies.

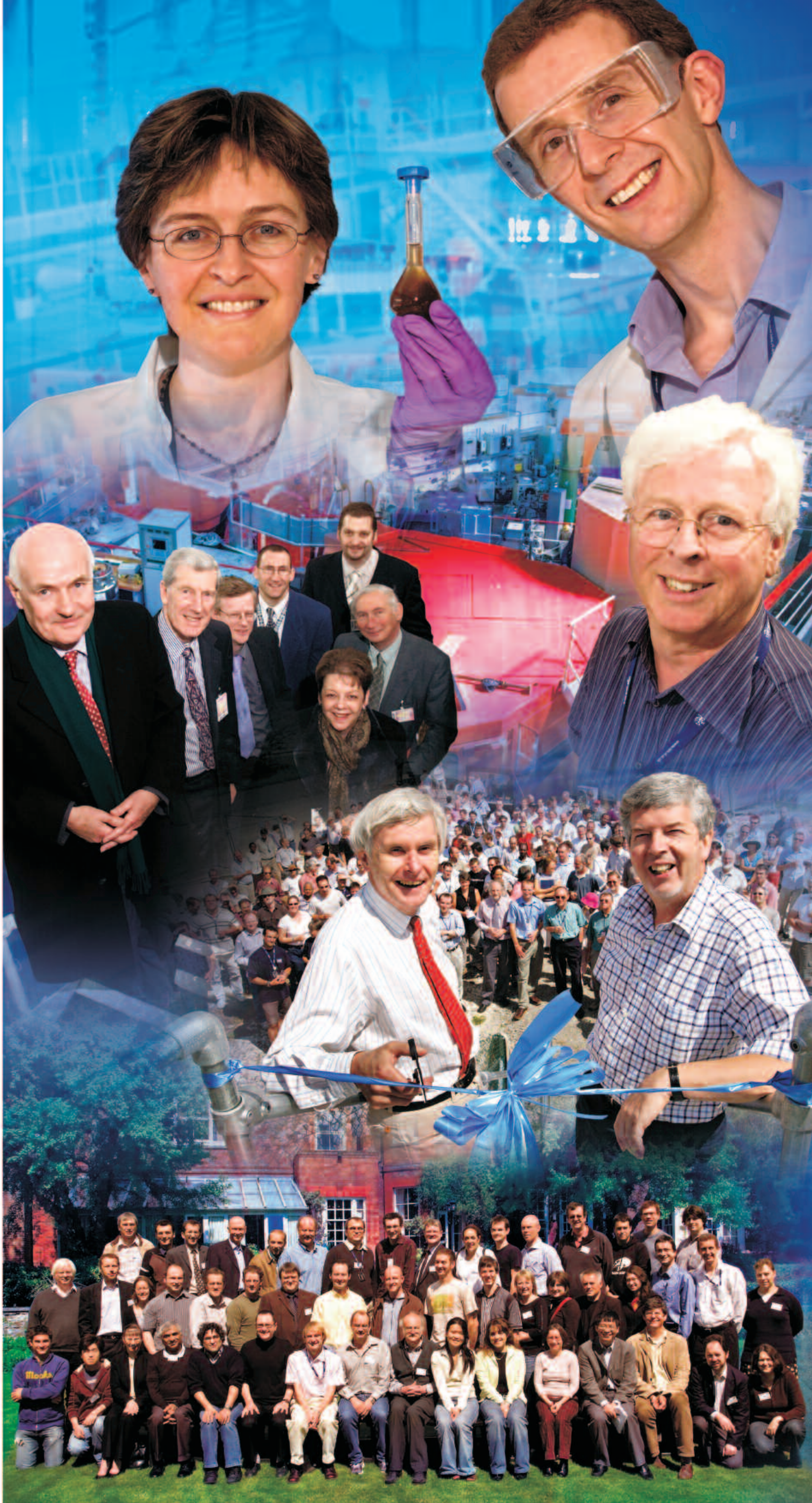
Instrument developments on the existing target station will also continue to provide new potential. Grants awarded this year from the CCLRC Facility Development Fund to ISIS and its user community will enable provision of advanced sample environment magnets, development of the POLARIS diffractometer and incorporation of neutron polarisation techniques on to ISIS instruments.

But in addition to developments in new instrumentation areas, the efficient and enhanced operation of the ISIS accelerators is high priority. The long facility shut-down in 2007 will see essential work on the extracted proton beam and hydrogen moderator transfer lines, systems which have been in operation for over 20 years and whose refurbishment is critical to ongoing operations.

Such work paves the way for the long-term use of ISIS. The review of UK neutron strategy completed by the CCLRC at the end of last year recognised the importance of neutron scattering and the world-leading nature of both ISIS and the ILL, including the need to ensure their continued competitiveness for at least the next 10-15 years. Other challenges lie ahead. We can look forward to neutron and muon investigations at ISIS encompassing an ever-increasing diversity of key science and technology areas well into the future.

Andrew Taylor

The ISIS facility, with the second target station building now complete. 06EC2711



Helen Jarvie (Centre for Ecology and Hydrology), the first environmental scientist from the Natural Environment Research Council to use ISIS, with Steve King (ISIS) during their LOQ experiment studying natural aquatic colloids. 06EC2459

MERLIN is the latest ISIS instrument and took its first neutrons this year. Prof. Keith McEwen (University College London) is one of the MERLIN grant principal investigators, here visiting the instrument during its construction. 06EC2880

Alec Osborne, President of the Institute of Mechanical Engineers, with members of the ImechE Thamesway Area committee, being shown the ISIS experimental hall by James Treadgold of the ISIS Project Engineering Group. 06EC1502

John Wood, CCLRC Chief Executive, and Andrew Taylor, ISIS Director, opening the walkway up to the 'mound', the area created by earth removal for the ISIS Second Target Station building. 06EC2770

User meetings are an important part of ISIS life, allowing discussion of latest facility scientific and instrument developments. The Large Scale Structures User Group met at the Cosener's House in May. 06EC2359

Students from the Materials Science Department at Oxford University visited ISIS at the end of 2005. 05EC4250

The seven Facility Access Panels meet twice per year to review all the proposals submitted to ISIS for beamtime. Here we see the muon FAP hard at work. 06EC2842

Ferdie Erasmus, Costain contracts director (right) with Andrew Taylor during a celebration to mark the Second Target Station building being weather-tight earlier this year. 06EC1592

The Foundation for Science and Technology visited ISIS in November. The Foundation provides a forum for debate of policy issues that have a science, engineering or technology element. Following their tour of ISIS, Foundation members held a lunchtime discussion chaired by the Rt Hon the Lord Jenkin of Roding. 05EC4332

Don Rej, Programme Director, Office of Science Programs at Los Alamos, USA, touring ISIS with Tim Broome (ISIS). 06EC2944

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.

Hydrogen behaviour in technological materials

New materials for hydrogen storage

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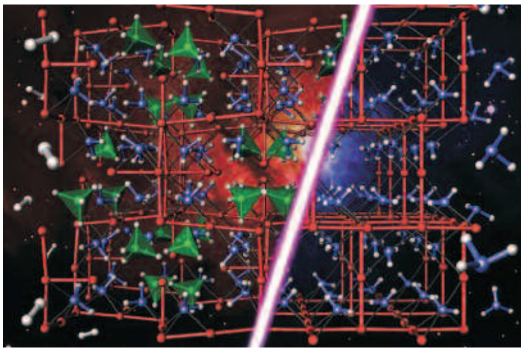
PA Chater et al.,
Chem. Comm.
23 (2006) 2439

There is worldwide interest in the use of hydrogen as the basis for a future sustainable energy system with low carbon emissions. Cars powered by hydrogen-based fuel cells are widely regarded as the first major inroad into the hydrogen economy. However, a suitable material for on-board storage should be able to store a high weight-percent and high volume density of hydrogen and, equally importantly, rapidly discharge and charge this same amount of hydrogen at acceptable temperatures (typically around 50 - 100°C). This represents a particular challenging set of credentials for an ideal storage material and at present no known material meets these critical requirements. The GEM diffractometer at ISIS has been used in conjunction with the high resolution powder diffractometer, ID31, at the ESRF to determine the crystal structure of a new candidate material for hydrogen storage, $Li_4BN_3H_{10}$. Importantly, the high count-rate of GEM enabled the material to be studied without any isotopic enrichment thus accelerating the ability to determine new hydride storage materials.



These ultra-lightweight materials, $Li_4BN_3H_{10}$ (left) and $LiNH_2$ (right), under development within the UK Sustainable Hydrogen Energy Consortium (UK-SHEC), offer significant hydrogen storage potential. Amazingly, they contain a higher density of hydrogen (illustrated as white spheres) than liquid hydrogen itself.

The binding of H_2 in zeolites

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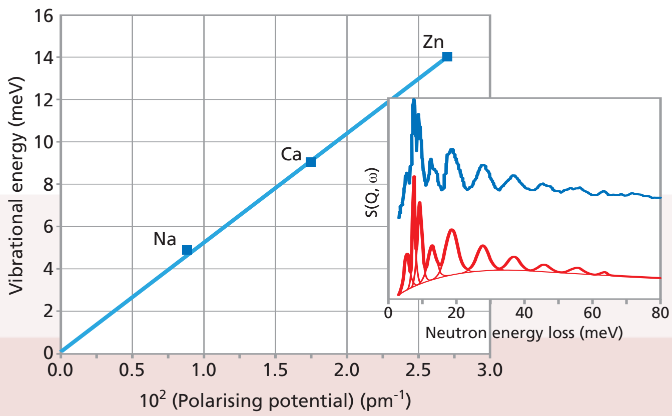
PCH Mitchell et al.,
Phys. Chem. Chem. Phys.
(2006, in preparation)

Zeolites are micro-porous materials with possible uses in hydrogen storage. Understanding the microscopic mechanisms of hydrogen interactions with zeolite materials is therefore important to develop their storage potential. Para-hydrogen adsorbed by cation (Na^+, Ca^{2+} and Zn^{2+}) – substituted zeolite X has been studied by inelastic neutron scattering (INS) on TOSCA. The INS spectrum reveals the rotational transition of H_2 (shifted and split by the interaction with the binding site) together with a series of equally-spaced peaks to higher energies which we assign to a vibrational transition (and its overtones). The vibration is that of the H_2 molecule against the binding site (X–H not H–H). This vibration frequency is directly proportional to the polarising power (z/r, z ionic charge; r ionic radius) of the cation concerned. This result is consistent with theoretical studies of the interaction of H_2 molecules with gaseous cations and zeolites, and to our knowledge is the first experimental proof of the importance of the polarisation of H_2 molecules in the binding of dihydrogen in a hydrogen storage material.



H_2-(zeolite) vibrational frequencies vs polarising potential of cations, with inelastic neutron scattering spectra of para-H_2 in Ca zeolite-X (experimental and simulation).

Hydrogen doping of colloidal quantum dots

AJ Houtepen, P Liljeroth, D Vanmaekelbergh (University of Utrecht, The Netherlands), JM Gil, HV Alberto (University of Coimbra, Portugal), J Gavartin (University College London), D Visser (ISIS-NWO), JS Lord, SFJ Cox (ISIS)

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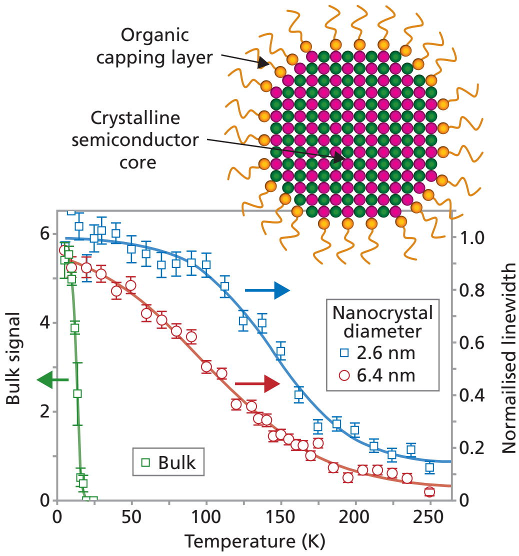
JM Gil et al., *Phys. Rev. B* 64 (2001) 075205

Semiconductor nanocrystals are of enormous interest due to their tunable properties and wide variety of promising applications, from quantum computing to bio-labelling and non-linear optics. The effect of size and shape on their characteristics has been subject to intense investigation. The introduction of dopants can also be explored, and a relevant question is whether doping in nanocrystals influences their properties when the size leads to strong quantum confinement.

Hydrogen can act as a dopant in many semiconductors, often forming a shallow-donor state in bulk material with an extended electron wavefunction. Muons are used to model hydrogen atoms, and can be used to study shallow-donor behaviour and characteristics – in the present case, to explore the effects of reducing the semiconductor crystal size to the nanoscale.



Temperature dependence of the muonium shallow donor fraction in nanocrystalline CdTe compared with bulk material. Inset – nanocrystalline CdTe.

In nanocrystalline samples of II-VI semiconductors the shallow-donor state is still observed, but is significantly affected by the variation of muon sites within the nanocrystal structure. The shallow donor state now persists to higher temperature than in the bulk material due to the higher binding-energy of the donor state limited by the onset of inter-nanocrystal conductivity.

Hydrogen conduction in oxide materials

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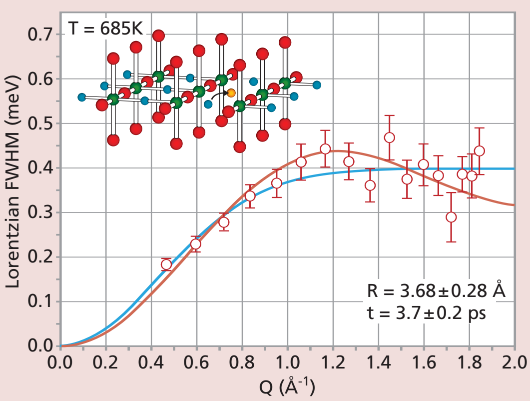
CA Bridges et al., *J. Am. Chem. Soc.* 92 (2005) 5996.

Compounds which exhibit high hydrogen conduction are currently of considerable interest due to potential applications in devices such as fuel cells and hydrogen sensors. Protonic conduction in perovskite-type oxides (e.g. $SrCe_{0.95}Yb_{0.05}O_{3-\delta}$) has been extensively examined, while similar information on hydride conduction in oxides is lacking. Quasi-elastic neutron scattering (QENS) has provided quantitative information on hydride diffusion in the novel transition metal oxide hydride $LaSrCoO_3H_{0.7}$. Variable temperature, high resolution QENS data reveal the onset of hydride anion mobility above 675 K via a jump process involving long-range diffusion of individual hydride anions. The site-to-site hopping distance is equal to the length of the *a* axis of the crystal unit cell, suggesting that diffusion occurs between vacancies in the hydride anion sublattice. Furthermore, diffusion coefficients have been used to obtain an estimate of the conductivity, which is significantly higher than has been observed in proton conducting materials.



Quasielastic energy widths versus momentum transfer at 685 K and derived diffusion parameters. Inset shows a schematic of the proposed hopping mechanism for hydride diffusion along the a axis within the perovskite-type layer of $LaSrCoO_3H_{0.7}$.

Nanoscale science

Superconductivity and magnetism meet

J Chakhalian, J Strempfer, G Khaliullin, C Bernhard, G Cristiani, H-U Habermeier, B Keimer (Max Planck Institute, Germany), T Charlton and R Dalgliesh (ISIS), JW Freeland and G Srajer (Argonne National Lab, USA), J Cezar (ESRF, France)

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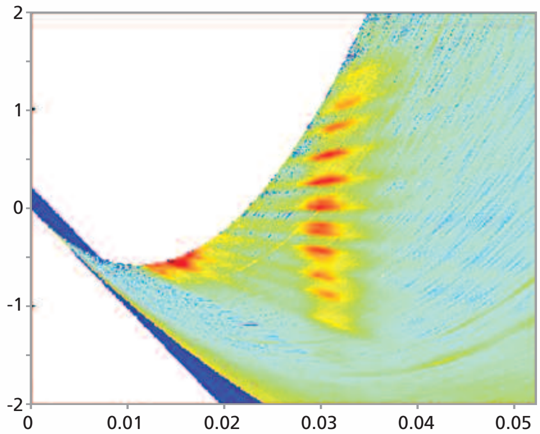
J Chakhalian et al., *Nature Physics* 2 (2006) 244

Superconductivity and ferromagnetism are very rarely found to co-exist in natural materials. However, artificially fabricated nanostructures can now be produced where a superconductor, $YBa_2Cu_3O_{7-x}$ (YBCO) and colossal magneto-resistance magnetic material, $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) are grown in alternating layers on a $SrTiO_3$ substrate. These structures exhibit novel quantum states that do not exist in the constituent materials, and such systems are of potential interest for spintronics applications. Off-specular neutron reflectivity measurements performed on CRISP have revealed rich in-plane magnetisation behaviour. On cooling through the cubic to tetragonal phase transition of the $SrTiO_3$ subphase, the Bragg peak resulting from the multilayer structure splits due to the twinning of the $SrTiO_3$ crystal. On cooling further, through the superconducting transition temperature of the film, the Bragg feature splits again as shown in the figure. This is indicative of the formation of a stripe domain structure with a length scale of tens of microns. This large length scale gives clues as to the mechanism driving the interaction between superconductivity and magnetism in these films, providing a tantalising glimpse into the interplay between these two effects in the multilayer structure.

Specular and off-specular neutron intensity around the first superlattice Bragg reflection taken at 10 K revealing the formation of a stripe domain structure.



Water at the leading edge: a new look at interfacial fluids

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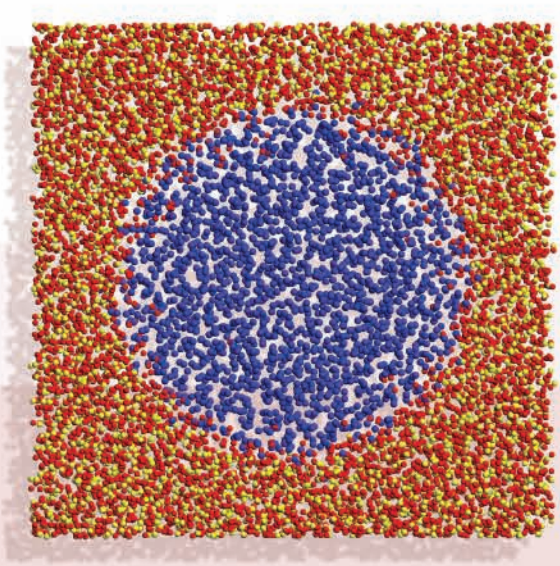
F Bruni et al., *J Chem Phys* **109** (1998) 1478

Water confinement occurs widely in nature, in areas ranging from biophysics (protein folding, enzyme activity) to geology (water in clays, hydrate formation in sediments). Confinement substantially modifies the bulk properties of water, e.g. lowering the freezing point and raising the boiling point. Hitherto, surprisingly little was known about water structure in confinement. We have therefore investigated the structure of confined water, using vycor, a silica glass with a random network of ~40 Å pores, as the confining medium. Earlier neutron diffraction measurements have been coupled with a new Empirical Potential Structure Refinement simulation which includes a model of both the confined water and the surrounding amorphous silica. There are on average only ~2.2 hydrogen bonds per water molecule in confined water, as compared to ~3.6 in bulk water. The second water coordination shell also moves markedly inwards by ~0.6 Å. It appears that confined water structure is dominated by the surface layer, where hydrogen bonding to the vycor OH groups causes a dramatic reorientation of the water molecules.



Confined water (blue) in a silica (red and yellow) pore. Water near the pore edge has reduced density, caused by the strong orientational surface interaction.

Holey hematite! Transforming magnetism in α-Fe_2O_3 through mesostructure

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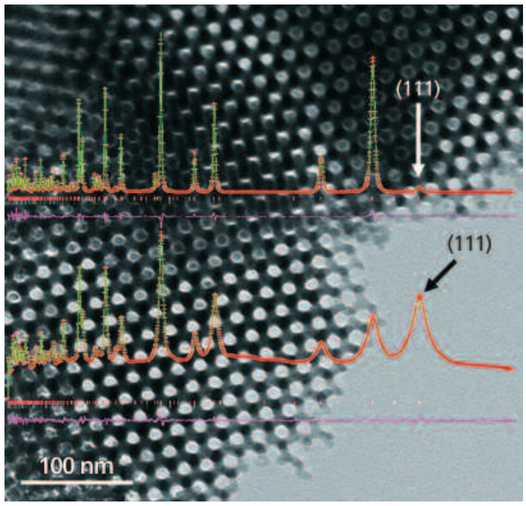
F Jiao et al., J. Am. Chem. Soc. 128 (2006) 5468.

One of the most fascinating recent developments in solid-state chemistry is the use of liquid crystal templates to make moulds in which mesostructured forms of a wide range of materials may be grown. One such material is α-Fe_2O_3 (hematite), which may be synthesised in an ordered crystalline mesoporous form with 3.85 nm diameter pores. Neutron powder diffraction studies on OSIRIS have shown that its collective magnetic properties are quite different from the standard, fully-dense form.

Bulk hematite undergoes the characteristic Morin transition at ~265 K, transforming from a canted antiferromagnet with a weak ferromagnetism to a fully antiferromagnetic form with no spontaneous moment. In contrast, this particular mesoporous form displayed no such transition down to 1.5 K, retaining its weakly ferromagnetic structure. The suppression of the Morin transition is also seen in nano-particulate hematite, but there the long-range magnetic order is also lost.

This change in the collective magnetic behaviour of hematite poses interesting questions about the influence of the mesostructure, and may also provide a means of conferring useful functionality on this and wider range of magnetic materials.



HRTEM image of mesoporous Fe_2O_3 with neutron diffraction patterns of bulk (top) and mesoporous forms (bottom) at 150 K. The (111) reflection characterises different magnetic structures.

Waxy molecules exhibit a special shine for metal oxide nanocubes

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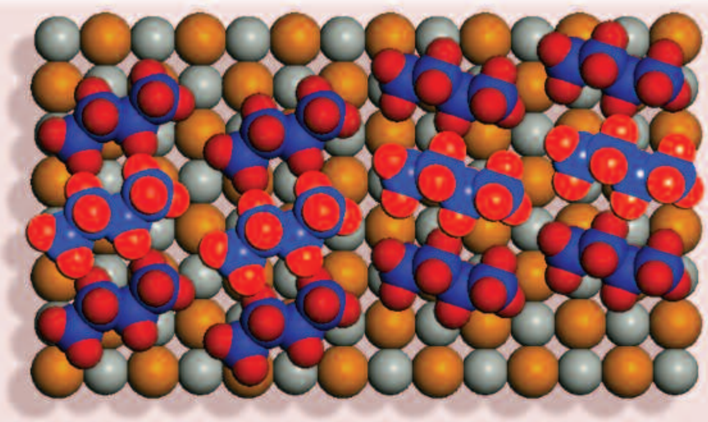
T Arnold et al., Phys Rev B (2006, accepted)

Metal oxides (MO) play a leading role in nanotechnology where nanometer-sized particles are routinely used as pigments for paints, supports for catalysts, as base components in cosmetics, medical ointments and lubricants, and in opto-magneto electronic materials e.g. as MEMS devices and novel sensors. Understanding how waxy molecules interact with and modify MO materials will unquestionably enhance their technological usage. We have used neutron diffraction to study the arrangement of molecular species on MO surfaces. We have found that a single '2D' layer of butane (C_4H_{10}) on MgO is sawtooth shaped. The structure results from the attractive force of the MgO surface 'pulling' the molecules into registry with it. MgO has a similar 'attraction' for longer-chain pentane (C_5H_{12}) and hexane (C_6H_{14}) molecules. This work is part of a comprehensive investigation into the adsorption, structural and dynamical properties of alkane films on nanocubes of MgO and represents a key step towards developing accurate and realistic models of the interplay between adsorbate-adsorbate and adsorbate-substrate interactions. Knowledge of these forces will ultimately lead to the production of nanomaterials that have predictable physical and chemical properties.

The structure of a monolayer butane film on MgO (100) surface.



Fundamental molecular studies

Four new polymorphs of formamide at high pressure

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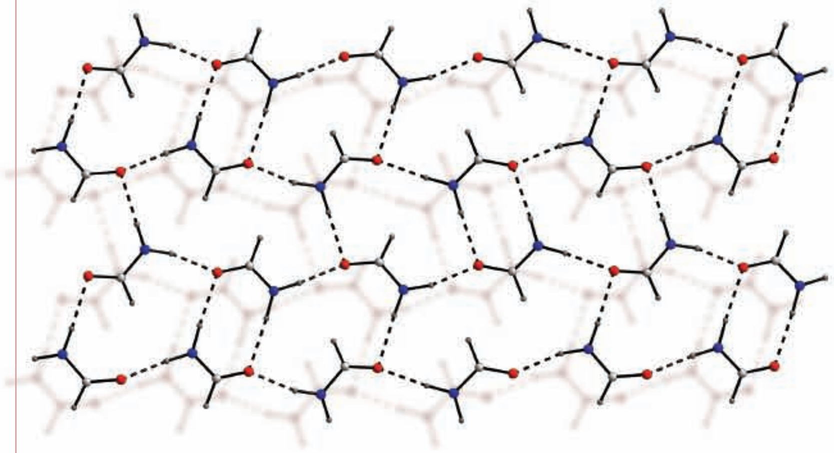
SA Moggach et al., *Acta Cryst*. B62 (2006, In press)

The properties of solids depend critically on structure. Some materials can crystallise in more than one structural form, a phenomenon referred to as polymorphism. Some very simple molecular systems are highly polymorphic: water for example has 19 solid forms, and research to find more is still being carried out. Formamide is the simplest amide, with formula $H_2NCH{=}O$. It has recently been implicated in the photocatalytic formation of nucleoside bases, and it may have been a precursor to biological compounds required for life. Upon cooling, formamide crystallises into a structure which remains essentially unchanged down to 2 K, and until recently this was the only crystalline form of formamide known. Following recent neutron diffraction experiments on PEARL, we have shown that formamide forms no fewer than four different polymorphs at room-temperature and pressures between 0.1 and 3 GPa. The structures can be understood in terms of the different conformations of hydrogen-bonded chains of molecules, and the ways in which these chains interact.



Formamide-IV showing H-bonded chains of molecules, running left to right, connected into a layer by more H-bonding interactions with other chains.

Effects of temperature and pressure on deuterium migration in urea – phosphoric acid

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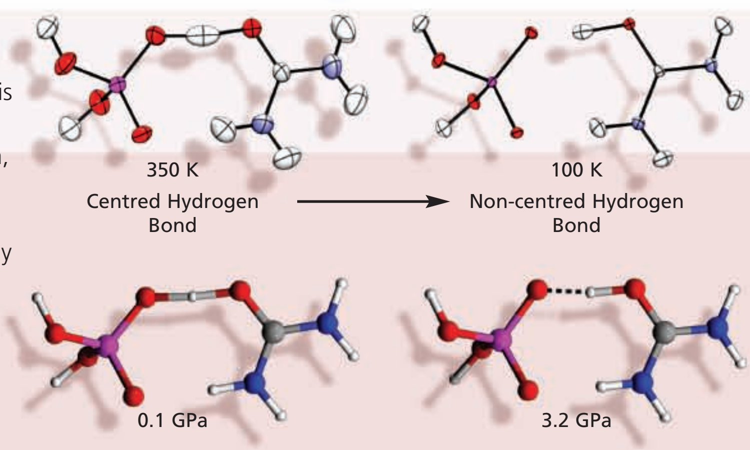
CA Morrison et al., *J. Am. Chem. Soc.* 127 (2005) 4042

Urea and phosphoric acid form an adduct (UPA) in which a strong hydrogen bond is formed involving the hydrogen atom of the acid and the carbonyl oxygen of the urea. Previous studies have shown that at low temperatures this proton is localised on the urea molecule, but as temperature increases the proton migrates to a position midway between the two O atoms. We aimed to explore the effect on this migration phenomenon of replacing hydrogen for deuterium, especially as computational studies had suggested that coupling of vibrational modes may be important. Experiments performed on SXD and HIPR for perdeuterated-UPA showed migration of deuterium towards urea with either decreasing temperature or increasing pressure. Our explanation is that a reduction in temperature or an increase in pressure results in a contraction (and hence strengthening) of the other hydrogen-bonded contacts involving phosphoric acid molecules. This increases the acidity of the phosphoric acid and so the deuterium moves towards the urea. Support for this hypothesis comes from computational studies that assess the charges on each atom.



Structure of perdeuterated urea – phosphoric acid at 100 K and 350 K (ambient pressure), and at 0.1 and 3.2 GPa (ambient temperature) showing migration of deuterium atom.

Evidence of the presence of optic-like collective modes in a liquid

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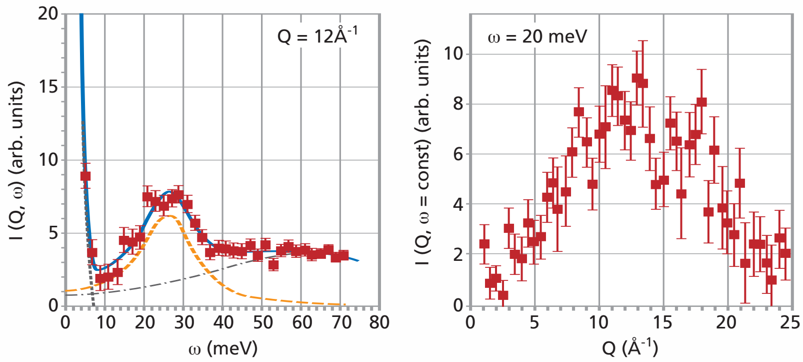
FJ Bermejo et al., Phys. Rev. Lett. 96 (2006) 235501

The dynamics within hydrogen bonded liquids are key to understanding the fundamental interactions which give rise to the cohesion energy being governed by strongly directional electrostatic forces.

Hydrogen bonded systems significantly differ from ionically bonded solids in the sense that the heavy atoms bridged by the hydrogen bonds approach each other more closely than expected given their ionic radii. Also, these systems are known to exhibit strong cooperative behaviour such as the appearance of small clusters in the gas phase.

Inelastic neutron scattering data taken on MARI from liquid deuterium fluoride (DF) close to the melting point show, in addition to quasielastic and heavily damped acoustic motions, an intense band centered at about 27 meV along with a broader higher energy feature. Observation of the former band provides the first direct verification of the existence within the liquid state of collective optic-like excitations as predicted by molecular dynamics simulations. The latter corresponds to mainly reorientational motions also predicted by simulation.



The energy and wave vector dependence (Q) of collective optic-like modes in liquid DF.

Accurate molecular structures for crystal structure prediction

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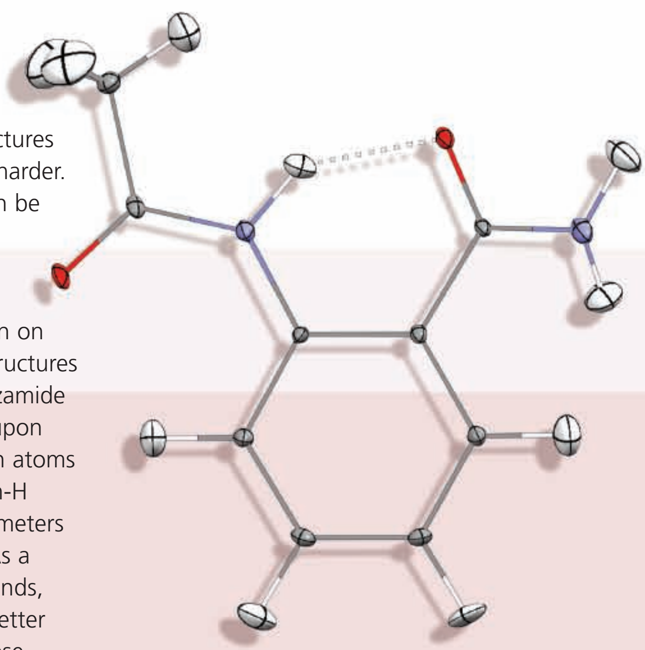
CK Broder et al., *Acta Cryst* B (2006, submitted)

Computational methods of crystal structure prediction (CSP) can easily generate a great many trial structures for any given molecule; predicting which structures actually occur in the solid state is notably harder. Fortunately, a great deal of uncertainty can be removed from CSP by employing accurate molecular starting models, particularly in respect of hydrogen atom positions. By employing single-crystal neutron diffraction on SXD, we have obtained accurate crystal structures for the α and β forms of *o*-acetamidobenzamide that represent a significant improvement upon existing X-ray derived structures. Hydrogen atoms are located with the same accuracy as non-H atoms and the thermal displacement parameters are refined anisotropically for all atoms. As a consequence, intra- and intermolecular bonds, including weak H-bonds, are now much better defined than was previously the case. These crystal structures are now being used in a CSP study into the energy difference between the two forms which is larger than that normally observed for two polymorphs of the same compound.



The molecular structure of the α form of o-acetamidobenzamide at 30 K, with thermal ellipsoids drawn at the 50% level.

Biomolecular science

Interfacial behaviour of the naturally occurring surfactant surfactin

HH Shen, RK Thomas, CY Chen, R Darton (University of Oxford)

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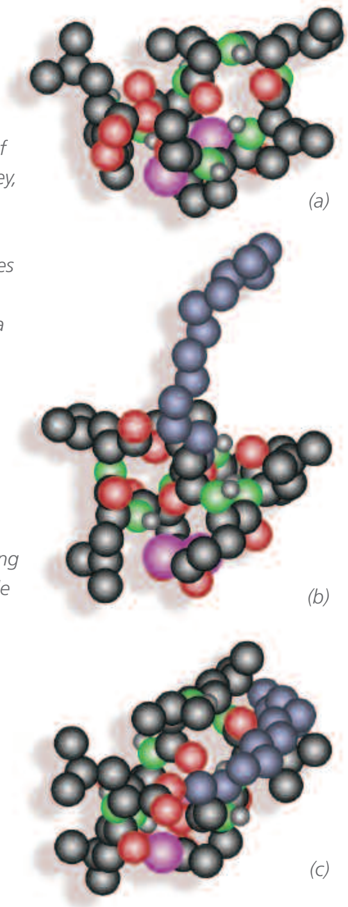
Surfactin is a naturally occurring surface active molecule produced from bacteria. Like many other biosurfactants, its biological function is not understood but it is extremely surface active at very low concentrations and is a powerful disrupter of phospholipid membranes. The chemical structure of surfactin, from NMR data, does not reveal how it possesses such surface activity. The charged groups are the only units capable of conferring water solubility on surfactin and yet are so buried in the generally hydrophobic surroundings that this part of the molecule bears little resemblance to a normal amphiphile's typical hydrophilic group. Neutron reflectivity measurements have allowed determination of the distribution of the three component fragments (hydrocarbon chain, leucines, and remaining part of the ring) in the structure of surfactin at the air/water interface. The structure accentuates the hydrophobic ball-like nature of the surfactin whose solubility in water is only maintained by the double charge, leading to its high surface active at such low concentrations, without self-assembly.



(a) The peptide ring of surfactin (carbons: grey, nitrogens: green, oxygens: red) which contains seven residues closed by two functional groups of a β-hydroxy-fatty acid. The two charged groups are drawn larger in pink. (b) A structure of surfactin with the hydrocarbon chain of the fatty acid projecting away from the peptide ring, the presumption being that the ring is hydrophilic. (c) The structure of surfactin most consistent with the neutron reflectivity data.

Nanoreactors formed from self-assembled protein cages

M Comellas-Aragones, FD Sikkema, JJLM Cornelissen, MC Feiters, RJM Nolte (Nijmegen University, The Netherlands), D Visser (NWO, The Netherlands), AE Terry, RK Heenan (ISIS)

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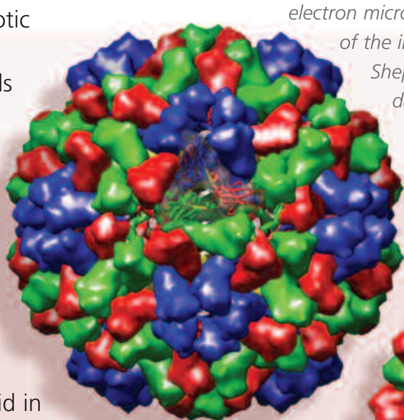
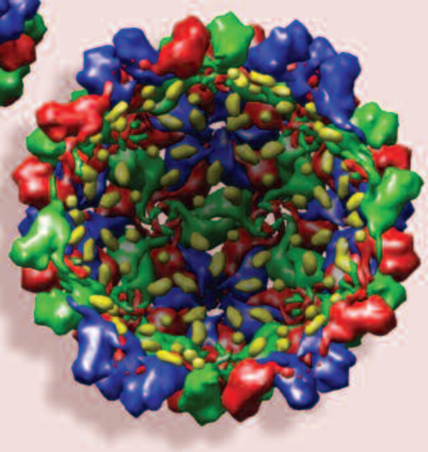
DM Vriezema et al., *Chem. Rev.* 105 (2005) 1445

At the interface of biology, chemistry and materials science we are developing novel approaches to the formation of materials, e.g. exploiting biomolecular self-assembly and organisation for the templated construction of new materials. Viruses such as the well-characterised Cowpea Chlorotic Mottle Virus (CCMV) are intrinsically attractive scaffolds because they consist of a highly stable, symmetrical, protein shell (called capsid), which is self-assembled from small proteins and encloses the viral RNA.

By Small Angle Neutron Scattering on LOQ, we have examined the sensitivity of the CCMV capsid in D_2O to pH and ionic strength of the surrounding environment. Fitting using a core-shell spherical model shows that there is almost no change in the outer diameter going from the virus to the capsid at pH 5 (27 vs. 26 nm) but that it decreases upon going to higher pH (pH 6.5, 23 nm; pH 7.5, 17 nm) with a concomitant increase in polydispersity.





Reconstruction of the structures of the Cowpea Chlorotic Mottle Virus determined by X-ray crystallography and cryo-electron microscopy. Full capsid structure (left) and view of the inner cavity of the virus (right). (From CM Shepherd et al., (2006). VIPERdb: a relational database for structural virology. Nucl. Acids Res. 34, D386. http://viperdb.scripps.edu/).

The structure of amino acids in solution

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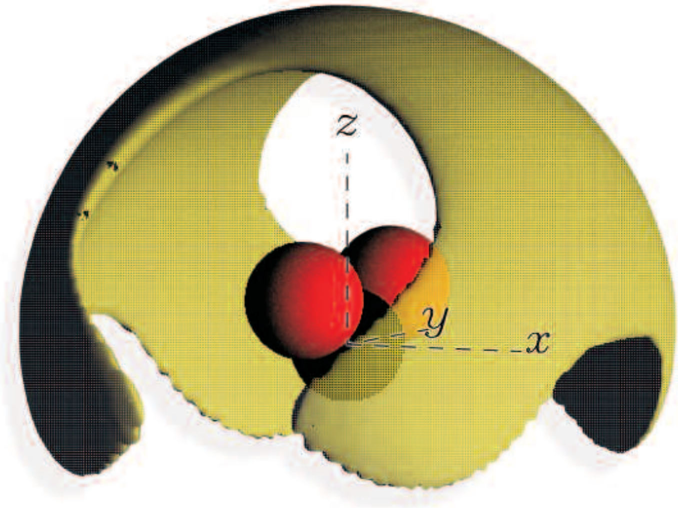
SE McLain et al.,
J. Chem. Phys. B110 (2006) 21251

Understanding how the self-organisation of a protein in solution is affected by its aqueous environment is a major challenge which has a long history. Unlike recent studies which have determined atomic-scale structural information in solid state proteins, the application of diffraction techniques to the study of protein hydration and conformation in solution at atomic-scale resolution is limited. In preparation for a wider programme to look at the conformation of oligopeptides and other biological molecules in solution, we have initiated a study of single amino acids, glutamic acid and proline, in solution. Glutamic acid is a neurotransmitter and the investigation provides information specific to receptor binding. Glutamic acid is also the precursor for proline, which was chosen as it occurs in most proteins and is believed to be the smallest known enzyme. These two systems have been investigated using neutron diffraction with isotopic substitution and combined with computer modelling, in order to elucidate the conformation of these amino acids in solution and their interaction with the aqueous environment.



Distribution of water around the carboxylate group in glutamic acid. Between the two oxygen atoms (red) a water molecule shares a hydrogen bond with both atoms.

Polarised neutrons to study protein/lipid nanostructures

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The development of sensors utilising both chemical and structural interactions between proteins and antibodies, bacteria, etc., requires the production of oriented protein arrays. In the present study, a membrane protein, OmpF, has been engineered to produce oriented arrays on gold. These arrays are multi-component devices with a number of assembly steps. Neutron Reflectometry (NR) offers in-situ characterisation throughout the assembly process. The characterisation of these complex structures requires contrast matching (the use of deuterated water / H_2O mixtures with the same contrast as part of the sample to highlight particular sample areas) and simultaneous data refinement. This particular problem does not lend itself to the use of deuterium labelling. Instead, we have used a different approach by inserting a magnetic reference layer between the gold electrode surface and the silicon substrate. NR is then performed with both up and down polarised neutrons after each assembly step. We are therefore certain that our contrast variation is performed on exactly the same system.

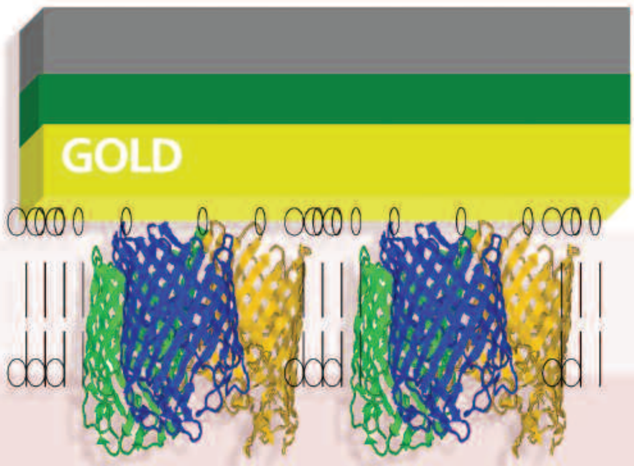

Diagram demonstrating the structural features of the device with the OmpF and lipids adsorbed to the gold electrode surface. The neutron beam passes through the magnetic reference layer (green) prior to and after reflecting from the device interface.

Technological materials – new… and old!

Materials ageing studies for current and future nuclear reactors

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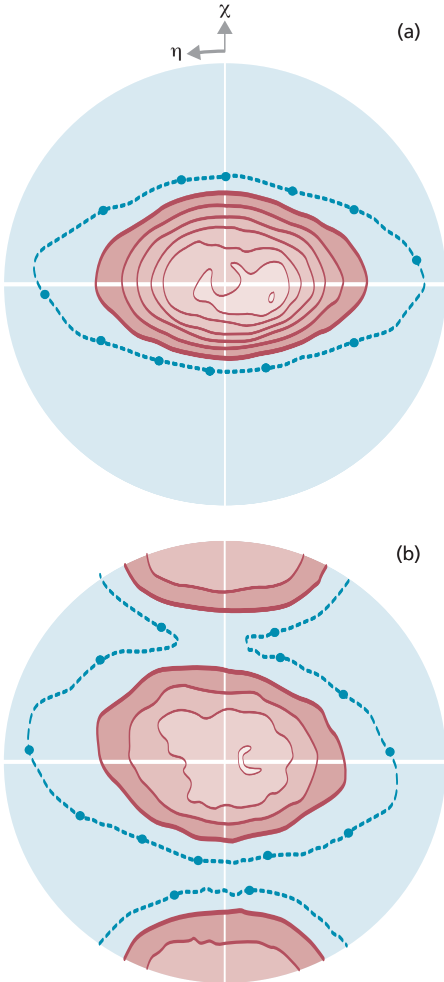
F Xu et al., *Acta Materialia* (2006, submitted)

Zirconium alloys are of critical importance to the nuclear power industry due to their combination of good mechanical properties, corrosion resistance in high temperature water and good neutronic properties – particularly important in the very high neutron fluxes of a reactor. The plastic and creep deformation of zirconium alloys thus has important technological applications, both in the deformation of components in the reactor itself – and hence predicting the safe life of existing reactors – and also in the optimisation of materials to be produced for the next reactor generation. The present study incorporates a comprehensive set of in-situ loading experiments on zirconium alloys exploring the relative contributions of different micromechanical deformation modes (different types of dislocation slip, and twinning) to the overall deformation. Comparisons of neutron diffraction data from ENGIN-X with theoretical models have – for the first time – given quantitative assessments of the relative importance of the interaction between these different modes. This information will feed into future models predicting the lifetime of components in the reactor.



Pole figure of Zircalloy-2 (a) before and (b) after compressive loading showing a clear signature of tensile twinning.

Negative thermal expansion in zirconium tungstate

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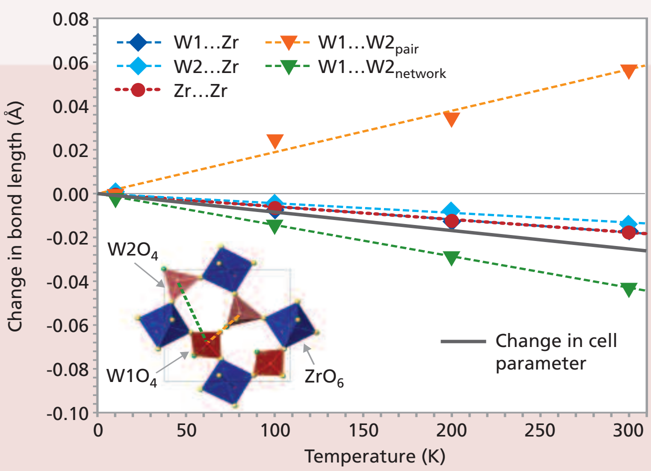
MG Tucker et al., Phys. Rev. Lett. 95 (2005) 255501

Negative thermal expansion (NTE), a property whereby a material contracts when it is heated, is important for varied applications from ceramic cooker hobs to high precision optical components. Zirconium tungstate (ZrW_2O_8) has one of the largest NTEs known over a wide temperature range. Its structure consists of a low-density, flexibly-hinged network of ZrO_6 octahedra and WO_4 tetrahedra. These structural units are able to rotate and translate more vigorously as the material is heated and this causes a net contraction of the crystal lattice. The mechanism for this is most clearly seen in the local changes within the structure – how an individual polyhedron moves with respect to its neighbours. Total neutron scattering (measuring and modelling Bragg and diffuse scattering together) is very sensitive to these changes and results from ZrW_2O_8 have been interpreted using computational modeling to show (for example) which atoms become closer and which become further apart on heating. Surprisingly, the locally-increased separation of pairs of WO_4 tetrahedra is a key structural feature for enabling NTE in ZrW_2O_8.

Various atom-to-atom distances from computer generated models of ZrW_2O_8 as a function of temperature.



Green solvents

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Prof. J.Eastoe,
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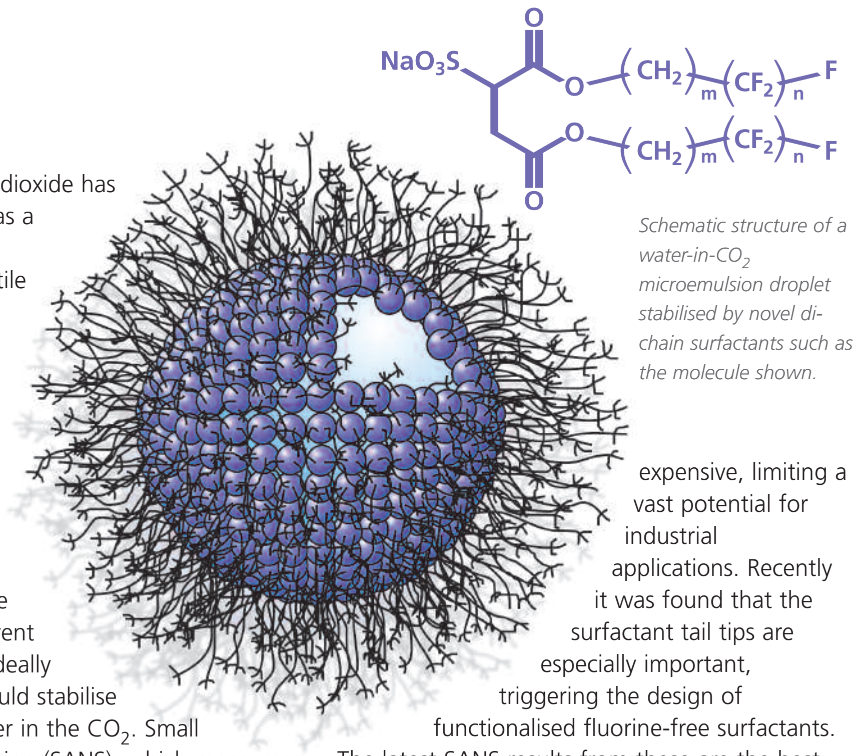
J Eastoe and S Gold, Phys. Chem. Chem. Phys., 7 (2005) 1353



Schematic structure of a water-in-CO_2 microemulsion droplet stabilised by novel di-chain surfactants such as the molecule shown.

Super-critical carbon dioxide has long been regarded as a potential 'green' replacement for volatile organic solvents. However, the truth is that sc-CO_2 is generally a poor solvent. For 15 years now groups in the USA and UK have been trying to create CO_2-compatible surfactants to achieve improvements in solvent properties of CO_2. Ideally these surfactants would stabilise nanodroplets of water in the CO_2. Small angle neutron scattering (SANS), which measures the size and interaction of particles, has provided key evidence for generation of nanoscale droplets in CO_2 using these stabilizers. Initial successes were with fluorocarbon molecules such as that shown in the figure, but unfortunately these are expensive, limiting a vast potential for industrial applications. Recently it was found that the surfactant tail tips are especially important, triggering the design of functionalised fluorine-free surfactants. The latest SANS results from these are the best yet, showing good levels of water solubilization and moderate stability. The next stage is optimisation of chemical structure to generate environmentally-acceptable and commercially-viable additives for this green solvent.

Ancient weapons technology studied on ENGIN-X

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E Godfrey et al., *The Conservation of Archaeological Materials conference proceedings*, Colonial Williamsburg, 2005

The Merovingian cemetery at Rhenen-Donderberg in the Netherlands, excavated in 1951, contained over 1100 graves. The cemetery was in use from around 375 AD to the first half of the 8th century AD. The population were not Christian: the majority of the burials included offerings. Apart from pottery, fibulae, jewellery and buckles, the most prominent grave-goods were iron weapons. The iron artefacts included a variety of Roman-style double-edged swords (*spathae*), Germanic-style single-edged swords (*seaxes*), shield-bosses, throwing-axes, and spearheads. The objects are now at the National Museum of Antiquities in Leiden, which allowed us to analyse two of the *seaxes* and 12 of the spearheads using ENGIN-X, with the aim of non-invasively characterising their chemical composition, level of technology, and current state of preservation. We found that ENGIN-X provided rapid identification and quantification of corrosion phases and preserved metal. We succeeded in mapping varying carbon contents across steel objects; this is crucially important, as we know from conventional destructive sampling methods that ancient iron artefacts are extremely heterogeneous.

E Godfrey with a Rhenen spearhead. The spearhead consisted mainly of corrosion and restoration, but had a preserved midrib of low carbon steel (ca. 0.1 wt% C).

Fundamental properties of materials

A step up the cuprate ladder?

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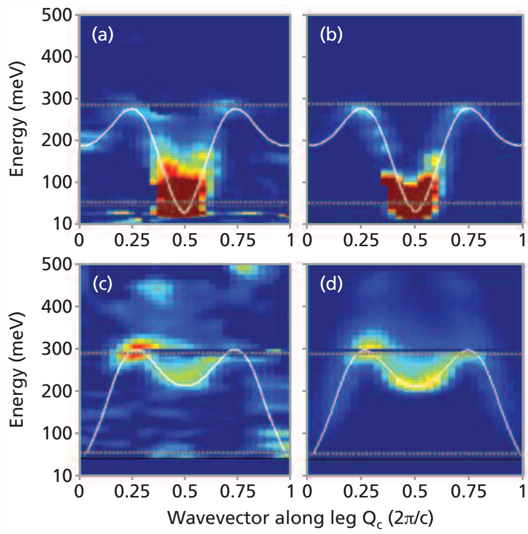
Cuprate ladders can be thought of as a strip cut out of a 2D square lattice, and therefore provide a link between magnetic behaviour in one and two dimensions. Additionally they share many features of the 2D high-temperature superconducting materials, and when doped and pressurised they become superconducting themselves.

We have investigated the ladder compound $La_4Sr_{10}Cu_{24}O_{41}$ and for the first time measured its complete magnetic excitation spectrum. A special feature of ladders is that the rung coupling decomposes scattering into separate one- and two-magnon contributions.

Utilising a powerful new computational method it has been possible for us to completely describe the quantum dynamics of the ladder. Our findings show not only that cyclic charge fluctuations are important in such systems but that oxygen tunnelling is essential to the description of the magnetic states. Our results provide a foundation for understanding strongly correlated states in this model cuprate.



(a) and (c) show the measured one and two magnon data respectively from $La_4Sr_{10}Cu_{24}O_{41}$ with the non-magnetic background subtracted. (b) and (d) show the simulated data. The white curves show the one magnon dispersion curve and the lower boundary of the two magnon dispersion.

Coupling of orbital, spin, and lattice degrees of freedom in $Tl_2Ru_2O_7$

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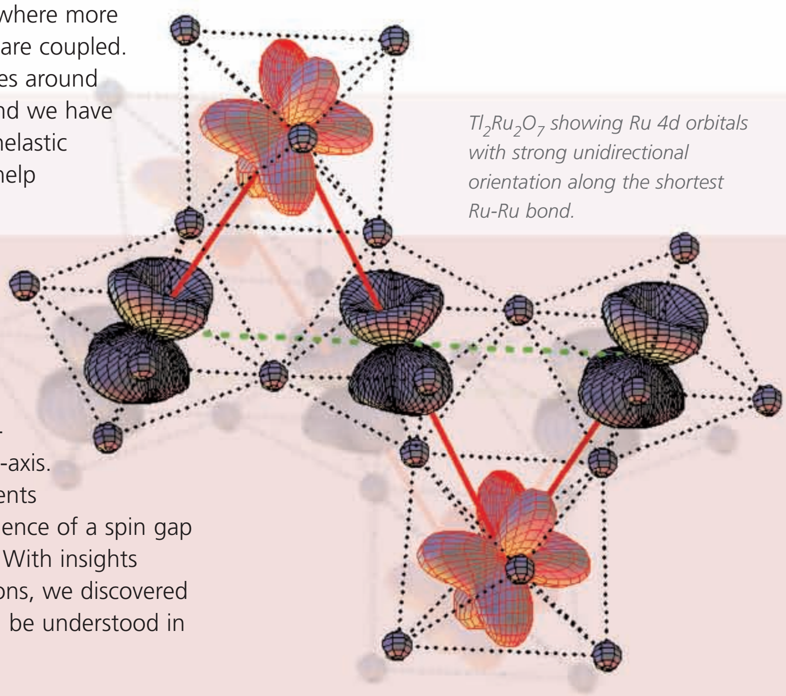
Seongsu Lee et al., Nature Materials 5 (2006) 471

A phase transition in a solid is produced by the order-disorder transition of any of the four fundamental degrees of freedom (orbital, spin, lattice and charge). Recently, there has been increasing interest in systems where more than two degrees of freedom are coupled. $Tl_2Ru_2O_7$ shows clear anomalies around 125 K in its bulk properties, and we have undertaken both elastic and inelastic neutron scattering studies to help understand this behaviour. According to our neutron diffraction experiments, $Tl_2Ru_2O_7$ undergoes a cubic-orthorhombic structural transition with three different types of Ru-Ru bond distances and the shortest zig-zag bond running along the b-axis. Our inelastic neutron experiments also revealed that there is evidence of a spin gap with a gap energy of 11 meV. With insights produced from band calculations, we discovered that all these observations can be understood in terms of one dimensional Ru 4d orbital ordering below 125 K. The coupling to its spin and lattice degrees of freedom then leads to the spin gap and structural distortion.



$Tl_2Ru_2O_7$ showing Ru 4d orbitals with strong unidirectional orientation along the shortest Ru-Ru bond.

New insights into INVAR systems through µSR

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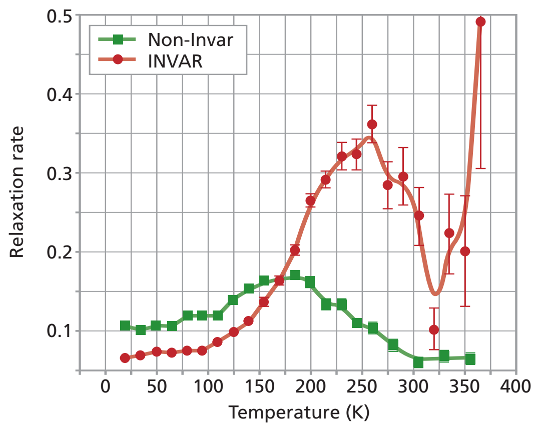
Khmelevskyi et al., Phys. Rev. Lett. 91 (2003) 037201

INVAR systems show near zero thermal expansion over a discrete temperature range. The discovery of the INVAR effect by Guillaume in 1897 won him the Nobel prize in 1920. However the underlying mechanism behind this phenomenon still remains unclear. Suggestions include a high-spin low-spin transition, or effects due to non-colinearity or disorder – but no experimental evidence has yet supported any particular model. µSR is an excellent probe of disorder in magnetic systems and furthermore is sensitive to a timescale that is difficult for neutron experiments to access. Here we studied $Fe_{1-x}Ni_x$ with $x = 0.35$ (INVAR, $T_c = 450$ K) and $x = 0.2$ (non-INVAR, $T_c = 400$ K). The INVAR system shows a dramatic change in muon relaxation rate compared with the non-INVAR case. The amplitude for this relaxational process is observed to decrease to zero for the INVAR system whereas for the non-INVAR material this component remains constant above 300 K. In elemental Fe and Ni the relaxation remains static over this temperature range as expected for an itinerant ferromagnetic below T_c. Here then we present the first observation of a two state dynamical transition in the INVAR system $Fe_{1-x}Ni_x$. This is commensurate with the idea that the large negative magneto-striction that dominates the lattice expansion in INVAR systems is driven by a dynamic process in the MHz range.



Muon spin relaxation rate as a function of temperature for the INVAR and non-INVAR systems studied.

Magnetic and molecular excitations in solid oxygen

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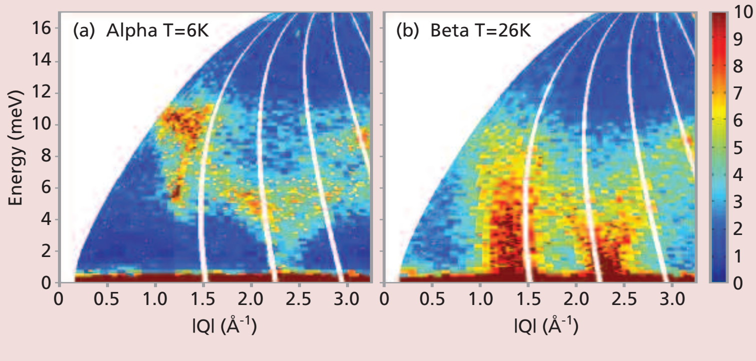
In spite of being the simplest molecular magnet, a self-consistent picture of the elementary excitations in solid oxygen remains semi-quantitative at best. This situation persists long after the first reported studies of its properties by Kamerlingh Onnes and Perrier back in 1910. Most spectroscopic results to date have been derived from infrared and Raman data and, as such, they can only provide a rather limited glimpse at the complex interplay between nuclear and spin motions in this seemingly simple molecular magnet. Using inelastic neutron scattering, we have carried out a comprehensive survey of the alpha and beta phases of solid oxygen. In addition to phonon and molecular (libron) modes common to both phases, we find that alpha oxygen ($T < 23.8$ K) also supports well-defined (solid-like) excitations of magnetic origin, the most prevalent being located at high energies ($E \sim 10$ meV) and low momentum transfers ($Q < 1.5$ Å^{-1}). As the alpha → beta transition is crossed from below, these well-defined magnetic modes give way to diffuse (quasielastic) scattering, indicative of a dynamically disordered (liquid-like) spin phase characterised by short-range magnetic order.



Inelastic neutron scattering contour maps for the alpha (a) and beta (b) phases of solid oxygen.

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 First Target Station instruments are described here, together with a summary of the day-1 instruments for the Second Target Station.

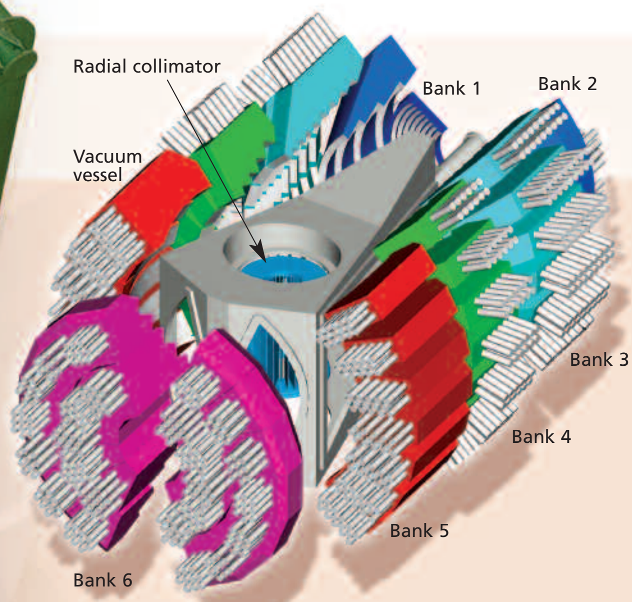
The TOSCA secondary spectrometer being lowered onto its kinematic mounts following improvements to the Be filters that led to dramatic improvements to the instrument background.

06EC1430

POLARIS

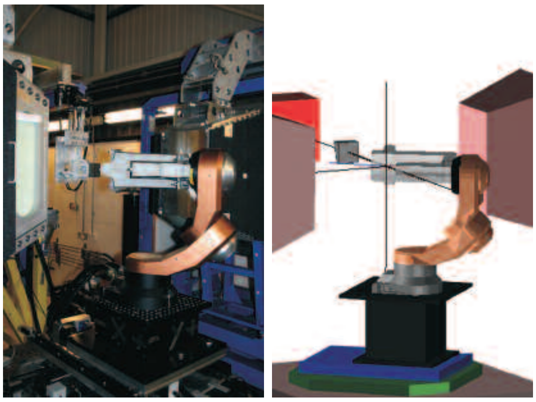
The ISIS Crystallography Group have been awarded £3M through the CCLRC Facility Development Grant scheme to undertake a major upgrade to the POLARIS diffractometer. Specifically, it is planned to replace the current detector banks with state-of-the-art, large solid angle ZnS scintillator modules. It is anticipated that the upgraded instrument will offer an approximately four-fold increase in count rate coupled with a modest improvement in $\Delta d/d$ resolution. In addition, fully adjustable collimation of the incident beam and an oscillating radial collimator will be installed, to reduce background scattering during experiments using complex sample environment equipment. The upgrade will allow expansion of the instrument's programme into new areas of science, including materials for energy production and storage, disordered and nanostructured solids, in-situ diffraction studies of chemical and electrochemical processes, high pressure investigations and rapid texture measurements of historical artefacts.

A schematic view of the upgraded POLARIS diffractometer, showing the 6 new detector banks.



Engineering Science Developments

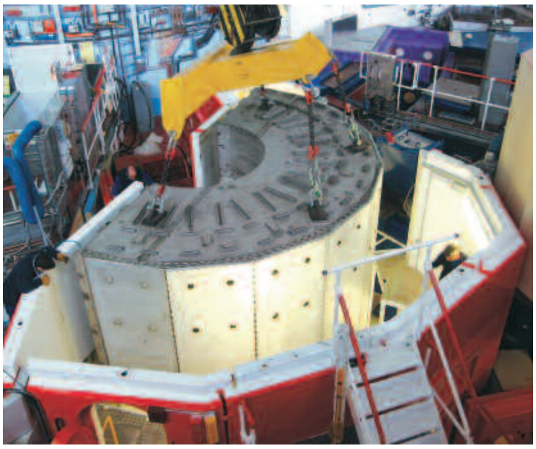
With ENGIN-X now a mature instrument, the focus this year has been on extending its capabilities and functionality. Final acquisitions from the Facility for Engineering Neutron Diffraction project have included a new pair of radial collimators defining 3 mm spatial resolution, and a novel cryogenic mechanical testing fixture. This latter equipment enables in-situ mechanical testing to temperatures as low as 70 K, opening up new opportunities for studies into temperature-dependent deformation mechanism transitions. A 100 kN stress rig has also extended the capabilities for in-situ experiments – for example, its frequency and load response have enabled some novel examinations of residual stress changes as a fatigue cracks are grown in-situ through weld stress fields.



The Cybaman rotary positioner (left) is now fully incorporated within the SSCANSS software (right) on ENGIN-X, providing a leap forward in positioning capabilities on the instrument.

MERLIN

MERLIN will be a high count rate, medium resolution chopper spectrometer, with a very large solid angle of detectors covering nearly 180° in the horizontal plane and ±30° in the vertical plane. This large solid angle and the incorporation of supermirror guides will mean that MERLIN will have a count rate some thirty times that of HET. MERLIN is now complete and has successfully measured its first neutrons. We will continue to install detectors and commission the instrument for the rest of the year with the aim of making it available after the long shutdown in 2007. We have secured funding to finish the detector coverage and MERLIN will start its first user run with complete detector banks.



The MERLIN vacuum tank is craned into position in the ISIS hall.

SANDALS

SANDALS was brought back into user operation in September 2005 after a short but successful commissioning period. Although the number of detectors installed is now smaller, their performance is sufficiently improved that the throughput on the instrument is if anything faster than before. In particular, the detector stability now means that fluctuations due to the small variations in target/moderator performance are readily detectable. The new electronics and the new blockhouse air conditioning system are all working extremely well compared to the previous performance that the instrument has seen.

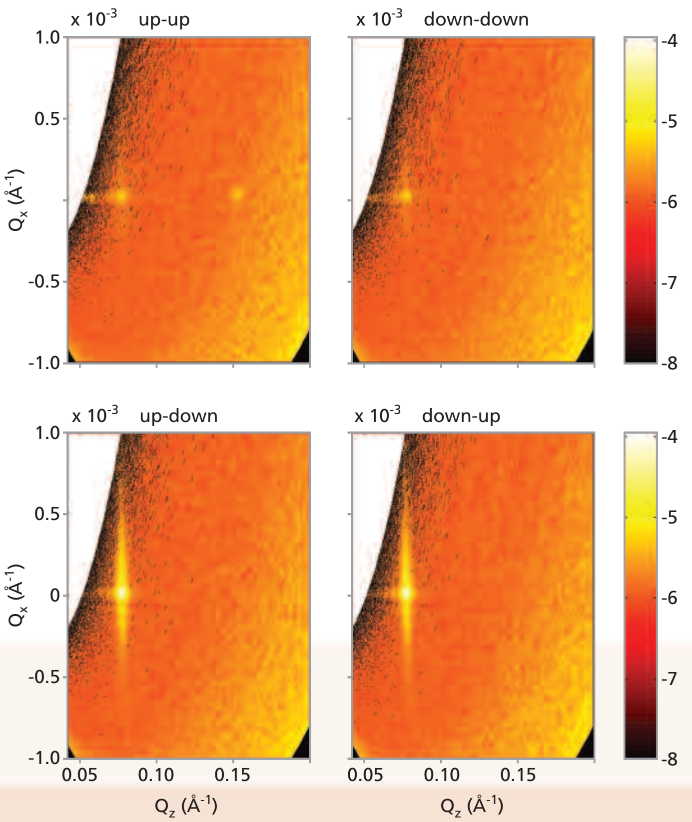
Erik Schooneveld (ISIS Detector Group) completing assembly of one of the very low angle detector (VLAD) rings for VESUVIO.

LOQ

Significant progress has being made on new sample environments for LOQ, which will also be used on SANS2D on TS-2. Delivery was taken of a new Anton Parr Rheometer, which is currently undergoing commissioning and will be installed ready for user experiments in cycle 06/5.

CRISP

The new CRISP supermirror analyser and linear scintillator detector are now fully commissioned and in routine use. The first experiment to combine the two devices was carried out in September 2005 in an investigation of the importance of interfacial roughness on the GMR effect on Iron/Chromium multilayers.



The measured scattering on CRISP from an iron/chromium multilayer system for the 4 spin cross-sections: up-up, down-down, up-down and down-up. The 'spin flip' scattering clearly visible in the up-down and down-up channels is purely magnetic in origin is thought to result from magnetic moments aligned perpendicular to the applied field at the interfaces between the layers in the sample.

SURF

A new m=3 super mirror has been installed to replace the existing mirror (m=1.75). The commissioning has been successful and it is possible to acquire the critical edge to background for an air/D_2O interface in 2 angles. Additionally, the motion control system has been updated with new flexible drive systems and control software. In preparation for TS-2, 'peltier' troughs are being developed, with Langmuir trough 'auto level' and script control.

HIFI

HIFI is the name of the new high field muon instrument that was funded through a £2.1M CCLRC Facility Development Award last year. The first year of the project has involved production of a detailed specification for the high field magnet itself, which is expected to operate up to around 5 T with good field homogeneity and very low stray field. The tender process for the magnet is underway at time of writing. In addition, simulations and tests of possible detector geometries are also ongoing to produce an efficient detector array which will work with the very tightly-curved positron trajectories that the high fields will produce. Detailed design work for the detectors, instrument framework and beamline elements will take place over the coming months. It is anticipated that construction of the new instrument will start at the beginning of 2008, with first muons in the latter part of that year.

Advanced Magnets

ISIS has been successful in its bid for a new suite of magnets for ISIS. This will include a wide angle 5-7 T magnet for the chopper spectrometers, a 14 T magnet for the diffraction instruments, a three-dimensional magnet for the reflectometers as well as a development programme for pulsed magnets in collaboration with Oxford University.

Polarised ^{3}He spin filters

ISIS has also secured funding to provide the equipment necessary to install ^{3}He spin filters on several of the instruments at ISIS, including WISH, LET and OSIRIS. This is being done in collaboration with the ILL and will ultimately see this technology used routinely on many other ISIS instruments.

TS-2 Instrument progress

There are seven first-phase instruments being built for the Second Target Station which will be available from late 2008:

LET: a very high count rate, low-energy, multi-chopper spectrometer. It will have excellent energy resolution, typically 5-6 μeV at 1 meV incident energy, as a well as a huge dynamic range. It is proposed to include a neutron polarisation option based around ^{3}He spin filter technology.

INTER: building upon the success of the world-leading SURF reflectometer, INTER will provide a unique facility for the study of air/liquid, liquid/liquid, air/solid and liquid/solid interfaces.

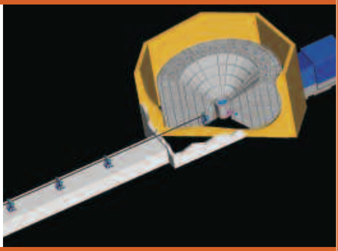
POLREF: a polarised neutron reflectometer designed for the study of the magnetic ordering in and between the layers and surfaces of thin film materials. Three-directional polarisation control will allow unique information to be obtained on the size and direction of the magnetism as a function of depth in multi-layer structures.

OFFSPEC: a reflectometer designed to characterise the increasingly important area of in-plane interface structure using the spin-echo technique. Through delicate manipulation of polarised neutrons, small structures with sizes from 10-1000 nm will be examined in thin-film samples.

SANS2D: representing a new concept in small angle scattering, SANS2D will use multiple position-sensitive detectors to give unsurpassed simultaneous data collection across a wide range of length scales. It will be well-placed to exploit the trend towards studying non-equilibrium and multi-component chemical systems.

WISH: a long-wavelength instrument optimised for studying magnetism at an atomic level. Designed for powder diffraction at long d-spacing in magnetic and large unit-cell systems, it will specialise in such topics as magnetic clusters, extreme conditions of magnetic field and pressure, and new designer magnetic systems tailored for specific applications.

NIMROD: a total scattering instrument that will offer greater insight into the subtle balance between short-, medium- and long-range interactions found in many materials.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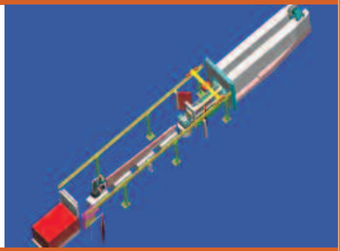
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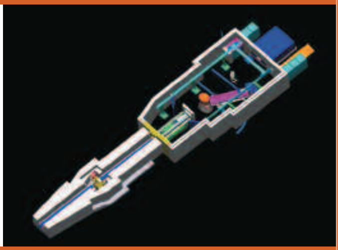
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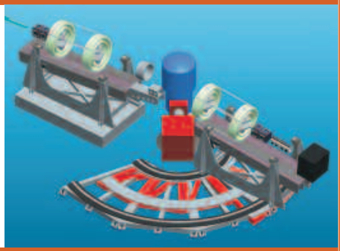
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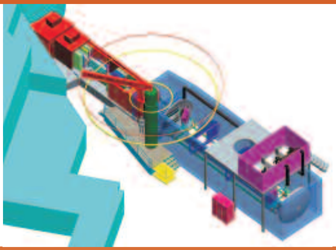
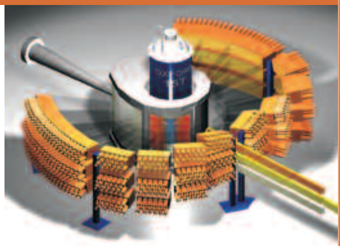
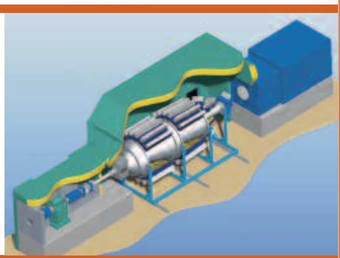

SANS2D


WISH


NIMROD


Keith Allum (ISIS Detector Group) checking the detector electronics on the prototype WISH detector assembly.

The Second Target Station

The Second Target Station Project is just over halfway to completion and activities on the ground are rapidly changing from building construction to the start of equipment installation. The main sections of the new experimental hall and link buildings were completed in April 2006 and there has been a substantial increase in the volume of components arriving on to site.

Proton beam

The extracted proton beamline for the Second Target Station Project will deliver a 60 μA proton beam to the new target station, steered and focused by 57 magnets along its path. Pulsed kicker magnets will take the beam from the synchrotron into the mouth of a septum magnet, diverting one proton pulse in five to the new target. The majority of the magnets are currently being manufactured across Europe by specialist engineering companies Scanditronix, Budker, Danfysik and SigmaPhi. The first components of the beamline will be laid on the ground in September 2006.

The considerable shielding requirements surrounding the proton beam line are becoming a significant feature in the link building between the ISIS synchrotron and the second target station. Approximately 50% of the 20,000 tonnes of steel and 2,000 tonnes of concrete has been installed to form the thick walls of the proton beam tunnel.

Members of the beam diagnostics group within the Proton Beam Task claimed the honour of getting the first components delivered to the Second Target Station Project site earlier in the year. The group's beam profile monitors will be used to report real-time beam position information to the accelerator control room.

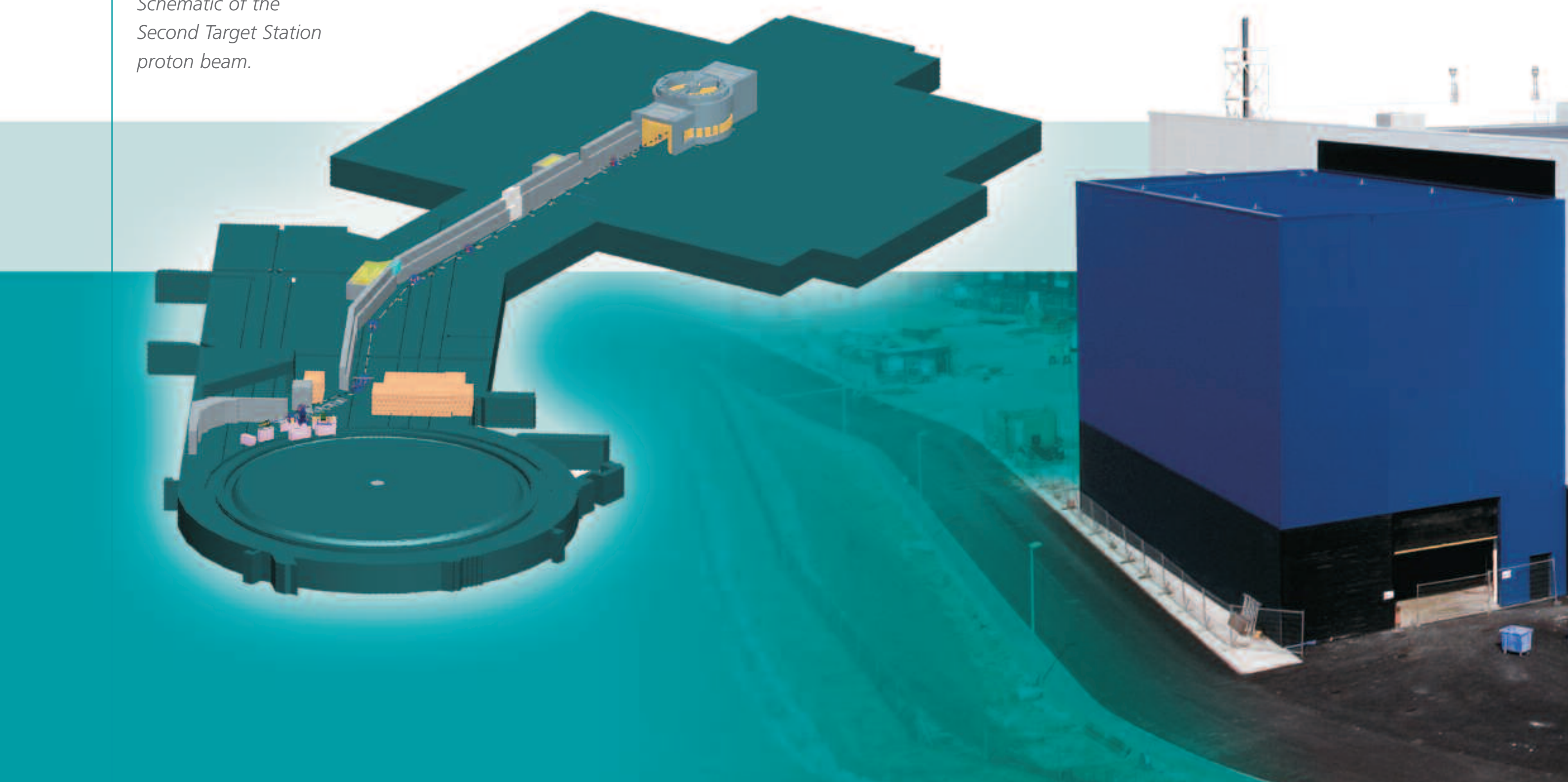
Target station

In July 2006, construction of the target station shield monolith commenced under the supervision of Corus Northern Engineering Services. This structure will eventually reach a size of 12 m diameter and 7 m height and will contain the tungsten target, two cold methane and hydrogen moderators, a beryllium reflector, a containment vessel and beam shutters to control the flow of neutrons to the instruments located around the target station.

Construction of the Second Target Station shield monolith.

06EC2556

Schematic of the Second Target Station proton beam.



The new target is a 6.6 cm diameter rod of tungsten, clad in tantalum to prevent corrosion, cooled from its surface with deuterated water. Prototypes of the target have been manufactured and tests of fluid flow and temperature gradients have been shown to be in good agreement with computational fluid dynamic simulations.

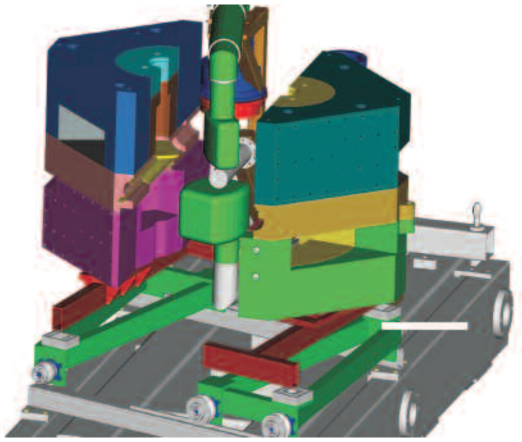
The target test facility. 06EC2643

Construction of the cryogenic systems for passing liquid methane and liquid hydrogen into the moderator vessels is progressing well in Grenoble at the premises of Air Liquide.

Instruments

Descriptions of the seven day-1 instruments can be found on page 21. Many of the instrument components for these, such as vacuum tanks, detector systems, neutron guides and choppers, have been designed and released to manufacture at companies across Europe. As well as the standard instrument design and safety reviews, operational reviews have also been held to ensure that the instruments can be easily used and efficiently serviced once completed and released to the user community.

A call for a proposals for a second phase of instruments was well-received by the user community and these were discussed at an open meeting of the Scientific Advisory Committee in October 2005. Proposals included a protein crystallography beamline, a spectrometer for extreme sample environments and a trio of small angle scattering instruments. The advisory committee has provided advice to the project on the second phase of instruments and identified further areas of instrumentation that should be developed. It is expected that new instruments will be funded through submissions to the UK Office of Science and Technology Large Facilities Fund supplemented by contributions from international partnerships.



Schematic of the TS-2 target and moderator assembly.

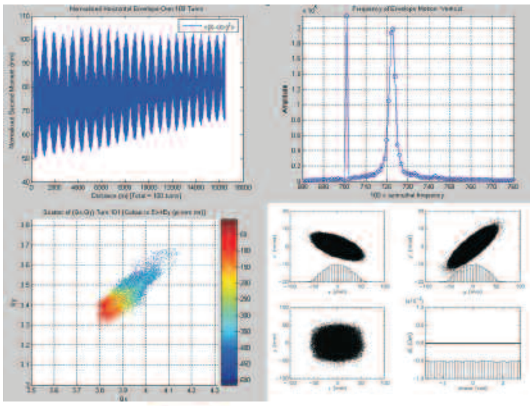
The Second Target Station building. 06EC1862

Accelerator and Target Developments

Accelerator and Target development activity is focused on performance and reliability improvements of existing systems, together with extending the accelerator and target capabilities including providing for the ISIS Second Target Station.

Synchrotron Group

Four new synchrotron RF accelerating cavities required for the second harmonic upgrade have been undergoing commissioning with full intensity beam. Together with the six fundamental RF cavities, the second harmonic system will allow the 50% extra current produced by the linac to be accelerated whilst keeping the absolute proton losses at the same level as before. The Group also has an ongoing programme of accelerator physics R&D to study the mechanisms causing beam loss at high intensities, work which will underpin future upgrades and new machines. This includes theoretical, computer simulation and experimental studies on the effects of transverse space charge, together with development of a more detailed understanding of beam diagnostics systems.



Computer simulation is helping the Synchrotron Group to better understand beam loss at high intensities. Here, the ORBIT code (from Oak Ridge) is used to model the ISIS ring near a high intensity loss condition.

Injector Group

The Injector Group has concentrated on replacing ageing high voltage power supplies in the four RF system modulators which were originally installed when ISIS was built. The work will be completed over the next 1 - 2 years, and the new supplies will be much more efficient and compact than those they are replacing. The Group is also at the forefront of H^- ion source development. Beam currents up to 70 mA have been achieved this year and efforts to improve the duty factor of the source have lead to the successful extraction of 1.2 ms-long beam pulses at 50 Hz.

Accelerator Engineering Group

As well as commissioning of the second harmonic RF systems and operational running of the radio frequency quadrupole, preparations have continued for the Muon Ionisation and Cooling Experiment (MICE) with a trial build of the target assembly. In addition, plans have been made to refurbish part of the extracted proton beam near the muon production target during the 2007 shutdown, following the failure of a quadrupole magnet earlier in the year. The installation of the new extracted proton beamline for the Second Target Station will also take place during the shutdown.

Tony Kershaw and Sarah Whitehead of the Diagnostic Section discussing a new LabView programme designed for the beam loss monitoring system installed inside dipole 2 of the synchrotron.

ISIS Synchrotron Diagnostics Section

The work of the Synchrotron Diagnostics Section is divided between the operation of existing diagnostics systems, and research and development into new diagnostics. Developments this year include plans for a new electron cloud monitor to study electron densities within the vacuum vessel which can lead to beam instabilities. New fast beam profile monitors are currently also being installed which will be used to observe, for the first time, the development of the profile of the proton beam in real time over the 10 ms acceleration cycle.

Experimental Halls Group

During the summer shutdown of 2005 the Target Station Section instigated the replacement of the neutron target, a complex procedure requiring remote manipulation due to the high radioactivity generated during the spallation process. In addition the team has been working on the development of a new hydrogen moderator, scheduled for installation during the 2007 shutdown. The present moderator has not been changed since ISIS came on-line more than 20 years ago.

Electrical Engineering Group

The Electrical Engineering Group have been preparing for installation of a new synchrotron extraction kicker system which will take place in the upcoming long shutdown. The kicker system extracts the proton beam from the synchrotron by raising the current in the kicker magnets to 5000 Amps within 100 ns. The new system will provide more efficient extraction for the higher intensity beam once TS-2 is operational.

New extraction kicker oil cooling systems.

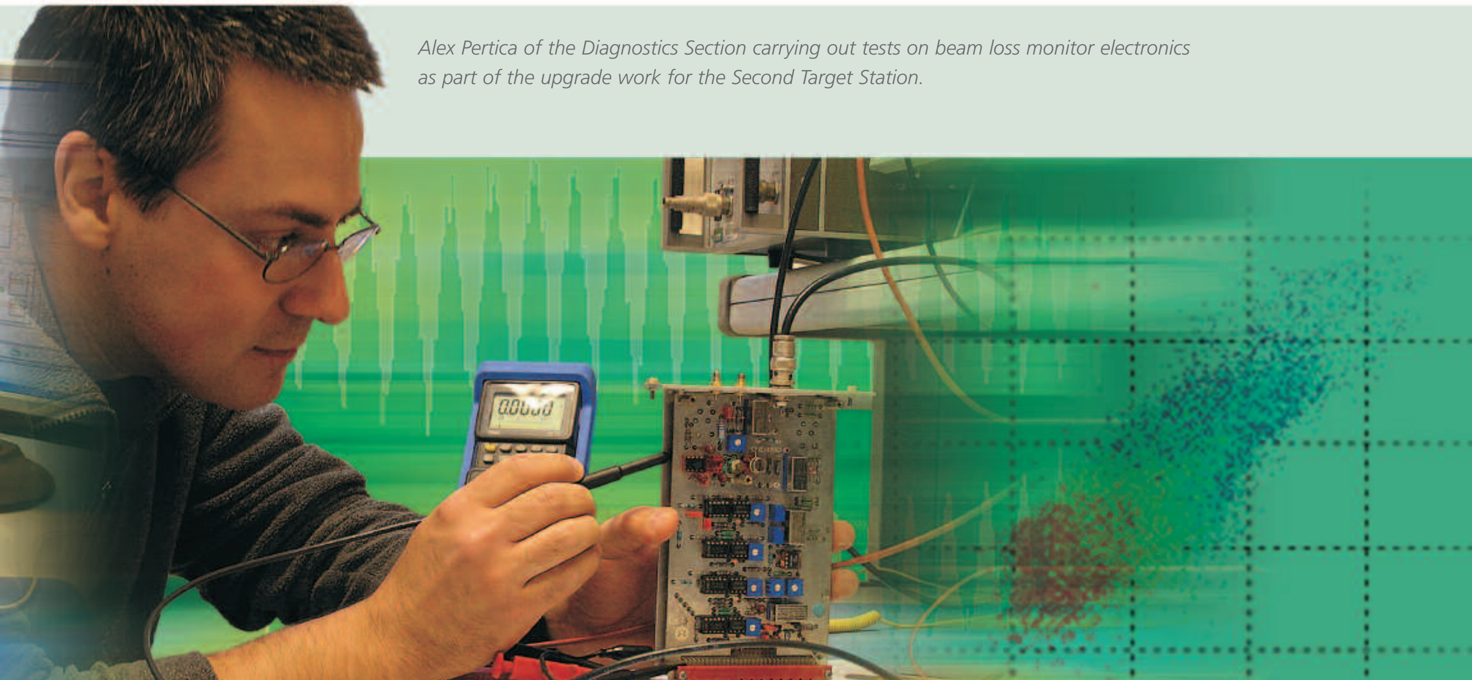
Controls Group

Controls Group work this year has included completion of the database for the new personnel protection and beam protection systems (~1000 channels in total) and successful initial testing of these systems; completion of the design for the new central timing distributor for two-target operation; the transfer of remaining legacy applications from the old control system, and significant reliability improvements. Maintenance of the old control system is scheduled for termination in November 2006.

Project Engineering Group

The Project Engineering Group has been involved in work across the facility for both first and second target stations. This has included detailed design of the Second Target Station target, moderators and reflector, shielding monolith, extracted proton beam line components and day-one instruments. Design and procurement of the MERLIN instrument vacuum vessel have also been completed.

Alex Pertica of the Diagnostics Section carrying out tests on beam loss monitor electronics as part of the upgrade work for the Second Target Station.



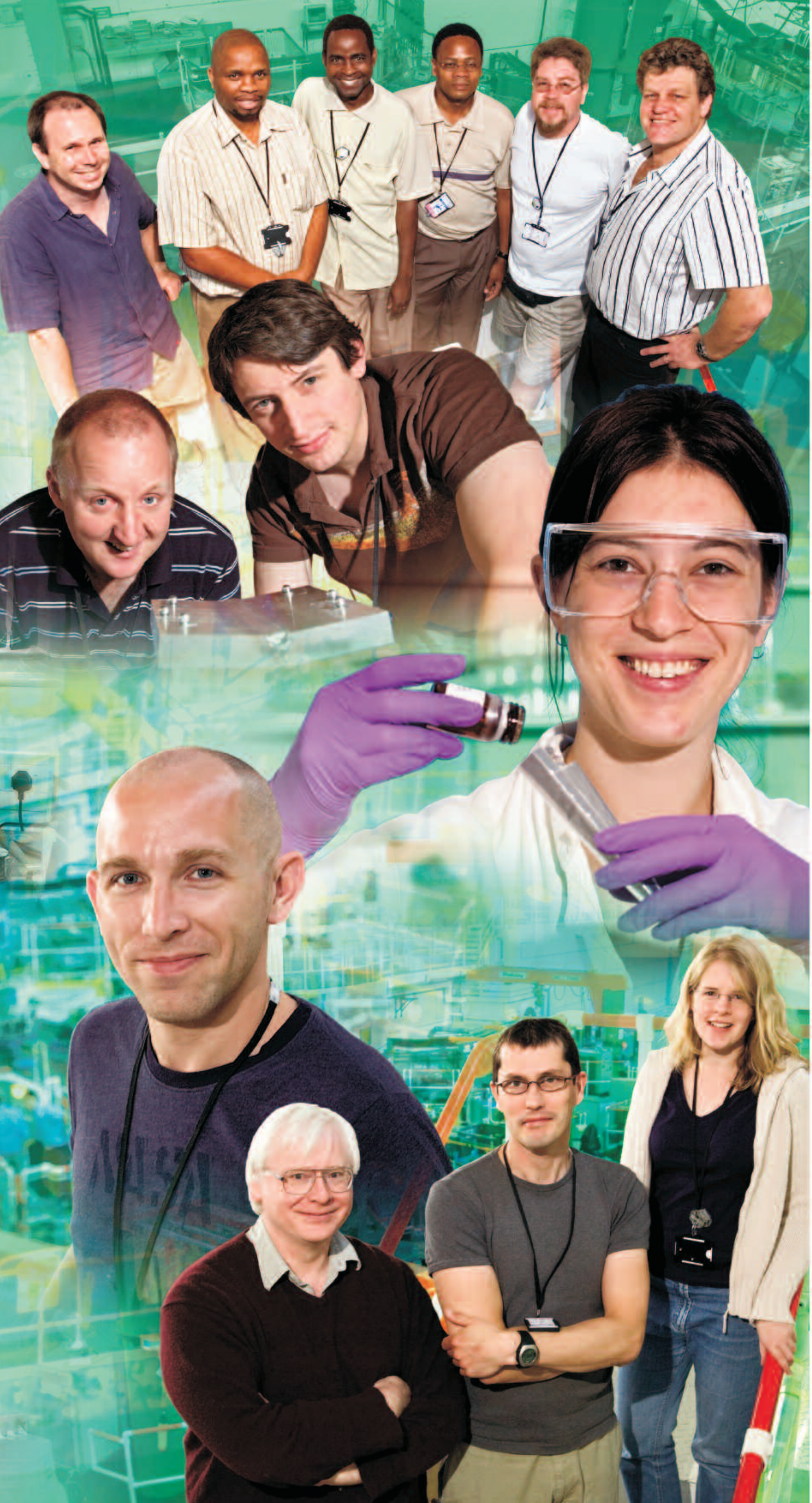
Dan Faircloth and Steve Jago with one of the Q11 qradrupole magnets for the ISIS Second Target Station.

Ben Pine and Bryan Jones discuss results from beam diagnostics modelling.

Steve Payne, assembling a new electron cloud detector. Electron 'clouds' can build up as a result of the passage of the proton beam around the synchrotron and can lead to beam instabilities, something which will be monitored as ISIS strives towards 300 µA and beyond.

Neal Leach of the ISIS Diagnostics Section winding a beam intensity toroid destined for the new TS-2 beam line.

Eamonn Quinn with one of the position monitors for the Second Target Station.



Simon Connell, Jonathan Keartland, Morgan Madhuku (University of Witwatersrand, South Africa), Isaac Machi (Ithemba Laboratories, South Africa), Dumisani Gxawu (Durban Institute of Technology, South Africa) with Philip King (ISIS) during their time on EMU using muons to explore hydrogen states in diamond. 06EC2875

Francis Fohn and Ben Grant (University of Manchester) using ENGIN-X to study the effect of mutliple welding passes on residual stresses in steel welds. 06EC2869

Jennifer Riesz (University of Queensland, Australia) mapping the vibrational structure of melanin precursors on TOSCA. 06EC2893

Dominic Fortes (University college London) studying the incompressibility and high-pressure behaviour of anhydrous $MgSO_4$ on POLARIS. 06EC2860

Emma Smith (Loughborough University), Karl Ryder and Andrew Glidle (Leicester University) during their time at ISIS using CRISP to compare the distribution of monomer species in conducting copolymer films prepared by electrodeposition. 06EC2902

A year around the facility

Future access to neutron sources: a strategy for the UK

Lord Sainsbury, the UK Minister for Science and Innovation, asked the CCLRC to prepare a report advising him on the UK's future requirements for neutron facilities and a plan to secure long-term access to leading-edge neutron facilities. A strategic review of the UK requirement for neutrons was therefore undertaken by CCLRC involving a consultation process with the UK academic, public and private sector communities. The report containing the recommendations was submitted to Lord Sainsbury in December 2005. It concludes that UK scientists will continue to require access to the best possible neutron facilities for the foreseeable future. It calls for enhanced investment in the ILL and ISIS neutron sources to sustain the international competitiveness of these world-leading facilities for the next ten to fifteen years, and recognises the future need of the UK research community for access to next generation neutron sources. The full report is available from the CCLRC website www.cclrc.ac.uk.

EPAC

The Tenth European Particle Accelerator Conference was held at the Edinburgh International Conference Centre earlier this year. The event was hosted by CCLRC, with a strong ISIS involvement from Freddie Akeroyd, Dan Faircloth, Andy Kimber, Matt North and John Thomason (as chairman) on the Local Organising Committee and David Findlay and John Thomason on the Organising Committee; staff from CCLRC's Accelerator Science and Technology Centre were also heavily involved. Over 1,400 attendees from 32 countries enjoyed a busy week of talks and poster sessions on all aspects of accelerator science, interspersed with the occasional dram of whisky. Plenary talks included an opening address from Sir Michael Atiyah, President of the Royal Society of Edinburgh, status reports on all major worldwide accelerator developments, and an invited presentation from Sir Roger Penrose. ISIS was represented by a talk on ISIS upgrades by David Findlay, 16 posters and an exhibition stand dedicated to the Second Target Station Project.

EPAC06 was held in the International Conference Centre, Edinburgh, UK.

Workshop on neutron and muon techniques in magnetism

A one-day workshop on neutron and muon techniques in magnetism, aimed at postgraduate students, was held at the Rutherford Appleton Laboratory on 1st February 2006. It attracted over 40 participants, including staff and students from various universities, CCLRC and DIAMOND. In

Areta Olariu and Philippe Mendels (Université Paris-Sud, France) preparing the MuSR dilution fridge for muon studies of pure and substituted sodium cobaltates. 06EC2873

Vladimir Kozhevnikov (Catholic University of Leuven, Belgium) using CRISP for a polarised neutron reflectivity study of the interface delocalisation transition in a type-I superconductor. 06EC2855 addition to talks on the experimental techniques and theory, the workshop provided an excellent networking opportunity for young members of the magnetism community.

Attendees at the workshop on neutron and muon techniques in magnetism. 06EC1264

9th Oxford School on Neutron Scattering, September 2005

From 6-15 September 2005 the 9th residential school in this series took place at Mansfield College, Oxford. Some 47 students attended the school, out of a total of 120 who applied, from the UK, other European countries, the USA and South Africa.

The mornings were busy with lectures in the Oxford Physics department. In the first week there was an emphasis on sources, instruments and science using diffraction. In the second week subjects such as inelastic scattering and polarised neutrons were covered, together with topics involving amorphous materials, engineering and biology. In the afternoons the students worked through a series of problems in neutron scattering, and were able to ask questions and discuss the fundamental points. CCLRC and the EC NMI3 are thanked for their funding of this event.

The attendees of the ninth Oxford Neutron Scattering Summer School.

Neutron Training Course

The demand for the latest ISIS Neutron Training Course, which was held successfully between 19-24 February, was again very high with 80 applicants for just 24 places. Students benefited from a combination of lectures on key aspects of the neutron technique, together with practical work on ISIS instruments. We plan to hold the next Training Course in early December 2006; more information can be found on the ISIS website (www.isis.rl.ac.uk/trainingcourse).

Toby Perring (ISIS) and Andrew Walters (UCL/ISIS) reviewing their MAPS data of high energy spin excitations in elemental iron. 06EC2916

Attendees at the ISIS neutron training course preparing samples. 06EC2014

Workshop on magnetic structure determination from neutron powder diffraction data

Following the success of a similar event held in December 2002, this workshop was aimed at providing the essential theoretical foundations and some working experience on solving and refining magnetic structures from neutron powder diffraction data. The meeting took place at the Cosener's House, 14-16 November 2005, with over half the 34 participants being from overseas, and was organised by Laurent Chapon and Aziz Daoud-Aladine from ISIS.

Attendees at the magnetic structure determination workshop at Cosener's House in November.

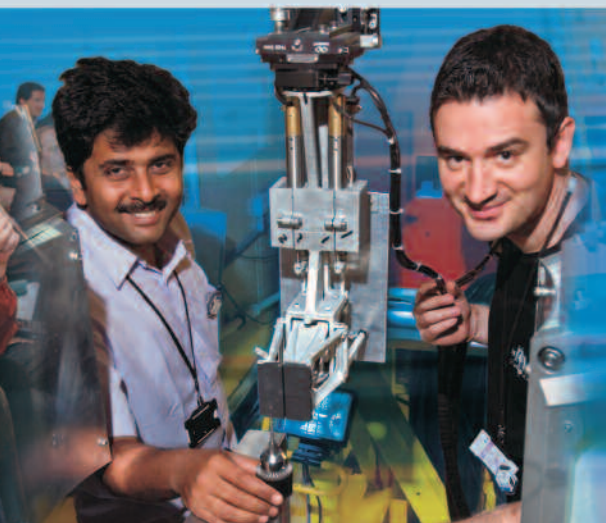
Neutron and Muon Integrated Infrastructure Initiative Meeting

The European Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (NMI3) brings together 23 partners from 14 countries, including 11 neutron or muon research infrastructures, together with other interested organisations. Activities include the provision of access for European researchers to neutron or muon facilities, the development of new technologies for neutron scattering or muon spectroscopy through joint research activities (JRAs), and networking events to promote neutron and muon science. The third NMI3 meeting took place in September at RAL. Over 200 participants gathered to swap ideas about neutron science and hear details of JRA progress in detectors, software, neutron optics, spin filters and polarised neutron techniques, deuterium labelling and muon techniques.

ISIS People

Each year sees the comings and goings of ISIS staff. Peter Gear retired as Head of Operations after 15 years service at ISIS, John Rice retired from his position as ISIS Duty Officer after 44 years service and David Bushnell, Senior Electrical Engineer, retired after 41 years of service. Ian Bailey, Section Leader Sample Environment retired after 25 years of service and Shirley Fortt, secretary to a number of division heads and CCLRC fellows retired after 16 years of service. Edith Knight retired following many years in ISIS administration and more recently as TS-2 Administrator, and Chris Cleverly left also after several years in the ISIS administration office. Their extensive knowledge and experience will be greatly missed.

Neutron scatterers and muon spectroscopists from around Europe gathered at the Rutherford Appleton Laboratory in September as part of the large NMI3 collaboration.



Supriyo Ganguly and Dimitrios Bakauos (University of Manchester) using ENGIN-X for determination of the 3-dimensional residual stress state in an electron beam welded bimetallic aircraft wing spar specimen. 06EC2918

We were saddened during the year by the passing away of two ISIS colleagues: Bryan Neville was a member of the ISIS computing group with great expertise in control software, and Michael Colley was a talented engineer working on the target assembly at the heart of the ISIS Second Target Station. We were also saddened to learn of the passing away of John Hirst shortly after his retirement from ISIS last year. All three are much missed by family and friends.

Instrument Scientists to join ISIS this year include Silvia Imberti on INES and Cameron Neylon, Large Scale Structures group. The TS-2 team has welcomed Bobby King, Colin Down, Gareth Powell, Mark Forrest, Detlev Riedel, Neil Schneider, Darryl Taylor, Matthew Fletcher and Richard Law. The Accelerator Division were joined by Jonathan Ranner, Garry Walsh, Steven Gray, Bryan Jones, Steve Bromwich, Mark Ashman, Jon Pile and Kenny Rodgers, and Jane Vickers has taken up the post of ISIS Safety Officer.

The Project Engineering Group were joined by Jim Nightingale, Nick Webb and Simon Waller. Oleg Kirichek joined the User Support Group as Sample Environment Section Leader, together with Richard Blight and Stephen Cox. Rowan White has joined the IDM Division as EC TS-2 Project Manager. New faces in the ISIS & CLF User Office are Evelyn Sanders, Iona Fletcher, Michelle King and Karen Briggs.

Congratulations are due to several ISIS staff. Andrew Taylor was awarded the Glazebrook Medal by the Institute of Physics for his contributions to neutron scattering physics, and he has also been elected a Fellow of the Royal Society of Edinburgh. Jeff Penfold was promoted to CCLRC Senior Fellow; Jeff is well known for his wide use of neutron reflectometry and small angle scattering at ISIS as a tool for studying soft matter, and is Project Scientist for the Second Target Station. Congratulations also to Matt Tucker of the ISIS Crystallography Group who has been awarded the Physical Crystallography Young Scientist Award at the BCA Spring Meeting in Lancaster, and to David Keen also of Crystallography who has been made a visiting professor to the Physics Department in Oxford.

Peter Gear retired as Head of Operations earlier this year. 06RC1708

Souleymane Diallo (University of Delaware, USA) during his time at ISIS using MARI to determine the Bose-Einstein condensate fraction of supersolid ^{4}He. 06EC2876

David Dobson and Cidunka Vocadlo (University College London) characterising the low temperature crystal and magnetic structure of FeO on GEM. 06EC2670

Publications

Publications relate to all work carried out at ISIS. Listed here are 337 publications resulting from work at the facility that have been published since ISIS 2005.

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.

T Abdul-Redah, C A Chatzidimitriou-Dreismann
Irreversible hydrogen quantum dynamics and anomalous scattering behaviour in liquids and solids
International Journal of Hydrogen Energy **31** 269-276 (2006)
[doi:10.1016/j.ijhydene.2005.04.037]

T Abdul-Redah, M Krzystyniak, J Mayers, C A Chatzidimitriou-Dreismann
Anomalous neutron Compton scattering cross section in zirconium hydride
J Alloys Comp **404-406** 790-793 (2005)
[doi:10.1016/j.jallcom.2005.05.003]

T Abdul-Redah, M Krzystyniak, C A Chatzidimitriou-Dreismann
Neutron Compton scattering from water studied with the double-difference technique
Phys Rev B **72** 052202 (2005) [doi:10.1103/PhysRevB.72.052202]

T Abdul-Redah, M Krzystyniak, C A Chatzidimitriou-Dreismann
Quantum entanglement and decoherence due to coupling of protons to electronic environment
in Decoherence, Entanglement and Information Protection in Complex Quantum Systems, eds. V M Akulin, A Sarfati, G Kurizki, S Pellegrin (Kluwer Academic Publisher, Boston/Dordrecht/London) (2005)

T Abdul-Redah, P A Georgiev, D K Ross, M Krzystyniak, C A Chatzidimitriou-Dreismann
Short lived protonic quantum entanglement and coupling to the electronic environment in LaH_2 and LaH_3
J Alloys Comp **404-406** 787-789 (2005)
[doi:10.1016/j.jallcom.2005.05.004]

J J Adkin, M A Hayward
Structure and magnetism of 4H-$BaMnO_{3-x}$ ($0 < x < 0.35$) and 4H-$Ba_{0.5}Sr_{0.5}MnO_{3-x}$ ($0 < x < 0.21$)
J Solid State Chem **179** 70 (2006) [doi:10.1016/j.jssc.2005.09.046]

A K Adya, M V Shcherbakov, A Zarbakhsh, J Bowers, J R P Webster
Neutron reflectivity study of grafted poly(ethylene glycol) in the presence of an aqueous bovine serum albumin solution
Journal of the Indian Chemical Society **82** 79-86 (2005)

F Affouard, P Bordat, M Descamps, A Lerbret, S Magazu, F Migliardo, et al
A combined neutron scattering and simulation study on bioprotectant systems
Chem Phys **317** (2-3) 258-266 (2005)
[doi:10.1016/j.chemphys.2005.05.033]

M Al-Jawad, P Manuel, C Ritter, S H Kilcoyne
Kinetic neutron diffraction study of Nb_3Sn phase formation in superconducting wires
J Phys Condens Matter **18** 1449-1457 (2006)
[doi:10.1088/0953-8984/18/4/028]

C Andreani, C Pantalei, R Senesi
Mean kinetic energy of helium atoms in fluid ^3He and ^3He–^4He mixtures
J Phys Condens Matter **18** 5587-5596 (2006)
[doi:10.1088/0953-8984/18/24/001]

C Andreani, S Imberti, A Pietropaolo, R Senesi, G Gorini, E Perelli-Cippo, et al
High energy inelastic neutron scattering on the VESUVIO spectrometer at ISIS
Neutron News **16** 30 (2005) [doi:10.1080/10448630500454304]

C Andreani, D Colognesi, J Mayers, G F Reiter, R Senesi
Measurement of momentum distribution of light atoms and molecules in condensed matter systems using inelastic neutron scattering
Advances in Physics **54** 377 (2005) [doi:10.1080/00018730500403136]

H N Bani-Salameh, Y G Celebi, S F J Cox, R L Lichti
Anisotropic muonium centres in aluminium nitride
Proc. *10th International Conference on Muon Spin Rotation, Relaxation and Resonance, Oxford, UK, August 2005,*
Physica B **374** 372-375 (2006) [doi:10.1016/j.physb.2005.11.104]

H N Bani-Salameh, Y G Celebi, K H Chow, B E Coss, S F J Cox, R L Lichti
Muonium states and dynamics in 4H and 6H silicon carbide
Proc. *10th International Conference on Muon Spin Rotation, Relaxation and Resonance, Oxford, UK, August 2005,*
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J Appl Phys **98** 103520 (2005) [doi:10.1063/1.2135888]

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Preliminary MuSR studies on the incorporation of steriodal drug molecules into liposomes
Physica B **374** 332 (2006) [doi:10.1016/j.physb.2005.11.089]

S A Barnett, C K Broder, K Shankland, W I F David, R M Ibberson, D A Tolcher
Single-crystal X-ray and neutron powder diffraction investigation of the phase transition in tetrachlorobenzene
Acta Cryst. B62, (2006), 287-295.

G D Barrera, S F Parker, A J Ramirez-Cuesta, P C H Mitchell
The vibrational spectrum and ultimate modulus of polyethylene
Macromolecules **39** (7) 2683-2690 (2006) [doi:10.1021/ma052602e]

G D Barrera, D Colognesi, P C H Mitchell, A J Ramirez-Cuesta
LDA or GGA? A combined experimental inelastic neutron scattering and ab initio lattice dynamics study of alkali metal hydrides
Chem Phys **317** (2-3) 119-129 (2005)
[doi:10.1016/j.chemphys.2005.04.027]

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Comment on 'hard-sphere-like dynamics in a non-hard-sphere liquid'
Phys Rev Lett **95** 269601 (2005) [doi:10.1103/PhysRevLett.95.269601]

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Experimental evidence for the presence of nonacoustic excitations in molten Ga
Phys Rev B **72** 104103 (2005) [doi:10.1103/PhysRevB.72.104103]

F J Bermejo, J W Taylor, S E McLain, I Bustinduy, J F C Turner, M D Ruiz-Martin, et al
Evidence of the presence of opticlike collective modes in a liquid from neutron scattering experiments
Phys Rev Lett (2006, in press)

F J Bermejo, I Bustinduy, S F J Cox, J S Lord, C Cabrillo, M A Gonzalez
Exploring the dynamics about the glass transition by muon spin relaxation and muon spin rotation
J Phys Condens Matter **18** 2871-2880 (2006)
[doi:10.1088/0953-8984/18/10/010]

F Bert, P Mendels, D Bono, A Olariu, F Ladieu, J C Trombe, et al
Dynamics in pure and substituted volborthite kagome-like compounds
Physica B **374** 134-137 (2006) [doi:10.1016/j.physb.2005.11.034]

R Bircher, G Chaboussant, S T Ochsenbein, F Fernandez-Alonso, H U Gudel, E K Brechin
Inelastic neutron scattering study of undeuterated $[Mn_9O_7(OAc)_{11}(thme)(py)_3(H_2O)_2]$
Polyhedron **24** 2455-2458 (2005) [doi:10.1016/j.poly.2005.03.062]

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Brief encounter at the molecular level: what muons tell us about molecule-based magnets
Synthetic Metals **152** 481 (2005) [doi:10.1016/j.synthmet.2005.07.200]

Eds. S J Blundell, P J C King, F L Pratt
Proceedings of the 10th International Conference on Muon Spin Rotation, Relaxation and Resonance
Proc *10th International Conference on Muon Spin Rotation, Relaxation and Resonance (µSR 2005), Oxford, UK, 08-12 Aug 2005*, Physica B **374-375** (2006) 1-507

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J Chem Phys **125** 014508 (2006) [doi:10.1063/1.2212421]

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Solvation shell of H^+ ions in water
J Mol. Liq. 117, 77-79 (2005)

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Solvation shell of OH^- ions in water
J Mol. Liq. 117, 81-84 (2005)

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Physica B (2006, in press)

A Bowman, R I Smith, D H Gregory
Synthesis and structure of the ternary and quaternary strontium nitride halides, $Sr_2N(X,X')$ (X, X' = Cl, Br, I)
J Solid State Chem **179** 130-139 (2006) [doi:10.1016/j.jssc.2005.10.006]

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Ternary and quaternary layered nitride halides, $Ca_2N(X,X')$ (X, X' = Cl, Br, I): evolution of structure with composition
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Phys Rev E 72 (4) (2005)

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ISIS Seminars 2005-2006

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

26th April 2005
Laurent Chapon (ISIS)
Magnetic diffraction: recent studies and future instrumentation at ISIS

12th May 2005
John Tranquada (Brookhaven National Laboratory, USA)
A universal magnetic excitation spectrum for cuprate superconductors

21st June 2005
C A Chatzidimitriou-Dreismann (Technical University Berlin, Germany)
Anomalous scattering of keV neutrons from H_2O, D_2O and their mixtures

24th June 2005
Dongfeng Chen (China Institute of Atomic Energy)
A new 60 MW research reactor for neutron scattering in CIAE

12th July 2005
Tom Griffin (ISIS)
Distributed Monte Carlo Instrument Simulations at ISIS

9th September 2005
Vadim Dudnikov (Brookhaven National Laboratory, USA)
Diagnostics for observation and damping of E-P instability

29th September 2005
Thomas Krist (HMI, Germany)
Neutron optics from HMI Berlin

4th October 2005
Brian Rainford (University of Southampton)
Anomalous ferromagnetism in CePdSb

18th October 2005
Paola Verrucchi (University of Florence, Italy)
Separability and quantum criticality in low-dimensional magnet systems

1st November 2005
Aziz Daoud-Aladine (ISIS)
Charge spin orbital ordering in manganites: novel insights from neutron diffraction

17th November 2005
Earl Babcock (ILL)
Polarizing ^3He for Neutrons and Fun

24th November 2005
Iain McKenzie (University of Stuttgart, Germany)
µSR of methyl and related radicals

28th November 2005
Aristides Mavridis (University of Athens, Greece)
Computational and interpretational problems of 3d-transition metal carbides MC, M=Sc,Ti,V, Cr, Mn, Fe, and Co

29th November 2005
Franz Demmel (ISIS)
Search for nanoclusters in liquid metals

13 December 2005
Matt Tucker (ISIS)
Studying disordered crystalline materials with total scattering

31st January 2006
Ann Terry (ISIS)
Use of synchrotron X-ray radiation to follow polymer crystallisation

14th February 2006
Cameron Neylon (University of Southampton and ISIS)
What is a molecular biologist doing in ISIS?

21st February 2005
Santiago Grigera (University of St Andrews)
Phase formation linked to quantum criticality in $Sr_3Ru_2O_7$

28th February 2005
Ted Forgan (University of Birmingham)
Experiments on vortex matter phase transitions in niobium

7th March 2005
David Manolopoulos (University of Oxford)
Quantum effects in molecular dynamics

14th March 2005
Arwel Hughes (ISIS)
Making models of membranes: neutron reflectivity from phospholipid bilayers

21 March 2006
Dario Stacchiola (MPI Berlin, Germany)
The role of surface hydrocarbon species during catalytic reactions

27th March 2006
Victor Efimov (ILL, France and Lancaster University)
Neutron scattering on impurity helium gel in superfluid helium

Tuesday 28th, March
Andrew Goodwin (University of Cambridge)
Exploiting powder diffraction with reverse Monte Carlo: excitations, modulations and some limitations

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
A Powell (Chair)	D Holland (Chair)	J Lawrence (Chair)	D Paul (Chair)	G Reiter (Chair)	A Harrison (Chair)	S Hainsworth (Chair)
R Angel	S Billinge	D Bucknall	S Bramwell	C Andreani	N Clayden	R Burguete
M Catti	L Cormier	P Doyle	R Coldea	F Cavatorta	J Davies	M Daymond
S Clarke	C Hardacre	R Felici	B Fak	R Ford	G Gehring	L Edwards
D Gregory	T Kanaya	J Goff	S Itoh	M Hayward	T Matsuzaki	M Preuss
W Harrison	P McMillan	P Griffiths	D McMorrow	M Johnson	P Mendels	R Tomlinson
P Hatton	K Refson	J Lu	K Prassides	E Karlsson	M Ricco	C Truman
T Koetzle	MA Ricci	F Mulder	A Schofield	D Lennon	R Scheuermann	
S Redfern	J Yarwood	P Olmsted	A Tennant	C Washington	J Stride	
J Rodriguez-Carvajal						
P Slater						
J Steed						
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*	*P King*	

ISIS Facility Access Panel Membership for the June 2006 meetings. The FAPs 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.

Chairman	S Kilcoyne	University of Salford
IUG1 Crystallography	P Battle R J Nelmes	University of Oxford University of Edinburgh
IUG2 Liquids & Amorphous	A Barnes D Holland N Skipper	University of Bristol University of Warwick University College London
IUG3 Large Scale Structures	R J Stewart R Thomas A Zarbaksh	University of Reading University of Oxford Queen Mary College London
IUG4 Excitations	D Mckenzie Paul A Boothroyd	Univesity of Warwick University of Oxford
IUG5 Molecular Spectroscopy	K Ross P Mitchell	University of Salford University of Reading
IUG6 Muons	T Lancaster S Kilcoyne	University of Oxford University of Leads
IUG7 Engineering	G Swallowe M Fitzpatrick	Loughborough University Open University

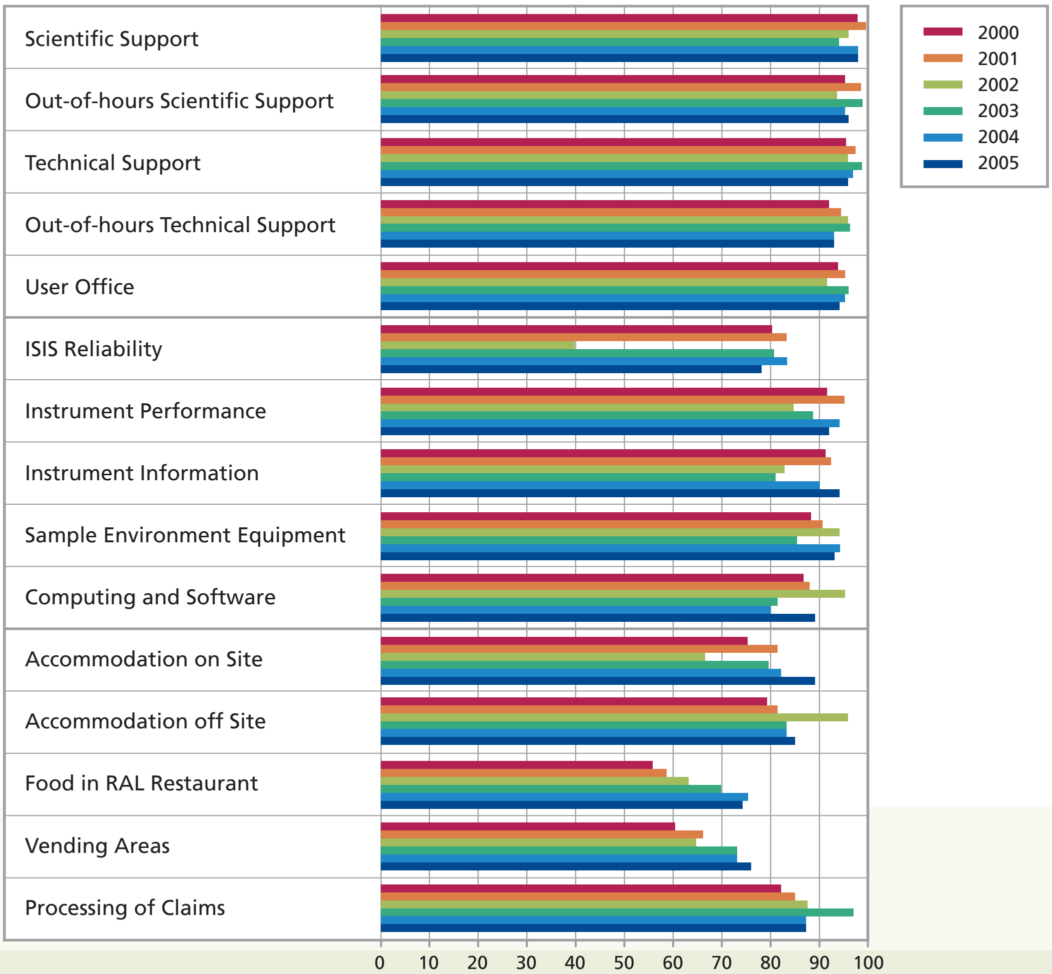
A D Taylor	Director ISIS
U Steigenberger	ISS Division Head
R Browning	ISIS User Programme Manager
R L McGreevy	IDM Division Head
Z A Bowden	ISIS User Support Group Leader

ISIS User Committee Membership. 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 2000 – 2005.



Beam Statistics 2005-2006

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 459 mA.hrs of user proton beam to the muon and neutron targets at an average current of 178 μA.

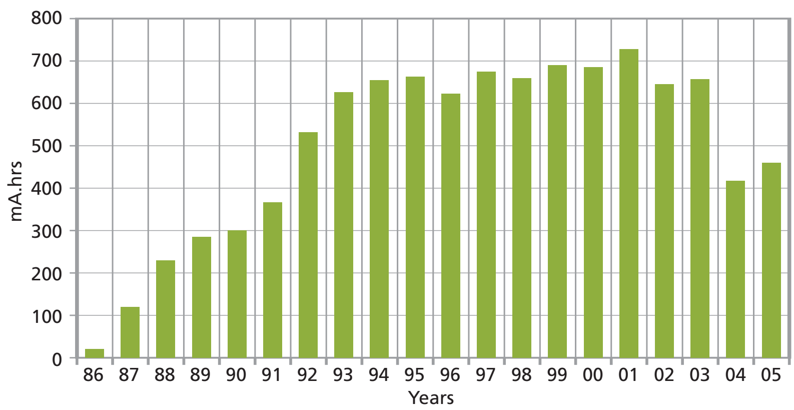
The tables below give beam statistics for the individual cycles in the year 2005-2006, together with year-on-year statistics for ISIS performance.

Cycle	05/1	05/2	05/3
Beam on target (hrs)	1066	735	778
Total beam current (mA.hr)	190	131	139
Average beam current for beam on target (μA)	178	178	178
Peak beam current (μA, average over 24 hrs)	179	185	181

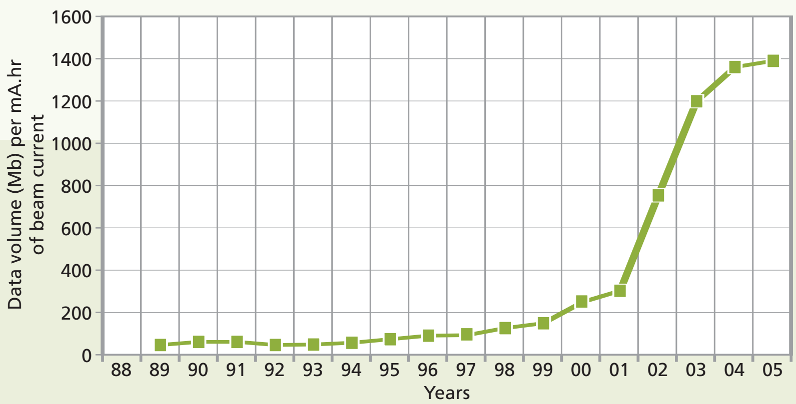
ISIS operational statistics for year 2005 - 2006.

Year	1998	1999	2000	2001	2002	2003	2004	2005
Total scheduled user time (days)	175	168	168	168	160	172	106	134
Total time on target (days)	160	153	154	158	148	154	96	107
Total integrated current (mA.hrs)	656	687	687	725	630	656	409	459
Average current on target (μA)	171	187	186	192	178	177	177	178
Peak current averaged over 24 hours	193	198	194	200	187	184	183	185
μA.hrs per trip	72	106	120	141	178	237	194	229

Year-on-year ISIS performance summary.



Average ISIS beam current per cycle.



As ISIS instrument performance has increased, the amount of data taken per mA.hr of proton current has risen sharply.

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