

ISIS 2003 Review of the Year



ISIS 2003 Review of the Year

Part of the ISIS Facility 2003 Annual Report

Review of the Year

was produced for ISIS,
CCLRC Rutherford Appleton Laboratory,
Chilton, DIDCOT,
OX11 0QX, UK

ISIS Director, Dr Andrew Taylor
01235 446681

ISIS User Office
01235 445592

ISIS Facility Web pages
<http://www.isis.rl.ac.uk>

October 2003

© Council for the Central Laboratory of
the Research Councils 2003

Enquiries about copyright, reproduction
and requests for additional copies of this
report should be addressed to:

CCLRC Library and Information Services,
Rutherford Appleton Laboratory, Chilton,
DIDCOT, OX11 0QX

email: library@rl.ac.uk

ISIS 2003 production team:

Philip King, Freddie Akeroyd,
John Thomason, David Clements,
Nigel Diaper, Katie Hopgood,
Spencer Howells.

Design and layout:
Ampersand Design Ltd, Ardington
01235 861444.

Printed by ???
and CCLRC Photographic and
Reprographic Services

Neither the Council nor the Laboratory
accept any responsibility for loss or
damage arising from the use of
information contained in any of their
reports or in any communication about
their tests or investigations.

ISIS 2003 Review of the Year

Review of the Year

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. This part of ISIS 2003 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 now-funded Second Target Station.

Contents

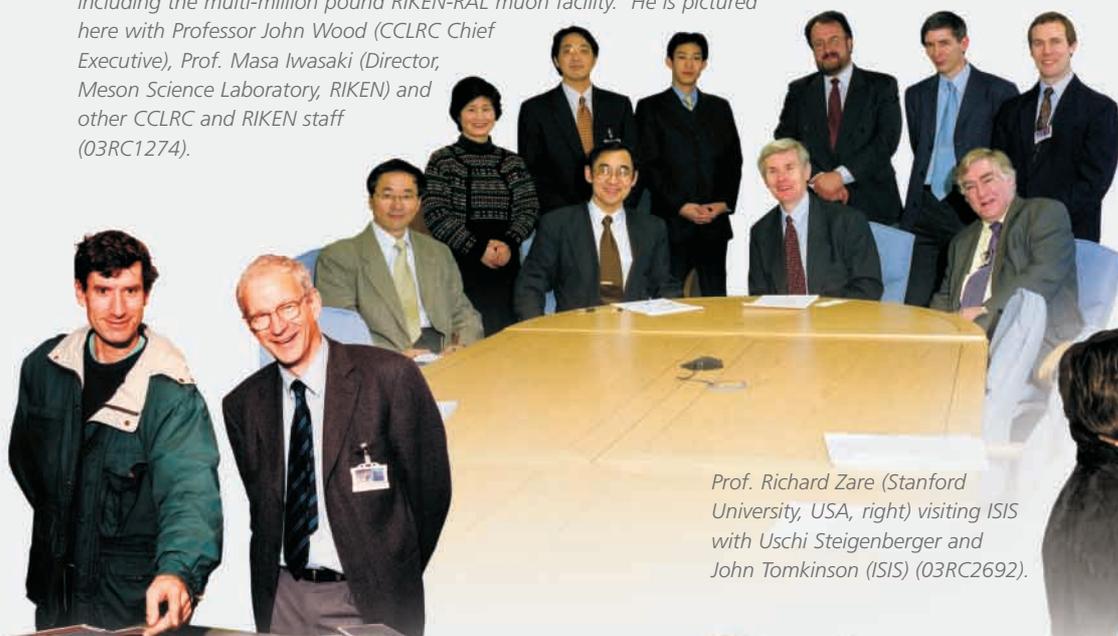
Foreword	3
Science Highlights	6
Advanced Materials and Engineering	6
Magnetism	8
Bio-molecular Materials and Soft Matter	10
Physics, Chemistry, Geology, Archaeology...a Broad Science Programme	12
Instrument Developments	16
Accelerator Developments	20
The Second Target Station	22
A year around the Facility	24
ISIS in Facts and Figures	28

Members of Parliament begin a tour of ISIS with John Wood (CCLRC Chief Executive), Bill David, Sean Langridge and John Webster (ISIS) (03RC1671).



Mr Masayasu Miyabayashi, Executive Director of the Japanese RIKEN Institute (centre left), visited the Laboratory in February. RIKEN has ongoing collaborations with ISIS in both neutron scattering and muon spectroscopy, including the multi-million pound RIKEN-RAL muon facility. He is pictured here with Professor John Wood (CCLRC Chief Executive), Prof. Masa Iwasaki (Director, Meson Science Laboratory, RIKEN) and other CCLRC and RIKEN staff (03RC1274).

Ray Orbach (Director, DoE, USA) and Todd Hanning (DoE) visiting ISIS with Andrew Taylor and Bill David (ISIS) (03RC1554).



Prof. Richard Zare (Stanford University, USA, right) visiting ISIS with Uschi Steigenberger and John Tomkinson (ISIS) (03RC2692).



Ralph Eichler, Director of PSI, Switzerland, touring ISIS with Bill Murray (Particle Physics Department) (02RC3823).



Members of the Scientific Advisory Committee (SAC), set up by Laboratory Chief Executive John Wood, visiting ISIS. The SAC advises the Chief Executive on current scientific and technical programmes and future research plans. It is chaired by Prof. Sir Peter Williams (far left) and includes (pictured here) Dominic Tildesley (Unilever), David Southwood (ESA), David Moncton (APS, Argonne), Alex Bradshaw (Max Planck Institute), Sune Svanberg (Lund Institute of Technology), Chris Llewellyn-Smith (Oxford), Keith Hodgson (SLAC) and Louise Johnson (Oxford), together with Francois Richard (Universite Paris-Sud) and John White (Australian National University). They are touring ISIS with Henry Hutchinson (Director, Central Laser Facility), and Bill David and Philip King (ISIS).

Foreword

The Earth moves at ISIS!

Without doubt, the highlight of the last twelve months has been the formal announcement of funding for the ISIS Second Target Station.

Together, the facility and user community have been working towards this goal for almost a decade. The announcement represents a critical milestone in the development of ISIS and a major achievement for all who have been involved. The announcement itself is not the end, nor even the beginning of the end – rather the end of the beginning! Since then, half a million tonnes of chalk have been removed to make way for the new target station building; after a very effective consultation process, seven priority instruments were selected by the Scientific Advisory Committee for the initial phase; and detailed costing of these instruments is now underway prior to the next hurdle – a Gateway Review in the late autumn.

Diamond construction is also making great progress. With first users expected at the new X-ray source in early in 2007, shortly before first neutrons on the Second Target Station, the RAL site is destined to become a major centre for condensed matter science. The Laboratory is further developing infrastructure to optimise the benefits of co-location for the effective delivery of science. The Research Complex project – led by the MRC – is the focus of considerable discussion and the present Science Networks have made a very positive start. These are promoting inter-facility activity and strengthening the scientific culture with the Laboratory by sponsoring productive and well-supported meetings, visiting scientists and other collaborative activities.

Compiling this report gives an opportunity to reflect on the substantial progress that the facility and community have made. In addition to the Second Target Station developments, the RFQ and dual harmonic upgrade to the source will produce benefits in terms of both reliability and performance within the next year. Instrument development remains one of our great strengths, and the new engineering instrument, ENGIN-X, was commissioned in January of this year and has



already demonstrated outstanding capability – perhaps ENGIN-X should be renamed ENGIN-XX!

Our primary output is, however, science and it is on the basis of the strength of scientific programme that the facility should be judged. As you read this report, I am sure that you will agree that the quality and increasing breadth of the science bears testament to the world-class stature of the ISIS facility and its user community.

My thanks to all who have contributed to yet another outstanding year!

Dr Andrew Taylor, ISIS Director

ISIS staff gather to hear the news that the Second Target Station has been funded (03RC1682).

A year around ISIS



Students from the University of Leiden visited ISIS in May (03RC1875).

Stewart Parker (ISIS) showing Oxford Particle Physics Masterclass students the TOSCA spectrometer (03RC1474).

Celebration of funding for the Second Target Station. Pete Surtell, Alan Stephens, Zoe Bowden and Dave Maxwell (ISIS) working out where it's going to be built (03RC2378).



Science teachers visiting the facility in November learning about how samples are mounted in ISIS cryostats (02RC3863).

Prof. Ken Nagamine (KEK), Paul Williams (former CCLRC Chief Executive) and Junko Nakai, pictured at a celebration in April at The Cosener's House. The event was held in recognition of the award to Paul Williams of the 'Minister's Commendation for Meritorious Service in the Field of International Exchange' by the Japanese Minister of Education, Culture, Sports, Science and Technology, and the award to Prof. Nagamine of the Toray Science and Engineering Prize by the Toray Science Foundation, Japan. Both awards are measures of the success of the RIKEN-RAL muon collaboration at ISIS (03RC1933).



ISIS Facility Access Panels

The ISIS Facility Access Panels (FAPs) are comprised of some 70 international experts. They meet twice per year over two days to review all beamtime proposals submitted to the facility.



Marco Zoppi (IFAC-CNR, Italy) in discussion with Roberto Trioli (Palermo, Italy) (03RC2127).



Bill Clegg (University of Newcastle Upon Tyne) during the Crystallography FAP meeting (03RC2140).



Brian Rainford (University of Southampton) and Sue Kilcoyne (University of Leeds) (03RC2137).



Paul Raithby (Bath) and Alberto Albinati (Milan, Italy) during proposal assessment (03RC2144).



Javier Bermejo (Bilbao, Spain) talking with Steve Bennington (ISIS) (03RC2134).



The Muon FAP at work. The panel consists of experts in muon science from six countries who review proposals based on scientific merit and timeliness, together with advisors from the facility (who do not take part in the reviewing process) (03RC2170).

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 scientific highlights; more detailed accounts can be found in the highlight article sheets accompanying ISIS 2003.

Advanced Materials and Engineering

Magnetic field distributions in thin-film superconductors

In a bulk superconductor in high fields, microscopic vortex currents induced deep inside the sample generate fields in the same direction as the applied field and create an ordered, periodic array of vortex lines. Future electronic devices could include superconductors with very small dimensions in which the flux structures can be very different from those found in bulk

material. Polarised neutron reflectometry is proving an effective method to investigate flux behaviour in thin-film superconductors with dimensions of order of the superconducting penetration depth. Variations in film thickness allow observation of a transition from a Meissner state, where flux is excluded, to a state where vortex lines form in the middle of the film. Such observations are useful for comparison with theoretical models, as well as providing input into studies of more complex systems such as superconducting-magnetic hybrid materials.

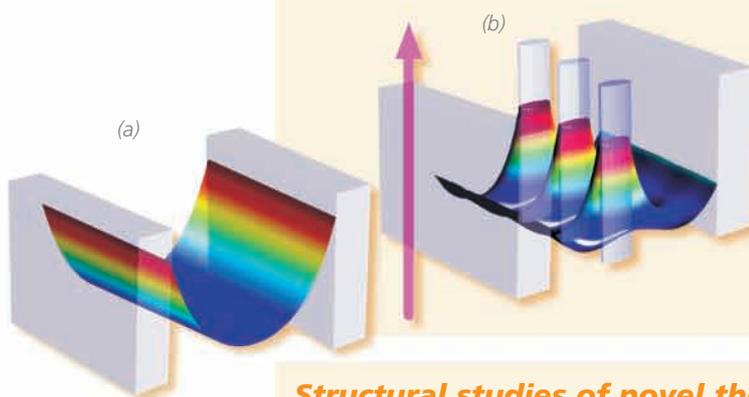


Fig. 1: The magnetic flux-density profile across a sample in the (a) Meissner state and (b) vortex state.

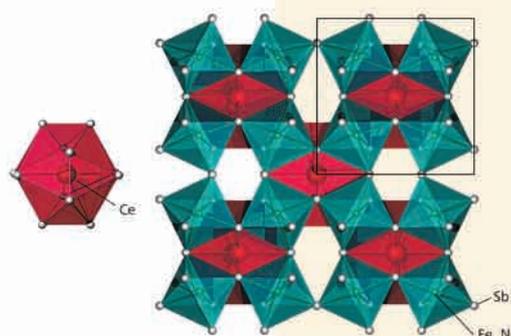
'Magnetic field distributions in thin film superconducting samples'

S.L. Lee et al, ISIS 2003 highlights.

Structural studies of novel thermoelectric materials

Thermoelectric materials presently find applications primarily in the high-technology market. Devices are reliable and environmentally-friendly, but suffer from poor efficiency, so there is interest in the exploration of potential new thermoelectric materials. An ideal thermoelectric should have the

vibrational modes interact with those of the lattice, reducing thermal conductivity. Filled skutterudites are one such class of material, and neutron diffraction is being used to study the vibrational motion of the guest atoms. In the case of partially-filled skutterudites, measurements of the guest atom displacement reveal a large residual contribution at low temperatures, and this positional disorder may be a factor in producing a lower thermal conductivity compared with the filled materials.



electronic transport properties of a heavily-doped semiconductor, but the thermal conductivity of a glass. These criteria can be met in compounds which have large voids in their structure that can be filled with atoms of a heavy element whose

Fig. 2: Crystal structure of a filled skutterudite type $\text{Ce}(\text{Fe}, \text{Ni})_4\text{Sb}_{12}$.

'Why are partially-filled skutterudites such promising thermoelectrics?'

L. Girard et al., ISIS 2003 highlights.

Modeling hydrogen behaviour in semiconductors

Hydrogen has a significant influence on the electronic properties of many semiconducting materials, and in the light of current attempts to develop new materials for electrical and optical devices, it is important to know in what capacity incorporated hydrogen will act. Direct spectroscopic study of hydrogen behaviour is difficult; however, investigations using positive muons as hydrogen mimics have been very successful in building up models of hydrogen states. For example, it has been found that muonium – a positive muon plus an electron, the equivalent of a hydrogen atom – forms a shallow donor state in InN at low temperatures. This is the first III-V compound in which muonium – and by analogy hydrogen – has been found to exhibit this behaviour, although similar states have also recently been found in some II-VI materials. Prior to these findings, hydrogen was always assumed to give rise to deep states, and these discoveries have implications for the suitability and doping of these materials for applications.

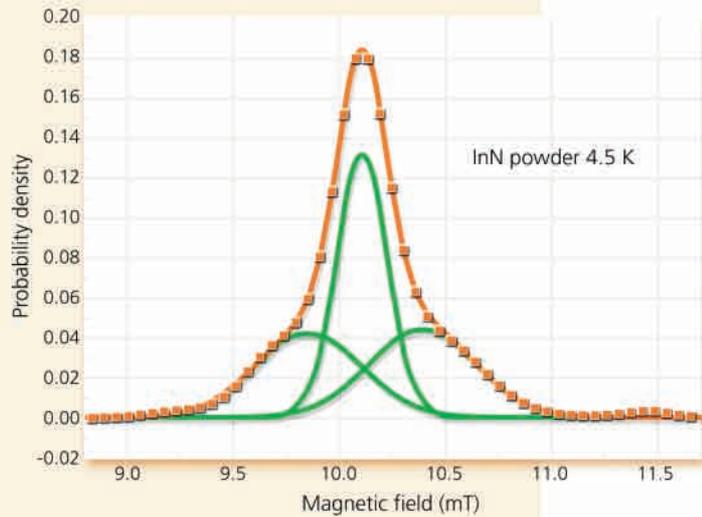


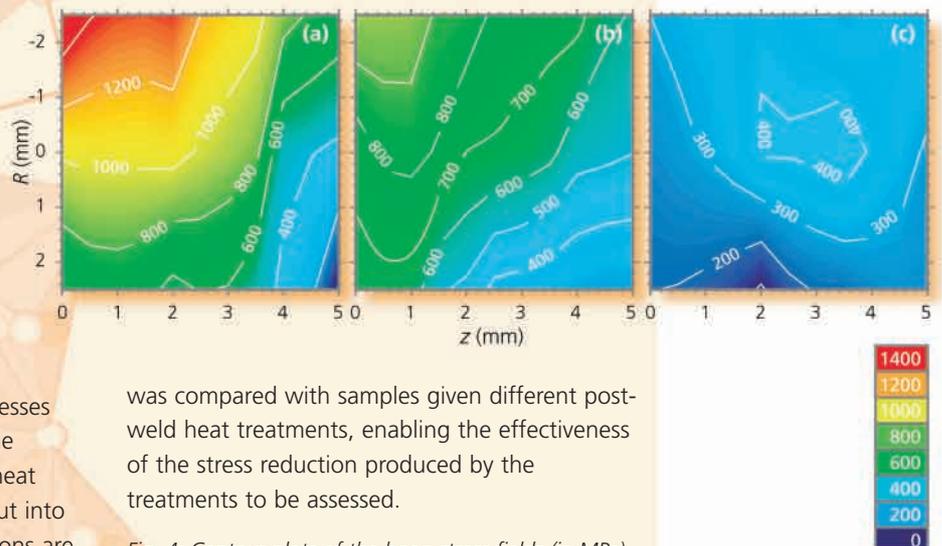
Fig. 3: Muon spectrum from InN at 4.5 K.

'Shallow or deep? Electronic states of hydrogen in indium nitride deduced from muonium experiments',

E.A. Davis et al., ISIS 2003 highlights.

Stress measurement in advanced engineering materials

In many advanced engineering applications the ability to weld components reliably, reproducibly and with high joint efficiencies is key. As materials improve, the challenges of welding become ever more demanding and, for the new generation of high performance, high temperature alloys, friction-based solid state welding techniques are fast becoming the industrial method of choice. It is important to characterise the residual stresses generated during friction welding and the degree of stress relief during post-weld heat treatment before such a component is put into commercial application. Such considerations are important for Rolls-Royce plc, who are planning to use friction welding in the very near future in their production processes. Measurements on the ENGIN diffractometer have been used to characterise stress distributions of friction welds in a nickel-based superalloy. As-welded material



was compared with samples given different post-weld heat treatments, enabling the effectiveness of the stress reduction produced by the treatments to be assessed.

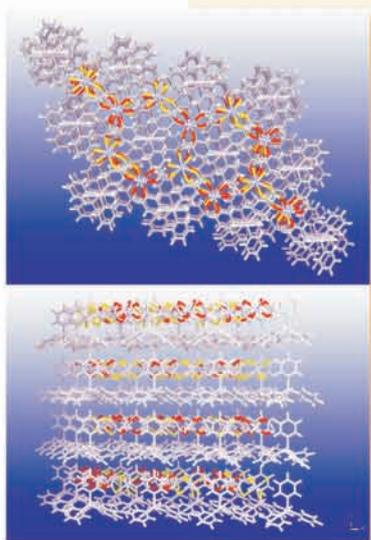
Fig. 4: Contour plots of the hoop stress fields (in MPa) in an inertia friction weld measured in the (a) as-welded, (b) conventional and (c) modified post-weld heat treated material.

'Residual stresses in inertia friction welded aeroengine materials',

M. Preuss et al., ISIS 2003 highlights.

Magnetism

Structural and magnetic studies of organic magnets



Magnets have been around for several millennia, but it is only in the last decade or so that chemists have begun to take a serious interest in synthesising magnetic materials from molecular building blocks in order to widen the spectrum of possible magnetic solids and, potentially, to incorporate other properties – to create, for example, a soluble magnet or one with a chiral crystal structure. Neutron diffraction has been applied

to compounds consisting of layers of metal ions bridged by oxalate or thio-oxalate anions, including measurement of inter- and intra-layer expansion coefficients, together with investigation of the nature of the (ferro)magnetic transition. A further set of organic charge transfer salts which show a ferrimagnetic transition have also been studied using neutrons and muons, the latter technique revealing an unexpected transition at low temperatures.

Fig. 5: Two views of the structure of the metal-organic magnet based on oxalate or thio-oxalate anions.

*'Neutrons and muons probe molecule-based metal-organic magnets',
P. Day et al., ISIS 2003 highlights.*

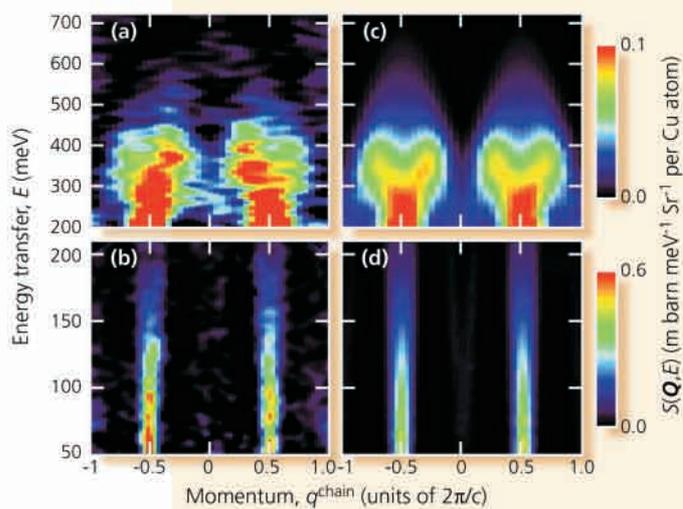
Investigation of fundamental magnetic system

Experimental exploration of model magnetic systems provide a basis for understanding more complex materials in which magnetism plays an important role, such as colossal magnetoresistive oxides or high temperature superconductors. As the dimensionality of a magnetic insulator and as the spin on the magnetic ions is reduced, quantum fluctuations become ever more important in the description of the magnetism.

When the interactions are only along a one-dimensional chain, quantum fluctuations destroy the long-range order that is otherwise expected when there is antiferromagnetic exchange between the ions. The most extreme case of this is when the ions have spin $S=1/2$, in which case the elementary excitations are spinons. SrCuO_2 is a good candidate material for investigating such spin excitations in a case where the magnetic interactions have similar energy to that required to excite a charge from one ion to another. The MAPS spectrometer is essential for such studies, which require measurement to high excitation energies. It has been shown that a model based on an antiferromagnetic chain reproduces the neutron data well even in this case where the charge and magnetic excitation energies are comparable.

Fig. 6: Maps of the scattering intensity in SrCuO_2 taken on MAPS with incident neutron energy (a) 848 meV, (b) 240 meV, with corresponding simulations in (c) and (d).

*'Spinons in strongly correlated copper oxide chain',
H. Woo et al., ISIS 2003 highlights.*



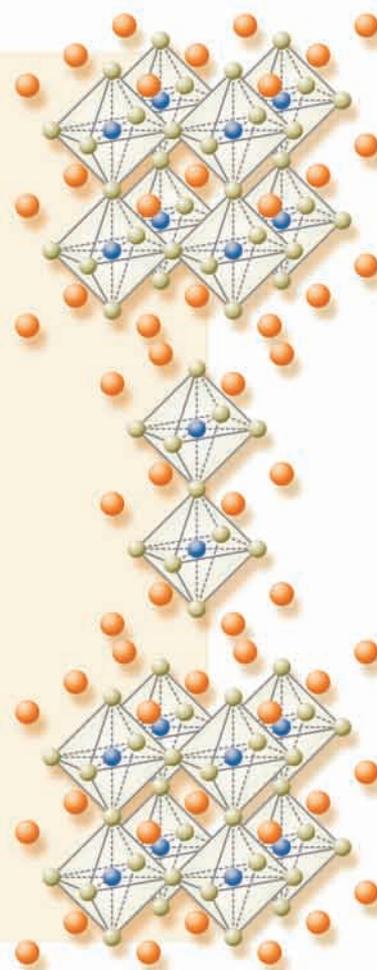
Exploring the phase diagram of colossal magnetoresistive perovskite

Magnetoresistance, the change of resistance following the application of a magnetic field, is usually an extremely small effect but in various manganese perovskites, the effect is so large that it has been termed 'colossal' magnetoresistance (CMR). The phenomenon has attracted attention both because of the possible sensor and device applications but also because the underlying physics appears intriguing. The properties of the bilayer manganese perovskites that exhibit CMR can be adjusted by chemical doping, producing a rich phase diagram. Neutron scattering has been used for their exploration, but additional muon information has also proved extremely useful in the $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ system for compositions where no long-range order was found using neutrons. In this case, muon results showed evidence for short-range order developing below T_f , the 'spin-freezing' temperature. Muon studies point to the spin freezing beginning with the formation of magnetic clusters at high

temperatures which grow as the temperature is reduced. The muon work thus provides evidence for magnetic order, phase separation and spin freezing, and has proved complementary to neutron studies of these materials.

Fig. 7: The structure of bilayer manganites.

'Spin freezing in a family of bilayer manganites',
A.I. Coldeira et al.,
ISIS 2003 highlights.



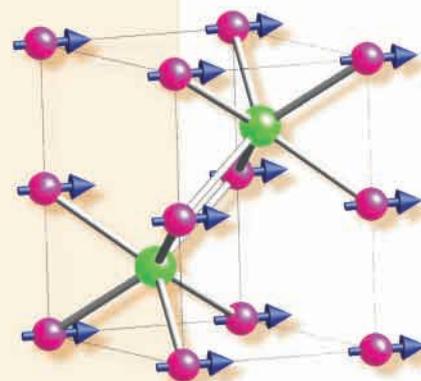
Structural studies of CMR materials

The discovery in the mid-1980s of high temperature superconductivity in perovskite cuprates, followed by the observation of colossal magnetoresistive effects in the manganites, has focused significant attention on these strongly correlated materials. Neutron diffraction studies of magnesium arsenide have now revealed the first coupled magnetoresistive / crystallographic transition induced by a magnetic field that involves the breaking of metal-metal bonds. MnAs is a ferromagnet with a Curie temperature of $T_c=313$ K. At T_c , a structural change also occurs from hexagonal to orthorhombic, along with a metal-like to insulator-like change in electrical transport. Neutron diffraction studies in the orthorhombic phase just above T_c have revealed a smooth transition back to the

hexagonal phase as a function of applied field, a transition involving the breaking of metal-metal bonds. The change is also accompanied by colossal magnetoresistance; that this occurs near room temperature may make MnAs attractive for device applications.

Fig. 8: The nuclear and magnetic structures of MnAs at low temperatures.

'Field-induced bond-breaking in MnAs',
T. Guidi et al., ISIS 2003 highlights.



Bio-molecular Materials and Soft Matter

Interfacial structure of biological proteins

In humans and other mammals the fluid that forms the interface between lung tissue and the atmosphere is an aqueous mixture of phospholipids, known as natural lung surfactant. The mesostructures formed by these lipids and their transport and interfacial properties are altered by surfactant-associated proteins and it is known that absence or mutation of one of these surfactant proteins, SP-B, leads to severe

respiratory problems. However, the mechanism by which SP-B operates remains speculative, and neutron and X-ray reflectometry have been used to investigate the structure of SP-B at the air-water interface together with its interaction with the dominant phospholipid with which it is commonly associated. The interfacial structure is modified as a function of surface pressure, with hysteresis effects being seen in mixtures with the phospholipid, and the results have enabled an initial model of the interfacial behaviour of the mixed system as a function of pressure to be generated.

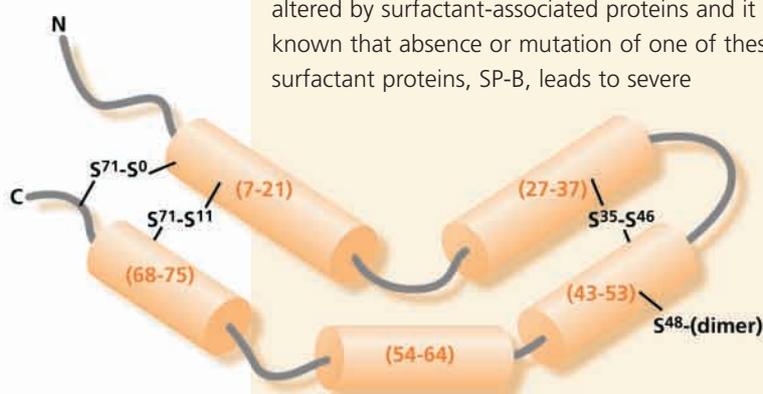


Fig. 9: Possible unfolded state of the SP-B protein at the air-water interface (barrels represent alpha helices).

*'Lung surfactant 'squeeze-out',
W.K. Fullagar et al., ISIS 2003 highlights.*

Microstructure of complex fluids

Many everyday household and personal care products are complex formulations which exhibit a rich behaviour. The processing and formulation of such products – which include fabric conditioners, shampoos and shower gels – are more controllable if their microstructure is understood. Small angle neutron scattering at ISIS has proved to be a valuable tool for investigation of such fluids, and results are now being applied to optimisation of processing

protocols. Specifically, many of these formulations are in the form of lamella phase dispersions and undergo structural phase transitions and changes in orientational order with shear flow. These lamella phase dispersions exhibit a liquid-like to semi-solid transition as a function of temperature, and this transition has a significant impact upon the in-use microstructure. SANS measurements during shear flow above and below the transition temperature of a di-chain cationic surfactant have enabled energy and time savings during in-production product processing.

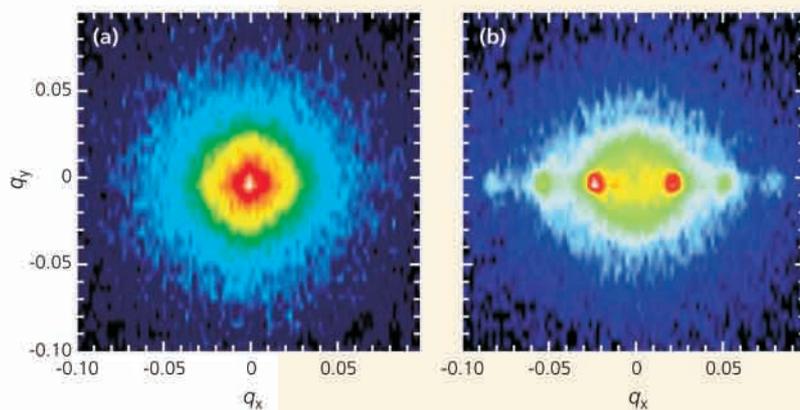


Fig. 10: SANS scattering patterns from the di-chain cationic surfactant di-octadecyl dimethyl ammonium chloride at 58 °C and 42 °C.

*'From small angle neutron scattering to the production line: optimising the industrial processing of personal care products',
I Tucker et al., ISIS 2003 highlights.*

Structural studies of adsorbed surfactants

Gemini surfactants are an interesting class of surfactant molecule with two hydrophilic tails connected to two or three hydrophobic heads. Their structure, together with their low critical micellar values, make them very efficient at reducing surface tension, leading to potential applications such as detergents and fabric softeners. Understanding their interface adsorption behaviour is important for future uses, and neutron reflectometry has been used to directly measure the adsorbed amount of a commonly-studied series of Gemini surfactants at the air-water interface. The unusual adsorption behaviour observed has implications for the structure of the adsorbed surfactant layer. Further neutron measurements using deuterium labelling for different molecule fragments have revealed structural features not normally observed in simpler surfactants at low concentrations that are manifestations of the unique properties of this surfactant class.

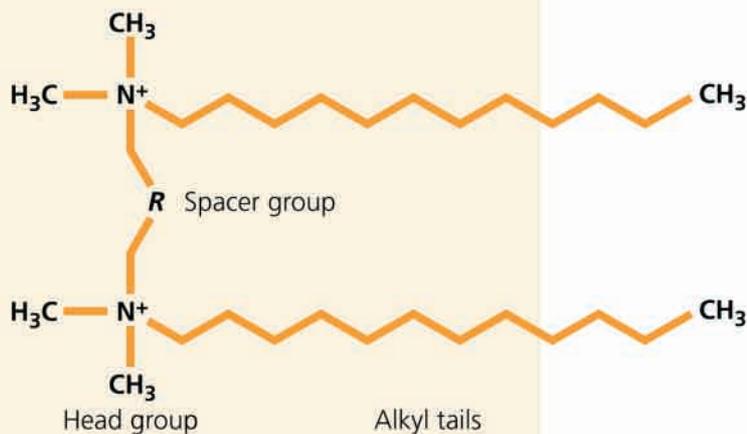


Fig. 11: General structure of $C_nC_mC_n$ Gemini surfactants.

'Unusual surface structure in cationic Gemini surfactants',
R.K. Thomas et al., ISIS 2003 highlights.

Behaviour of complex polymer systems

When polymers, surfactants and cyclic sugars in solution interact, the polymer chain structure changes dramatically as the polymer is snared by the guest molecules. Small-angle neutron scattering (SANS) has revealed the detailed structural rearrangements that occur in two systems – a star polymer and a polymer that has been tethered to a surface – which find applications in drug delivery and personal care products. In the former case, where several polymer arms are attached to a central entity, NMR measurements can divulge the effects of surfactant addition on the size of the complex. However, SANS measurements are necessary to reveal information on the complex shape and have enabled detailed models of star polymer-surfactant complexes to be developed. Inclusion complexes are remarkable structures caused by cyclic sugar molecules spontaneously threading

themselves on to polymer chains. They may appear as a grafted layer, and SANS measurements have revealed the effects on polymer chain behaviour as a function of sugar concentration.

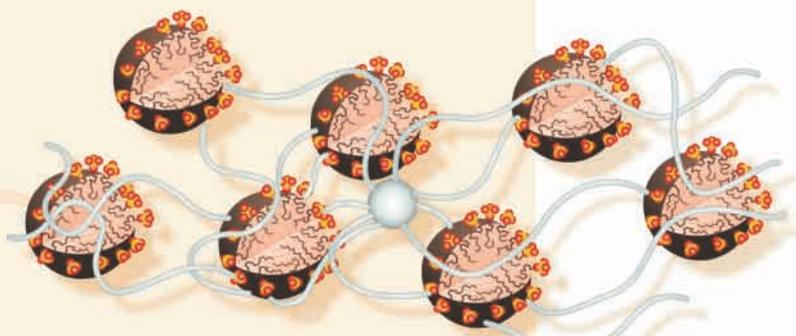


Fig. 12: Schematic of PEO star polymer saturated with surfactant micelles.

'Snared polymer chains',
T. Cosgrove et al., ISIS 2003 highlights.

Physics, Chemistry, Geology, Archaeology – a Broad

High pressure studies of amorphous ice

Although water is ubiquitous in our every-day lives, many interesting questions remain about its structure as a function of temperature and pressure. For example, there is a proposal that there are two distinct forms of supercooled water which themselves are experimentally inaccessible, but which have glassy analogues in the forms of ice known as high-density and low-density amorphous (HDA and LDA respectively) ice. HDA

is formed at pressures above 1.1 GPa below 100 K, and neutrons have been used to probe its structure under in-situ conditions for the first time, using the Paris-Edinburgh pressure cell. Spatial distribution functions of the oxygen atoms reveal the effects of pressure on the first and second co-ordination shells of water molecules around a central molecule. There are strong co-ordination changes with pressure, and at 2 GPa it is found that HDA shares structural similarities with high-pressure forms of crystalline ice. This provides important information on how the amorphous and crystalline phases are related and demonstrates the value of in-situ investigations.

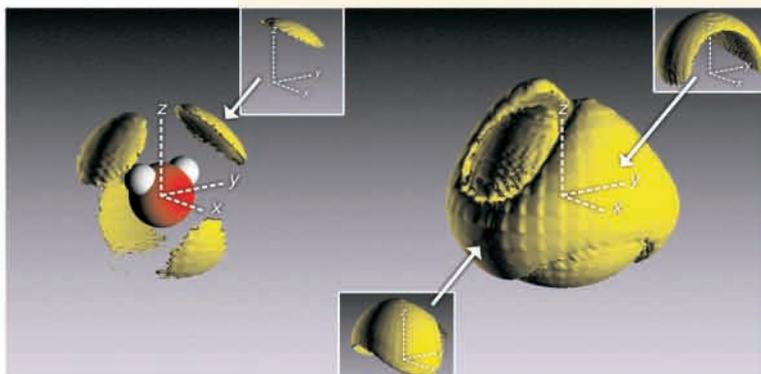


Fig. 13: Spatial distribution function of oxygen atoms at 2.0 GPa for first (left) and second (right) coordination shells in high density amorphous ice.

*'The structure of high density amorphous ice at high pressure',
S. Klotz et al., ISIS 2003 highlights.*

Non-destructive testing of archaeological materials

Neutron diffraction can be used to characterise archaeological artefacts and museum objects. The phase and microstructural information obtained – without damaging an object of value – can help answer questions of authenticity, as recent investigations of 16th-century silver/copper coins and an obviously repaired 7th-century BC

Greek bronze helmet show. In the former case, six coins were examined using neutron diffraction to distinguish between those that were minted (genuine) and those that were cast (fake).

Consideration of the metal composition of the coins and maps of grain orientation distributions corroborated suspicions that only three of the six were original. Neutron diffraction data were also collected from a 7th-century BC Greek helmet in order to examine whether the nose-guard was original or a later add-on. Composition measurements reveal a different bronze composition of the nose-guard compared with the rest of the helmet, suggesting the nose-guard was not part of the original structure.

Fig. 14: Corinthian-type bronze helmet being put into position on the ROTAX instrument by Roy Garner from The Manchester Museum.

*'Genuine or fake? Neutron diffraction for non-destructive testing of museum objects',
W. Kockelmann et al., ISIS 2003 highlights.*



Science Programme

Neutron diffraction and high performance computing probe the Earth's core

Surprisingly little is known about the Earth's deep interior. Although the Earth's core may seem not seem relevant to our daily lives, the fluid outer core is responsible for generation of the Earth's magnetic field which shields us from harmful solar radiation. One of the driving forces behind this geodynamo is the heat released during crystallisation as the inner core grows and solidifies. Whilst the inner core is primarily composed of iron, density measurements point to lighter alloying elements also being present, and it has been suggested that cementite, Fe_3C , is a possible core constituent. To test this hypothesis, neutron powder diffraction has been used to measure cementite's thermal expansion coefficient. Additionally, high-performance computing methods have been used to investigate the effect of pressure on the properties of Fe_3C . Both studies suggest that Fe_3C cannot be a major core-forming phase; further measurements of cementite's thermo-elastic properties are being carried out to validate this conclusion further.

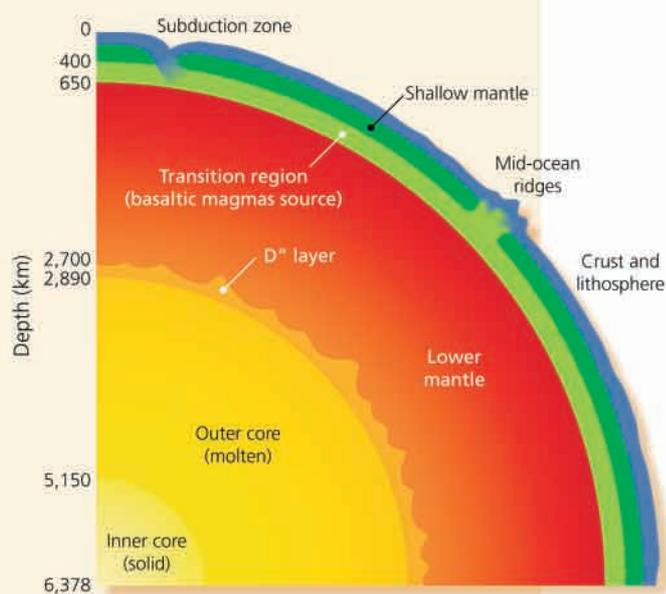


Fig. 15: Cut-away of the Earth.

'The equation of state of Fe_3C – the carbon in the Earth's core?'

L. Vočadlo et al., ISIS 2003 highlights.

Observation of phonon modes during zeolite collapse

Zeolites are microporous aluminosilicates which can be envisaged as being formed from SiO_4 and AlO_4 tetrahedra. The amorphisation of these low-density crystalline materials results from the excitation of low energy phonon excitations known as 'floppy' modes which leave the structure susceptible to shear deformations. Inelastic neutron scattering has been used to reveal floppy modes during the amorphisation process for the first time. Results show low energy phonons that are not present in the starting zeolite or the final glass state, but which appear as a function of pressure during the collapse of the zeolite cage, revealing floppy modes and suggesting that similar behaviour might be expected in other microporous materials when they are compressively amorphised.

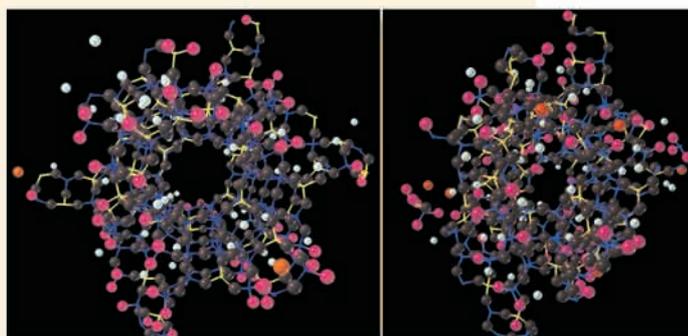


Fig. 16: Zeolite supercage structure (left) before amorphisation and (right) after collapse.

'Direct observation of floppy modes generated during zeolite amorphisation'

G.N. Greaves et al., ISIS 2003 highlights.



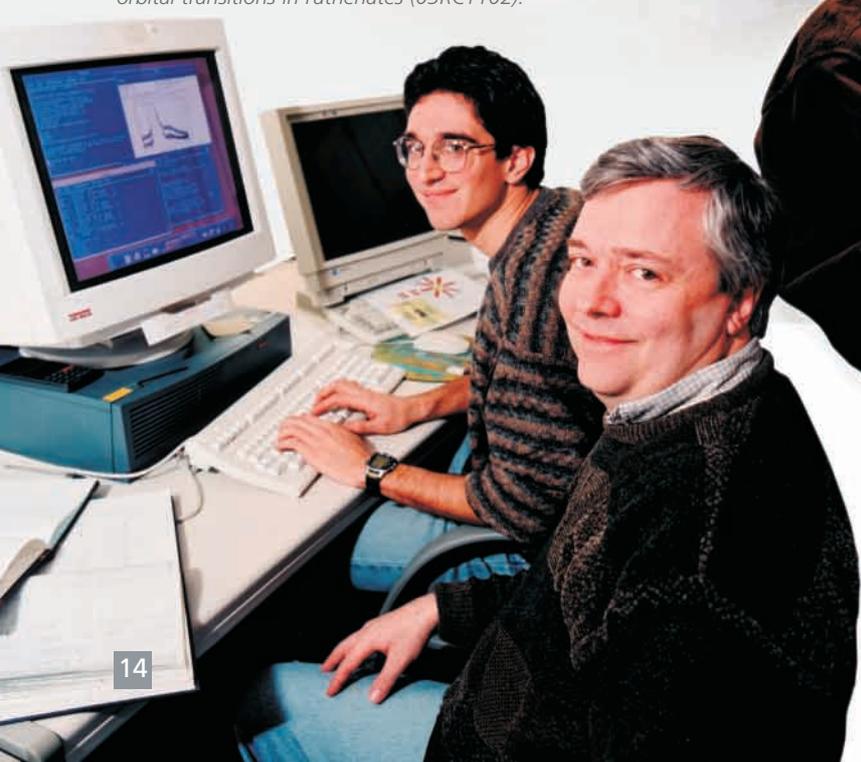
Lorna Dougan (University of Edinburgh) analysing her methanol in water data from SANDALS (02RC3919).

Don Fleming (University of British Columbia, Canada) by the muon beamlines during his radio-frequency μ SR investigations of noble gases (03RC2502).



David Scott and Darren Gowers (University of Bristol) with Richard Heenan (ISIS) during studies of biological enzymes on LOQ (02RC3922).

Ray Osborn (Argonne National Laboratory, USA) and Peter Khalifah (Oak Ridge, USA) during their investigation of orbital transitions in ruthenates (03RC1102).



Wilfred Fullagar (University of Queensland, Australia) analysing his CRISP data from synthetic peptides used to model surfactant protein behaviour (02RC3925).



Dave Pickup (University of Kent) checking his sample of Ti-silica sol-gels for GEM experiments (03RC1110).



David Narehood (Pennsylvania State University, USA) using MARI for investigations of H₂ in activated carbon (03RC2442).

Maria Ariza-Camacho (Montpellier, France) using muons to study ionic conduction in Li-based battery electrode materials (02RC3890).



Karen Edler (University of Bath) and Arach Goldar (CEA-Saclay, France) exploring polyelectrolyte-surfactant solutions on SURF (03RC2518).



Anne-Katrin Klehe (University of Oxford) using SXD to explore the structure of an organic superconductor under pressure at low temperatures (03RC1119).

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 improvements over the past year are described here.

ENGIN-X

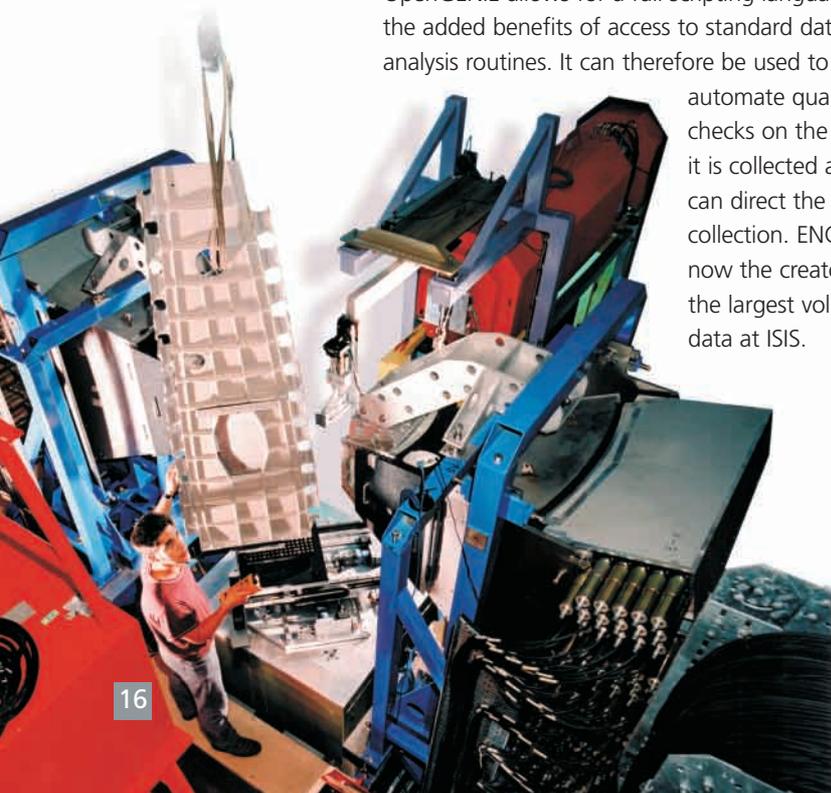
The Engineering user programme was transferred this year on to ENGIN-X, the new ISIS time of flight neutron diffractometer optimised for engineering measurements. After technical commissioning the scientific programme on the instrument has begun, and the anticipated order of magnitude improvement over the old ENGIN instrument has been demonstrated.

The new ENGIN-X detectors are fibre coupled ZnS⁶Li scintillators covering 1.4 m² and composed of 2400 individual detector elements. The scintillator arrangement is based on a 'Venetian' geometry specifically developed for this instrument, with individual elements having 3 mm spatial resolution, significantly higher than previously achieved.

ENGIN-X is the first ISIS instrument to have all its data acquisition and device control performed by Windows PCs. The new system uses a combination of Labview, for the control of individual devices, and OpenGENIE (the ISIS in-house data analysis and visualisation package) for data acquisition control. OpenGENIE allows for a full scripting language with the added benefits of access to standard data analysis routines. It can therefore be used

to automate quality checks on the data as it is collected and so can direct the data collection. ENGIN-X is now the creator of the largest volume of data at ISIS.

Fig. 17: Preparations for a collaborative ENGIN-X experiment between The Open University, Airbus UK and ISIS, aimed at optimising the fabrication of large aluminium alloy wing components. A wing-box typical of that which may be used on the very large aircraft presently under development is being loaded on to the instrument (03RC1746).



OSIRIS

OSIRIS is now able to operate as a quasi/inelastic neutron scattering spectrometer and/or a high-resolution neutron diffractometer. Development of spectroscopy on the instrument over the last 6 months has been an involved process, but first QENS results from the instrument were submitted for publication in February. In addition, the installation of magnetically-insensitive ³He detectors for spectroscopy now enables use of high magnetic fields, and a highly successful investigation of quantum magnetism has been performed involving 70 mK temperatures and fields in excess of 7 T.

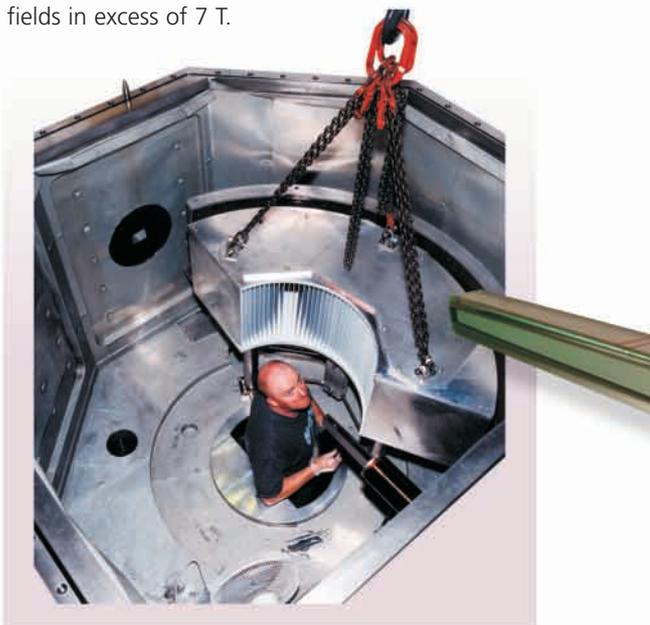


Fig. 18: Dave Maxwell (ISIS) oversees installation of the new OSIRIS collimator (02RC3294).

Effort is now being focused on further improving the sensitivity of the spectrometer by cooling the graphite analyser bank close to liquid helium temperatures. This will not only reduce the effect of thermal diffuse scattering but also significantly improve the signal to noise ratio of the spectrometer. Installation of the cooling circuit will commence in August 2003.

PRISMA

During the year PRISMA has undergone a major revamp of its secondary spectrometer. The aim of this work was to improve both reliability of operation and ease of use. One of the major problems with PRISMA in the past has been the poor reproducibility in the positioning of its analysers, so that it has been difficult to perform reliable energy scans. Now all the motors and encoders have now been replaced and the first experiments successfully completed. In a second project, the detector banks were attached to a concentric rail system, enabling the switch between diffraction and spectroscopy options to take a few minutes rather than a whole day.

SXD

The second stage of the major project to upgrade the SXD instrument, to add to the initial provision of a 2π sr solid angle detector array by improving the beamline optics, has essentially been completed. This has involved incorporation of both collimation and focusing options along with laser-assisted sample alignment (of particular benefit for the study of small samples). Initial commissioning of the 400 mm-long 2D supermirror focusing device ('trumpet') has been very promising, indicating substantial flux gains at longer wavelengths.



Fig. 19: The new SXD supermirror focusing 'trumpet' (03EC2743, 03EC2745).

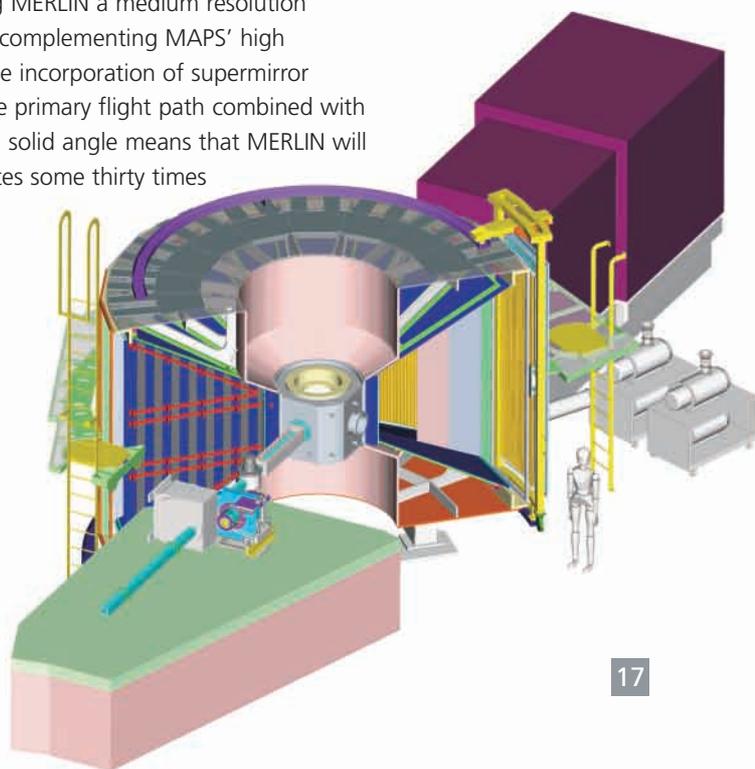
GEM

The GEM user programme is operating in parallel with further installation and commissioning on the instrument; for example, detectors for the remaining EPSRC-funded low angle banks are being installed on a continuous basis. The 90° detector bank, with its low background, excellent resolution and superb count rate, has proved to be very successful for both crystallographic and disordered materials experiments alike. The oscillating radial collimator has been installed and offers dramatic reductions in background levels (by as much as a factor 1000). In addition, the incident beam scraper immediately before the sample is now fully automated, allowing the incident beam dimensions to be altered easily and remotely. The RIKEN/JREI funded cryomagnet has been tested on the instrument and promises to enhance this important component of the programme.

MERLIN

MERLIN is now under construction and is on-target for completion in 2005. It will be a high count rate, medium energy resolution, direct geometry chopper spectrometer, with a very large solid angle of detectors covering nearly 180° in the horizontal plane and $\pm 30^\circ$ in the vertical plane. All the detectors will be position-sensitive, similar to those on MAPS, making it ideal for studies of single crystals. To achieve such a large solid angle the sample-to-detector distance is relatively small at 2.5 m, making MERLIN a medium resolution spectrometer, complementing MAPS' high resolution. The incorporation of supermirror guides into the primary flight path combined with the increase in solid angle means that MERLIN will have count rates some thirty times those of HET.

Fig. 20: Cutaway diagram of the MERLIN vacuum tank. The detectors are three meter long ^3He tubes mounted inside the vacuum.



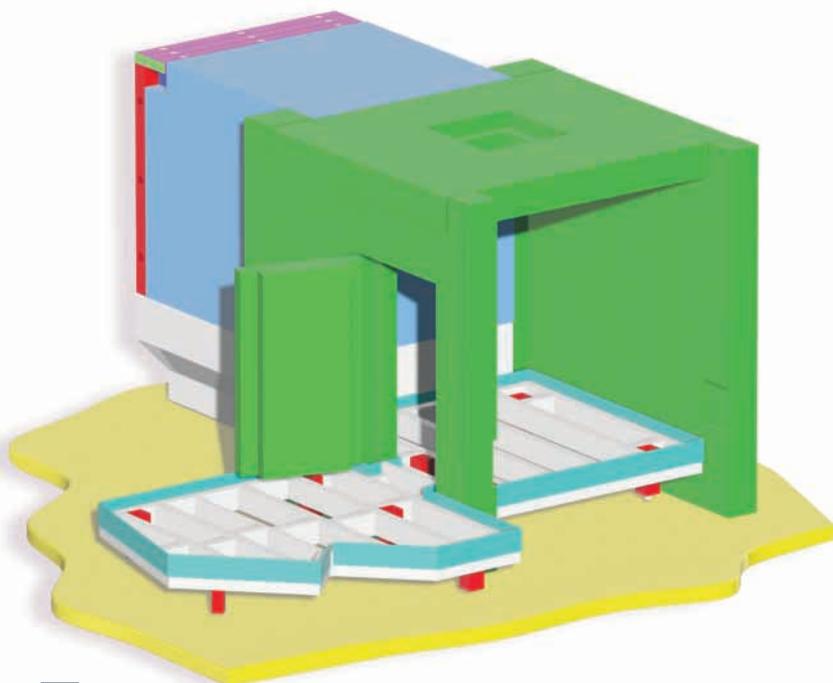
eVERDI

The eVERDI project is a collaboration between ISIS and the universities of Rome, Milan and Kent, aimed at developing a very low angle scattering capability for VESUVIO, so that low momentum transfers ($1 < q < 10 \text{ \AA}^{-1}$) and high energy transfers ($1 < \omega < 5 \text{ eV}$) can be accessed. It is hoped that this will enable the first study of very high energy magnetic excitations. The University of Milan are developing new detectors, based on the resonance detector technique, and early results are very encouraging. eVERDI will also improve the VESUVIO detection system for studies of protons, and the first new detector module, based on the current VESUVIO forward scattering detectors, has been designed.

INES

INES is a new instrument that is being funded by CNR (Italy). The instrument will be located on a beamline beyond TOSCA at 22 m from the moderator. The aim is to provide a highly flexible working environment that will allow investigation of novel scattering geometries and methods. The basic design is a medium resolution powder diffractometer but the detectors will be a moveable array that will enable some flexibility in their configuration. The instrument will also be used for training in neutron scattering, and first neutrons are expected in winter 2004.

Fig. 21: Initial designs for the INES instrument blockhouse.



Muons

The three EC muon instruments have seen a variety of developments over the past year, focused in particular on sample environment facilities. A liquid de-gassing rig is now available for direct loading of liquid samples into a flow cryostat, and new gas-handling facilities enable gas phase measurements at pressures up to 50 bar. Both gas and liquid samples have been studied with the radio-frequency (RF) μ SR technique this year. RF- μ SR is now being used by a range of user groups across a wide variety of science areas and an ongoing, EPSRC-funded project is aimed at developing the technique further.

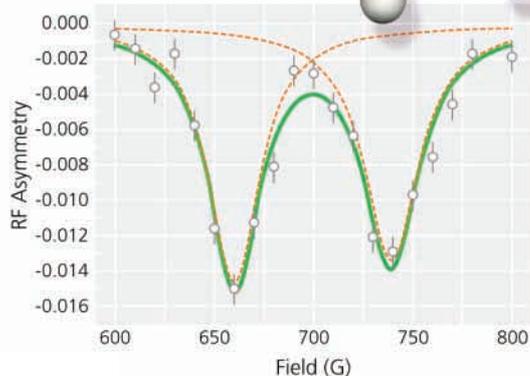
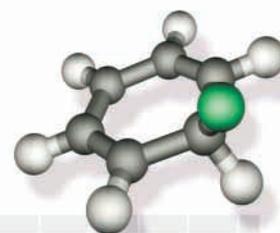


Fig. 22: The cyclohexadienyl muonic radical resonance signal obtained by RF- μ SR. The signal could only be obtained by de-gassing the sample to remove dissolved oxygen. Inset: model of the radical state with the muon in green.

Autumn 2003 will see the first laser-excitation μ SR experiments at ISIS, including investigation of the motion of induced charge carriers in conducting polymers and of the reactivity of muonium (and hence hydrogen) with water molecules in a vibrationally excited state. Finally, by the time next year's annual report appears, the MuSR instrument will have been equipped with twice its present complement of detectors, a relatively simple but very effective project to enable a doubling of the instrument count rate.

High pressure

The development of the ISIS high pressure programme is still largely carried out on the HiPr high pressure instrument on the PEARL beamline exploiting the Paris-Edinburgh (P-E) cell. The most recent major development of this system, the Cambridge/NERC-funded internal heating system for the cell, offers a convenient way of carrying out high temperature/high pressure experiments to 1500 K and 25 GPa. The HiPr instrument itself is also being improved, including an automated pressure control system for the P-E cell and a major upgrade to the front-end collimation.

Further sample environment developments

SXD experiments now benefit from a unique piece of sample environment equipment allowing the in-situ re-orientation of crystal samples at cryogenic temperatures within a vacuum environment. The new crystallographic goniometer provides both a zero to 45° angular change of sample orientation at 20 K, as well as crystal centre rotation about a fixed point in space.

A group from KCL led by Carolyn Koh, in collaboration with Alan Soper from ISIS, have had a long-standing interest in methane hydrates, and recently a rig has been developed which promotes the absorption of methane by water. Methane hydrate consists of hydrogen-bonded water molecules which form cage-like structures in which are trapped significant amounts of methane. Its preparation involves a complex off-line apparatus which vigorously agitates a water-filled sample preparation cell to which a pressure of up to 18 MPa of deuterated methane is applied whilst being held at a controlled temperature of ~18 °C. The apparatus then allows transfer of the methane-water system into a special cell for study on SANDALS.

Further sample environment developments include a major initiative on reactive chemistry to enable in-situ studies of materials as they are formed or of reaction intermediates. There has been a rapid growth in the development of such in-situ apparatus at ISIS over recent years,

Fig. 23:
Gwenaëlle Rouse
(Universite P et M
Curie, Paris) with the
Paris-Edinburgh
pressure cell
(02RC3901).

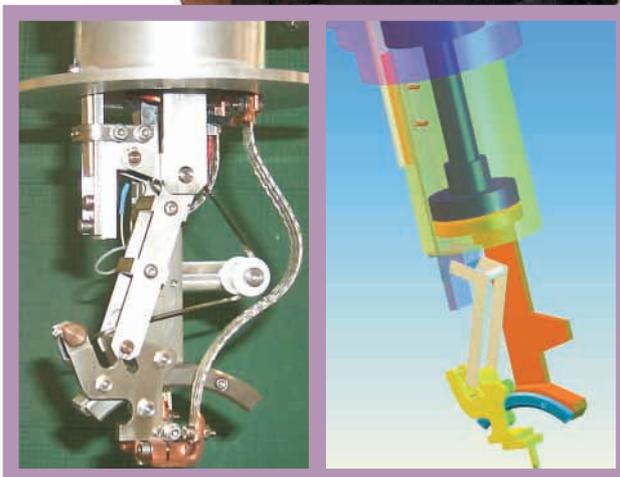


Fig. 24:
The SXD crystallographic
goniometer and its
CAD
representation.

including provision of the RI catalytic cell, the Oxford-ISIS hydrothermal cell and the ISIS reaction cell. Recent initiatives have seen delivery of an in-situ conductivity rig and construction of an electrochemical cell.

Accelerator and Target Developments

The Accelerator and Target Divisions have continued to maintain the high reliability of the ISIS neutron source during the past year. Much of the focus of development activity has been on the 300 μA accelerator upgrade, a vital part of the preparations for the ISIS Second Target Station.

ISIS Injector

Part of the 300 μA upgrade programme includes replacing the present Cockcroft-Walton pre-injector with a 665 keV, 202.5 MHz, radio-frequency quadrupole (RFQ) accelerator. This requires full testing of the new RFQ system, and an experimental programme to put the new accelerator through its paces has been completed ready for its installation in the long shutdown in 2004.

Development of the world-class ISIS H^- ion source has begun in earnest, both to meet future ISIS requirements and to increase performance towards specifications for next generation high power proton accelerators. A programme of measurements on the ion source development rig and extensive computer modelling are yielding encouraging results.

Fig. 25:
Mark Whitehead
operating the ISIS ion
source development rig.



Synchrotron accelerator

The 300 μA upgrade requires insertion of four new RF accelerating cavities into the synchrotron ring. Two of these cavities were installed during the 2002 shutdown, and in early 2003 two high power drives (HPD) were installed, together with electrical and mechanical services. Commissioning of these two complete systems is now underway. A further two cavities, two HPDs and services are planned for installation during 2004.



Fig. 26: A second harmonic cavity and high power drive installed in Super-period 6 of the ISIS synchrotron.

A prototype upgraded, high voltage kicker power supply system (for kicking the accelerated proton beam from the synchrotron to the neutron and muon targets) is about to be commissioned. Successful completion of these tests and the building and installation of six systems (there are three extraction kicker magnets, each with two drives) will be another step towards the ISIS 300 μA upgrade.

Neutron and Muon Targets

Plans for the 300 μA upgrade also concern the neutron and muon production targets. The cooling system on the latter will be inadequate for the increased ISIS current, so a new target has been designed and will be ready for installation in 2004. Similarly, the neutron target reflector will also need replacing, and this will also be ready for the long 2004 shutdown.

Recent target development work has also included complete redesign of the controls for the hydrogen and methane moderators, and design of replacement controls for the target ventilation systems.

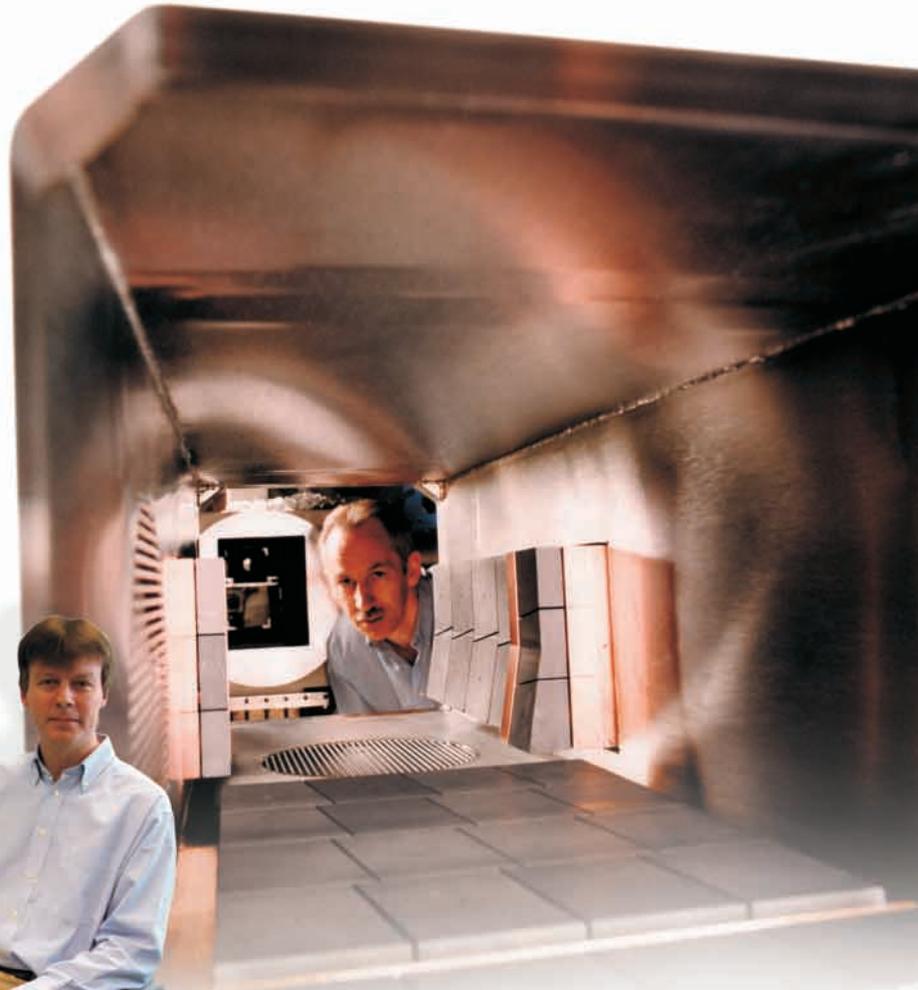
Fig. 27: Clive Lambourne of the Controls Group with the compact PCI system intended to replace the present STEbus system.



Control systems

The ISIS control system has continued its record as one of the most reliable parts of the accelerator. Further work to provide monitoring of the new collectors has completed the controls part of the straight 1 replacement project in the synchrotron. Much effort is being put into the controls and monitoring for the second harmonic RF project, and on the preparation for the installation of the RFQ.

The Controls Group has started major developments on a new compact PCI-based front-end i/o system and analogue waveform switching system – essential for long term operation. This requires new skills, upgraded CAE tools and a move to more outsourcing and better production methods.



Future Projects – the Ion Beams Group

Studies of solid targets for a proposed neutrino factory have concentrated on the problems of material strength and fatigue associated with the thermal shock wave induced by repeated proton pulses. Calculations have shown that intense high power electron beams can simulate the conditions, and experiments using tantalum have been performed in a commercial welding facility with encouraging results. A 40 kW electron beam was used to deliver fast pulses of energy at a density comparable to that expected at the neutrino factory, demonstrating that material lifetimes of at least a million cycles are possible. The group has also been working on the Muon Ionisation Cooling Experiment (MICE), a technology demonstration experiment which has been proposed to be based at ISIS.

Fig. 28: Mike Krendler of the Operations and Installations Group inspects the collectors for the Straight 1 replacement (02RC2104).

The Second Target Station

8th April 2003 was an important date for the development of ISIS, when formal approval for the construction of a Second Target Station was announced in a press release from the UK Minister for Science and Innovation, Lord Sainsbury. This major new investment (£100M) will greatly extend the capability and capacity of the facility.

The Second Target Station will be optimised for the production of cold neutrons, providing exciting new opportunities in the key areas of Soft Matter, Bio-materials, Advanced Materials and Nanotechnology. Taking one in five pulse from the ISIS synchrotron, the lower proton power (48 kW) and low repetition rate (10 Hz) will enable the use of a compact, well-coupled target, moderator, and

reflector assembly for the efficient production of long wavelength neutrons with a particularly broad range of simultaneously usable wavelengths.

The project is now well underway, and important progress is being made on all fronts, led by the Project Sponsor, Tim Broome, the Project Manager, Harry Jones, and the Project Scientist, Jeff Penfold. Work on site preparation, which involves moving some 300,000 m³ of the existing chalk mounds to make way for the new experimental hall, has started. Following Local Authority planning approval in March, the contract for the major earth moving was awarded to VHE Construction and commenced on the 1st July.

The design and build contract for the new support building to accommodate workshops, offices, assembly areas and mess facilities displaced by the construction of the Second Target Station, will go out to tender in August, for completion towards the end of 2004. The specification for the new experimental hall will be completed this summer, and will go to tender for design in late September. Construction should then start in early 2004.

A small international workshop was held at RAL in February to discuss the status of the neutronic calculations for the proposed target / moderator / reflector assembly. Experts from the

Fig. 29:

The Second Target Station (dark blue building) alongside the existing facility buildings.

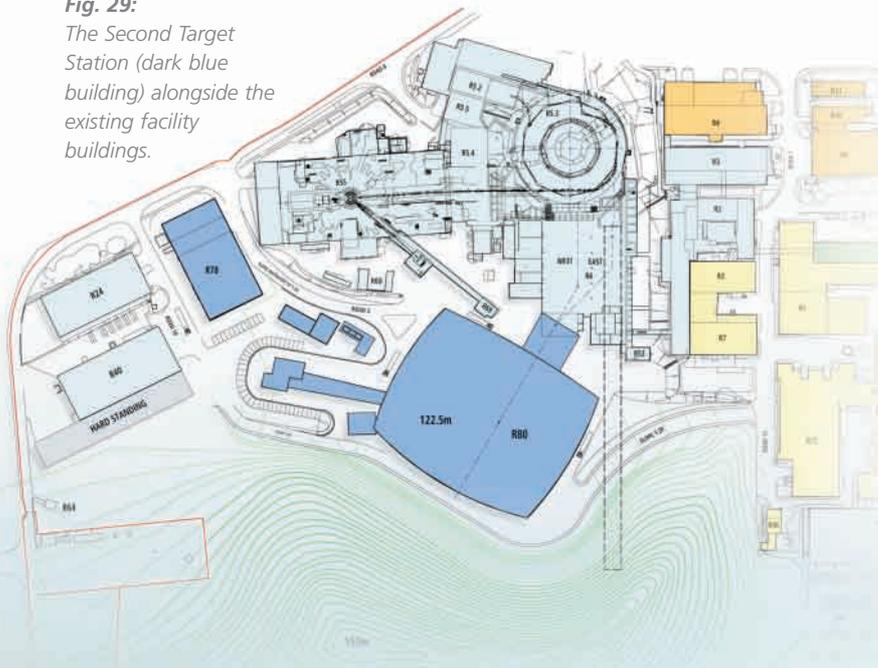


Fig. 30: Earth-moving work for the second target station site almost complete (03RC2616).



major pulsed neutron sources (KEK, SNS, Los Alamos, and IPNS) broadly endorsed the concepts employed and the predicted performance. The neutronic calculations, optimisation and design of the target station are now at an advanced stage, and the detailed engineering design work is also underway.

Schemes for the extracted proton beam from the ISIS synchrotron are now being refined. The main technical committee of the project, TRIM, which provides the forum to develop and co-ordinate all the technical issues relating to the target, moderators and instruments, has been formed and meets monthly.

Substantial progress has been made on the development of the instrument suite for the Second Target Station, and its scientific opportunities and potential instruments were the focus of the ISIS User Meeting on the 14th April. The original science case was broadly endorsed and updated, and ideas for the instrument suite discussed and refined.

On 26th June the Scientific Advisory Committee, SAC, met to prioritise the proposed instrumentation for 'day one'. 11 instruments were presented during the morning 'open' session (INTER, polREF, offSPEC, SANS2a, SANS2b, NIMROD, LMX, WISH, HRPD-II, LET and HERBI), and the SAC were impressed by the quality of all the proposals. Using the criteria of scientific quality, exploitation of the Second Target Station neutron characteristics, user support, and technical challenge and feasibility, the instruments were prioritised into a first phase (LET, offSPEC, SANS2b, WISH, INTER, polREF and NIMROD) and a later phase (HERBI, HRPD-II, LMX, and SAN2a). This recommendation will be used as the basis of the Gateway 2 review that is required for the instrument suite, and work will now begin on the detailed costing and technical design of the first phase of instrumentation.

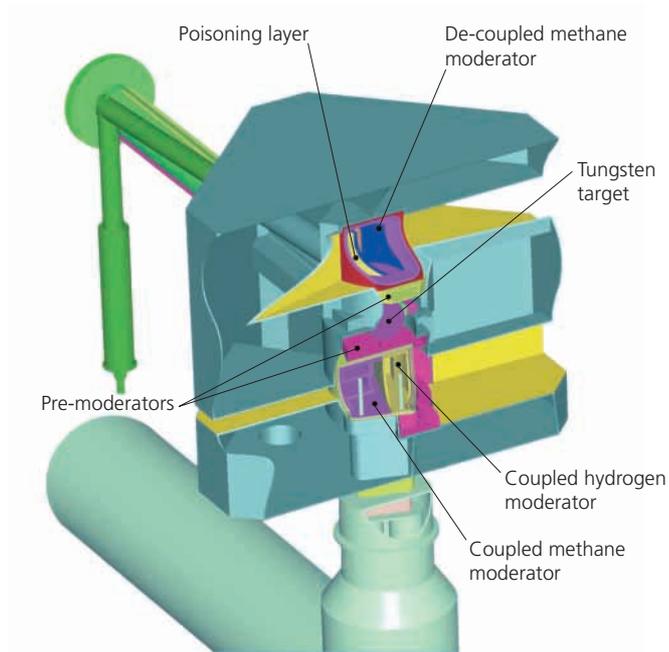


Fig. 31: Proposed layout of the Second Target Station target / moderator / reflector assembly.

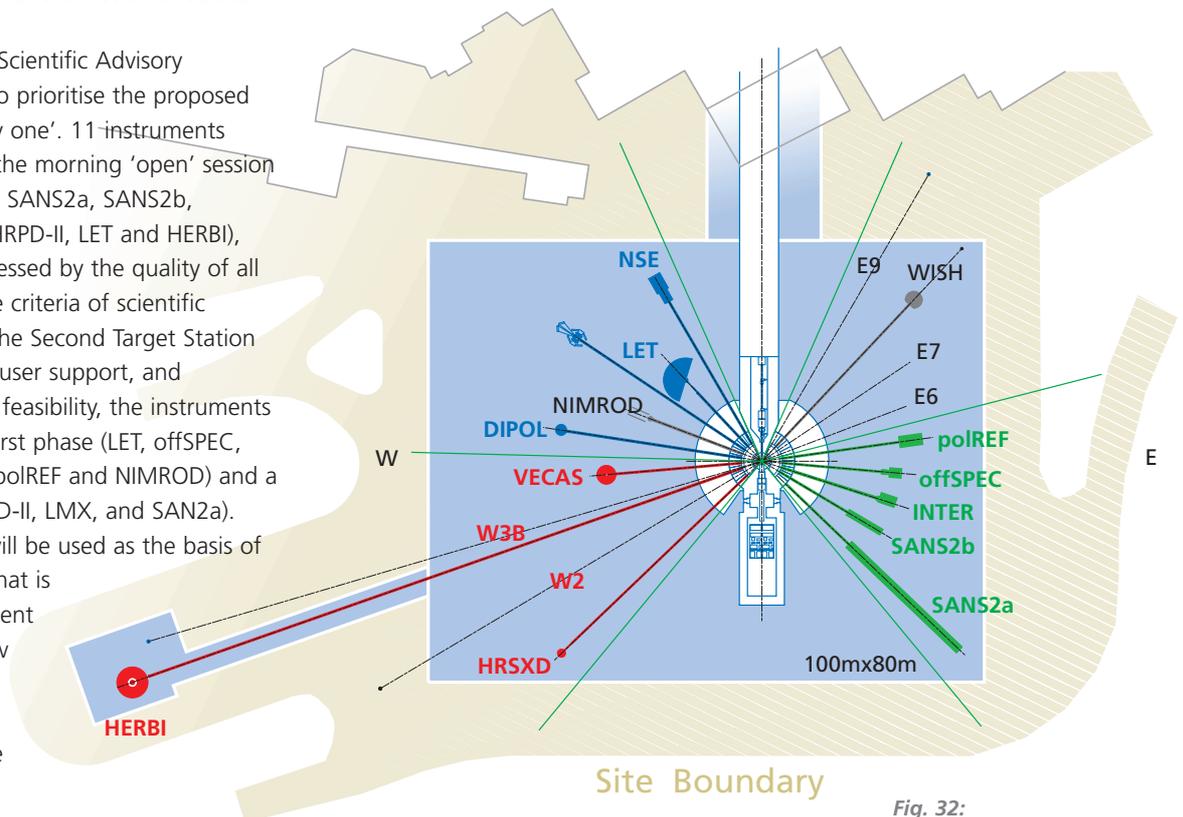


Fig. 32: Current layout for the reference instrument suite.

Regular updates on the progress of the project can be found on the Second Target Station website, www.isis.rl.ac.uk/targetstation2/

A Year Around the Facility Year

ISIS Spring User Meeting

ISIS hosted a very successful Spring User Meeting on 14th April 2003. The day was focused around the user requirements for the initial instrumentation on the ISIS Second Target Station, giving an opportunity for members of the ISIS Science Advisory Committee to informally ask individuals and groups what they needed from TS-II and how it might best be delivered.

The day was opened by a welcome from the SAC chairman, Bob Thomas (Oxford) who stressed the information gathering nature of the meeting. This was followed by an overview of the current status of ISIS and the recent technical developments on TS-II. Armed with this up-to-date information the community broke out into discussion groups chaired by the SAC members: *Soft Matter*, Randal Richards (Durham); *Hard Advanced Materials*, Paul Madden (Oxford); *Biomolecular Systems*, Tony Watts (Oxford); *Magnetic and Quantum Systems*, Mike Gunn (Birmingham) and *Chemical Structure Kinetics and Dynamics*, Andrew Harrison (Edinburgh).

These discussions were continued over lunch after which there was a lively reporting back session. Several common themes were brought out and important experimental parameters were identified. This provided useful input for the traditional User Groups, which met later in the afternoon to discuss specific instrument designs.

Fig. 33:
The ISIS User Meeting, held in April, focused on the scientific and instrument possibilities that will be provided by the Second Target Station (03RC1627).

UK Strategy for Neutron Scattering Facilities

In April 2003 the CCLRC published and invited comments on an outline UK strategy for neutron scattering. The strategy has been developed within the framework of the Office of Science and Technology Large Facilities 'road-map' which takes a broad look at the range of potential new developments in research facilities of priority interest to the UK. The UK strategy for neutrons has also drawn on the OECD Megascience Forum recommendations, namely:

- in the short to medium term, maximise the utilisation and potential of the current front rank facilities – the Institut Laue Langevin (ILL) and the ISIS spallation neutron source;
- develop, in a timely manner, a next generation neutron source for Europe.

European co-operation and investment in neutron scattering has resulted in Europe having a strong position for continued development of neutron facilities, one in which the UK will continue to be a key player. In 2004 the UK will return to a full (33%) contribution to the ILL; in recent years, the UK alongside the other ILL partners, has made a series of direct investments in instrumentation under the ILL Millennium Programme, with plans for further investments over the next several years. Investment in the Second Target Station at ISIS will also increase capability, focusing on soft condensed matter, advanced materials and biomolecular science.

A project of special European interest over the past ten years has been work on the development of the design for a next generation neutron source, the 'European Spallation Source' project. The UK, through the CCLRC Rutherford Appleton Laboratory, has been a long-standing partner in this international endeavour, and many UK scientists and engineers have contributed to the scientific and technical studies for this new source. In January 2003, the European Strategy Forum for Research Infrastructure (ESFRI) considered a report from its Working Group on 'Neutron scenarios within Europe'. It is clear from the outcome of that meeting that there is, across Europe, not now likely to be sufficient high level support to enable the European Spallation Source project to be realised in the short term. This accords with the view of the



UK where the current priority is continued investment in the ILL and in ISIS.

In the short term, therefore, the UK will focus its energies on successful delivery of new investment in the ILL Millennium Programme and in the ISIS Second Target Station, through international partnership. Beyond this, planning is required for the medium term and the CCLRC will continue to explore with the UK research communities the developing scientific requirements for access to neutron facilities. The CCLRC will also explore with wider interests at the European level the opportunity for strengthening collaboration in Europe on planning for a next generation neutron source and the associated timeline for decision making. The UK research community has a tremendous record of success in designing, building, operating and exploiting neutron research facilities and should be at the forefront of planning for the future of these within Europe.

Empirical Potential Structure Refinement Workshop

Funded in part by the CCLRC Centre for Molecular Structure and Dynamics, a workshop was held at The Cosener's House in November 2002 to enable users to gain hands-on experience of running Empirical Potential Structure Refinement (EPSR) for disordered materials. Some 30 participants spent 3 days glued to their laptops learning how to run the EPSR suite of programs, from simple simulation

Fig. 34: Participants at the Empirical Potential Structure Refinement Workshop at The Cosener's House in November (02RC3771).

exercises to sophisticated simulation techniques enabling 3-dimensional representations of atom distribution functions to be plotted.

Materials for Energy Production and Storage

A 2-day meeting was hosted by the CCLRC Centre for Materials Physics and Chemistry at RAL in March 2003, exploring the atomistic understanding of materials involved in energy production and storage. The meeting focused on the characterisation, simulation and development of materials for applications in fuel cells, batteries and hydrogen storage materials, photovoltaics and catalysts. Its purpose was to provide a broad forum for users of CCLRC facilities to discuss common issues and as such it revolved primarily around the inter-relationship between bulk properties and the atomic and nano-scale structure and dynamics of the materials using computer simulation, X-ray and neutron scattering techniques, and muon spectroscopy. The meeting was lively and interesting and has sparked a variety of collaborations between CCLRC staff and external users.

Fig. 35: Energy workshop attendees (03RC1427).



EC Framework Programme 6

European researchers wishing to use ISIS have benefited from contracts that the facility has had with the European Commission which provide beam fees and travel and subsistence costs to fund their experiments. These contracts are run under so-called EC Framework Programmes; the present programme, FP5, is about to end, and FP6 will start at the beginning of 2004. ISIS will have new contracts to enable neutron and muon users to gain access to the facility under FP6, and will also be involved in several research and development networks also to be funded. New arrangements under FP6 mean that all neutron and muon facilities in Europe which receive funds from the EC now come under a single umbrella arrangement, called the Neutron and Muon Integrated Infrastructure Initiative (NMI3). This includes twelve facilities with access contracts and nine research and development networks, together with other activities of benefit to European neutron and muon science. Further information on NMI3 activities can be obtained from Robert McGreevy at ISIS (NMI3 co-ordinator). Details of the ISIS neutron and muon access contracts and how to apply can be obtained from Uschi Steigenberger and Philip King respectively.

Developing the Scientists of Tomorrow

This year saw the launch of the ISIS 'Living in A Materials World' CD-ROM for schools. Based around the technology and science of the facility, the CD-ROM has been jointly developed with teachers to meet the needs of the current A-Level physics curriculum. Funded by EPSRC under the Partnership for Public Awareness, the CD-ROM is being supplied free to schools and educational establishments. The project offers a fantastic opportunity for students who live too far away to come and 'visit' the facility; the virtual tour means that they can look around the particle accelerators and find out how they work, watch video interviews with some of the people who work at ISIS, and explore the latest research. The CD is packed with pictures and animations, plus a historical section about the developments of particle accelerators and neutron science, and there are lots of web links, other information

sources, and even A-Level questions based on ISIS. Chris Frost or Martyn Bull at the facility can be contacted for further information.

Nottingham MSc student visit

On March 11 ISIS played hosted a visit by 36 students from Nottingham University studying for an MSc in Biomolecular Technology. Part of the course syllabus covers techniques for studying the structure of biological molecules, an area in which neutron diffraction has a part to play! After a variety of talks describing neutron techniques and their applications to biological systems, the students toured the ISIS Experimental Hall before spending an hour analysing some SANS data.



Fig. 36: Nottingham University students studying biomolecular technology visited ISIS in March (03RC1428).

ISIS People

Congratulations are due to several ISIS staff members whose scientific achievements have been recognised during the past year. Professor Chick Wilson, head of the ISIS Crystallography Group, has recently been elected President of the British Crystallographic Association (BCA); Alex Hannon, of the Disordered Materials Group, has been appointed as a visitor professor at the Laboratoire de Physico-Chimie de l'Atmosphère of the Université du Littoral in Dunkerque, France; and Paolo Radaelli has been promoted to Band 2 in the Research Councils' Individual Merit Promotion Scheme. Congratulations also to Richard Nelmes on being elected as a Fellow of The Royal Society on 15th May. Richard, a long-term visiting scientist at ISIS, has been instrumental in pushing the limits of high pressure research using neutron scattering and synchrotron radiation.



Fig. 37: Andrew Taylor with (l to r) Gérard Hamel, Stefan Klotz, Richard Nelmes and John Loveday in Paris for a colloquium held in May this year to honour the memory of Michel Besson, who inspired the novel Paris-Edinburgh pressure cell developments at ISIS over the past decade. Michel established and led the renowned Paris high-pressure laboratory Physique des Milieux Condensés until his untimely death in 2001, and was recognised as one of the outstanding high-pressure scientists of his generation.



Fig. 38: Stephen Lovesey (left) retired in April after over 23 years at the Laboratory.

ISIS has also seen the comings and goings of people over the past year. Ian Gardner stepped down as Head of the ISIS Accelerator Division on 31 May 2003. Ian has not been lost to ISIS, though – he continues to be involved in the technical developments of the accelerator. David Findlay has been appointed Acting Head for the ISIS Accelerator Division. Prof. Stephen Lovesey retired as Head of the ISIS Theory Division on 30 April

2003 after an illustrious career in condensed matter theory encompassing neutrons, muons and X-rays. Stephen will also continue to have a presence at ISIS and be engaged in the scientific programme. Other retirements have included Pete Surtell from the ISIS Operations Group and Mike Yates from the Sample Environment Section, and Bjorn Fak left his role supporting the PRISMA instrument to pursue his neutron career elsewhere.

New arrivals during the year have included Felix Fernandez-Alonso, who will be working as an instrument scientist on the OSIRIS instrument.



Fig. 39: Training courses to introduce young researchers to the practicalities of the neutron and muon techniques were held at ISIS in January. Pictured here are the attendees at the two courses, plus some of the ISIS lecturers and demonstrators (03RC1078, 03RC1248).



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
W Clegg (CH) A Albinati G Artioli J Hriljac T Kamiyama P Lightfoot A Powell D Price P Raithby C Ritter P Stephens P Thomas R Ibberson C Wilson	P Smith (CH) M Bellissent-F T Fukunaga P Madden P Salmon K Seddon N Skipper J Swenson	A Rennie (CH) J Andrew N Clarke J Eastoe I Gentle B Hickey F Mulder S Roser F Tiberger R Triolo	R Cowley (CH) A Boothroyd C Broholm D Edwards J Gunn S Julian A Krimmel D Noreus K Yamada	J Larese (CH) J Bradshaw S Kilcoyne D O'Hare C Rhodes R Simmons D Timms M Zoppi	S Blundell (CH) J Campos Gil P Carretta A Fisher M Iwasaki R Lichti P Mitchell E Morenzoni B Rainford	M Fitzpatrick (CH) J Bouchard M Johnson R L Peng D Smith G Swallowe
	D Bowron A Soper	J Webster J Penfold	T Perring S Bennington	J Mayers J Tomkinson	S Cottrell P King	J Dann M Daymond

Table 1: ISIS Facility Access Panel Membership. The FAPs meet twice per year to review all proposals submitted to the facility based on scientific merit and timeliness.

Chairman	R J Stewart	University of Reading	A D Taylor	Director ISIS
IUG1 Crystallography	P Battle R J Nelmes	University of Oxford University of Edinburgh	J Green	EPSRC
IUG2 Liquids & Amorphous	A Barnes N Skipper	University of Bristol University College London	U Steigenberger	ISIS Division Head
IUG3 Large Scale Structures	R J Stewart R Thomas	University of Reading University of Oxford	J Tomkinson	ISIS User Office Co-ordinator
IUG4 Excitations	D Mckenzie Paul	University of Warwick	R S Eccleston	ISIS Division Head
IUG5 Molecular Spectroscopy	K Ross	University of Salford	R L MCGreevy	IDM Division Head
IUG6 Muons	J Jayasooriya S Kilcoyne	University of East Anglia University of Leeds	Z A Bowden	ISIS User Support Group Leader
IUG7 Engineering	G Swallowe M Fitzpatrick	Open University Open University		

Table 2: ISIS User Committee Membership. The IUC exists to represent the user community on all aspects of facility operation.

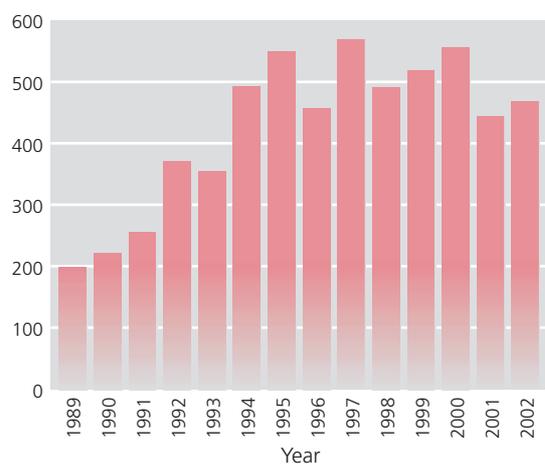


Fig. 42: Year-on-year publication numbers resulting from work carried out at ISIS.

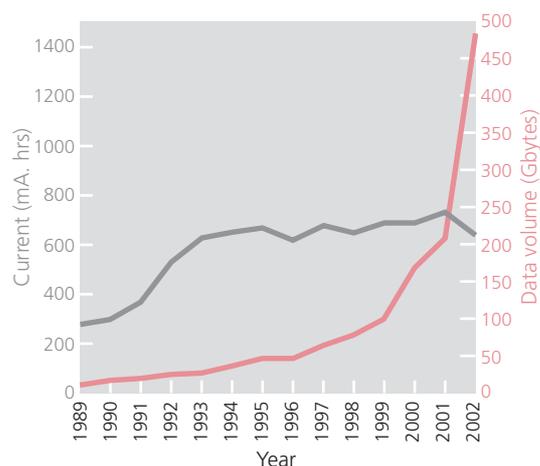


Fig. 43: Comparison of ISIS data taken year-on-year with proton beam current. In the past year, the new ENGIN-X instrument has added significantly to the volume of data taken at the facility.

Beam Statistics 2002 - 2003

ISIS continues to be the world's most intense pulsed spallation neutron source, and for the period of this report and during scheduled operating cycles, the facility delivered a total of 630 mA.hrs of user proton beam to the muon and neutron targets at an average current of 165 μ A.

Table 3 gives beam statistics for the individual cycles in the year 2002-2003. Year-on-year statistics for ISIS performance are given in table 4. Figure 44 shows the total integrated current for each year since 1987.

Cycle	02/1	02/2	02/3	02/4	02/5
Beam on target (hrs)	170	389	1026	768	1068
Total beam current (mA.hr)	53	70	183	138	186
Average beam current on target (μ A)	168	179	178	180	176
Peak beam current (μ A, average over 24 hrs)	179	185	187	184	178
Current averaged over cycle (μ A)	87	137	155	162	157
Average beam trips per day	17	21	18	18	24

Table 3: ISIS operational statistics for year 2002-2003.

Year	1996	1997	1998	1999	2000	2001	2002
Total scheduled user time (days)	168	168	175	168	168	168	160
Total time on target (days)	152	153	160	153	154	158	148
Total integrated current (mA.hrs)	621	672	656	687	687	725	630
Average current on target (μ A)	171	183	171	187	186	192	178
Peak current averaged over 24 hours	204	197	193	198	194	200	187
Current averaged over year (μ A)	153	167	156	171	165	171	165
μ A.hrs per trip	115	81	72	106	120	141	178
Total power consumption (GWh)	47	47	42	52	46	46	53
Energy efficiency (mA.hr/GWh)	13.1	14.9	14.9	13.2	14.9	15.7	12.1

Table 4: Year-on-year ISIS performance summary.

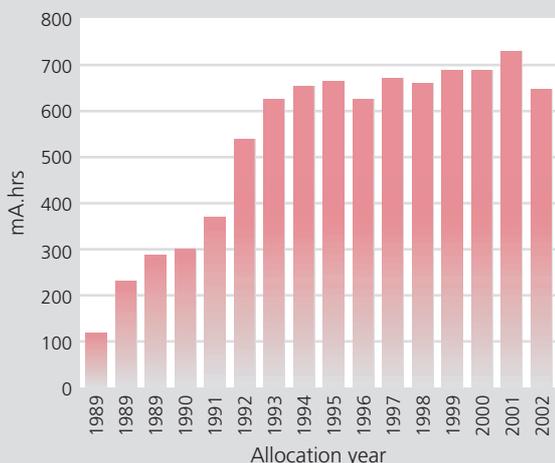


Fig. 44: Total integrated ISIS current.



The ISIS Facility, CCLRC Rutherford Appleton Laboratory, Chilton, DIDCOT OX11 0QX, UK
Tel: +44 (0)1235 821900 Fax: +44 (0)1235 445103 email: isisuo@rl.ac.uk

www.isis.rl.ac.uk