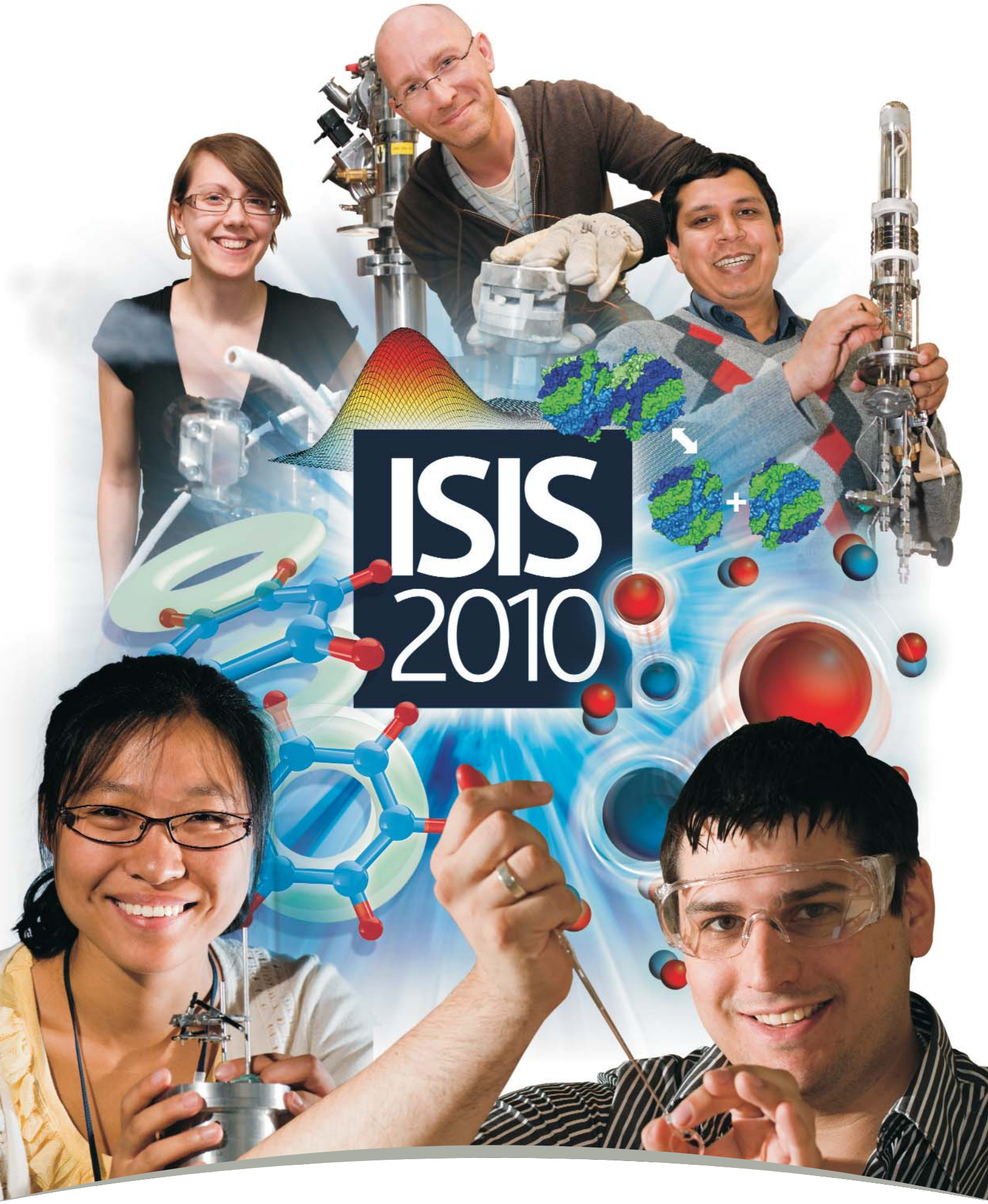
THE ISIS PULSED NEUTRON AND MUON SOURCE



Science & Technology Facilities Council

ISIS 2010

THE ISIS PULSED NEUTRON AND MUON SOURCE

ISIS 2010 was produced for the ISIS Facility,
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September 2010

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2010 details the work of the facility over the past year, including accounts of science highlights, descriptions of major instrument and accelerator developments and the facility's publications for the year.

ISIS 2010

Contents

▼ Dr Robert Kirby-Harris, Chief Executive, Institute of Physics, examining a single crystal array with Toby Perring (ISIS) during his visit in April.
10EC2808

▶ The ISIS Facility Board has been created to provide advice to STFC and ISIS on ISIS operational performance. The Board met for the first time in February. Seen here during their visit to ISIS are Prof Tom McLeish (Durham University, Chair), Mr Jonathan Flint (Oxford Instruments), Prof Andrew Harrison (Institut Laue Langevin), Dr Stuart Henderson (Oak Ridge National Laboratory), Dr David Lennon, (Glasgow University), Professor Peter Littlewood (Cambridge University) and Prof Bob Newport (Kent University).
10EC1255

▶ Prof Ryoji Noyori (President, RIKEN, Japan) and Prof Keith Mason (STFC Chief Executive) signing an agreement to renew the partnership between STFC and RIKEN for muon science. This year saw the 20th anniversary of the first RIKEN-RAL agreement, signed in 1990, which established the RIKEN-RAL muon facility at ISIS.
10EC2488

▼ New STFC Chairman Professor Michael Stirling visited ISIS in September. Left to right: Dr Andrew Taylor (ISIS Director), Mrs Sterling, Prof Stirling and Prof Keith Mason (STFC Chief Executive).
09EC3074

▶ New STFC council member Will Whitethorn (President of Virgin Galactic, right) being shown ISIS by Chris Frost during his visit in June.
10EC2809

▶ Ed Vaizey MP, Minister for Culture, Communications and the Creative Industries, visited the ISIS Second Target Station in July. Here he is making a thermocouple measurement of his temperature with ISIS's Julie Roberts, Andrew Chamberlain and Zoe Bowden.
10EC2753

Happy Birthday ISIS!

ISIS celebrated 25 years of successful neutron production last December.

What a long way we have come since 1984! Not just in terms of the instrument suite – a fully-developed first target station, and a brand-new second target station with seven operating instruments and potential for so much more – but in terms of the science we have delivered. And what advances in science! I doubt that we would have predicted, 25 years ago, that ISIS would be exploring materials used to repair cleft palates, or for drug delivery, or protein arrays for medical diagnosis. Or the myriad other applications that neutron scattering now has, in addition to the more traditional areas of superconductivity and magnetism. *Who knows what will the next 25 years hold!*

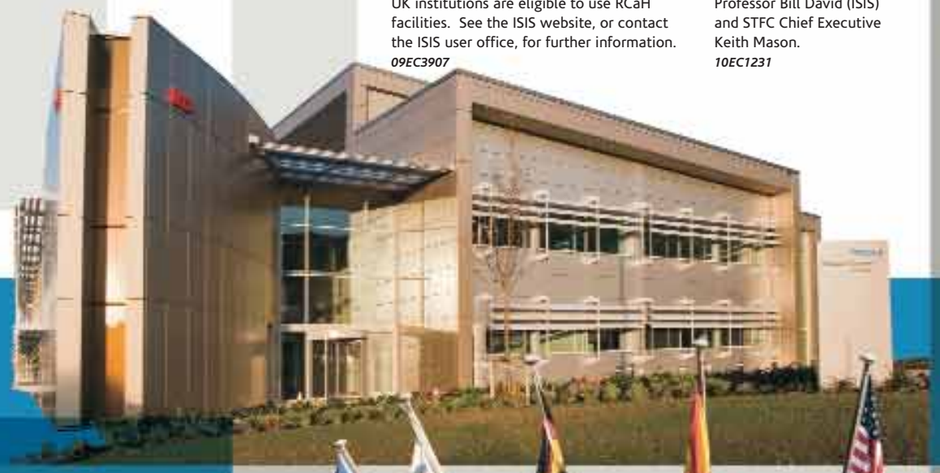
One sign of a mature science facility is the partnerships that it has fostered. ISIS is no exception: collaboration with researchers from The Netherlands to realise the Offspec reflectometer; or Nimrod developed with colleagues from Italy; or Spanish colleagues building the tank for LET and detectors for Pearl; or the upgrade of Polaris with scientists from Sweden – to name but a few. And this year we celebrated 20 years of muon science collaboration with the RIKEN institute of Japan through the RIKEN-RAL muon facility. Prof Ryoji Noyori, Nobel Laureate and President of RIKEN, signed an agreement which will continue our partnership for many years to come.

But it is people that enable all this to happen. Members of the user community become collaborators and close colleagues, working with ISIS staff to produce science of the highest quality. The ISIS team consists of hundreds of people – many seen here – each with individual skills and expertise that combine to make ISIS the world-leading facility that it is. It is invidious to single out any individual staff member, but recognition this year must be paid to Harry Jones, Head of the ISIS Target Division, who retired after a career spanning five decades. Awarded an MBE in the New Year Honours this year for his services to science, he exemplified the qualities needed to manage a project of the scale and complexity of the Second Target Station.

ISIS staff celebrating 25 years of ISIS running.
09EC4000

As I write, ISIS is within a long shut-down period. We are refurbishing parts of the accelerator and proton beamline systems to provide for many future years of running. And we are further developing our instrument suite through upgrades to Polaris and Pearl, and are eagerly awaiting the next phase of second target instruments. There are undoubtedly tough times ahead, and ISIS will not be immune from the current financial squeeze. But we are looking forward to further great science in 2011 – and for a long time beyond!

◀ A delegation from the Republic of Korea visited ISIS in July. Here we see Mrs Young-Ah Park, MP, Member of the Korean National Assembly, Mr Jong-Min Jeon, Policy Advisor to MP Park, Prof Dong-Pil Min, Chair of Korea Research Council of Fundamental Science and Technology (KRCF), Dr Chae-Jun Song, Research Fellow, KRCF, Prof Hong Thomas Hahn, President of Korea Institute of Science and Technology (KIST), Prof Young-Joon Kim, Vice President of Gwangju Institute of Science and Technology (GIST) and Hyeyoung Kim, Science and Innovation Manager, British Embassy, Seoul, with Andrew Taylor and Uschi Steigenberger (ISIS). ***10EC2803***



▼ The Research Complex at Harwell (RCaH) was formally opened in July. RCaH is a new, multidisciplinary laboratory at RAL that provides facilities for researchers in both life and physical sciences, particularly users of Diamond and ISIS. ISIS users from UK institutions are eligible to use RCaH facilities. See the ISIS website, or contact the ISIS user office, for further information. ***09EC3907***

▶ The Rt Hon Lord Drayson, Minister for Science and Innovation, visited ISIS in February. Here he is discussing hydrogen storage materials with Professor Bill David (ISIS) and STFC Chief Executive Keith Mason. ***10EC1231***

A year around ISIS

◀ The Offspec instrument on the ISIS Second Target Station has been built through a collaboration between ISIS and Technical University Delft in The Netherlands. Professor Tim van de Hagen, Director Reactor Institute Delft (left) and Professor Karel Luyben, Rector Magnificus Technical University Delft (Right) are seen inspecting the new instrument. ***09EC3106***

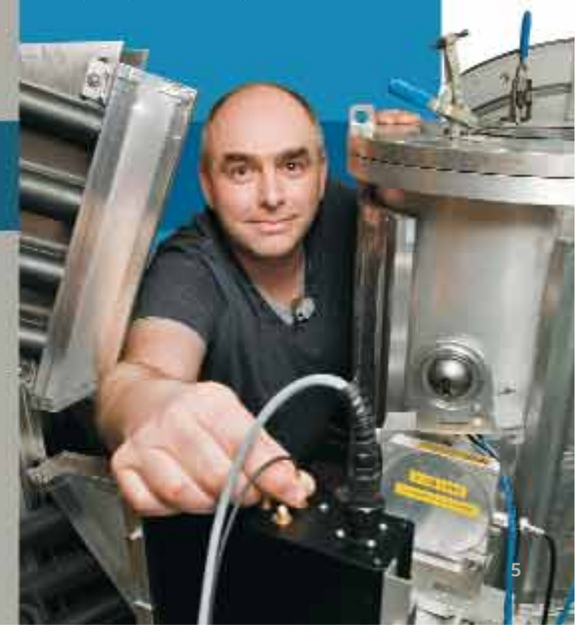
▲ A delegation from the Chinese Academy of Sciences visited ISIS in October. ***09EC3607***

▲ Members from the Japanese institute RIKEN visited ISIS in April. Seen here are Dr Hideto En'yo (Director, RIKEN Nishina Centre), Mr Motohide Yokota (Director, RIKEN Advanced Research Promotion Division), Dr Masa Iwasaki (Chief Scientist, RIKEN Advanced Meson Science Laboratory), Mr Koji Yokoyama (Chief, Planning section, Advanced Research Promotion Division) and Dr Tei Matsuzaki (Head, RIKEN-RAL Muon Facility), along with Andrew Taylor, Uschi Steigenberger and Philip King (ISIS). ***10EC2762***

▼ December 16, 2009 marked 25 years of running at ISIS. First neutrons were produced at the facility on 16 December 1984, and ISIS has been producing science ever since. ISIS users and staff met for a small celebration in the ISIS foyer.

▶ Dr Paul Williams and Dr Godfrey Stafford, former directors of the Rutherford Appleton Laboratory toured the ISIS facility with Dr Andrew Taylor, ISIS Director, in December. ***09EC4134***

▶ SEEDER is a collaborative study by industrial partners to try and establish how single event effects (SEEs), produced by cosmic-ray neutrons, impact on the workings of microchips and electronic systems. Richard Jenkins (BAE systems) is seen here performing initial studies of the effect on Vesuvio, preparing the way for a dedicated instrument on the ISIS Second Target Station. ***10EC2736***



Highlights of ISIS science

The advanced facilities provided by ISIS enable world-class research to be performed by scientists from around the world in partnership 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.

▶ Michael Pitcher and Dinah Parker (Oxford University) using Polaris to investigate the correlation of composition, structure and superconductivity in electron-doped pnictide LiFeAs.
10EC2501

Highlights of ISIS science

Mind the gap: interfaces, from nano to macro

… biological interfaces mimicking the physiological conditions found in cell membranes and ion channels can now be prepared and studied at ISIS using state-of-the-art equipment for the production of lipid bilayers.

A time-resolved study into the growth of large silica-surfactant particles

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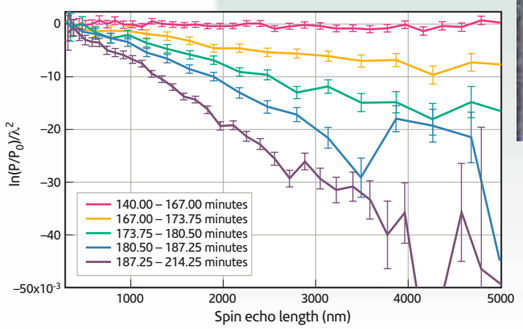
Further reading:

KJ Edler, Soft Matter 2 (2006) 284

Studying the growth of silica-surfactant architectures during the formation of mesoporous silicates is pivotal to understand how these materials may be used in catalysts, drug delivery, and nanotechnology. Small-angle neutron scattering (SANS) has been used to study the in-situ formation kinetics of these hierarchical structures. SANS can access a wide enough size range and has sufficient temporal resolution to follow how silica grows around the templating surfactant. Ultra-small-angle scattering and light scattering can access length scales larger than the hundreds of nanometres possible with SANS but, in this case, long data collection times and the turbidity of the solution prevent their use.

Recent developments in spin-echo-SANS techniques now allow studies of structures from hundreds to thousands of nanometres with a time resolution of a few minutes. We have used this approach on Offspec to monitor the condensation and aggregation of silica around surfactant micelles to form larger particles. The final structures were fitted to a sphere model with characteristic radii of approximately 2500 nm.



◀ Time-resolved spin-echo SANS profiles during the aggregation of surfactant template silica particles (see photograph). Each scan lasted for 7.5 minutes every 15 minutes.

Understanding flow in ice-rock mixtures

CA Middleton, PM Grindrod, AD Fortes, SA Hunt, J Bowles, IG Wood (University College London), SJ Covey-Crump (Manchester University), S-Y Zhang (ISIS)

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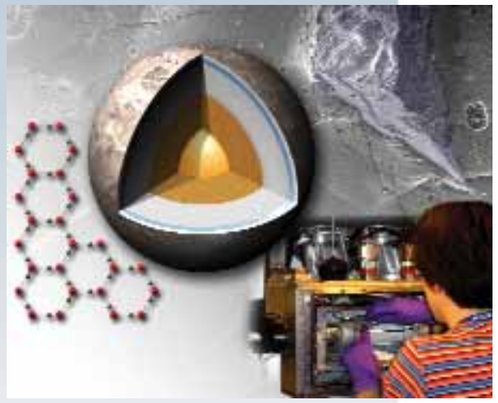
Further reading:

Durham et al., J Geophys Res 102 (1997) 16293

The rheology of multi-phase materials is of relevance to a broad range of applications. Our recent work has focused on the properties of ice-rock mixtures, which are likely to occur in the outer solar system's icy satellites – e.g., Ganymede, Callisto, Titan – and to have played a role in their geological evolution. Rocky particles may pin ice grain boundaries, hindering the flow of the icy matrix, thereby reducing the efficiency of convection. We have carried out tests upon ice-fluorite mixtures (an 'ice-rock' proxy) using neutron diffraction on Engin-x to measure the strain partitioning between the phases. We have observed unusual behaviour in that, under certain conditions, increased load leads to reduced stress on the fluorite. We hypothesise that this may be due to pressure melting of ice around points on the fluorite grains. These data show that the ice-rock fabric has a more complex behaviour than hitherto thought, and this may have unexpected consequences for the evolution of icy planetary bodies.



▲ Measurement and applications of flow in ice-rock mixtures: atomic arrangement in ice; scanning-electron micrograph of ice-rock fabric; possible icy-moon interior; and experiment on Engin-x.

How neutrons can improve orthopaedic implants

R Ahmed (Heriot-Watt University), AM Paradowska (STFC), M Fitzpatrick (Open University)

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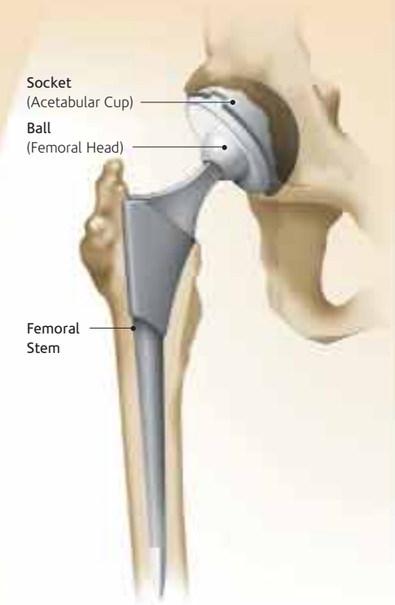
Further reading:

R Ahmed et al., Mater Sci Forum 652 (2010) 309

The use of surface coatings in orthopaedic and dental implants has significantly improved the quality of human life. Modern implants provide improved recovery times and lower implant rejection rates. Early implants were expensive, and often failed because the bonding between the implant and the bone, a process known as osteo-integration, was poor. Several designs have been formulated to date but many failed to achieve a strong enough bond. A solution involves coating the metal with a layer of hydroxyapatite (HA). Hydroxyapatite forms almost three-quarters of natural bone. Coating the metal first with HA gives a stronger metal-bone bond. Even with this improvement, one in five implants can still fail. One of the main reasons of failure is the residual stress developed at the metal-HA interface. Neutrons offer significant advantages to analyse this critical interface, enabling measurements to be made in-depth and non-destructively. This unique capability enables us to improve our understanding of how HA bonds to the metal and bone.



ISIS 2010

Highlights of ISIS science

Getting on top of calcite

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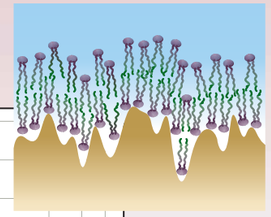
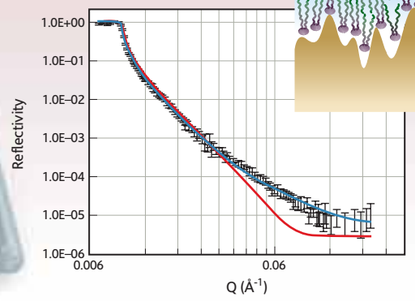
Further reading:

FC Meldrum et al., Chem Rev 108 (2008) 4332

Calcite is an extremely important mineral in sedimentary deposits and in many industrial processes. This is particularly evident in water heating where it forms 'scale' in hard water areas due to its retrograde solubility (solubility falls on heating). This precipitation leads to major process difficulties including pipe blockage. We have successfully used neutron reflection on Crisp to address the surface behaviour of calcite, particularly adsorption of surface active agents including those that inhibit calcite crystal formation and growth. The adsorbents studied include surfactants and polymers of different molecular weights adsorbed from both water and oil, reflecting the wide range of systems of interest. The results are complex with mono, bi and multilayer formation together with surface dissolution in some cases. Similarly, this approach can be used to probe adsorption of biopolymers on to the surface of calcite which in nature leads to the formation of beautiful, complex calcite architectures that are still perfect single crystals.





▶ Left: optical birefringence of calcite (Iceland spar). Middle: reflectivity profile and fit (blue) for a surfactant (AOT) in water at the calcite interface compared to a bare surface (red). Right: schematic illustration of the structure deduced.

Solution structure of **proteasome activators**

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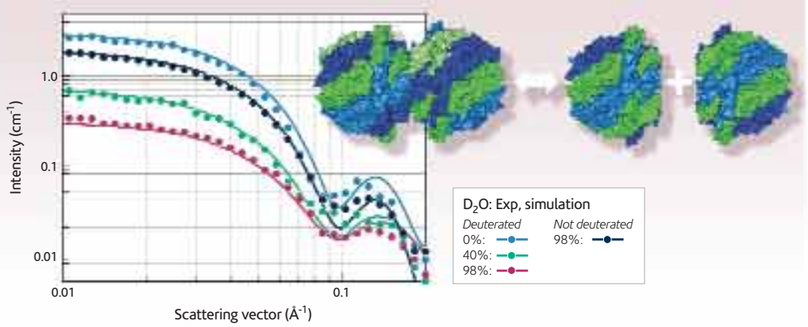
Further reading:

M Sugiyama, in preparation

In biological cells, the so-called '20S proteasome' is responsible for breaking down damaged or unneeded proteins so they can be recycled into new ones. Its function is regulated by several Proteasome Activators (PAs). For example, PA28 binds to proteasomes and the resulting complex promotes the production of immune-response peptides. PA28 is known to comprise seven-membered rings containing two very similar subunits, named α and β, each of molecular weight ~28 kDa. Novel insight into the structure of PA28 has been obtained in small-angle neutron scattering (SANS) experiments carried out on the recently commissioned Second Target Station instrument Sans2d. Employing water-solvent contrast variation with deuterated α subunits was key to this study. Initial modeling efforts having as starting point the crystal structure of homologue PA28 indicate that PA28 heptamer rings are made up of three α and four β subunits in an alternating zig-zag arrangement. The SANS intensities also reveal that there is a well-defined solution equilibrium between heptamer and its double-ring dimer, making the analysis more intricate than anticipated.



▶ Sans2d data for PA28 (points) and initial simulations (lines) allowing for dimer–monomer equilibrium. D_2O/H_2O contrast variation with deuterated α subunits shows that the rings comprise three α and four β units.

Nimrod gives quantitative insight into the **structural kinetics of polymer crystallisation**

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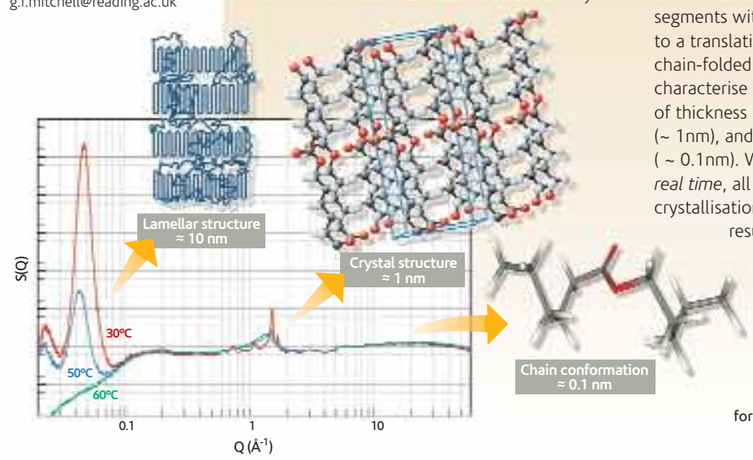
Many technologically important polymers are partially crystalline and their crystalline structure and morphology are critical to delivering the required properties. Although the process whereby polymers crystallise by folding into thin lamellae was discovered some fifty years ago, the existence of a transition in which a randomly coiled polymer chain in the melt reorganises to form a chain-folded lamellar phase remains a subject of much debate and conjecture. Crystallisation involves conformational changes to produce chain segments with a regular conformation leading to a translationally ordered crystal containing chain-folded surfaces. Three key length scales characterise this process: chain-folded lamellae of thickness ~ 10nm, the crystal unit cell (~ 1nm), and chain-conformation details (~ 0.1nm). We have used Nimrod to follow, *in real time*, all three length scales during the crystallisation process. These experimental results are being used to develop detailed multiscale models of polymer crystallisation.



◀ Time-resolved neutron scattering data for poly(e-caprolactone) during cooling from the melt. The observed structural variations are linked to the three key length scales for crystallisation.

Big and alive: biology and supramolecular science

… the high flux on the ISIS Second Target Station enables kinetic studies, from polymer crystallisation to protein binding, down to millisecond timescales.

Exploring membrane activity of **plant seed defence proteins**

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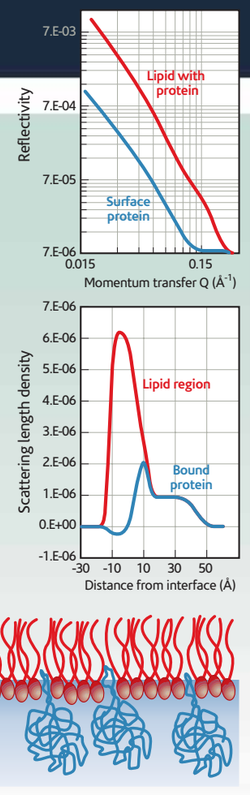
Further reading:

LA Clifton et al., J Phys Chem B 112 (2008) 15907

Plants are constantly exposed to pathogens and, in response, have developed multiple defence mechanisms that include the expression of antimicrobial proteins. These are characterised by having high structural and thermodynamic stability, but their precise mechanism of action is not known. However, it is widely accepted that these proteins act at the level of the cell membrane.

We have investigated the membrane interactions of the puroindolines, a family of antimicrobial proteins found in wheat. The puroindolines are unique among plant proteins as they contain a tryptophan-rich domain and play an additional role in determining wheat endosperm texture, an economically important quality that determines the milling characteristics of wheat.

The tryptophan-rich domain is thought to be implicated in the membrane interactions of puroindolines. Using air/liquid monolayer and solid/liquid floating bilayer models, we have used neutron reflectivity to explore how single amino-acid residue substitutions affect a protein's ability to penetrate lipid membranes, as well as how these findings relate to antimicrobial effectiveness.



▶ Neutron reflectivity data and associated scattering length density profile for the interaction of puroindoline-a with an anionic phospholipid monolayer. The schematic shows the interfacial layer structure.

Optimising polymer solutions for **printed electronics**

A Urbina, **N Espinosa**, **R García-Valverde** (Universidad Politécnica de Cartagena, Spain), **V García-Sakai**, **SE Rogers** (ISIS), **F Batallan**, **C Díaz-Paniagua** (Instituto de Ciencia de Materiales, Spain), **M Jiménez** (ILL, France), **J Abad** (Universidad de Murcia, Spain)

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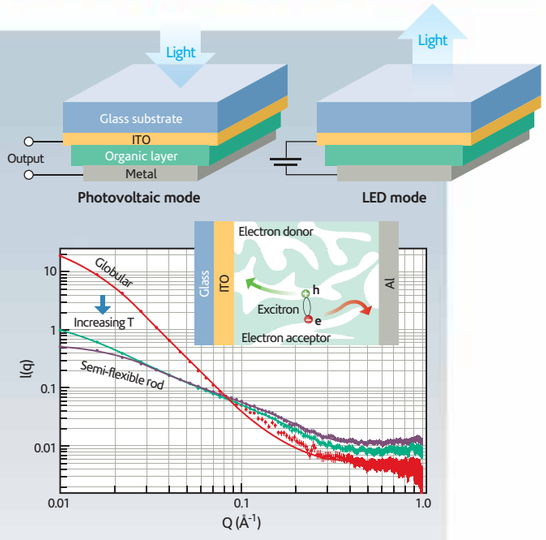
Further reading:

A Urbina et al., Phys Rev B 78 (2008) 045420; R García-Valverde et al., Prog Photovolt: Res Appl 18 (2010) 535

The development of polymer-based optoelectronic devices (or 'plastic solar cells') that could deliver electricity at a competitive cost is a key area of research. Solutions of conjugated polymers can be 'printed' to produce the active layer of low-cost solar cells by means of technologies such as screen and ink-jet printing or spray coating. The properties of this 'ink' need to be controlled to ensure that the self-assembled nanostructures formed in the process are electrically conducting. Small angle neutron scattering (SANS) measurements were made on LOQ on a range of solutions of conjugated pure and blended polymers at different temperatures. From these studies, we are able to determine how solvent interaction, temperature, polymer molecular weight, and polydispersity influence the structural properties of the polymer assemblies in solution. A temperature-induced shape change (from globular to semi-flexible rod) and solvent-induced size changes have been observed. These findings will be used to improve the layer fabrication procedure which, in turn, will increase the efficiency of the resulting solar-cell.



▲ SANS data demonstrating a temperature-induced shape change from globular to semi-flexible rod for P3HT in toluene. The inset shows an organic light-emitting diode and an organic solar cell.

Proton harmonic **motion in ice**

D Flammini, A Pietropaolo, R Senesi, C Andreani (Università di Roma Tor Vergata, Italy), F McBride, A Hodgson (Liverpool University), L Lin, R Car (Princeton University USA), MA Adams (ISIS)

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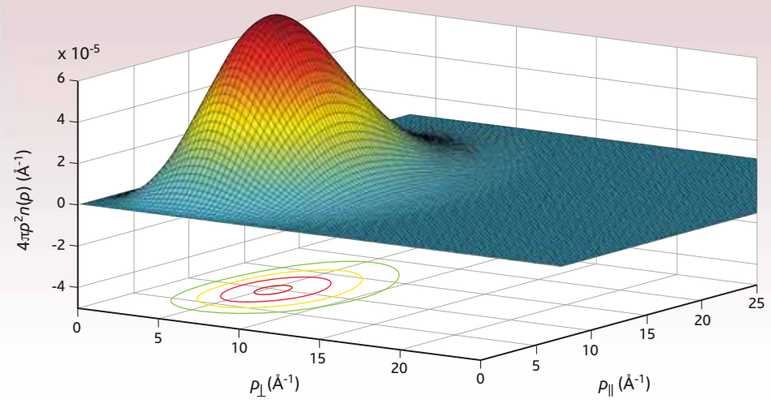
Further reading:

C Andreani et al., Adv Phys 54 (2005) 377

There is currently great interest in probing the quantum state of the proton in ice. This can be revealed from the momentum distribution $n(p)$, which is a very sensitive probe of the potential of mean force experienced by the protons in hydrogen-bonded systems. We have explored the details of $n(p)$ in ice at T=271 K using a combination of deep inelastic neutron scattering and path-integral Car-Parrinello molecular dynamics simulations. The neutron data have been interpreted within the framework of the impulse approximation, which allows us to extract the three-dimensional $n(p)$. Experimental and simulation data have been successfully interpreted with an anisotropic Gaussian model in which the proton essentially moves in a harmonic well along each direction, but with a marked anisotropy between motions parallel and perpendicular to the bond-stretching direction.



▶ The proton momentum distribution in ice parallel ($p_{||}$) and perpendicular ($p_{\perp}$) to the bond-stretching direction.

$\pi - \pi$ **interactions** in aromatic liquids

TF Headen, CA Howard, NT Skipper, MA Wilkinson (University College London), DT Bowron, AK Soper (ISIS)

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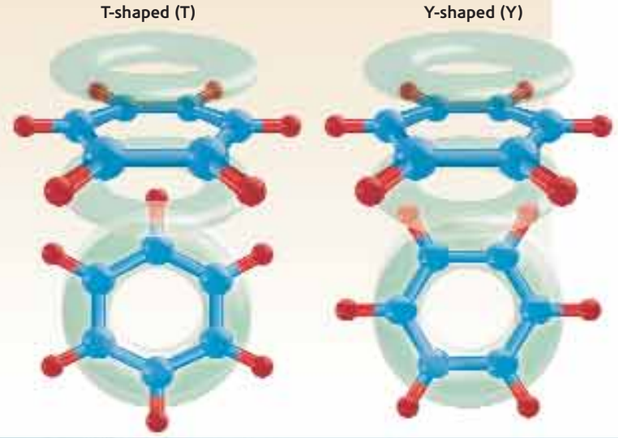
Further reading:

TF Headen et al., J Am Chem Soc 132 (2010) 5735

Aromatic $\pi - \pi$ interactions between benzene-like chemical groups play a key role in many important scientific phenomena, including the stereochemistry of organic reactions, organic host-guest chemistry and crystal packing, protein folding and structure, DNA and RNA base stacking, protein-nucleic acid recognition, drug design, and asphaltene (heavy crude oil) aggregation and fouling. We have used isotopic labelling and neutron diffraction to measure the structure in two archetypal aromatic liquids: benzene and toluene. Our results call for a significant rethink of the way we model π-orbital interactions. We have found that the so-called 'T-shaped' arrangement between aromatic groups, which had previously been proposed as a dominant motif in $\pi - \pi$ interactions, in is in fact absent in our liquids. Instead, we have observed an entirely new geometry, which we have christened 'Y-shaped'. In this configuration molecules direct hydrogen atoms towards the π-orbitals themselves, rather than towards the centre of the aromatic ring.



▶ A slight shift in molecule orientation affects how the benzene molecules interact chemically with other molecules such as proteins. The 'T-shaped' arrangement has a single hydrogen atom pointing into the centre of the pair benzene molecule. The 'Y-shaped' arrangement is slightly rotated so that two hydrogen atoms are pointing to the other molecule's delocalised electron ring.

Back to square one: rethinking chemistry

… the time window accessed by the ISIS spectroscopy suite spans eight orders of magnitude, from attoseconds to hundreds of picoseconds. Larmor, one of the next instruments planned for the Second Target Station, will boost current capabilities by an additional factor of 1000, approaching the microsecond domain.

Towards controlled proton transfer: **tuning proton behaviour in a ternary molecular complex**

LH Thomas, AA Kallay, A Parkin, CC Wilson (Glasgow and Bath Universities), N Blagden (Bradford University), CC Seaton (Manchester University), MJ Gutmann (ISIS)

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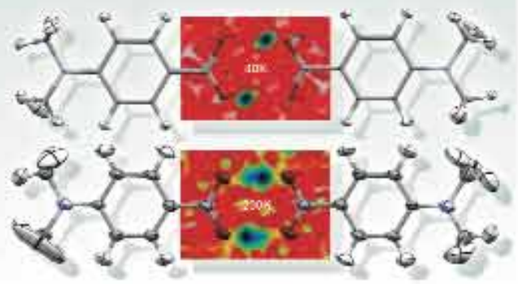
Further reading:

LH Thomas et al., Cryst Growth Design 10 (2010) 2770

Intermolecular proton transfer through hydrogen bonds has wide-ranging implications in fields as diverse as ferroelectrics, electrochemical processes, and enzymatic activity. In the solid state, the environment around a hydrogen bond is known to alter the behaviour of the proton, leading to effects such as proton disorder or migration across bonds as a function of temperature. However, it is difficult to control and predict when this may happen. 4-dimethylaminobenzoic acid (4DABA) contains dimeric building blocks in its pure form and also exhibits hydrogen disorder.However, introducing the second component 3,5-dinitrobenzoic acid into the crystalline lattice removes this disorder within the 4DABA unit. Using SXD at ISIS, we have shown that introducing a third component, 4,4'-bipyridine, further perturbs the local environment, and hydrogen disorder is again observed. These results show that the behaviour of hydrogen atoms can be tuned by modifying the molecular and crystalline environment around the 4DABA dimer building block, with implications for the general control of proton transfer processes.

▼ Temperature evolution of hydrogen disorder in 4-dimethylaminobenzoic acid dimer embedded in a ternary molecular complex.



Twists, bends, and stretches in $Li(NH_3)_4$, **the lightest metal known**

MTJ Lodge, PP Edwards (Oxford University), WIF David, AJ Ramirez-Cuesta (ISIS)

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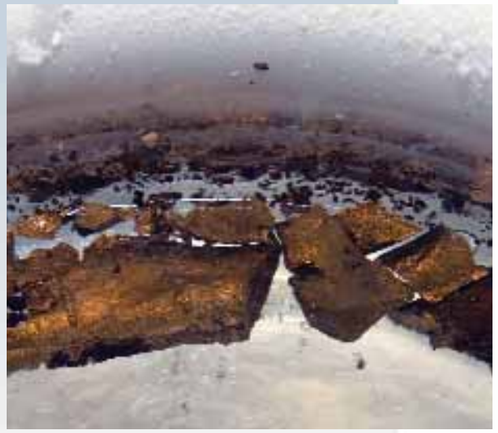
Further reading:

E Zurek et al., Ang Chem Int Ed 48 (2009) 8198

When alkali metals are dissolved in anhydrous liquid ammonia they give up their outer-shell electrons to the solvent producing solvated electrons and metal ions. At low metal concentrations, the solutions are electrolytic in nature and deep blue in colour. As the concentration is increased, the solutions transform to a fine bronze colour with metallic lustre.

Lithium-ammonia solutions are unique amongst the alkali metal systems in that they form a highly conductive crystalline compound $Li(NH_3)_4$ at low temperature.

The metallic nature of these systems makes recording of vibrational spectra particularly challenging! Our inelastic neutron scattering measurements on Tosca represent the first look into the vibrational modes of this fascinating metallic material, revealing unique insights into the vibrational characteristics of this molecular system, the lightest metal known.



▲ Metallic $Li(NH_3)_4$ photographed in liquid nitrogen in the open lab. This ultra-light bronze metal even floats!

Confinement phenomenon observed in **spin ladders**

B Lake (Helmholtz Zentrum Berlin, Technical University Berlin), **AM Tsvelik** (Brookhaven National Laboratory, USA), **S Notbohm** (Helmholtz Zentrum Berlin, St Andrew's University), **DA Tennant** (Helmholtz Zentrum Berlin, Technical University Berlin), **TG Perring** (ISIS), **M Reehuis** (Helmholtz Zentrum Berlin), **C Sekar** (Periyar University), **G Krabbes**, **B Büchner** (IFW Dresden)

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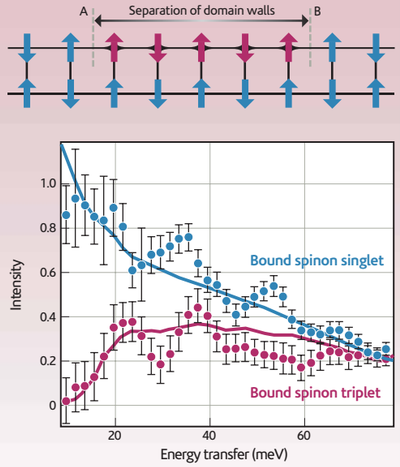
Further reading:

B Lake et al., Nat Phys 6 (2010) 50-55

Confinement is the binding of particles by an interaction whose strength grows with separation. The most famous example is that of three quarks confined by the strong nuclear force to form protons or neutrons. As this force becomes stronger with increasing separation, free quarks do not exist and can only be observed indirectly. An analogous confinement process is predicted in condensed matter systems known as spin ladders. Ladders consist of two parallel chains of spin-1/2 ions magnetically bonded together. A remarkable feature of a single chain is that the individual electrons separate into independent spin and charge parts. The spin parts, or spinons, have spin 1/2. By coupling two chains together to form a ladder, spinon pairs form composite spin 0 or 1 particles in a way analogous to how protons and neutrons emerge from quarks. This phenomenon was investigated on the spin-ladder compound $CaCu_2O_3$ where the interchain coupling is weak enough to allow the observation of confinement effects. Using Maps, the excitation spectrum was measured and found to agree well with the theoretical model, confirming the confinement picture.



▲ Top: Region between two spinons on a chain consists of reversed spins (red); reversed spins cost energy due to their parallel alignment with the spins on the neighbouring chain. Bottom: Bound spinon spectra. The lines are theoretical predictions for the weakly coupled ladder.

Strongly correlated **alkali fullerides**

K Prassides (Durham University), **MJ Rosseinsky** (University of Liverpool), **PJ Baker** (ISIS)

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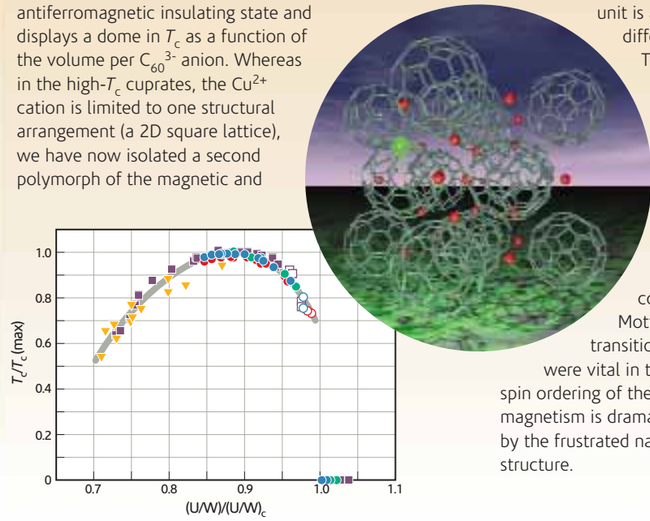
Further information:

AY Ganin et al., Nature 466 (2010) 221

Alkali-doped fullerides are the simplest type of high-T_c superconductors. In the hyperexpanded bcc-structured A15 Cs_3C_{60}, superconductivity emerges upon applied pressure out of an antiferromagnetic insulating state and displays a dome in T_c as a function of the volume per C_{60}^{3-} anion. Whereas in the high-T_c cuprates, the Cu^{2+} cation is limited to one structural arrangement (a 2D square lattice), we have now isolated a second polymorph of the magnetic and superconducting fulleride Cs_3C_{60} with an fcc structure. This enables a comparison between these two cooperative electronic states when the same electronically active unit is arranged differently in space. The dominant role of electron correlations is then shown by a simple structure-independent scaling of T_c according to proximity to the correlation-driven Mott metal-insulator transition. ISIS muons were vital in the discovery of spin ordering of the fcc variant, where magnetism is dramatically suppressed by the frustrated nature of the lattice structure.



▶ Universal trend in the superconducting transition temperature as a function of the proximity to the Mott transition. The inset shows a muon (green) implanted in fcc Cs_3C_{60}.

Weird is beautiful: strongly correlated quantum matter

… it is possible to perform measurements from 20 μeV up to 80 meV with a continuous position-sensitive detector coverage of 1 steradian, and up to 9 Tesla magnetic field. All this on just one instrument – LET – not to mention the other spectroscopy instruments!

Quantum melting of magnetic order in an Ising spin chain

R Coldea (Oxford University), **DA Tennant** (Helmholtz Zentrum Berlin, Technical University Berlin), **EM Wheeler** (Oxford University), **E Wawrzynska** (Bristol University), **D Prabhakaran** (Oxford University), **M Telling** (ISIS), **K Habicht**, **P Smeibidl**, **K Kiefer** (Berlin)

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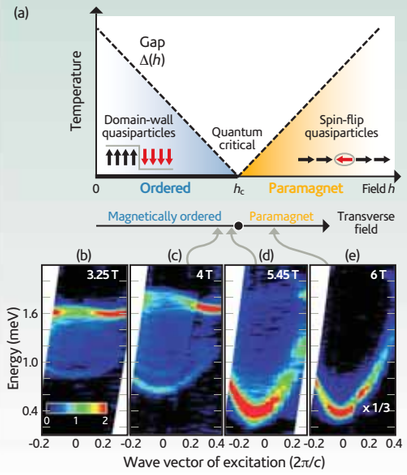
Further reading:

R Coldea et al., Science 327 (2010) 177

Quantum systems have zero-point fluctuations even at zero temperature. When such fluctuations become strong, they can drive transitions between distinct phases of matter.

One of the most theoretically studied paradigms for such a quantum phase transition is the one-dimensional (1D) chain of Ising spins in a transverse magnetic field. The field stimulates quantum tunneling between the 'up' and 'down' spin orientations and, above a critical field, these quantum fluctuations become strong enough to 'melt' the spontaneous magnetic order and stabilise a paramagnetic state.

We have realised this system experimentally for the first time by applying strong magnetic fields to the quasi-1D Ising ferromagnet $CoNb_2O_6$. Using high-resolution single-crystal neutron scattering on Osiris and Iris we have observed a dramatic change in the fundamental quantum character of spin quasiparticles as the magnetic field quantum melts the spontaneous magnetic order. Our results emphasise that quantum criticality opens up new avenues to experimentally realise and explore otherwise inaccessible and novel correlated quantum states of matter.



▶ Top: Schematic phase diagram and cartoon of the spin excitations in the ordered and paramagnetic phases of $CoNb_2O_6$. Bottom: Evolution of the spin excitation spectrum as a function of applied field.

Magnetic excitation spectrum of $Fe_{1+y}Te_{1-x}Se_x$

MD Lumsden, AD Christianson, SE Nagler, HA Mook, C de la Cruz, MB Stone, DL Abernathy, GJ MacDougall, AS Sefat, MA McGuire, BC Sales, D Mandrus (Oak Ridge National Laboratory, USA), EA Goremychkin (ISIS, Argonne National Laboratory), T Guidi (ISIS)

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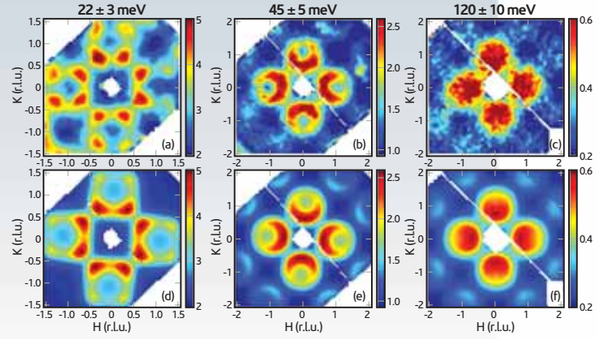
Further information:

MD Lumsden et al., Nat Phys 6 (2010) 182

The recent discovery of superconductivity with T_c up to 55 K in Fe-based materials has generated much excitement, yet the mechanism underpinning superconductivity in these 'unconventional' superconductors remains elusive. Of the mechanisms proposed, spin-fluctuation-mediated superconductivity is among the most promising. As such, studies of magnetic excitations by means of inelastic neutron scattering are crucial. The simple crystal structure and availability of large crystals makes $Fe_{1+y}Te_{1-x}Se_x$ particularly interesting. We have performed detailed inelastic neutron scattering studies of the magnetic excitations in $Fe_{1+y}Te_{1-x}Se_x$ crystals with x=0.27 (non-superconducting) and x=0.49 (superconducting). These measurements reveal incommensurate 2d magnetic excitations up to energies of at least 300 meV. The spectrum exhibits four-fold symmetry about the (π,π) wave vector showing that a square lattice constitutes the fundamental unit cell for the magnetic interactions, as also found in the cuprates. The presence of incommensurate excitations and their evolution with energy are also similar to previous observations in the cuprates, which may suggest a common origin of superconductivity in both classes of materials.



▲ Constant-energy plots of the magnetic excitations projected onto the H–K plane for the x=0.27 sample (panels a-c) as measured on Merlin. Panels d-f are fits to the data.

Tomorrow is today: materials for emerging technologies

… many experiments, from catalysis to gas storage, batteries to fuel cells, need to measure a physical property (e.g., conductivity, weight change, gas uptake, or Raman spectrum) in conjunction with the collection of neutron and muon data. All of the above are possible at ISIS.

Metal-organic polyhedral frameworks by powder neutron diffraction

IPL Telepeni, GS Walker, Y Yan, X Lin, M Schröder (Nottingham University), W Kockelmann (ISIS)

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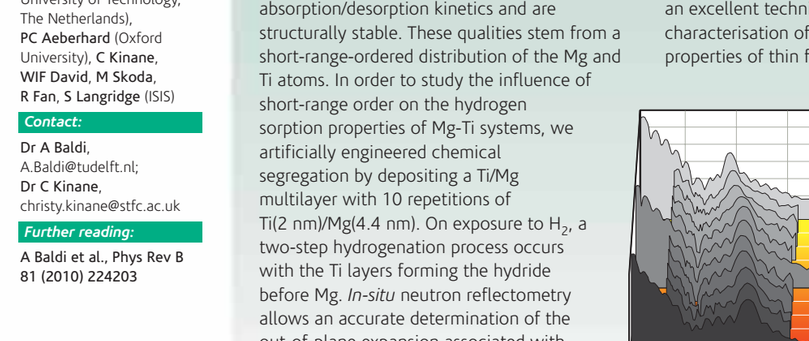
Prof GS Walker, Gavin.Walker@nottingham.ac.uk

Further information:

Y Yan et al., J Am Chem Soc 132 (2010) 4092

Metal-organic frameworks (MOFs) are excellent candidates for solid state hydrogen storage. Our aim was to determine the preferred position of hydrogen adsorption sites within one of the most promising Cu-MOFs: NOTT-112. The intrinsic scattering properties of hydrogen and its isotopes make neutron powder diffraction a useful tool for monitoring the hydrogen adsorption mechanism. The sample was exposed to aliquots of D_2 gas at 50 K allowing us to populate sequentially different adsorption sites. Data were collected after each dosing on Gem. The figure shows the adsorption site distribution revealing positions within NOTT-112. For the first time, we have been able to demonstrate preferential adsorption to the two Cu atoms in the paddlewheel coordination unit (the sorption site within the cage) filling before the exo-cage site (i.e. A_1 and A_2). Future work will apply inelastic neutron scattering techniques with the same experimental procedure in order to investigate the nature of the interaction between the hydrogen molecule and these two Cu sites.



▲ D_2 sites in NOTT-112 cages A (a) and B (b). (c) shows five possible D_2 sites: A_1, lavender; A_2, blue; A_3, yellow; A_4, orange; A_5, green.

Hydrogen absorption in Ti/Mg multilayers studied by neutron reflectometry

A Baldi, H Schreuders, B Dam, R Griessen (Delft University of Technology, The Netherlands), PC Aeberhard (Oxford University), C Kinane, WIF David, M Skoda, R Fan, S Langridge (ISIS)

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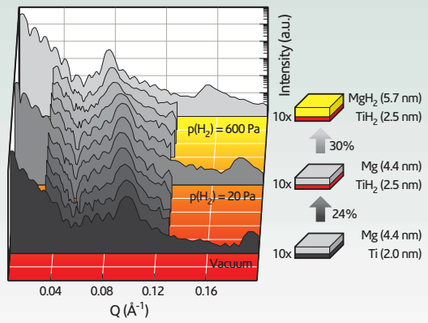
Dr A Baldi, A.Baldi@tudelft.nl; Dr C Kinane, christy.kinane@stfc.ac.uk

Further reading:

A Baldi et al., Phys Rev B 81 (2010) 224203

Mg-Ti thin film alloys have large hydrogen storage capacities, fast hydrogen absorption/desorption kinetics and are structurally stable. These qualities stem from a short-range-ordered distribution of the Mg and Ti atoms. In order to study the influence of short-range order on the hydrogen sorption properties of Mg-Ti systems, we artificially engineered chemical segregation by depositing a Ti/Mg multilayer with 10 repetitions of Ti(2 nm)/Mg(4.4 nm). On exposure to H_2, a two-step hydrogenation process occurs with the Ti layers forming the hydride before Mg. *In-situ* neutron reflectometry allows an accurate determination of the out-of-plane expansion associated with each hydrogenation step. The volume expansion expected for the hydrogenation of both Ti and Mg is transferred completely along the vertical direction, indicating that large plastic deformations have to occur upon hydrogen uptake. Owing to the large negative neutron scattering length of hydrogen, neutron reflectometry proves to be an excellent technique for the *in situ* characterisation of the hydrogen absorption properties of thin films.



▲ Neutron reflectometry patterns measured during the hydrogenation of a 10x{Ti/Mg} multilayer at 333 K in vacuum and after exposure to 20 and 600 Pa of H_2.

Tipping the magneto-elastic balance

A Barcza (Cambridge University), Z Gercsi (Imperial College London), KS Knight (ISIS), KG Sandeman (Imperial College London)

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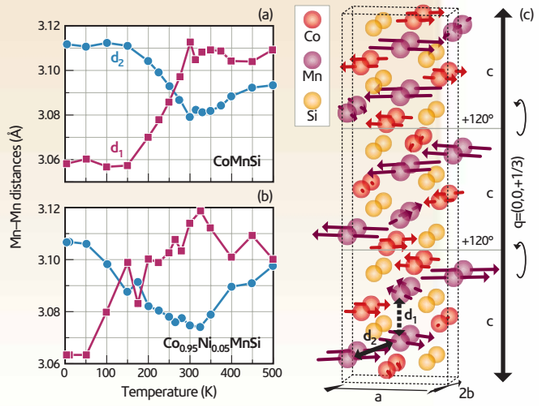
Further information:

A Barcza et al., Phys Rev Lett 104 (2010) 247202

'Smart' materials display a plethora of potentially useful properties, and these can interact with each other giving rise to new phenomena. In magnetic systems such as ferrromagnetic shape memory materials and magnetic refrigerants, magnetism and crystal structure are intimately linked with each other; that is, a change in one can alter the other.

This feedback mechanism – known as magneto-elastic coupling – is usually quite weak, with atomic separations changing by fractions of a percent as the temperature of the material changes. However, using the high resolution powder diffractometer (HRPD) at ISIS, we see that the separation of magnetic centres in CoMnSi can change by up to 2% as it is heated.

Such large changes in crystal structure have urged us to postulate a novel mechanism for large magneto-elastic coupling. We conclude that the manganese atoms experience a competition between energetically similar magnetic states resulting in quite different atomic separations. Thus, temperature (or magnetic field) can 'tip the balance' in these novel materials.



▼ Temperature dependence of Mn-Mn nearest-neighbor distances in (a) CoMnSi and (b) $Co_{0.95}Ni_{0.05}MnSi$. Crystallographic positions are shown in (c), together with the closest commensurate version of the helical spin Co and Mn sublattices.

Magnetricity

SR Giblin (ISIS), ST Bramwell, S Calder, R Aldus (University College London), D Prabhakaran (Oxford University), and T Fennel (ILL)

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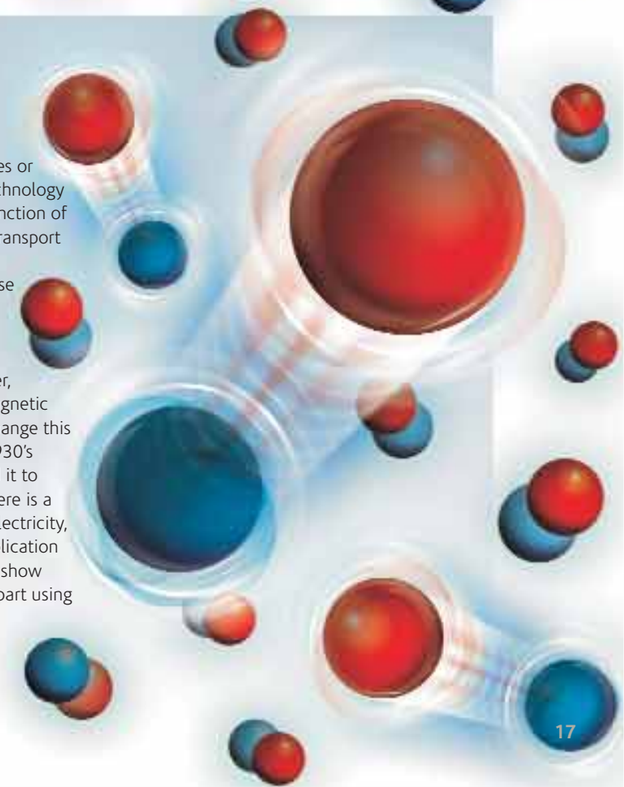
Further information:

ST Bramwell et al., Nature 461 (2009) 956

The transport of electrically charged quasiparticles (based on electrons, holes or ions) plays a pivotal role in modern technology as well as determining the essential function of biological organisms. In contrast, the transport of magnetic charges has barely been explored experimentally, mainly because magnetic charges are generally considered to be, at most, convenient macroscopic parameters rather than sharply defined quasiparticles. However, the recent proposition of emergent magnetic monopoles in certain materials may change this point of view. We have dusted off a 1930's theory of electrochemistry and applied it to demonstrate that in some materials there is a magnetic equivalent of electricity. In electricity, charges can be driven apart by the application of an electric field. We used muons to show that magnetic charges can be driven apart using magnetic fields, creating a magnetic current.



▶ Magnetic charge moving apart under the influence of an applied magnetic field.

Characterisation of **nickel-based superalloys** as used in aero-engine turbine discs

DM Collins, HJ Stone (Cambridge University), RK Heenan (ISIS)

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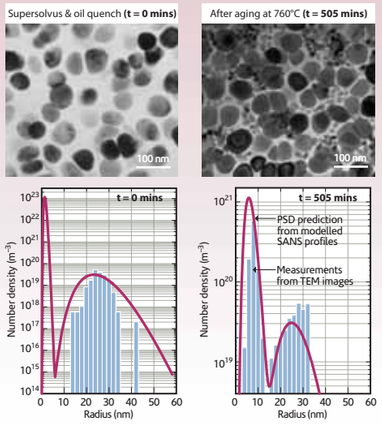
Further information:

DM Collins, Met Trans A (accepted, 2010)

Nickel-based superalloys are a family of materials designed to exhibit both exceptional mechanical properties and superior corrosion resistance at very high temperatures. Typically, they are the material of choice for the most demanding applications in modern gas turbines.



▶ ***Top:*** Transmission electron images of carbon replicas used to image the γ' precipitates in RR1000 at the start and end of the heat treatment. ***Bottom:*** measured particle size distributions and SANS predictions.

The presence of γ′ Ni_3(Al,Ti,Ta) precipitates accounts for their exceptional material performance. The precipitate size and distribution are carefully controlled by heat treatments during manufacturing so as to attain optimal properties.

To investigate γ′ particle size distributions, microscopy is often used, though this technique can only be used before and after heat treatment. An in situ experiment investigating the temporal evolution of γ′ particle size distributions in a RR1000 nickel-based superalloy during aging at 760°C has been performed using small angle neutron scattering (SANS) on LOQ. Due to the high γ′ volume fraction, our data analysis had to account for the scattering from both within and between each distribution. The SANS results will help to validate computer models of precipitates and improve our understanding of these important class of alloys.

Structural studies of **Ca-Mg-Zn bulk metallic glasses**

ON Senkov, DB Miracle (Air Force Research Laboratory), YQ Cheng, E Ma (John Hopkins University), ER Barney, and AC Hannon (ISIS)

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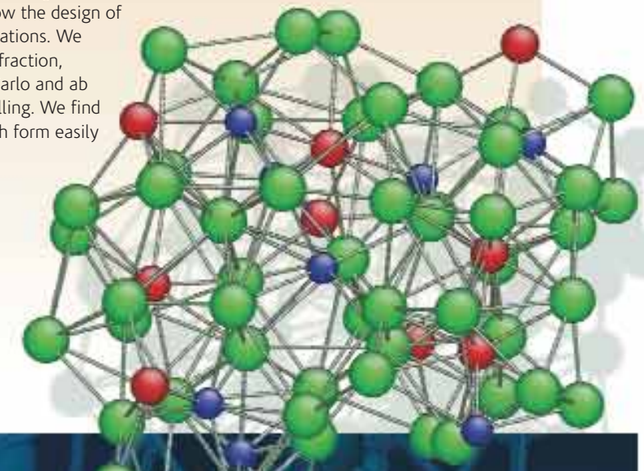
Further information:

ON Senkov et al., Phys Rev B 82 (2010) 104206

Bulk metallic glasses have unique properties which offer potential developments for a wide range of technological applications. CaMgZn glasses have extremely good glass-forming ability, whilst exhibiting low densities (1.6 – 2.4 g/cm^3) and extremely low Young's (~20-30 GPa) and shear (~9-14 GPa) moduli. Relating the structural characteristics of these glasses to their physical properties will allow the design of new materials for specific applications. We have used neutron and X-ray diffraction, combined with Reverse Monte Carlo and ab initio molecular dynamics modelling. We find that those CaMgZn glasses which form easily have zinc- and magnesium-centred clusters, around which calcium atoms are packed efficiently to give high coordination numbers. As the composition of the glass is altered, the arrangement of the atoms in the clusters changes dramatically. A decrease in the glass-forming ability is linked to the formation of clusters similar to those found in Ca_2Cu crystals, as well as to an increase in Zn-Zn clustering.

▼ Zinc (blue) and magnesium (red) centred clusters formed by the close packing of calcium atoms (green) in the $Ca_{60}Mg_{20}Zn_{20}$ glass.



Knowing is doing: enabling technologies

… ISIS scientists develop new processes, technologies, and equipment in close collaboration with a wide range of industrial R&D teams in the UK and abroad, from small and medium enterprises to large multinational corporations.

Low-temperature cryogenics based on pulse-tube technology

CR Chapman, BE Evans, MP Dudman, J Keeping, RBE Down, O Kirichek, ZA Bowden (ISIS)

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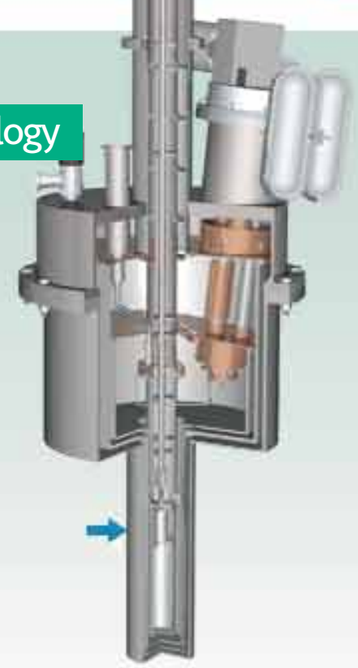
Further information:

Cryogenics, submitted

Every large neutron facility uses liquid helium cryostats for scattering experiments at very low (cryogenic) temperatures. The ISIS Sample Environment Group has designed, assembled, and successfully tested a prototype of a liquid-cryogen-free system based on a pulse-tube refrigerator. Equipped with a 50 mm diameter top-loading port for neutron scattering experiments, the sample temperature range achieved in our tests is 1.35 – 300 K, with a maximum cooling power of 55 mW at 1.8 K. All cryostat parameters are similar to those of the classic 'Orange' cryostat, yet this system does not require any liquid cryogens. This new cryostat design can also house ultra-low temperature inserts such as the Kelvinox VT dilution refrigerator, so as to reach temperatures as low as 30 mK.



▲ Cryogen free top-loading cryostat based on a pulse-tube refrigerator. The arrow indicates the height of the beam.

Prize-winning **accelerator diagnostic systems**

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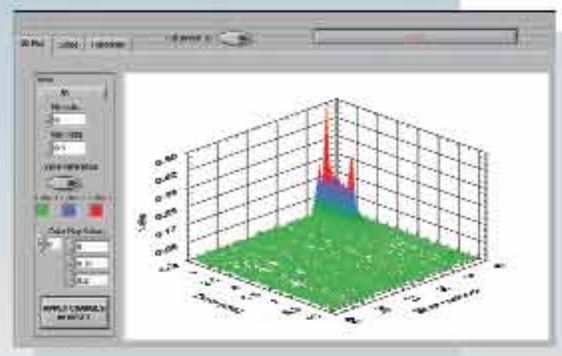
Further reading:

The ISIS Proton Synchrotron: Beam Data Acquisition and Analysis Using NI PXI and LabVIEW (http://sine.ni.com/cs/app/doc/p/id/cs-12422)

The ISIS synchrotron accelerates a beam of 2.8 x 10^{13} protons to 85% of light speed, 50 times per second. Each cycle lasts 10 ms, during which the beam makes 12,000 revolutions in a 163 m circumference, with the proton energy gradually rising from 70 to 800 MeV.

The amount of beam the synchrotron can accelerate is limited by beam losses. A new monitoring system has been developed to analyse data from thirty-nine gas ionization tubes distributed around the synchrotron. Beam losses are identified in individual monitors at any time during acceleration.

Accurate determination and correction of the position of the proton beam is also a major factor in reducing losses. To this end, data acquisition and analysis systems for the fourteen horizontal and seventeen vertical beam position monitors have been installed in the synchrotron. The new system can closely monitor and correct the beam position to within 2 mm of the machine centre.



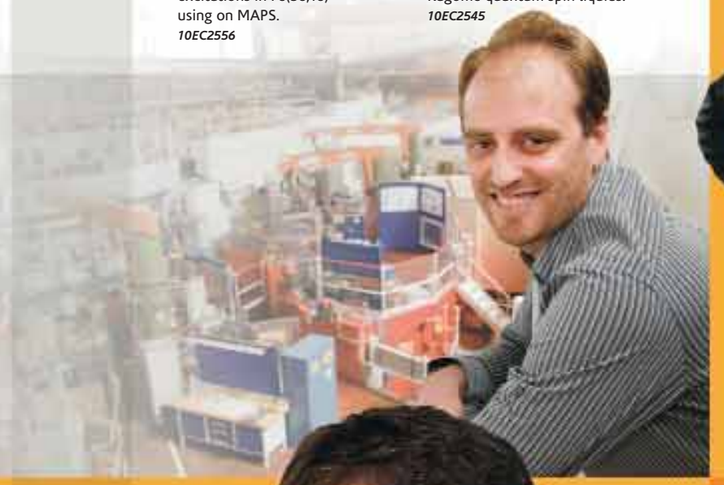
▲ LabVIEW-based user interface displaying beam loss levels in the synchrotron.

These developments have helped set new records for maximum beam current from the ISIS synchrotron. The record average current for 24 hours of operation now stands at 217.1 μA.

ISIS users at work

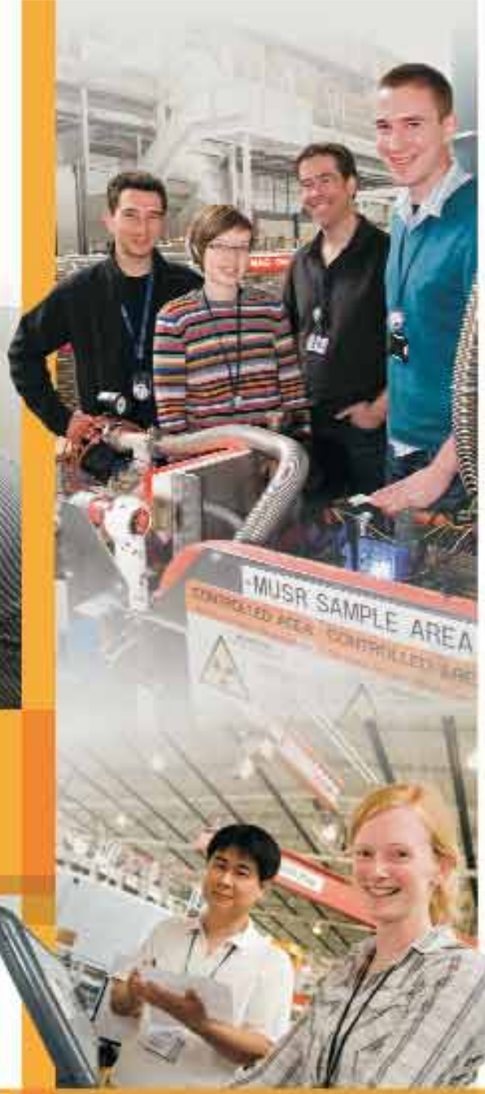
◀ Bella Lake, Alan Tennant and Elisa Wheeler (Helmholtz Zentrum Berlin) using Mari and Merlin to determine orbital ordering in ZnV_2O_4. ***10EC2515***

▼ Andrew Hodgson, Fiona McBride (Liverpool University) and Carla Andreani (Università di Roma – Tor Vergata) studying the proton momentum distribution in oriented ice films on Vesuvio. ***10EC2555***

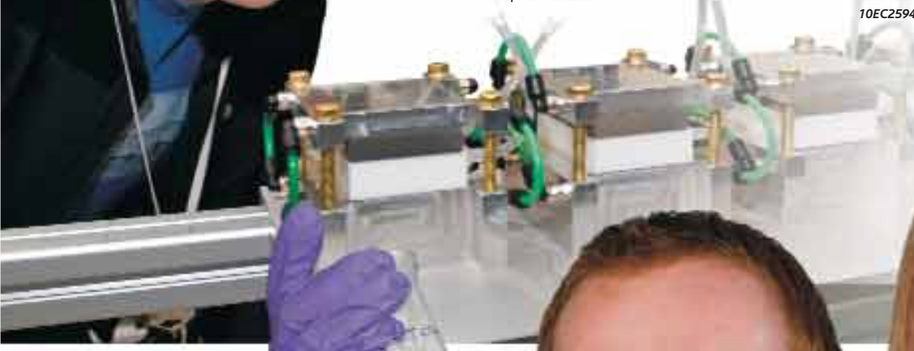


▼ Andrew Christianson (Oak Ridge National Laboratory, USA) prepares to examine high energy magnetic excitations in Fe(Se,Te) using on MAPS. ***10EC2556***

▶ Ross Colman, Andrew Wills (University College London), Fabrice Bert (CEA-Saclay) and Laura Fenner (Université de Paris-Sud) using MuSR to continue their studies on Kagome quantum spin liquids. ***10EC2545***



◀ Simon Titmuss (Oxford University) employing off-specular reflectivity to probe the characteristic lateral length-scales in responsive polyelectrolyte brushes on Offspec. ***10EC2530***

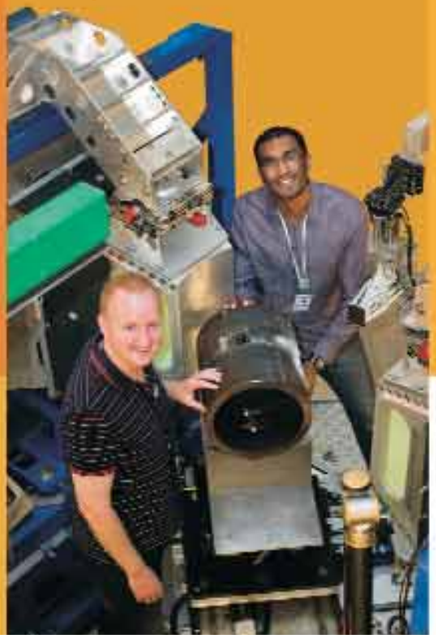


▼ Jacqueline Edge and Michael Wilkinson (UCL) making preparations for studies of the dynamics of an important water soluble pesticide molecule, paraquat, in solution and in hydrated clay on IRIS. ***10EC2594***

▲ Andrew Quirk (Newcastle University) preparing samples for Polref studies of the assembly of antibody binding proteins as part of a programme to develop wireless medical diagnostic sensors. ***10EC2533***

▶ Sanjooram Paddea and John Francis (Open University) using Engin-x to measure residual stress distributions and stress relaxation due to post weld heat treatment in P91 (9Cr-1Mo) steel welds. ***10EC2573***

▲ Samantha Callear (ISIS) and Kazuya Kamazawa (Toyota, Japan) performing in-situ inelastic neutron spectroscopy studies of metal-hydride hydrogen storage materials on Tosca. ***10EC2587***



Technology and training

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

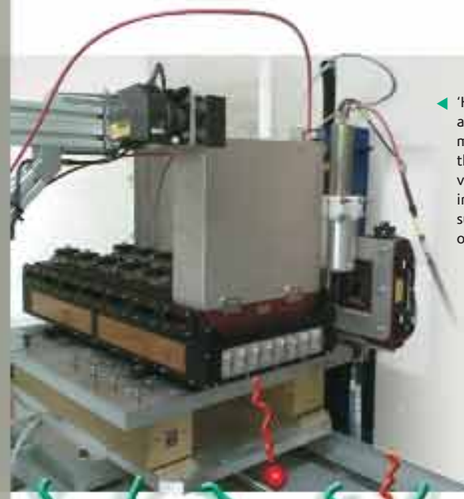
The past year has seen first users on several new ISIS instruments, and a variety of other technique and instrument enhancements. Alongside technical development comes a wide range of education and training activities – from training courses and workshops for the user community, to projects run with teachers and schools.

▶ Emma McCabe (Durham University) preparing her oxyselenide sample to examine its crystal and magnetic structures on HRPD. *10EC2525*

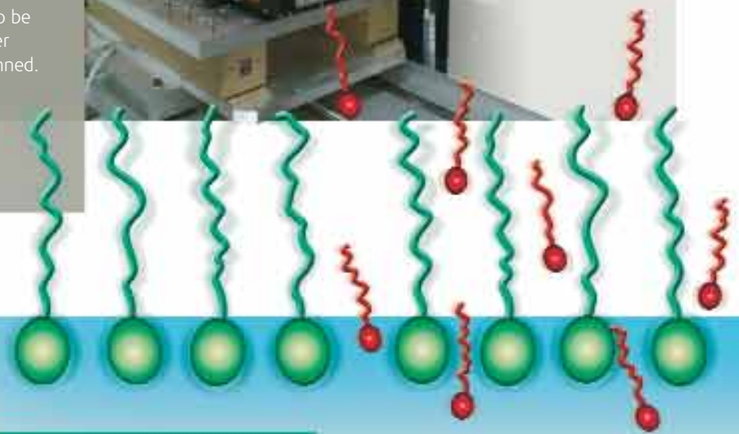
Technology and training

Inter

Over the past year, Inter has hosted a range of experiments from electrochemistry to biocompatible surfactants and 'designer' DNA adsorption. A new stream of research enabled by the reflectometer has been the study of kinetics and complexity. As an example, the figure shows a recent experiment to measure the evaporation of volatile molecules incorporated into surfactant layers. Inter's high flux allows the kinetics of such transport mechanisms to be investigated with a time resolution better than 30s, with further improvement planned.



◀ 'Head space' apparatus for measurement of the evaporation of volatile molecules incorporated into surfactant layers on Inter.



▶ Studies of the incorporation of volatile molecules into surfactant layers on Inter.

▼ First users of Offspec. David Bucknall (Georgia Institute of Technology and Oxford University), Jinhyun Hannah Lee and Zamri Radzi (Oxford University) with Rob Dalgleish (ISIS) investigating hydrogels for their prospective role in cleft pallet repair. ***09EC3928***

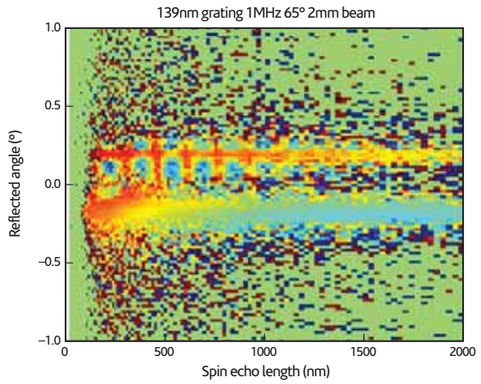
Science with Second Target Station instruments

Polref

◀ Soumya Ray and Steve Lister (University of St Andrews) using Polref to study the interaction between superconductivity and magnetism in iron-lead thin films. The newly commissioned 3D vector cryomagnet is visible behind them. Polref is a neutron reflectometer exploiting state of the art sample environment and flexible polarisation to study a wide range of nanomagnetic and superconducting systems. It delivers significantly reduced data acquisition times compared to current instrumentation. Increasingly, the instrument also enables the application of polarised neutrons to studies on soft matter and biology resulting in important improvements in data analysis.
10EC2562

Offspec

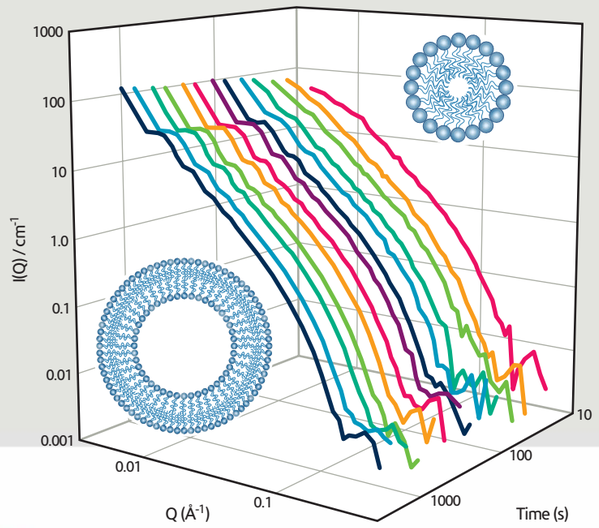
Offspec has started its user programme with successful experiments in both Spin Echo Small Angle Neutron Scattering (SESANS) and Spin-Echo Resolved Grazing Incidence Scattering modes (SERGIS), the only regularly operating user instrument in the World with these techniques. Grating samples have shown that it is possible to access length scales of order 100 nm for some samples. In standard reflectivity mode, using two incident angles and a resolution of ~3%, measurement times of around 1 hour produce high quality data with extremely low background.



▲ Offspec SERGIS data from a 139nm repeat silicon grating.

Sans2d

Commissioning of the Sans2d beam line started in the summer of 2009 and has continued in parallel with an initial user program and development of new data reduction software. Recently, complex sample environment, such as shear, pressure and stopped-flow cells, has started to be used.

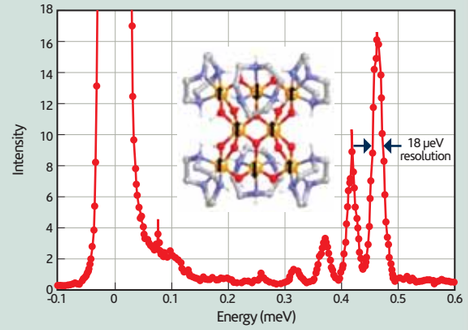


▶ Stopped-flow kinetic data taken on Sans2d (collaboration with TU-Berlin). The data show a micelle-vesicle transition followed by an increas in vesicle monodispersity measured with 15s time resolution.

Science with Second Target Station instruments

LET

LET has completed the commissioning of all seven disk choppers, and 4 detector panels out of the final detector complement of 12. The massive 4 m long detectors perform excellently with a 20 mm position resolution along the length and very low background noise. The first inelastic measurements, performed in May 2010, confirmed the top class performance in good agreement with simulations.

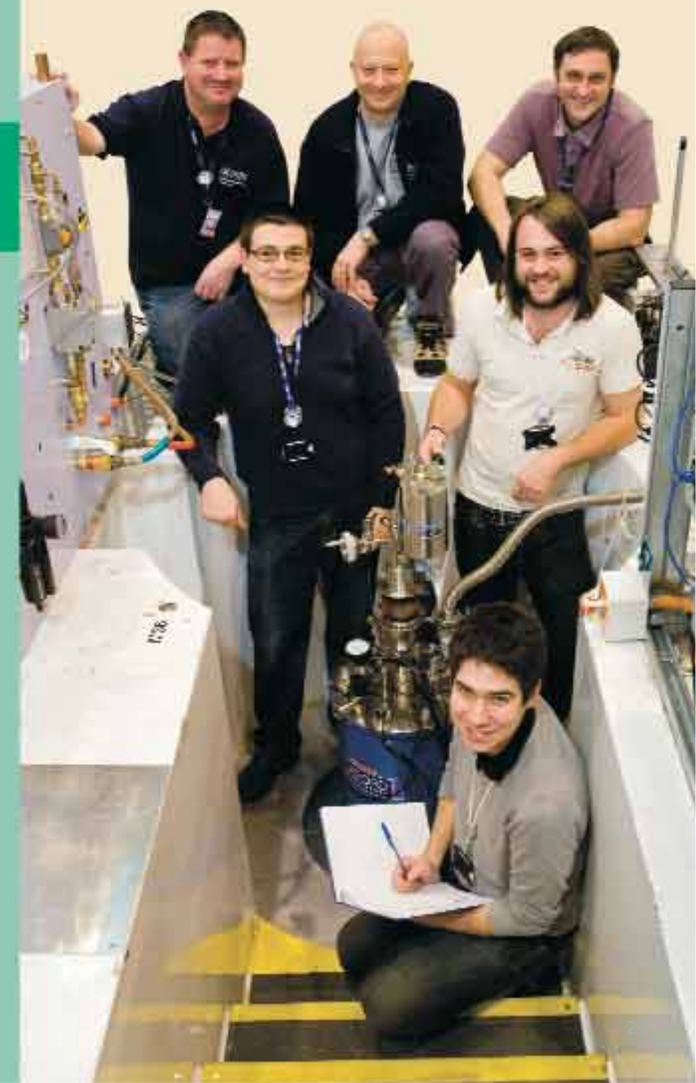


▲ LET measurements of excitations in the Fe_8 single molecule magnet demonstrating the instrumental resolution.

Wish

From the moment it received beam in June 2009, the Wish diffractometer started producing very high quality data. The high cold neutron flux, good Q-resolution and low background have already made an impact in the study of magnetic systems with weakly ordered moments which had not been resolved anywhere previously (as low as 0.1 μ_B) and routinely allow work on 100 mg samples. On larger samples, a collection time of minutes provides good statistics for Rietveld refinement. Wish is also used in areas such as hydrogen storage materials with large unit cells. The first experiment using the dedicated 14T cryomagnet gave excellent results, showing that the radial collimator eliminates the Al contamination in a wide angular range.

▼ The team for the first Wish experiment. Roger Johnson and Tom Frawley (Durham University) working with Pascal Manuel and Dmitry Khalyavin, Wish instrument scientists, and Jeff Keeping and Richard Down of the ISIS user support group, to determine the magnetic structures of Er_2CoGa_8 and Tm_2CoGa_8. ***09EC4179***



Nimrod

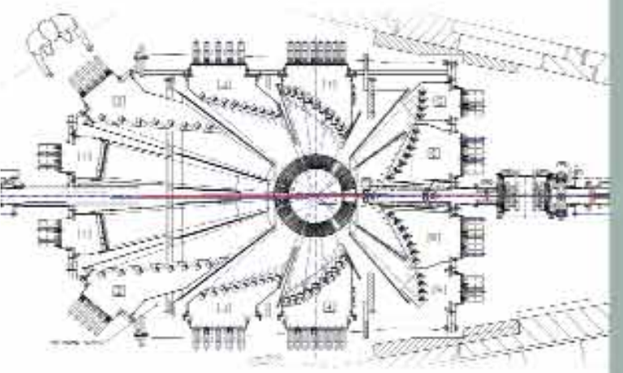
Nimrod has been developed for atomic-resolution structural characterisation of liquid and disordered material systems on a single continuous measurement length scale up to tens of nanometres. The instrument is built around a pixellated small angle detector bank that consists of 756 neutron scintillation elements, fibre-coupled to an array of 120 photomultiplier tubes. This array covers scattering angles of 0.5°-2.2°, which in combination with the instrument's wider angle detector modules, allow Nimrod to access a Q-range from 0.02Å^{-1} to 50Å^{-1} giving a structural resolution of 0.1Å out to length scales of 300Å. This performance is unique in the world.

◀ Beau Webber (University of Kent, right) was the first user on Nimrod. He is seen here with Daniel Bowron and Alan Soper (ISIS) during their experiment to study the wall structure of pores in templated silcas. ***09EC3548***

Advances in instruments and techniques

Polaris

Polaris will be completely upgraded during the ISIS 2010 long shutdown. When complete, its 38 modules of fibre-coupled scintillation detectors will contain some 400,000 m of fibre optic light guide and will give Polaris a gain of up to a factor of 20 in count rate. Manufacture of the main vacuum tank at Cadinox has been completed, and production of the Debye-Scherrer collimator is currently underway at RAL.



▲ The upgraded Polaris will have a primary flight path of 14 m. Thirty eight detector modules will give a total coverage of ~44% of the maximum possible solid angle.

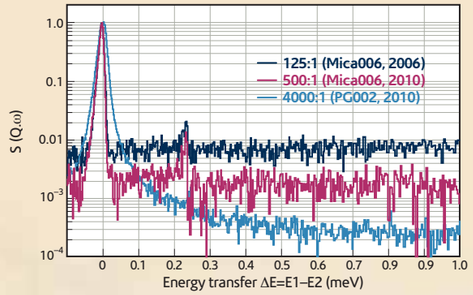
Pearl

During the long 2010 ISIS shutdown the high pressure neutron diffraction facility, Pearl, will undergo a major upgrade. The aim is to provide the option of tuning the resolution of the diffraction data while maintaining as large as possible d-spacing range. To this end the full detector compliment is being replaced with a new design of ZnS scintillator detector developed in collaboration with Spain. The secondary flight path is being slightly increased and, combined with the new detectors, this will improve the resolution and the counting stability of the instrument. In addition, a new incident beam collimation system is being installed which will enable neutron flux to be traded for a further increase in resolution. This project is being funded by the Spanish government and being designed and constructed by ISIS in partnership with AVS and Scientifica in Spain.

▼ Olatz and Natxo Carrera with the Pearl 90° detector in production at Scientifica, Deba, Spain.

Iris detector upgrade

The detector bank upgrade on the Iris spectrometer was successfully completed in May this year. Following the installation and commissioning of the detector manifold for the pyrolytic graphite bank in March 2008, the upgrade of the detectors for the mica bank is now also finished. Iris is now equipped with state-of-the-art detector electronics and new photomultiplier manifolds with μ-metal shielding to avoid stray field interference from magnet operation on Osiris. We see a much increased detector stability, a strong reduction in stray fields and, in the case of the Mica bank, significant improvements in signal to noise.



▲ Iris results from a vanadium calibration standard for the new mica detector bank, showing improved signal-to-noise and resolution.

▲ Helen Jarvie (Centre for Hydrology and Ecology), Steve King (ISIS), pictured here, and Jayne Lawrence (King's College London) have been looking at the behaviour of man-made nanoparticles in sewage treatment processes. Because sewage contains potentially harmful bacteria and viruses, ISIS engineers designed and constructed a robust hermetically-sealed containment vessel for the LoQ small angle neutron scattering experiment. ***09EC3847***

EMU Upgrade

This year has seen a significant upgrade to the EMU muon spectrometer. EMU has been given a new detector array, with three times the number of detector elements providing significant improvements in data rates. It also has enhanced performance for small samples, and is now equipped for dilution refrigerator use. The new instrument has been commissioned and is performing extremely well.

◀ The refurbished EMU instrument provides three times the previous data rate together with other experiment improvements.

First users on HiFi

HiFi is the new ISIS high-field muon spectrometer. The instrument opens up new possibilities for muon studies at ISIS by providing an order of magnitude increase in applied field (up to 5T) compared with existing ISIS muon spectrometers. HiFi took four years to design and build. It is based around a state-of-the-art superconducting split-pair magnet that is cryogen-free and has very high field homogeneity. The instrument is now fully available to the ISIS user programme.

◀ First users on the HiFi muon instrument. (left to right) Dr Alan Drew, Dr Laura Nuccio, Leander Schulz, Maureen Willis (Queen Mary University of London) and Dr Iain McKenzie (ISIS) using the instrument to explore spin scattering processes in organic materials relevant to spintronics. ***09EC3991***

Advances in instruments and techniques

High fields and low temperatures

The combination of high magnetic field and ultralow temperatures is indispensable for a broad range of neutron scattering experiments. However, problems with the global helium supply have raised significant concerns about the affordability of conventional cryogenic equipment. Oxford Instruments, in collaboration with ISIS, have designed, produced and tested 9T and 14T superconducting magnets which can be combined with a dilution refrigerator producing a base temperature of 60 mK. The systems can be operated continuously with zero helium boil-off. This significantly reduces liquid helium consumption as well as having operational simplicity. The two magnets have been used on Wish and Merlin.

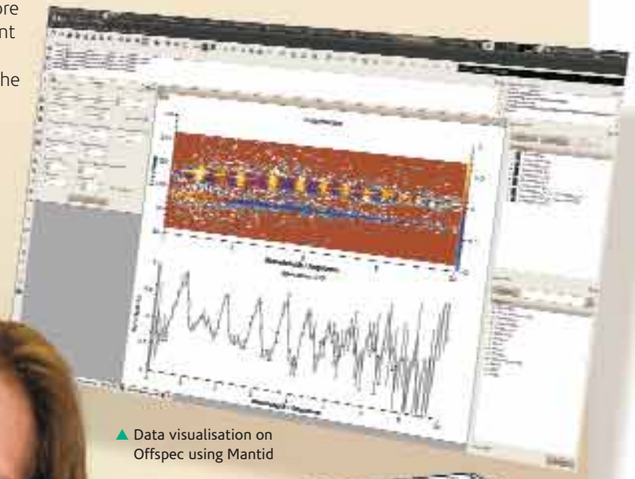
▶ Oleg Kirichek (ISIS) with the new superconducting magnet systems. *08EC3821*

Software

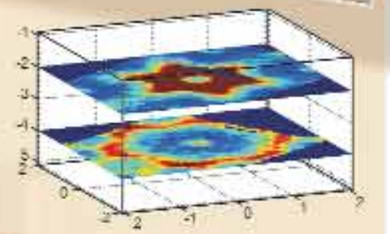
As ISIS instruments become more complex and capable of taking increasingly large data sets in a single run or across multiple runs, so tools for handling data also need to grow accordingly. ISIS has ongoing projects to ensure that software for data reduction and analysis keeps pace with instrument hardware developments.

Mantid is an open-source, multiplatform project for neutron data reduction, analysis and visualisation. The package supports an increasing number of ISIS instruments, soon to include all Crystallography instruments and progressively the instruments of the Excitations Group. It will eventually be used for all ISIS instruments. ISIS staff are working with developers from Tessella on the project, which now consists of more than 260,000 lines of code. Recently an agreement has been signed with the US Spallation Neutron Source for joint Mantid development – doubling the size of the development team. Mantid supports data reduction for the time-of-flight diffractometer EXED at the Helmholtz Zentrum Berlin, and the Institut Laue Langevin in France is also considering piloting Mantid over the next year.

A major sub-project within Mantid is the development of multi-dimensional visualisation software for inelastic and diffraction data. Exploring four dimensional data sets from the Merlin instrument, which can be as large as 100GB, is a challenge, and is one that is set to become greater as instruments such as LET and Wish come online. Capabilities will be built into Mantid to visualise such massive datasets using established open-source libraries that take advantage of multi-core and distributed computing environments. Model fitting of inelastic scattering data will also be integrated into the Mantid framework, allowing users to fit their own models or select from a models library.



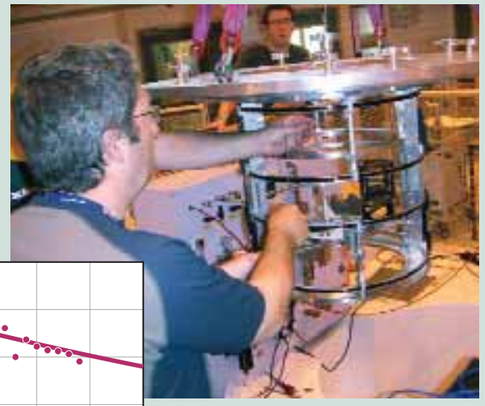
▲ Data visualisation on Offspec using Mantid



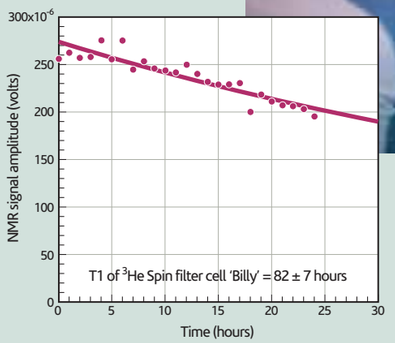
▲ Merlin data showing excitations in $YBaCo_4O_7$. The image shows a 3d plot at fixed energy extracted from the original 4d dataset.

Polarised Neutrons

The ISIS polarisation group is on course to deliver polarised neutron capability on both the LET and Wish instruments. This year saw the construction of the LET polariser and analysis systems, and the LET spin-filter cells, designed to reduce background contamination, are in production. A compact polariser and analyser insert has been constructed for use on Wish. Tests on the Wish beamline showed the device to be working well, with a ^{3}He spin-relaxation time of 82 hours. When the new ISIS ^{3}He optical pumping station is delivered early in 2011, we will be in a position to run wide-angle neutron polarization analysis experiments on both LET and Wish, adding a new dimension to the ISIS instrument suite.



▲ The polarisation analysis insert being lowered into the Wish sample tank.



◀ Plot showing a relaxation time of 82 hours for the ^{3}He cell in the Wish sample tank.

Biolabs

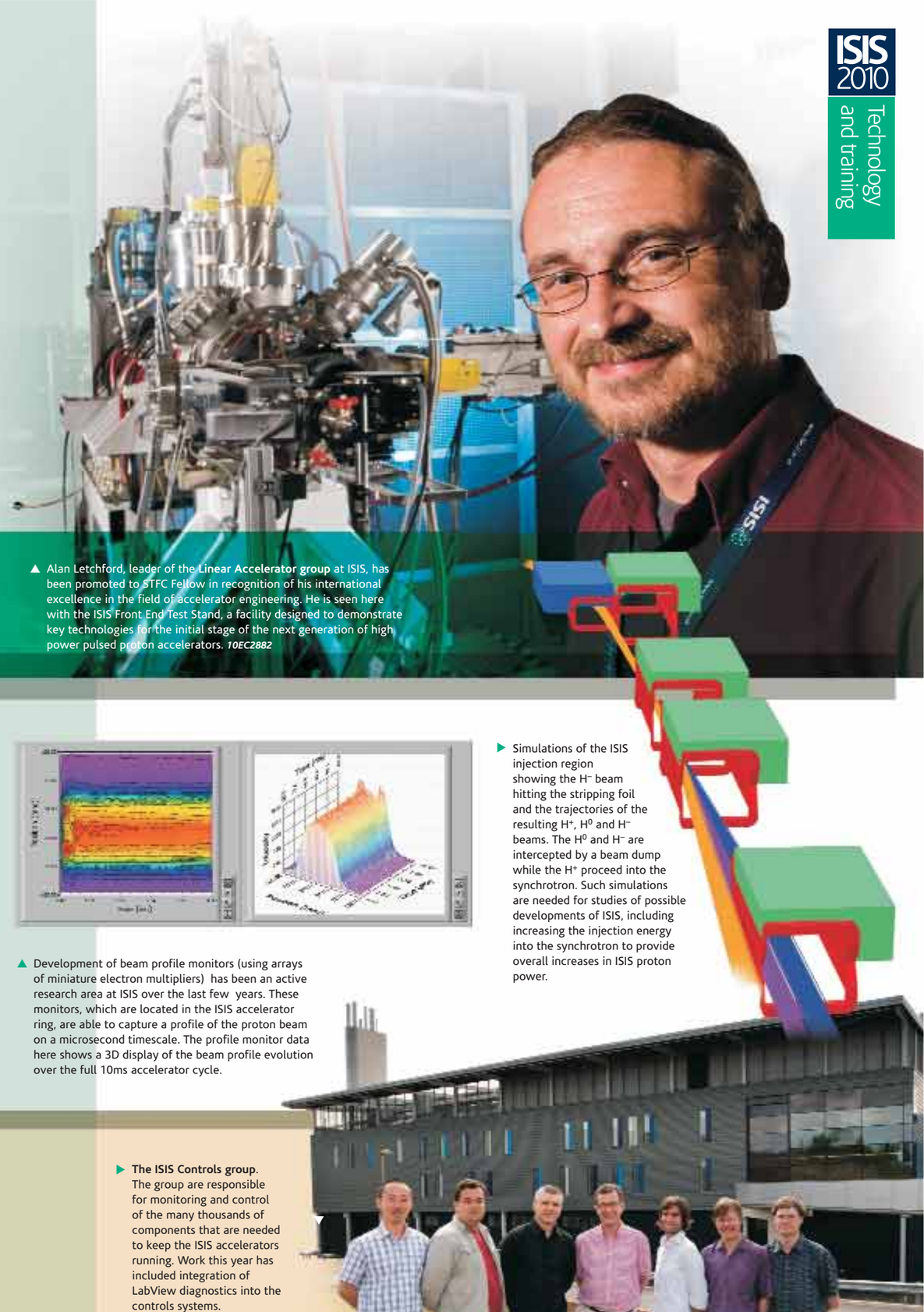
ISIS houses two biology Laboratories, one in each target station. Both labs provide basic biochemical, biological and biophysical facilities. They are equipped with general lab equipment as well as several more specialised instruments.

◀ Luke Clifton (ISIS) prepares for studies of bacterial membranes on Polref in an ISIS biolab. *10EC1962*

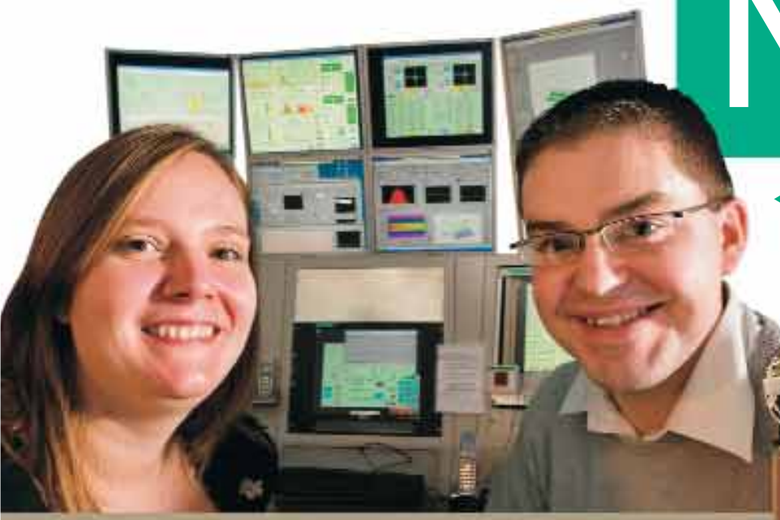
▲ Jim Ellis (ISIS) is monitoring power supplies for EPB2 magnets. ***09EC1453***

◀ The Second Target Station extracted proton beamline (EPB2) transports protons from the ISIS synchrotron to the Second Target Station hall. Steve Jago (ISIS) is seen here with quadrupole magnets for the EPB2 line which he designed. ***09EC1819***

Accelerator and Target News



▲ Alan Letchford, leader of the **Linear Accelerator group** at ISIS, has been promoted to STFC Fellow in recognition of his international excellence in the field of accelerator engineering. He is seen here with the ISIS Front End Test Stand, a facility designed to demonstrate key technologies for the initial stage of the next generation of high power pulsed proton accelerators. ***10EC2882***



◀ Bryan Jones and Sarah Whitehead of the **ISIS Diagnostics group**, pictured here in the ISIS control room, were awarded first prize in a competition run by National Instruments for their paper describing their work on ISIS synchrotron diagnostics. A highlight on Sarah and Bryan's work can be found on page19. ***09EC3834***

▲ Development of beam profile monitors (using arrays of miniature electron multipliers) has been an active research area at ISIS over the last few years. These monitors, which are located in the ISIS accelerator ring, are able to capture a profile of the proton beam on a microsecond timescale. The profile monitor data here shows a 3D display of the beam profile evolution over the full 10ms accelerator cycle.

▶ Simulations of the ISIS injection region showing the H^- beam hitting the stripping foil and the trajectories of the resulting H^+, H^0 and H^- beams. The H^0 and H^- are intercepted by a beam dump while the H^+ proceed into the synchrotron. Such simulations are needed for studies of possible developments of ISIS, including increasing the injection energy into the synchrotron to provide overall increases in ISIS proton power.

▶ **The Electrical Engineering group** deal with all the power supplies and motors required to drive ISIS. The group are presently taking delivery of and testing over ninety new power supplies for the synchrotron and extracted proton beam to target station 1. Here group members are seen with one of twelve new energy storage chokes for the synchrotron main magnet power supply. ***08EC3909***

▶ **The ISIS Controls group**. The group are responsible for monitoring and control of the many thousands of components that are needed to keep the ISIS accelerators running. Work this year has included integration of LabView diagnostics into the controls systems. ***10EC2804***

Daniel Bowron (ISIS) discussing solution chemistry with Prof Ryoki Noyori, President of RIKEN and Nobel Laureate in Chemistry, during Prof Noyori's visit to sign a new agreement between ISIS and RIKEN for muon science. *10EC2451*

Prof Ken Nagamine was instrumental in creating the RIKEN-RAL muon facility at ISIS. Here he is leading the toast to celebrate 20 years of successful collaboration and the further renewal of the RIKEN-RAL agreement. *10EC2497*

A year around ISIS

Neutron Training Course

The ISIS Neutron Training Course took place in May. The course is designed to provide practical experience of setting up and running neutron scattering experiments on a wide range of instruments at ISIS, and is aimed at researchers new to neutron science. 24 students and post-docs took part in the course. The 8-day event included practicals on Engin-x, HRPD, Merlin and other instruments, plus the first use of the new LET spectrometer on the Second Target Station.

Muon Training School

ISIS also runs a muon training school to give postgraduate and postdoctoral students practical experience in running muon experiments. The course also includes lectures and workshops in the principles and applications of the technique given by experts in the field. This year, 18 students from nine countries came to ISIS for six days in May. Each had the opportunity of running two experiments on the ISIS muon instruments.

Students on the ISIS muon training course viewing the new Chronus spectrometer on the RIKEN-RAL muon facility. *10EC2151*

Students on the neutron training course preparing samples for a reflectometry experiment. *10EC2800*

Attendees at the Disordered Materials Data Analysis Workshop held in March at The Cosener's House. *10EC1774*

Attendees at the one day workshop on Strongly Correlated and Interacting Electron Systems organised by ISIS and held at The Cosener's House in January. *10EC1083*

Small Angle Scattering Conference held in Oxford

SAS-2009, the XIV IUCr International Conference on Small-Angle Scattering (SANS) was jointly organized by the ISIS SANS team and their counterparts from Diamond under the chairmanship of Steve King and Nick Terrill. A total of 434 delegates from 32 different countries attended. A vast range of science and technology was presented in 10 plenary presentations, 144 contributed oral presentations and 308 posters, testament to the continuing broad appeal of small-angle scattering as a technique.

Delegates at SAS-2009 listening to talks at the Examination Schools in Oxford. *09EC3270*

ISIS People

Congratulations to Harry Jones, Project Manager for the ISIS Second Target Project, who was awarded an MBE in Her Majesty the Queen's New Year Honours List. *"No-one could deserve this award more than Harry Jones,"* said ISIS Director Andrew Taylor. *"His contribution to delivering this world-leading project was absolutely key. Just as importantly, throughout his career Harry has developed and mentored successive generations of young engineers, contributing to the engineering skills base not only in this laboratory but more widely across the different sectors of UK industry where many of them now work."*

Congratulations are also due to Andrew Taylor, ISIS Director, who was awarded an Honorary Degree of Doctor of Science from the University of Glasgow in recognition of the major contributions he has made in Chemistry and Physics.

Harry Jones MBE inside the ISIS Second Target Station. *10EC1309*

▶ ISIS held a 'friends and family' afternoon in January. Five hundred visitors were able to learn about ISIS and see what their ISIS friends or family members get up to in their work at the facility. ***10EC1138, 10EC1140***

▼ Pupils from Didcot Girls School learning about superconductivity at ISIS as part of a schools 'triple science conference' in January. ***10EC1175***

▶ A teacher training weekend was held at ISIS in July. Participants learned about science at ISIS and its relevance to science in schools. Here we see them during a tour of the ISIS Second Target Station. ***10EC2728***

◀ ISIS regularly takes work experience pupils, who come for up to two weeks to learn about the world of work and get valuable experience working in a large science facility. Here we see Matthew Izzard from King Alfred's School, Wantage, working with a design for a shutter lift mechanism for the Second Target Station. ***10EC2689***

▼ Pupils from Marling School, Stroud, visited ISIS in February with French exchange students they were hosting. ***10EC1292***

Inspiring the next generation of scientists!

▼ ISIS staff helped Harwell Primary School Year 6 pupils to build an electric car. Here we see the ISIS and school team following assembly of the car in July, together with pupils visiting the ISIS Second Target Station with Chris Frost (ISIS). ***10EC2653, 10EC2424***

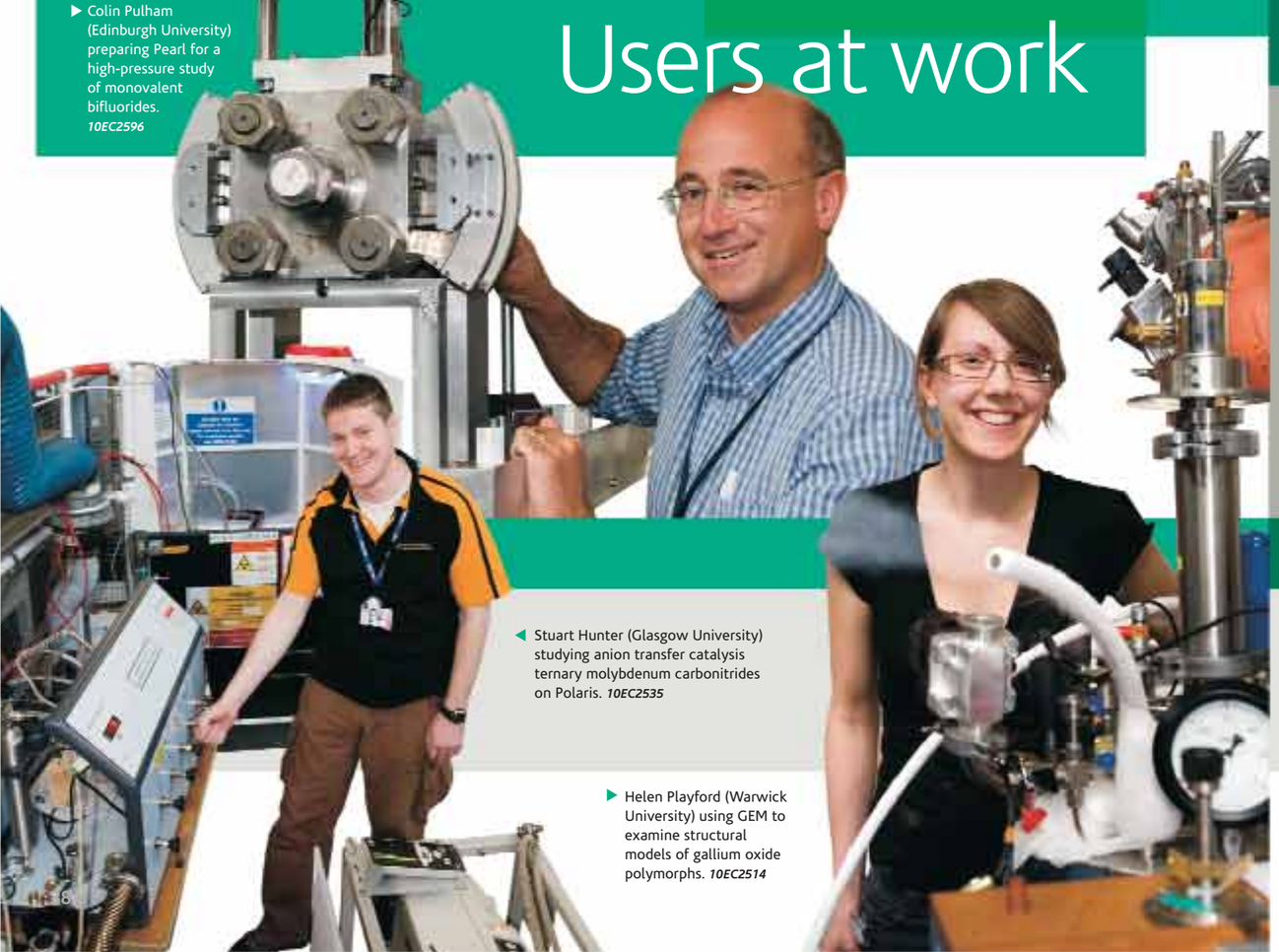
◀ A Particle Physics Masterclass for around 400 sixth form students is held every year at RAL. Here, students from Tiffin School for boys, Kingston upon Thames, are being shown ISIS by Adrian Hillier (ISIS). ***10EC1460***

▼ Sarah Norman and Tristan Youngs (Queens University Belfast) in the ISIS Second Target station during Nimrod studies of atomic and mesoscale structural correlations in 1-alkyl-3-methylimidazolium ionic liquids. ***10EC2527***

▲ Samantha Ford (ILL, Grenoble) and Ivana Evans (Durham University) exploring pressure effects on proton migration in 3,5-pyridinedicarboxylic acid on SXD. ***10EC2554***

ISIS
Users at work

▶ Colin Pulham (Edinburgh University) preparing Pearl for a high-pressure study of monovalent bifluorides. ***10EC2596***



◀ Stuart Hunter (Glasgow University) studying anion transfer catalysis ternary molybdenum carbonitrides on Polaris. ***10EC2535***

▶ Helen Playford (Warwick University) using GEM to examine structural models of gallium oxide polymorphs. ***10EC2514***

◀ Bella Lake (Helmholtz Centrum Berlin) and Toby Perring (ISIS) studying Excitations proposals. ***09EC4266***

◀ Rod Macrae (Marian College, USA) and Ray Osborn (Argonne National Laboratory, USA) during the Muon FAP meeting. ***09EC4276***

▲ Crystallography FAP members: Duncan Gregory (Glasgow University), John Claridge (Liverpool University), Peter Slater (Surry University) and Lawrence Falvello (Universidad de Zaragoza). ***09EC4281***

▶ Milva Celli (Istituto dei Sistemi Complessi) of the Disordered Materials FAP. ***09EC4296***

Facility Access Panels (FAPs)

There are seven ISIS FAPs covering the variety of science areas studied by neutrons and muons. Each FAP consists of experts in their subject field from the international research community. The FAPs meet roughly six weeks after each ISIS proposal deadline. They rigourously review all proposals received based on their scientific merit and timeliness.

▲ The Large Scale Structures FAP at work. ***09EC4225***

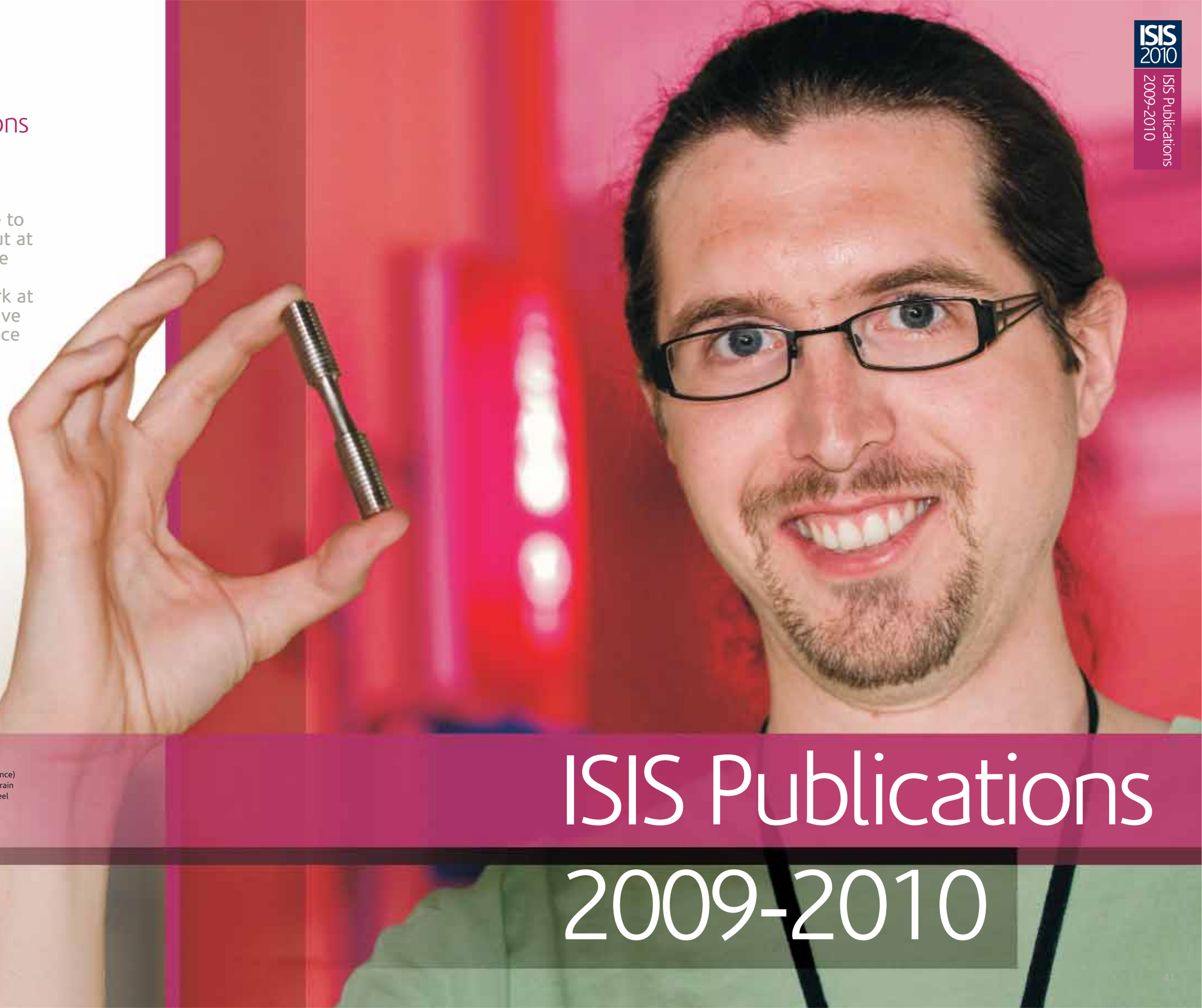
▶ Jon Goff (Royal Holloway and Bedford New College) during Large Scale Structures FAP discussions. ***09EC4235***

▲ Howard Stone (Cambridge University) discussing Engineering proposals. ***09EC4246***

◀ Chris Hardacre (Queen's University Belfast) chairing the Disordered Materials FAP. ***09EC4292***

ISIS Publications 2009-2010

Publications relate to all work carried out at ISIS. Listed here are 345 publications resulting from work at the facility that have been published since ISIS 2008.



▶ Vincent Legrand (Rennes University, France) employing Engin-x for in-situ internal strain measurements in textured austenitic steel under strain-path changes.
10EC2560

ISIS Publications 2009-2010

B Abbey, S Zhang, W Vorster and A Korsunsky

Feasibility study of neutron strain tomography

Mesomechanics **1** 185 (2009)

I Abrahams, X Liu, S Hull, ST Norberg, F Krok, A Kozanecka-Szmigiel, MS Islam and SJ Stokes

A combined total scattering and simulation approach to analysing defect structure in Bi_3YO_6

Chemistry of Materials **22** 15 4435 (2010)

M Acar, P Bouchard, JQ de Fonseca, M Fitzpatrick and S Gungor

Intergranular strains in pre-strained and welded pipes

5th International Conference on Mechanical Stress Evaluation by Neutron and Synchrotron Radiation (2009)

M Adam

An investigation of hydrogen bonded molecular systems using X-ray and neutron diffraction

Thesis (2009)

M Adam, M Gutmann, C Leech, D Middlemiss, A Parkin, L Thomas and C Wilson

Stability and cooperativity of hydrogen bonds in dihydroxybenzoic acids

New Journal of Chemistry **34** 85-91 (2010)

D Adams, B Jones, S Payne, B Pine and R Williamson

Studies of space charge loss mechanisms associated with half integer resonance on the ISIS RCSS

Particle Accelerator Conference (2009)

D Adroja, A Hillier, P Deen, A Strydom, Y Muro, J Kajino, W Kockelmann, T Takabatake, V Anand and JAT Stewart

Long-range ordering of reduced magnetic moments in the spin-gap compound $CeOs_2Al_{10}$ as seen via muon spin relaxation and neutron scattering

Physical Review B **82** 104405 (2010)

I Ahmed, S Rahman, P Steegstra, S Norberg, S Eriksson, E Ahlberg, C Knee and S Hull

Effect of co-doping on proton conductivity in perovskite oxides $BaZr_{0.9}In_{0.05}M_{0.05}O_{3-\delta}$ ($M = Yb^{3+}$ or Ga^{3+})

International Journal of Hydrogen Energy **35** 6381-6391 (2010)

H Alberto, A Weidinger, R Vilao, J Duarte, J Gil, N de Campos, J Lord and S Cox

Muonium as a probe of electron spin polarisation in CdTe

Physica B Condensed Matter **404** 5110-5112 (2009)

H Alberto, A Weidinger, R Vilao, J Duarte, J Gil, J Lord and S Cox

Mechanisms of electron polarisation of shallow muonium in CdTe and CdS

Physical Review B **81** (2010)

S Alessandroni, A Paradowska, EP Cippo, R Senesi, C Andreani, P Montedoro, F Chiti, D Sala, D Spinelli and C Mannini

Investigation of residual stress distribution of wheel rims using neutron diffraction

8th European Conference on Residual Stresses (2010)

G Alexander, S King, R Richardson and H Zimmermann

Determination of the translational order parameter for smectic liquid crystals using small-angle neutron scattering

Liquid Crystals **37** 961-968 (2010)

D Allan, W Marshall, D Francis, I Oswald, C Pulham and C Spanswick

The crystal structures of the low-temperature and high-pressure polymorphs of nitric acid

Dalton Transactions **39** 3736-3743 (2010)

H Al-Obaidi, M Bowes, M Lawrence, A Drake, M Green and P Dobson

Fate of silica nanoparticles in simulated primary wastewater treatment

Environmental Science & Technology **43** 8622-8628 (2009)

DC Arnold, KS Knight, G Catalan, SAT Redfern, JF Scott, P Lightfoot and FD Morrison

The beta-to-gamma transition in $BiFeO_3$: a powder neutron diffraction study

Advanced Functional Materials **20** 13 2116-2123

M Bacci, M Picollo and D Colognesi

The vibrational spectroscopy of Indigo: a reassessment

Vibrational Spectroscopy **50** 268-276 (2009)

T Baikie, S Pramana, C Ferraris, Y Huang, E Kendrick, K Knight, Z Ahmad and T White

Polysomatic apatites

Acta Crystallographica Section B Structural Science **66** 1-16 (2010)

P Baker, I Franke, T Lancaster, S Blundell, L Kerslake and S Clarke

Two-dimensional magnetism in the pnictide superconductor parent material SrFeAsF probed by muon-spin relaxation

Physical Review B **79** (2009)

P Baker, S Giblin, F Pratt, R Liu, G Wu, X Chen, M Pitcher, D Parker, S Clarke and S Blundell

Heat capacity measurements on FeAs-based compounds: a thermodynamic probe of electronic and magnetic states

New Journal of Physics **11** (2009)

P Baker, T Lancaster, I Franke, W Hayes, S Blundell, F Pratt, P Jain, Z Wang and M Kurmoo

Muon spin relaxation investigation of magnetic ordering in the hybrid organic-inorganic perovskites $[(CH_3)_2NH_2]$ $M(HCOO)_3$ (M=Ni,Co,Mn,Cu)

Physical Review B **82** 12407 (2010)

P Baker, H Lewtas, S Blundell, T Lancaster, I Franke, W Hayes, F Pratt, L Bohaty and P Becker

Muon-spin relaxation and heat capacity measurements on the magnetoelectric and multiferroic pyroxenes $LiFeSi_2O_6$ and $NaFeSi_2O_6$

Physical Review B **81** (2010)

J Ballin, J Crooks, P Dauncey, B Levin, M Lynch, A Magnan, Y Mikami, O Miller, M Noy, V Rajovic, M Stanitzki, K Stefanov, R Turchetta, M Tyndel, E Villani, N Watson and J Wilson

A MAPS-based readout for a Tera-Pixel electromagnetic calorimeter at the ILC

Nuclear Physics B – Proceedings Supplements 342-345 (2009)

M Barbagallo, N Hine, J Cooper, N Steinke, A Ionescu, C Barnes, C Kinane, R Dalgliesh, T Charlton and S Langridge

Experimental and theoretical analysis of magnetic moment enhancement in oxygen-deficient EuO

Physical Review B **81** (2010)

A Barbour, M Telling and J Larese

Investigation of the behavior of ethylene molecular films using high resolution adsorption isotherms and neutron scattering

Langmuir **26** 8113-8121 (2010)

A Barcza, Z Gercsi, K Knight and K Sandeman

Giant magnetoelastic coupling in a metallic helical metamagnet

Physical Review Letters **104** (2010)

E Barney, A Hannon and D Holland

A multi-technique structural study of the tellurium borate glass system

Physics and Chemistry of Glasses – European Journal of Glass Science and Technology Part B **50** 156-164 (2009)

L Bartoli, F Civita, A Paradowska, A Scherillo and M Zoppi

Nondestructive characterisation of phase distribution and residual strain/stress map of two ancient (Koto) age Japanese swords

Materials Science Forum **652** 167-173 (2010)

J Bateman, R Dalgliesh, D Duxbury, S Holt, D McPhail, A Marsh, N Rhodes, E Schooneveld, E Spill and R Stephenson

The FastGas detector

Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment **616** 59-64 (2009)

AMT Bell, KS Knight, CMB Henderson and AN Fitch

Revision of the structure of $Cs_2CuSi_5O_{12}$ leucite as orthorhombic Pbca

Acta Crystallographica Section B-Structural Science **66** 51-59 (2010)

CG Bell, CJW Breward, PD Howell, J Penfold and RK Thomas

A theoretical analysis of the surface tension profiles of strongly interacting polymer-surfactant systems

Journal of Colloid and Interface Science **350** 2 486-493 (2010)

T Bennett, A Goodwin, M Dove, D Keen, M Tucker, E Barney, A Soper, E Bithell, J Tan and A Cheetham

Structure and properties of an amorphous metal-organic framework

Physical Review Letters **104** (2010)

P Berastegui, S Hull and S Eriksson

A high temperature superionic phase of $CsSn_2F_5$

Journal of Solid State Chemistry **183** 373-378 (2010)

P Mendels and F Bert

Quantum Kagome antiferromagnet $ZnCu_3(OH)_6Cl_2$

Journal of the Physical Society of Japan **79** 011001 (2010)

S Betouras, J Carr and J Quintanilla

Deconfinement and quantum liquid crystalline states of dipolar fermions in optical lattices

International Journal of Modern Physics B **23** 4074-4086 (2009)

H Billetter, T Wallraff, U Schwarz, RI Smith and U Ruschewitz

Ternary transition metal acetylides A(2)(I)M(0)C(2) (A(I) = K, Rb; M-0 = Pd, Pt): neutron diffraction studies and electronic properties

Zeitschrift Fur Anorganische Und Allgemeine Chemie **636** 9-10 1834-1838 (2010)

P Biswas, G Balakrishnan, D Paul, C Tomy and MLA Hillier

Muon-spin-spectroscopy study of the penetration depth of $FeTe_{0.5}Se_{0.5}$

Physical Review B **81** (2010)

G Blake, A Nugroho, M Gutmann and T Palstra

Competition between Jahn-Teller coupling and orbital fluctuations in $HoVO_3$

Physical Review B **79** (2009)

M Bloksma, S Rogers, U Schubert and R Hoogenboom

Secondary structure formation of main-chain chiral poly(2-oxazoline)s in solution

Soft Matter **6** 994-1003 (2010)

S Blundell, T Lancaster, F Pratt, P Baker, W Hayes, J Ansermet and A Comment

Phase transition in the localised ferromagnet EuO probed by muSR

Physical Review B **81** (2010)

H Bordeneuve, C Tenailleau, S Guillemet-Fritsch, R Smith, E Suard and A Rousset

Structural variations and cation distributions in $Mn_{3-x}Co_xO_4$ (0 =< x =< 3) dense ceramics using neutron diffraction data

Solid State Sciences **12** 379-386 (2010)

L Bove, S Klotz, A Paciaroni and F Sacchetti

Anomalous proton dynamics in ice at low temperatures

Physical Review Letters **103** (2009)

L Bove, S Klotz, A Paciaroni and F Sacchetti

Concerted proton tunelling in ordinary ice

Notiziario Neutroni e Luce di Sincrotrone **15** 4-11 (2010)

D Bowron

Comprehensive structural modelling of aqueous solutions using neutron diffraction and X-ray absorption spectroscopy

14th International Conference on X-Ray Absorption Fine Structure (XAFS14), Journal of Physics Conference Proceedings **190** (2009)

D Bowron, C D'Agostino, L Gladden, C Hardacre, J Holbrey, M Lagunas, J McGregor, M Mantle, C Mullan and T Youngs

Structure and dynamics of 1-ethyl-3-methylimidazolium acetate via molecular dynamics and neutron diffraction

The Journal of Physical Chemistry B **114** 7760-7768 (2010)

D Bowron, A Soper, K Jones, S Ansell, S Birch, J Norris, L Perrott, D Riedel, N Rhodes, S Wakefield, A Botti, M Ricci, F Grazzi and M Zoppi

NIMROD: the Near and InterMediate Range Order Diffractometer of the ISIS second target station

Review of Scientific Instruments **81** (2010)

J Bradley, A Lang, P Lindenbaum, C Neylon, A Williams and E Willighagen

Beautifying data in the real world

Beautiful Data 259-278 (2009)

S Bramwell, S Giblin, S Calder, R Aldus, D Prabhakaran and T Fennell

Measurement of the charge and current of magnetic monopoles in spin ice

Nature **461** 956-U211 (2009)

M Brogan, R Hughes, R Smith and D Gregory

Structural and compositional tuning of layered subnitrides; new complex nitride halides

2010 Dalton Transactions **39** 7153-7158 (2010)

MA Brogan, RW Hughes, RI Smith and DH Gregory

Structural and compositional tuning of layered subnitrides; new complex nitride halides

Dalton Transactions **39** 30 7153-7158 (2010)

C Bull, M Guthrie, R Nelmes, J Loveday, H Hamidov and M Gutmann

Low-temperature neutron single-crystal diffraction studies of samples grown at high pressure

International Journal of High Pressure Research **29** 644-648 (2009)

C Bull, M Guthrie, R Nelmes, J Loveday, K Komatsu, H Hamidov and M Gutmann

Time-of-flight single-crystal neutron diffraction to 10GPa and above

International Journal of High Pressure Research **29** 780-791 (2009)

DJ Bull, E Weidner, IL Shabalin, MTF Telling, CM Jewell, DH Gregory and DK Ross

Pressure-dependent deuterium reaction pathways in the Li-N-D system

Physical Chemistry Chemical Physics **12** 9 2089-2097 (2010)

A Bungau, R Cywinski and J Lord

Geant4 simulations of the ISIS muon target at Rutherford Appleton Laboratory

23rd Particle Accelerator Conference (2009)

A Bungau, R Cywinski and J Lord

Development and optimisation of the muon target at the ISIS-RAL Muon Facility

23rd Particle Accelerator Conference (2009)

A Bungau, R Cywinski, J Lord, P King, M Poole, S Smith, R Barlow, PD d Reotier, F Pratt, R Edgecock, K Clausen, T Shiroka and et al

Exploring the feasibility of a stand alone muon facility for MUSR research

23rd Particle Accelerator Conference (2009)

R Burton, E Ferrari, R Davey, J Finney and D Bowron

Relationship between solution structure and phase behavior: a neutron scattering study of concentrated aqueous hexamethylenetetramine solutions

The Journal of Physical Chemistry B **113** 5967-5977 (2009)

R Burton, E Ferrari, R Davey, J Finney and D Bowron

Relationship between solution structure and phase behavior: a neutron scattering study of concentrated aqueous hexamethylenetetramine solutions

Journal of Physical Chemistry B **113** 5967-5977 (2009)

S Calder, T Fennell, W Kockelmann, G Lau, R Cava and S Bramwell

Neutron scattering and crystal field studies of the rare earth double perovskite Ba_2ErSbO_6

Journal of Physics Condensed Matter **22** (2010)

S Calder, X Ke, F Bert, A Amato, C Baines, C Carboni, R Cava, A Daoud-Aladine, P Deen, T Fennell, A Hillier, H Karunadasa, J Taylor, P Mendels, P Schiffer and S Bramwell

Magnetic properties of Ba_2HoSbO_6 with a frustrated lattice geometry

Physical Review B **81** (2010)

C Candolfi, J Leszczynski, P Masschelein, C Chubilleau, B Lenoir, A Dauscher, E Guilmeau, J Hejtmanek, SJ Clarke and RI Smith

Crystal structure and high-temperature thermoelectric properties of the $Mo_{3-x}Ru_xSb_7$ compounds

Journal of Electronic Materials **39** 9 2132-2135 (2010)

MA Carpenter, REA McKnight, CJ Howard and KS Knight

Symmetry and strain analysis of structural phase transitions in $Pr_{0.48}Ca_{0.52}MnO_3$

Physical Review B **82** (2009)

S Carretta, P Santini, G Amoretti, T Guidi, Y Qiu, J Copley, G Timco, C Muryn and R Winpenny

Rotational bands in open antiferromagnetic rings: a neutron spectroscopy study of Cr_8Zn

Physical Review B **79** 144422 (2009)

B Carroll, R Lichti, Y Celebi, K Chow, P King and I Yonenaga

Evidence for a shallow muonium acceptor state in Ge-rich Cz-$Si_{1-x}Ge_x$

Physica B Condensed Matter **404** 5113-5116 (2009)

Y Celebi, R Lichti, H Bani-Salameh, A Meyer, B Carroll, J Vernon, P King and S Cox

Muonium transitions in 4H silicon carbide

Physica B-Condensed Matter **404** 845-848 (2009)

M Chambrier, R Ibberson and F Goutenoire

Structure determination of alpha-$La_6W_2O_{15}$

Journal of Solid State Chemistry **183** 1297-1302 (2010)

L Chapon

Origin of the long-wavelength magnetic modulation in $Ca_3Co_2O_6$

Physical Review B **80** (2009)

A Chiba, M Tomomasa, S Bennington, A Hannon and K Tsuji

Pressure-induced suppression of the Peierls distortion of liquid As and GeX (X=S,Se,Te)

Physical Review B **80** (2009)

H Choo, P Liaw, E Oliver and A Paradowska

In situ neutron diffraction study of internal strain evolution around a crack tip under variable-amplitude fatigue-loading conditions

Scripta Materialia **60** 866-869 (2009)

O Ciftja and J Quintanilla

Effective interaction potentials in the uppermost Landau level

Journal of Low Temperature Physics **159** 189-192 (2010)

EP Cippo, A Borella, W Kockelmann, A Pietropaolo, H Postma, N Rhodes, P Schillebeeckx, E Schooneveld, M Tardocchi, R Wynants and G Gorini

A detector system for Neutron Resonance Capture Imaging

Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment **623** 693-698 (2010)

J Claridge, H Hughes, C Bridges, M Allix, M Suchomel, H Niu, X Kuang, M Rosseinsky, N Bellido, D Grebille, O Perez, C Simon, D Pelloquin, S Blundell, T Lancaster, P Baker, F Pratt and P Halasyamani

Frustration of magnetic and ferroelectric long-range order in $Bi_2Mn_{4/3}Ni_{2/3}O_6$

Journal of the American Chemical Society **131** 14000-14017 (2009)

R Coldea, D Tennant, E Wheeler, E Wawrzynska, D Prabhakaran, M Telling, K Habicht, P Smedibidl and K Kiefer

Quantum criticality in an Ising chain: experimental evidence for emergent E 8 symmetry

Science **327** 177-180 (2010)

F Coneri, S Sanna, K Zheng, J Lord and R de Renzi

Magnetic states of lightly hole-doped cuprates in the clean limit as seen via zero-field muon spin spectroscopy

Physical Review B **81** (2010)

R Cortes-Gil, D Parker, M Pitcher, J Hadermann and S Clarke

Indifference of superconductivity and magnetism to size-mismatched cations in the layered iron arsenides $Ba_{1-x}NaxFe_2As_2$

Chemistry of Materials **22** 4304-4311 (2010)

M Cote, T Nicholls, D Knight, I Morgan, P Rogueda, S King, R Heenan and P Griffiths

Self-assembling chiral gelators for fluorinated media

Langmuir **25** 8678-8684 (2009)

S Cox

Muonium as a model for interstitial hydrogen in the semiconducting and semimetallic elements

Reports on Progress in Physics **72** (2009)

F Damay, C Martin, V Hardy, A Maignan, G Andre, K Knight, S Giblin and L Chapon

Zigzag ladders with staggered magnetic chirality in the S=3/2 compound beta-$CaCr_2O_4$

Physical Review B **81** (2010)

A Daoud-Aladine, B Kundys, C Martin, P Radaelli, P Brown, C Simon and L Chapon

Multiferroicity and spiral magnetism in $FeVO_4$ with quenched Fe orbital moments

Physical Review B **80** (2009)

V de Haan, J Plomp, T Rekveldt, W Kraan, A van Well, R Dalgliesh and S Langridge

Observation of the Goos-Hanchen Shift with Neutrons

Physical Review Letters **104** (2010)

M de Vries, A McLaughlin and J-W Bos

Valence bond glass on an fcc lattice in the double perovskite Ba_2YMoO_6

Physical Review Letters **104** 177202 (2010)

P Deen, A Strydom, S Paschen, D Adroja, W Kockelmann and S Rols

Quantum fluctuations and the magnetic ground state of $Ce_3Pd_{20}Si_6$

Physical Review B **81** (2010)

F Demmel, S Howells, C Morkel and W Pilgrim

Slow dynamics in liquid metals as seen by QENS

Zeitschrift fur Physikalische Chemie-International Journal of research in Physical Chemistry & Chemical Physics **224** 83-99 (2010)

F Demmel, T Seydel and S Jahn

Sodium diffusion in cryolite at elevated temperatures studied by quasielastic neutron scattering

Solid State Ionics **180** 1257-1260 (2009)

A Deriu, M di Bari and Y Gerelli

Dynamics of nanostructures for drug delivery: the potential of QENS

Z Phys Chem **224** 227-242 (2010)

S Diallo, D Pratt, R Fernandes, W Tian, J Zarestky, M Lumsden, T Perring, C Broholm, N Ni, S Bud'ko, P Canfield, H-Li, D Vaknin, A Kreyssig, A Goldman and R McQueeney

Paramagnetic spin correlations in $CaFe_2As_2$ single crystals

Physical Review B **81** (2010)

D Dini, X Song, S Zhang and A Korsunsky

Residual strain analysis in polycrystalline aggregates using diffraction measurement and finite element modelling

Journal of Strain Analysis for Engineering Design **44** 55-70 (2009)

D Dobson, IIG Wood, J Brodholt, J Mecklenburgh and E Oliver

Deformation of olivine at 5GPa and 350-900 degrees C

Physics of the Earth and Planetary Interiors **172** 84-90 (2009)

R Doubble, S Hayden, P Dai, H Mook, J Thompson and C Frost

Direct observation of paramagnons in palladium

Physical Review Letters **105** (2010)

L Dougan, J Crain, JL Finney and AK Soper

Molecular self-assembly in a model amphiphile system

Physical Chemistry Chemical Physics **12** 35 10221-10229 (2010)

J Dreiser, O Waldmann, C Dobe, G Carver, S Ochsenbein, A Sieber, H Guedel, J van Duijn, J Taylor and A Podlesnyak

Quantised antiferromagnetic spin waves in the molecular Heisenberg ring $CsFe_8$

Physical Review B **81** (2010)

A Drew, M Wisemayer, D Heron, S Lister, S Lee, A Potenza, C Marrows, R Dalgliesh, T Charlton and S Langridge

Using spin-polarised neutron reflectivity to probe mesoscopic vortex states in a Pb thin-film superconductor

Physical Review B **80** (2009)

A Dunbar, P Mokarian-Tabari, A Parnell, S Martin, M Skoda and R Jones

A solution concentration dependent transition from self-stratification to lateral phase separation in spin-cast PS:d-PMMA thin films

The European Physical Journal E-Soft Matter **31** 369-375 (2010)

D Dye, J Coakley, V Vorontsov, H Stone and R Rogge

Elastic moduli and load partitioning in a single crystal nickel superalloy

Scripta Materialia **61** 109-112 (2009)

J Eastoe, L Hudson, S Gold, R Heenan and I Grillo

Fluorocarbon – hydrocarbon incompatibility in micellar polymerisations

Journal of Colloid and Interface Science **330** 437-442 (2009)

K Eblagon, K Tam, K Yu, S Zhao, X Gong, H He, L Ye, L Wang, A Ramirez-Cuesta and S Tsang

Study of catalytic sites on ruthenium for hydrogenation of N-ethylcarbazole: implications of hydrogen storage via reversible catalytic hydrogenation

Journal of Physical Chemistry **114** 9720-9730 (2010)

N Emery, EJ Wildman, JMS Skakle, G Giriat, RI Smith and AC McLaughlin

Giant magnetoresistance in oxypnictides (La,Nd)OMnAs

Chemical Communications **46** 36 6777-6779

D Eshchenko, V Storchak, S Cottrell and E Morenzoni

Electric-field-enhanced neutralisation of deep centers in GaAs

Physical Review Letters **103** (2009)

A Evans, A Paradowska, T Etter and HV Swygenhoven

Residual strain measurements in a monocrystalline Ni-based superalloy turbine blade using neutron diffraction

15th International Conference on Strength of Materials (2009)

D Faircloth, M Kronberger, D Kuechler, J Lettry and R Scrivens

Finite element thermal study of the Linac4 plasma generator

Review of Scientific Instruments **81** (2010)

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

The front end test stand high performance H^- ion source at Rutherford Appleton Laboratory

Review of Scientific Instruments **81** (2010)

N Faisal, S Knupfer, A Paradowska, M Fitzpatrick, K Khor and J Cizek

Neutron diffraction residual strain measurements in plasma sprayed nanostructured hydroxyapatite coatings for orthopaedic implants

Materials Science Forum **652** 309-315 (2010)

I Fallis, P Griffiths, T Cosgrove, C Dreiss, N Govan, R Heenan, I Holden, R Jenkins, S Mitchell, S Notman, J Platts, J Riches and T Tatchell

Locus-specific microemulsion catalysts for sulfur mustard (HD) chemical warfare agent decontamination

Journal of the American Chemical Society **131** 9746-9755 (2009)

F Fernandez-Alonso, F Bermejo and M Saboungi

Molecular hydrogen in carbon nanostructures

Handbook of Nanophysics **5** 47119 (2010)

J Fernandez-Rodriguez, V Scagnoli, C Mazzoli, F Fabrizi, S Lovesey, J Blanco, D Sivia, K Knight, F de Bergevin and L Paolasini

Experimental evidence of anapolar moments in the antiferromagnetic insulating phase of V_2O_3 obtained from X-ray resonant Bragg diffraction

Physical Review B **81** (2010)

G Festa, A Pietropaolo, E Reali, F Grazzi and E Schooneveld

A gamma-ray detector with a silicon photomultiplier (SiPM) readout for neutron diffraction experiments at spallation neutron sources

Measurement Science and Technology **21** (2010)

F Fillaux, A Cousson and M Gutmann

Evidence of macroscopically entangled protons in a mixed isotope crystal of $KH_pD_{1-p}CO_3$

Journal of Physics Condensed Matter **22** (2010)

D Flannery, B Matthews, T Griffin, J Bicarregui, M Gleaves, L Lerusse, R Downing, A Ashton, S Sufi, G Drinkwater and K Kleese

ICAT: Integrating data infrastructure for facilities based science

5th IEEE International Conference on e-Science (2009)

A Fortes, I Wood and K Knight

The crystal structure of perdeuterated methanol hemiammoniate ($CD_3OD.0.5ND_3$) determined from neutron powder diffraction data at 4.2 and 180 K

Journal of Applied Crystallography **43** 328-336 (2010)

M Francisco, C Malliakas, P Piccoli, M Gutmann, A Schultz and M Kanatzidis

Development and loss of ferromagnetism controlled by the interplay of Ge concentration and Mn vacancies in structurally modulated $Y_4Mn_{1-x}Ga_{12-y}Ge_y$

Journal of the American Chemical Society **123** 8998-9006 (2010)

C Frost, S Ansell and G Gorini

A new dedicated neutron facility for accelerated SEE testing at the ISIS facility

47th Annual Reliability Physics Symposium 2009 **1 & 2** 952-955 (2009)

C de la Fuente, A del Moral, D Adroja, A Fraile and J Arnaudas

Study of 4f hybridization in CeNiX with $X = Sn_\delta Ge_{1-\delta}$, $0 <= \delta <= 1$

Journal of Magnetism and Magnetic Materials **322** 1059-1063 (2010)

NP Funnell, A Dawson, D Francis, AR Lennie, WG Marshall, SA Moggach, JE Warren and S Parsons

The effect of pressure on the crystal structure of L-alanine

Crystengcomm **12** 9 2573-2583

C Gabor, D Faircloth, D Lee, S Lawrie, A Letchford and J Pozimski

Diagnostic experiments at a 3 MeV test stand at Rutherford Appleton Laboratory (United Kingdom)

Review of Scientific Instruments **81** (2010)

A Ganin, Y Takabayashi, P Jeglic, D Arcon, A Potocnik, P Baker, Y Ohishi, M McDonald, M Tzirakis, A McLennan, G Darling, M Takata, M Rosseinsky and K Prassides

Polymorphism control of superconductivity and magnetism in Cs_3C_{60} close to the Mott transition

2010 Nature **466** 221-U93 (2010)

J Garcia-Munoz, C Frontera, P Beran, N Bellido, J Hernandez-Velasco and C Ritter

Consequences of embedding Ti^{4+} 3d(0) centers in $Pr_{0.50}Ca_{0.50}MnO_3$: Phase competition in $Pr_{0.50}Ca_{0.50}Mn_{1-x}Ti_xO_3$

Physical Review B **81** (2010)

J Gardner, M Gingras and J Greedan

Magnetic pyrochlore oxides

Reviews of Modern Physics **82** 53-107 (2010)

A Giannasi, D Colognesi, L Ulivi, M Zoppi, A Ramirez-Cuesta, E Bardaji, E Roehm and M Fichtner

High resolution Raman and neutron investigation of $Mg(BH_4)_2$ in an extensive temperature range

The Journal of Physical Chemistry A **114** 2788-2793 (2010)

J Gil, J Duarte, R Vilao, H Alberto, N de Campos and S Cox

Spin exchange of muonium in CdS

Physica B-Condensed Matter **404** 834-836 (2009)

E Godfrey and W Kockelmann

Neutron-based analytical methods for the non-invasive characterisation of iron artefacts

International Symposium on Archaeometry (2009)

A Goodwin, F Michel, B Phillips, D Keen, M Dove and R Reeder

Nanoporous structure and medium-range order in synthetic amorphous calcium carbonate

Chemistry of Materials **22** 3197-3205 (2010)

D Goossens and T Welberry

Approaches to modeling diffuse scattering from molecular crystals: Para-Terphenyl ($C_{18}H_{14}$)

2010 Metallurgical and Materials Transactions **41** 1119-1129 (2010)

P Gorria, D Martinez-Blanco and R Smith

Neutron powder thermo-diffraction in mechanically alloyed $Fe_{64}Ni_{36}$ invar alloy

Journal of Alloys and Compounds **495** 495-498 (2010)

B Gray, A Hector, W Levason, G Reid, M Webster, W Zhang and M Jura

Synthesis, spectroscopic and structural characterisation of vanadium(IV) and oxovanadium(IV) complexes with arsenic donor ligands

Polyhedron **29** 1630-1638 (2010)

F Grazzi, A Scherillo and M Zoppi

A neutron imaging device for sample alignment in a pulsed neutron scattering instrument

Review of Scientific Instruments **80** (2009)

R Gremaud, Z Lodziana, P Hug, B Willenberg, A Racu, J Schoenes, A Ramirez-Cuesta, S Clark, K Refson, A Züttel and A Borgschulte

Evidence for hydrogen transport in deuterated $LiBH_4$ from low-temperature Raman-scattering measurements and first-principles calculations

Physical Review B **80** (2009)

P Griffiths, I Fallis, C James, I Morgan, G Brett, R Heenan, R Schweins, I Grillo and A Paul

Structure-property relationships in metallosurfactants

Soft Matter **6** 1981-1989 (2010)

P Griffiths, P Occhipinti, C Morris, R Heenan, S King and M Gumbleton

PGSE-NMR and SANS studies of the interaction of model polymer therapeutics with Mucin

Biomacromolecules **11** 120-125 (2010)

PC Griffiths, R Nilmini, E Carter, P Dodds, DM Murphy, Z Khayat, E Lattanzio, P Ferruti, RK Heenan, SM King and R Duncan

Interaction of an endosomolytic polyamidoamine ISA23 with vesicles mimicking intracellular membranes: a SANS/EPR study

Macromolecular Bioscience **10** 8 963-973 (2010)

M Guignard, L Cormier, V Montouillout, N Menguy, D Massiot and A Hannon

Environment of titanium and aluminum in a magnesium alumino-silicate glass

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

M Guignard, L Cormier, V Montouillout, N Menguy, D Massiot, A Hannon and B Beuneu

Rearrangement of the structure during nucleation of a cordierite glass doped with TiO_2

Journal of Physics Condensed Matter **22** (2010)

M Gutmann

Accelerated computation of diffuse scattering patterns and application to magnetic neutron scattering

Journal of Applied Crystallography **43** 250-255 (2010)

V d Haan, J Plomp, M Rekveldt, A v Well, R Dalgliesh, S Langridge, A Bottger and R Hendrikx

Coherence approach in neutron, X-ray, and neutron spin-echo reflectometry

Physical Review B **81** (2010)

V d Haan, J Plomp, T Rekveldt, W Kraan, A v Well, R Dalgliesh and S Langridge

Comment on 'Observation of the Goos-Hanchen Shift with Neutrons' Reply

Physical Review Letters **105** (2010)

A Hall, J Swenson, D Bowron and S Adams

Structure of $Li_xRb_{1-x}PO_3$ glasses near the glass transition

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

A Hannon, E Barney and D Holland

The structure of tin borate based glasses

Physics and Chemistry of Glasses – European Journal of Glass Science and Technology Part B **50** 271-283 (2009)

J Haraldsen, M Stone, M Lumsden, T Barnes, R Jin, J Taylor and F Fernandez-Alonso

Spin-lozenge thermodynamics and magnetic excitations in Na_3RuO_4

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

C Hardacre, J Holbrey, C Mullan, M Nieuwenhuyzen, T Youngs, D Bowron and S Teat

Solid and liquid charge-transfer complex formation between 1-methylnaphthalene and 1-alkyl-cyanopyridinium bis{(trifluoromethyl)sulfonyl}imide ionic liquids

Physical Chemistry Chemical Physics **12** 1842-1853 (2010)

C Hardacre, JD Holbrey, CL Mullan, TGA Youngs and DT Bowron

Small angle neutron scattering from 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquids ([C(n)mim][PF6], n=4, 6, and 8)

Journal of Chemical Physics **133** 7 (2010)

T Headen, C Howard, N Skipper, M Wilkinson, D Bowron and A Soper

Structure of pi-pi interactions in aromatic liquids

Journal of the American Chemical Society **132** 5735-5742 (2010)

A Hill, A Harrison, C Dickinson, W Zhou and W Kockelmann

Crystallographic and magnetic studies of mesoporous eskolaite, Cr_2O_3

Microporous and Mesoporous Materials 280-286 (2010)

A Hillier, P Manuel, D Adroja, J Taylor, A Azad and J Irvine

Probing the superconducting ground state near the charge density wave phase transition in $Cu_{0.06}TiSe_2$

Physical Review **81** (2010)

A Hillman, K Ryder, E Madrid, A Burley, R Wiltshire, J Merotra, M Grau, S Horswell, A Glidle, R Dalgliesh, A Hughes, R Cubitt and A Wildes

Structure and dynamics of phospholipid bilayer films under electrochemical control

Faraday Discussions **145** 357-379 (2010)

J Hodges, P Bonville, A Forget, A Yaouanc, P Dalmas de Reotier, X Chaud and S Cottrell

Dynamic correlated Cu(2) magnetic moments in superconducting $YBa_2(Cu_{0.96}Ni_{0.04})_3O_y$ (y similar to 7)

Physical Review B **80** (2009)

M Hollamby, J Eastoe, A Chemelli, O Glatter, S Rogers, R Heenan and I Grillo

Separation and purification of nanoparticles in a single step

Langmuir **26** 6989-6994 (2010)

M Hollamby, J Eastoe, K Mutch, S Rogers and R Heenan

Fluorinated microemulsions as reaction media for fluorous nanoparticles

Soft Matter **6** 971-976 (2010)

M Hollamby, K Trickett, A Mohamed, J Eastoe, S Rogers and R Heenan

Surfactant aggregation in CO_2/Heptane solvent mixtures

Langmuir **25** 12909-12913 (2009)

R Hoogenboom, S Rogers, A Can, C Becer, C Guerrero-Sanchez, D Wouters, S Hoeppener and U Schubert

Self-assembly of double hydrophobic block copolymers in water-ethanol mixtures: from micelles to thermoresponsive micellar gels

Chemical Communications 5582-5584 (2009)

S Hosokawa, F Demmel, W Pilgrim, M Inui, S Tsutsui and A Baron

Acoustic phonons in molten NaI

Electrochemistry **77** 608 (2009)

S Hossain, C Truman, A Paradowska, D Hughes, R Wimpory and M Fox

Residual stress in 7449 aluminium alloy forgings

Materials Science and Engineering A **527** 2603-2612 (2009)

S Hunter, D McKay, R Smith, J Hargreaves and D Gregory

Topotactic nitrogen transfer: structural transformation in cobalt molybdenum nitrides

Chemistry of Materials **22** 2898-2907 (2010)

L Ianeselli, F Zhang, M Skoda, R Jacobs, R Martin, S Callow, S Prevost and F Schreiber

Protein-protein interactions in ovalbumin solutions studied by small-angle scattering: effect of ionic strength and the chemical nature of cations

The Journal of Physical Chemistry B **114** 3776-3783 (2010)

RM Ibberson

Design and performance of the new supermirror guide on HRPD at ISIS

Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment **600** 47-49 (2009)

RM Ibberson, A Fowkes, M Rosseinsky, WI David and P Edwards

Structure and Phase Behavior of the Expanded-Metal Compound $Li_7(ND_3)_4$

Angewandte Chemie International Edition **48** 1435-1438 (2009)

Y Ikedo, H Nozaki, M Harada, J Sugiyama, T Sato, Y Matsuo, K Nishiyama, J Lord, Y Qiu and J Copley

Study of hydrogen diffusion in superprotonic ionic conductors, $MHXO_4$, by muSR and QENS

Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment **600** 316-318 (2009)

R Inoue, T Kanaya, K Nishisa, I Tsukushi, M Telling, B Gabrys, M Tyagi, C Soles and W Wu

Glass transition and molecular mobility in polymer thin films

Physical Review E **80** 031802 (2009)

H Jarvie, H Al-Obaidi, S King, M Bowes, M Lawrence, A Drake, M Green and P Dobson

Fate of silica nanoparticles in simulated primary wastewater treatment

Environmental Science & Technology **43** 8622-8628 (2009)

HP Jarvie and SM King

Just scratching the surface? New techniques show how surface functionality of nanoparticles influences their environmental fate

Nano Today **5** 4 248-250 (2010)

RD Johnson, T Frawley, P Manuel, DD Khalyavin, C Adriano, C Giles, PG Pagliuso and PD Hatton

Magnetic structures of the anisotropic intermetallic compounds Er_2CoGa_8 and Tm_2CoGa_8

Physical Review B **82** 10 (2010)

K Johnston, C Tang, J Parker, K Knight, P Lightfoot and S Ashbrook

The polar phase of $NaNbO_3$: a combined study by powder diffraction, solid-state NMR, and first-principles calculations

Journal of the American Chemical Society **132** 8732-8746 (2010)

R Johnstone, A Lennie, S Parker, S Parsons, E Pidcock, P Richardson, J Warren and P Wood

High-pressure polymorphism in salicylamide

CrystEngComm **12** 1065-1078 (2010)

R Kajimoto, S Shamoto, M Arai, A Iyo, K Miyazawa, P Shirage, H Kito, H Eisaki, S Kim, H Hosono, T Guidi, R Bewley and S Bennington

Two-dimensional spin density wave state in LaFeAsO

Journal of the Physical Society of Japan **78** (2009)

A Keren

Evidence of magnetic mechanism for cuprate superconductivity

New Journal of Physics **11** (2009)

D Khalyavin, A Hillier, D Adroja, A Strydom, P Manuel, L Chapon, P Peratheepan, K Knight, P Deen, C Ritter, Y Muro and T Takabatake

Long-range magnetic order in $CeRu_2Al_{10}$ studied via muon spin relaxation and neutron diffraction

Physical Review B **82** 100405 (2010)

DD Khalyavin, P Manuel, JF Mitchell and LC Chapon

Spin correlations in the geometrically frustrated $RBaCo_4O_7$ antiferromagnets: Mean-field approach and Monte Carlo simulations

Physical Review B **82** 9 (2010)

M King, A Rennie, C Pfrang, A Hughes and K Thompson

Interaction of nitrogen dioxide (NO_2) with a monolayer of oleic acid at the air-water interface – A simple proxy for atmospheric aerosol

Atmospheric Environment **44** 1822-1825 (2010)

PDC King, IM McKenzie and TD Veal

Observation of shallow-donor muonium in Ga_2O_3: evidence for hydrogen-induced conductivity

Applied Physics Letters **96** (2010)

S King, L Bohlin and N Clarke

Apparatus for simultaneous rheology and small-angle neutron scattering from high-viscosity polymer melts and blends

Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment **620** 437-444 (2010)

E Kisi, J Zhang, O Kirstein, D Riley, M Styles and A Paradowska

Shear stiffness in nanolaminar Ti_3SiC_2 challenges ab initio calculations

Journal of Physics Condensed Matter **22** (2010)

K Knight, C Henderson and S Clark

Structural variations in the wesselsite-effenbergerite ($Sr_{1-x}Ba_xCuSi_4O_{10}$) solid solution

European Journal of Mineralogy **22** 411-423 (2010)

KS Knight

Analytical expressions to determine the isothermal compressibility tensor and the isobaric thermal expansion tensor for monoclinic crystals: application to determine the direction of maximum compressibility in jadeite

Physics and Chemistry of Minerals **37** 8 529-533

A Kovalevsky, L Hanson, S Fisher, M Mustyakimov, S Mason, V Forsyth, M Blakeley, D Keen, T Wagner, H Carrell, A Katz, J Glusker and P Langan

Metal ion roles and the movement of hydrogen during reaction catalysed by d-xylose isomerase: a joint X-ray and neutron diffraction study

Structure **18** 688-699 (2010)

M Krzystyniak and T Abdul-Redah

Proton momentum distribution in solid and liquid HF

Physical Review B **82** 6 (2010)

M Krzystyniak, R Lopez-Anton, A Chatzidimitriou-Dreismann, M Lerch and F Fernandez-Alonso

Dynamics of caged hydronium ions and super-protonic conduction in $(H_3O)SbTeO_6$

Z Phys Chem **224** 279-287 (2010)

Z Kurban, A Lovell, D Jenkins, S Bennington, I Loader, A Schober and N Skipper

Turbostratic graphite nanofibres from electrospun solutions of PAN in dimethylsulphoxide

European Polymer Journal **46** 1194-1202 (2010)

E Kutarski, R Dennis, J Price and T Finlayson

Comparison of residual stresses measurement with simulation for steel welded repairs EPRI

International Conference on Welds (2009)

B Lake, AM Tsvelik, S Notbohm, DA Tennant, TG Perring, M Reehuis, C Sekar, G Krabbes and B Buchner

Confinement of fractional quantum number particles in a condensed-matter system

Nature Physics **6** 1 50-55 (2010)

B Lake, E Wheeler, A Islam, T Guidi, K Rule, Z Izaola, M Russina, K Kiefer and Y Skourski

Magnetic excitations of the gapped quantum spin dimer antiferromagnet $Sr_3Cr_2O_8$

Physical Review B **81** 014415 (2010)

T Lancaster, S Blundell, P Baker, H Lewtas, W Hayes, F Pratt, H Yi and S Cheong

Spin freezing and dynamics in $Ca_3Co_{2-x}Mn_xO_6$ (x approximate to 0.95) investigated with implanted muons: Disorder in the anisotropic next-nearest-neighbor Ising model

Physical Review B **80** (2009)

T Lancaster, SJ Blundell, FL Pratt, I Franke, AJ Steele, PJ Baker, Z Salman, C Baines, I Watanabe, S Carretta, GA Timco and REP Winpenny

Relaxation of muon spins in molecular nanomagnets

Physical Review B **81** 14 (2010)

N Lathiotakis, N Gidopoulos and N Helbig

Size consistency of explicit functionals of the natural orbitals in reduced density matrix functional theory

The Journal of Chemical Physics **132** (2010)

S Lawrie, D Faircloth, A Letchford, C Gabor and J Pozimski

Plasma meniscus and extraction electrode studies of the ISIS H^- ion source

Review of Scientific Instruments **81** (2010)

A Lazim, J Eastoe, M Bradley, K Trickett, A Mohamed and S Rogers

Recovery of gold nanoparticles using pH-sensitive microgels

Soft Matter **6** 2050-2055 (2010)

G Lelong, W Howells, J Brady, C Talon, D Price and ML Saboungi

Translational and rotational dynamics of monosaccharide solutions

The Journal of Physical Chemistry B **113** 13079-13085 (2009)

S Lepadatu, J Claydon, D Ciudad, C Kinane, S Langridge, S Cavill, S Dhesi and C Marrows

Determination of domain wall depinning and driving currents in doped permalloy structures

IEEE Transactions on Magnetics **46** 1759-1761 (2010)

S Lepadatu, O Wessely, A Vanhaverbeke, R Allenspach, A Potenza, H Marchetto, T Charlton, S Langridge, S Dhesi and C Marrows

Domain-wall spin-torque resonators for frequency-selective operation

Physical Review B **81** (2010)

C Lester, J Chu, J Analytis, T Perring, I Fisher and S Hayden

Dispersive spin fluctuations in the nearly optimally doped superconductor $Ba(Fe_{1-x}Co_x)As_2$ (x=0.065)

Physical Review B **81** (2010)

J Lettry, M Kronberger, R Scrivens, E Chaudet, D Faircloth, G Favre, J Geisser, D Kuechler, S Mathot, O Midttun, M Paoluzzi, C Schmitzer and D Steyaert

High duty factor plasma generator for CERN's Superconducting Proton Linac

Review of Scientific Instruments **81** (2010)

I Levin, S Karimi, V Provenzano, C Dennis, H Wu, T Comyn, T Stevenson, R Smith and I Reaney

Reorientation of magnetic dipoles at the antiferroelectric-paraelectric phase transition of $Bi_{1-x}Nd_xFeO_3$ (0.15 <= x <= 0.25)

Physical Review B **81** (2010)

I Levin, JC Woicik, A Llobet, MG Tucker, V Krayzman, J Pokorny and IM Reaney

Displacive ordering transitions in perovskite-like $AgNb_{1/2}Ta_{1/2}O_3$

Chemistry of Materials **22** 17 4987-4995 (2010)

H Lewtas, T Lancaster, P Baker, S Blundell and D Prabhakaran and FL Pratt

Local magnetism and magnetoelectric effect in $HoMnO_3$ studied with muon-spin relaxation

Physical Review B **81** (2010)

R Lichti, K Chow and S Cox

Defect-level pinning and shallow states of the muonium isotope of hydrogen

Physica B: Condensed Matter **404** 5106-5109 (2009)

V Lopez-Flores, S Ansell, S Ramos, D Bowron, S Diaz-Moreno and A Munoz-Paez

Development of ReflEXAFS data analysis for deeper surface structure studies

J Phys: Conference Series **190** (2009)

T Lord, J Hobbs, A Terry, A Kvick and S Hanna

Variation of lattice parameters with fold state in the Ultralong n-Alkanes

Macromolecules **43** 3365-3375 (2010)

M Lumsden, A Christianson, E Goremychkin, S Nagler, H Mook, M Stone, D Abernathy, T Guidi, G MacDougall, Cde la Cruz, A Sefat, M McGuire, B Sales and D Mandrus

Evolution of spin excitations into the superconducting state in $FeTe_{1-x}Se_x$

Nature Physics **6** 182-186 (2010)

P Macchi, N Casati, WG Marshall and A Sironi

The alpha and beta forms of oxalic acid di-hydrate at high pressure: a theoretical simulation and a neutron diffraction study

Crystengcomm **12** 9 2596-2603

D MacLaughlin, A Hillier, J Mackie, L Shu, Y Aoki, D Kikuchi, H Sato, Y Tunashima and H Sugawara

Comment on 'Pronounced enhancement of the lower critical field and critical current deep in the superconducting state of $PrOs_4Sb_{12}$'

Physical Review Letters **105** (2010)

S Magazu, F Migliardo, F Affouard, M Descamps and M Telling

Study of the relaxational and vibrational dynamics of bioprotectant glass-forming mixtures by neutron scattering and molecular dynamics simulation

The Journal of Chemical Physics **132** (2010)

B Maier, R Angel, W Marshall, B Mihailova, C Paulmann, J Engel, M Gospodinov, A Welsch, D Petrova and U Bismayer

Octahedral tilting in Pb-based relaxor ferroelectrics at high pressure

Acta Crystallographica Section B Structural Science **66** 280-291 (2010)

C Malardier-Jugroot, D Bowron, A Soper, M Johnson and T Head-Gordon

Structure and water dynamics of aqueous peptide solutions in the presence of co-solvents

Physical Chemistry Chemical Physics **12** 382-392 (2010)

E Mamontov and D Neumann

A background suppression chopper for the high-flux backscattering spectrometer at NIST

Journal of Neutron Research **16** 65-74 (2009)

R Mancinelli, S Imberti, AK Soper, KH Liu, CY Mou, F Bruni and MA Ricci

Multiscale approach to the structural study of water confined in MCM41

Journal of Physical Chemistry B **113** 16169-16177 (2009)

J Manson, T Lancaster, S Blundell, Y Qiu, J Singleton, P Sengupta, F Pratt, J Kang, C Lee and M Whangbo

Spin fluctuations and orbital ordering in quasi-one-dimensional alpha-Cu(dca)$_2$(pyz);a = dicyanamide = N(CN)$_2$-; pyz = pyrazine, a molecular analogue of $KCuF_3$

Polyhedron **29** 514-520 (2010)

J Manson, K Stone, H Southerland, T Lancaster, A Steele, S Blundell, F Pratt, P Baker, R McDonald, P Sengupta, J Singleton, P Goddard, C Lee, M Whangbo, M Warter, C Mielke and P Stephens

Characterisation of the antiferromagnetism in Ag(pyz)$_2$(S$_2$O$_8$) (pyz = Pyrazine) with a two-dimensional square lattice of Ag_{2+} ions

Journal of the American Chemical Society **131** 4590 (2009)

P Manuel, L Chapon, I Todorov, D Chung, J Castellan, S Rosenkranz, R Osborn, P Toledano and M Kanatzidis

Incommensurate spin-density wave and magnetic lock-in transition in $CaFe_4As_3$

Physical Review B **81** (2010)

AJ Markvardsen and WIF David

Diffusion-equation method for crystallographic figure of merits

Acta Crystallographica Section A **66** 591-596

D Martínez-Blanco, P Gorria, J Blanco and R Smith

Temperature induced phase transformations and microstructural changes in nanostructured FeCu solid solutions using in situ neutron powder thermo-diffraction

Journal of Alloys and Compounds **483** 549-552 (2009)

B Matthews, A Duncan, C Jones, C Neylon, S Coles, M Borkum and P Hunter

A protocol for exchanging scientific citations

5th IEEE International Conference on e-Science (2009)

B Matthews, S Sufi, D Flannery, L Lerusse, T Griffin, M Gleaves and K Kleese

Using a core scientific metadata model in large-scale facilities

5th International Digital Curation Conference (2009)

F Meersman, D Bowron, A Soper and M Koch

Counteraction of urea by trimethylamine N-oxide is due to direct interaction

Biophysical Journal **97** 2559-2566 (2009)

DIA Millar, WG Marshall, IDH Oswald and CR Pulham

High-pressure structural studies of energetic materials

Crystallography Reviews **16** 2 115-132

DIA Millar, HE Maynard-Casely, AK Kleppe, WG Marshall, CR Pulham and AS Cumming

Putting the squeeze on energetic materials-structural characterisation of a high-pressure phase of CL-20

Crystal Engineering Comm **12** 9 2524-2527

DIA Millar, IDH Oswald, C Barry, DJ Francis, WG Marshall, CR Pulham and AS Cumming

Pressure-cooking of explosives-the crystal structure of epsilon-RDX as determined by X-ray and neutron diffraction

Chemical Communications **46** 31 5662-5664

M Mito, M Pitcher, W Crichton, G Garbarino, P Baker, S Blundell, P Adamson, D Parker and S Clarke

Response of superconductivity and crystal structure of LiFeAs to hydrostatic pressure

Journal of the American Chemical Society **131** 2986-2992 (2009)

M Moglianetti, JRP Webster, S Edmondson, SP Armes and S Titmuss

Neutron reflectivity study of the structure of pH-responsive polymer brushes grown from a macroinitiator at the sapphire-water interface

Langmuir 26 **15** 12684-12689

A Mohamed, K Trickett, SY Chin, S Cummings, M Sagisaka, L Hudson, S Nave, R Dyer, SE Rogers, RK Heenan and J Eastoe

Universal surfactant for water, oils, and CO_2

Langmuir **26** 17 13861-13866

R Moss, EA Neel, D Pickup, H Twyman, R Martin, M Henson, E Barney, A Hannon, J Knowles and R Newport

The effect of zinc and titanium on the structure of calcium-sodium phosphate based glass

Journal of Non-Crystalline Solids **356** 1319-1324 (2010)

F Mulder, B Assfour, J Huot, T Dingemans, M Wagemaker and A Ramirez-Cuesta

Hydrogen in the metal-organic framework Cr MIL-53

Journal of Physical Chemistry **114** 10648-10655 (2010)

O Muransky, M Barnett, D Carr, S Vogel and E Oliver

Investigation of deformation twinning in a fine-grained and coarse-grained ZM20 Mg alloy: Combined in situ neutron diffraction and acoustic emission

Acta Materialia **58** 1503-1517 (2010)

D Muransky, D Carr, P Sittner and E Oliver

In situ neutron diffraction investigation of deformation twinning and pseudoelastic-like behaviour of extruded AZ31 magnesium alloy

International Journal of Plasticity **25** 1107-1127 (2009)

K Mutch, Jv Duijneveldt, J Eastoe, I Grillo and R Heenan

Scaling the structure factors of protein limit colloid-polymer mixtures

Langmuir **26** 1630-1634 (2010)

O Myakonkaya, B Deniau, J Eastoe, S Rogers, A Ghigo, M Hollamby, A Vesperinas, M Sankar, S Taylor, J Bartley and G Hutchings

Recovery and reuse of nanoparticles by tuning solvent quality

Chemsuschem **3** 339-341 (2010)

DE Nanu, MG Tucker, WG Haije, JF Vente and AJ Bottger

Atom configurations in Pd-Au and Pd-Au-D alloys: a neutron total scattering and Reverse Monte Carlo study

Acta Materialia **58** 16 5502-5510

K Nemkovski, P Alekseev, J- Mignot, E Goremychkin, A Nikonov, O Parfenov, V Lazukov, N Shitsevalova and A Dukhnenko

Spin dynamics in the electron-doped Kondo insulator $Yb_{1-x}Zr_xB_{12}$ (x=0.2)

Physical Review B **81** (2010)

C Neylon

Head in the clouds: reimagining the laboratory record for the web-based, networked world

Automated Experimentation **1** (2009)

C Neylon

Stitching science together

Nature **461** 881 (2009)

C Neylon and S Wu

Article-level metrics and the evolution of scientific impact

PLOS Biology **7** (2009)

ST Norberg, S Hull, R Mathieu and SG Eriksson

Local structural properties of $0.5BiMnO_3$-$0.5ATiO_3$ (A = Ba or Sr)

Chemical Communications **46** 9 1455-1457 (2010)

J O'Callaghan, H McNamara, M Copley, J Hanrahan, M Morris, D Steytler, R Heenan and J Holmes

Swelling of ionic and nonionic surfactant micelles by high pressure gases

Langmuir **26** 7725-7731 (2010)

K Omoto, S Norberg, S Hull, A Aoto and T Hashimoto

Neutron diffraction study of the crystal structure and structural phase transition of $La_{0.7}Ca_{0.3-x}Sr_xCrO_3$ (0 <= x <= 0.3): the relationship between thermodynamic behavior and crystal structure changes at the phase transition

Journal of Solid State Chemistry **183** 392-401 (2010)

I Oswald, D Millar, A Davidson, D Francis, W Marshall, C Pulham, A Cumming, A Lennie and J Warren

High-pressure structural studies of energetic compounds

International Journal of High Pressure Research **30** 280-291 (2010)

S Paddea, J Francis, A Paradowska, P Bouchard and I Shibli

Characterisation of residual stresses in a welded P91 pipe section using neutron diffraction

High Temperature Defect Assesment 5 (2010)

S Paddea, J Francis, A Paradowska, P Bouchard and I Shibli

Residual stresses in as-welded P91 steel pipe

8th European Conference on Residual Stresses (2010)

S Pagnotta, S McLain, A Soper, F Bruni and M Ricci

Water and trehalose: flow much do they Interact with each other?

The Journal of Physical Chemistry B **114** 4904-4908 (2010)

F Pan, X Zhao, S Perumal, T Waigh, J Lu and J Webster

Interfacial dynamic adsorption and structure of molecular layers of peptide surfactants

Langmuir **26** 5690-5696 (2010)

B Panicaud, A Baczmanski, M Francois, C Braham and A Paradowska

Large deformation and mechanical effects of damage in aged duplex stainless steel

Materials Science Forum **652** 155-161 (2010)

A Paradowska, O Kirstein and A Moor

Investigation of residual stress in laser formed mild steel plates using neutron diffraction

Materials Science Forum **652** 123-128 (2010)

AM Paradowska, JWH Price, TR Finlayson, U Lienert and R Ibrahim

Comparison of neutron and synchrotron diffraction measurements of residual stress in bead-on-plate weldments

Journal of Pressure Vessel Technology-Transactions of the Asme **132** 1 (2010)

AM Paradowska, JWH Price, B Kerezsi, P Dayawansa and XL Zhao

Stress relieving and its effect on life of welded tubular joints

Engineering Failure Analysis **17** 1 320-327

D Parker, M Pitcher, P Baker, I Franke, T Lancaster, S Blundell and S Clarke

Structure, antiferromagnetism and superconductivity of the layered iron arsenide NaFeAs

Chemical Communications **16** 2189-2191 (2009)

D Parker, M Smith, T Lancaster, A Steele, I Franke, P Baker, F Pratt, M Pitcher, S Blundell and S Clarke

Control of the competition between a magnetic phase and a superconducting phase in cobalt-doped and nickel-doped NaFeAs using electron count

Physical Review Letters **104** (2010)

S Parker

Reactions of iron atoms with benzene

The Journal of Physical Chemistry A **114** 1657-1664 (2010)

S Parker

Spectroscopy and bonding in ternary metal hydride complexes: potential hydrogen storage media

Coordination Chemistry Reviews **254** 215-234 (2010)

SF Parker, DT Bowron, S Imberti, AK Soper, K Refson, ES Lox, M Lopez and P Albers

Structure determination of adsorbed hydrogen on a real catalyst

Chemical Communications **46** 17 2959-2961 (2010)

SF Parker, K Refson, AC Hannon, ER Barney, SJ Robertson and P Albers

Characterisation of hydrous palladium oxide: implications for low-temperature carbon monoxide oxidation

Journal of Physical Chemistry C **114** 33 14164-14172

A Parnell, A Dunbar, A Pearson, P Staniec, A Dennison, H Hamamatsu, M Skoda, D Lidzey and R Jones

Depletion of PCBM at the cathode interface in P3HT/PCBM thin films as quantified via neutron reflectivity measurements

Advanced Materials **22** 2444 (2010)

S Parnell, M Deppe, S Ajraoui, J Parra-Robles, S Boag and J Wild

Measurement of laser heating in spin exchange optical pumping by NMR diffusion sensitisation gradients

Journal of Applied Physics **107** (2010)

E Pascual, J Amores, R Puche, M Castro, N Taira, J d Paz and L Chapon

Zircon to scheelite phase transition induced by pressure and magnetism in $TbCrO_4$

Physical Review B **81** (2010)

A Paul, I Fallis, C Cooper, T Wess, K Thomas, R Heenan, S King and P Griffiths

A contrast variation small-angle scattering study of the microstructure of 2,5-dimethyl-7-hydroxy-2,5-diazaheptadecane-toluene-butanol oil-in-water metallomicroemulsions

Soft Matter **6** 2552-2556 (2010)

A Paul, C James, RK Heenan and R Schweins

Drug mimic induced conformational changes in model polymer-drug conjugates characterised by small-angle neutron scattering

Biomacromolecules **11** 8 1978-1982 (2010)

B Peplinski, A Fitch, A Evans, R Ibberson, D Toebbens, L Cranswick, I Doerfel, F Emmerling and R Matschat

Structural characterisation of a coarse-grained transparent silicon carbide powder by a combination of powder diffraction techniques

Zeitschrift für Kristallographie 61-66 (2009)

V Peterson, G Kearley, Y Wu, A Ramirez-Cuesta, E Kemner and C Kepert

Local vibrational mechanism for negative thermal expansion: a combined neutron scattering and first-principles study

Angewandte Chemie International Edition **49** 585-588 (2010)

O Pieper, T Guidi, S Carretta, J v Slageren, F Hallak, B Lake, P Santini, G Amoretti, H Mutka, M Koza and M Russina et al

Inelastic neutron scattering and frequency-domain magnetic resonance studies of S=4 and S=12 Mn6 single-molecule magnets

Physical Review B **81** 174420 (2010)

B Pine and C Warsop

Longitudinal dynamics studies for ISIS upgrades

Particle Accelerator Conference (2009)

MJ Pitcher, T Lancaster, JD Wright, I Franke, AJ Steele, PJ Baker, FL Pratt, WT Thomas, DR Parker, SJ Blundell and SJ Clarke

Compositional control of the superconducting properties of LiFeAs

Journal of the American Chemical Society **132** 30 10467-10476 (2010)

H Postma, L Amkreutz, A Borella, M Clarijs, H Kamermans, W Kockelmann, A Paradowska, P Schillebeeckx and D Visser

Non-destructive bulk analysis of the Buggenum sword by neutron resonance capture analysis and neutron diffraction 2010

Journal of Radioanalytical and Nuclear Chemistry **283** 641-652 (2010)

V Poulopoulou, F Fernandez-Alonso and JF Garcia

Perfil Cientifico de Charles Darwin

Trabajos Dedicados a Charles Darwin por Medicos y Cientificos Asturianos con Motivo del 200 Aniversario de su Nacimiento 83-138 (2009)

A Powell, J Lord, D Gregory and J Titman

Muon spin relaxation studies of lithium nitridometallate battery materials: muon trapping and lithium ion diffusion

Journal of Physical Chemistry C **113** 20758-20763 (2009)

A Prag, R Garner, E Pantos, S Bennett, J Mosselmans, M Tobin, W Kockelmann, L Chapon, N Salvado and T Pradell

How the Greeks got ahead: technological aspects of manufacture of a Corinthian type Hoplite bronze helmet from Olympia

History of Mechanism and Machine Science **6** (2009)

F Pratt, P Baker, S Blundell, T Lancaster, H Lewtas, P Adamson, M Pitcher, D Parker and S Clarke

Enhanced superfluid stiffness, lowered superconducting transition temperature, and field-induced magnetic state of the pnictide superconductor LiFeAs

Physical Review B **79** (2009)

J Price and T Finlayson

Comparison of residual stresses measurements techniques applicable to the steel welded components

Welding and Welded Structures **3** 119-127 (2009)

J Price, T Finlayson and R Ibrahim

Evaluation of residual stress measurements before and after post-weld heat treatment in the weld repairs

Journal of Physics: Conference Series (2009)

J Price, T Finlayson, U Lienert and R Ibrahim

Comparison of neutron and synchrotron measurements of residual stress in bead-on-plate weldments

Journal of Pressure Vessel Technology **132** 1-8 (2010)

J Price, T Finlayson, U Lienert, P Walls and R Ibrahim

Residual stress distribution in steel butt welds measured by neutron and synchrotron diffraction

Journal of Physics: Condensed Matter **21** 1-8 (2009)

J Price, B Kerezsi, P Dayawansa and X-L Zhao

Stress relieving and its effect on life of welded tubular joints

Engineering Failure Analysis **17** 320-327 (2010)

D Procissi, P Arosio, F Orsini, M Marinone, A Cornia and A Lascialfari

Muon spin relaxation investigation of tetranuclear iron(III) $Fe_4(OCH_3)_6(dpm)_6$ molecular cluster

Physical Review B **80** (2009)

DL Quintero-Castro, B Lake, EM Wheeler, A Islam, T Guidi, KC Rule, Z Izaola, M Russina, K Kiefer and Y Skourski

Magnetic excitations of the gapped quantum spin dimer antiferromagnet $Sr_3Cr_2O_8$

Physical Review B **81** 1 (2010)

A Remhof, R Gremaud, F Buchter, Z Lodziana, J Embs, T Ramirez-Cuesta, A Borgschulte and A Zuettel

Hydrogen dynamics in lightweight tetrahydroborates

Journal of Research in Physical Chemistry **224** 263-278 (2010)

F Roosen-Runge, M Hennig, T Seydel, F Zhang, M Skoda, S Zorn, R Jacobs, M Maccarini, P Fouquet and F Schreiber

Protein diffusion in crowded electrolyte solutions

Biochimica et Biophysica Acta (BBA) – Proteins & Proteomics **1804** 68-75 (2010)

VG Sakai and A Arbe

Quasielastic neutron scattering in soft matter

Current Opinion in Colloid & Interface Science **14** 381-390 (2009)

VG Sakai and M Telling

ISIS Molecular Spectroscopy User Group Meeting 2008

Neutron News **20** 5-6 (2009)

K Sasai, M Kofu, RM Ibberson, K Hirota, J Yamaura, Z Hiroi and O Yamamuro

A novel isomorphic phase transition in beta-pyrochlore oxide KOs_2O_6: a study using high resolution neutron powder diffraction

Journal of Physics-Condensed Matter **22** 1 (2010)

M Schmidtmann, L Farrugia, D Middlemiss, M Gutmann, G McIntyre and C Wilson

Experimental and theoretical charge density study of polymorphic isonicotinamide-oxalic acid molecular complexes with strong O...H...N hydrogen bonds

Journal of Physical Chemistry **113** 13985-13997 (2009)

P Schofield, C Wilson, K Knight and C Kirk

Proton location and hydrogen bonding in the hydrous lead copper sulfates linarite $PbCu(SO_4)_2(OH)_2$, and Caledonite, $Pb_5Cu_2(SO_4)_3CO_3(OH)_6$

American Mineralogist **47** 649-662 (2009)

E Schooneveld, M Tardocchi, G Gorini, W Kockelmann, T Nakamura, E Perelli-Cippo and N Rhodes

A position-sensitive transmision detector for epithermal neutron imaging

Journal of Physics D Applied Physics **42** (2009)

AG Seel, A Sartbaeva, AJ Rammirez-Cuesta and PP Edwards

Inelastic neutron scattering of Na-zeolite A with in situ ammoniation: an examination of initial coordination

Physical Chemistry Chemical Physics **12** 33 9661-9666 (2010)

S Shalev, S Shilstein, A Paradowska, W Kockelmann and Y Levy

Neutron diffraction study of Levantine Middle Bronze Age cast axes

Journal of Physics: Conference Series (2009)

K Shankland, T Griffin, J van de Streek, J Cole, N Shankland, A Florence and W David

Large-scale distributed computing for accelerated structure solution

Zeitschrift für Kristallographie 227-232 (2009)

K Shankland, A Markvardsen, C Rowlatt, N Shankland and W David

A benchmark method for global optimisation problems in structure determination from powder diffraction data

Journal of Applied Crystallography **43** 401-406 (2010)

J Sharma, SM King, L Bohlin and N Clarke

Apparatus for simultaneous rheology and small-angle neutron scattering from high-viscosity polymer melts and blends

Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment **620** 2-3 437-444 (2010)

N Sharma, R Withers, K Knight and C Ling

Structure, crystal chemistry and thermal evolution of the delta-Bi_2O_3-related phase Bi_9ReO_{17}

Journal of Solid State Chemistry **182** 2468-2474 (2009)

H Shen, R Thomas, J Penfold and G Fragneto

Destruction and solubilisation of supported phospholipid bilayers on silica by the biosurfactant surfactin

Langmuir **26** 7334-7342 (2010)

HH Shen, RK Thomas and P Taylor

The location of the biosurfactant surfactin in phospholipid bilayers supported on silica using neutron reflectometry

Langmuir 26 1 320-327

I Silverwood, N Hamilton, C Laycock, J Staniforth, R Ormerod, C Frost, S Parker and D Lennon

Quantification of surface species present on a nickel/alumina methane reforming catalyst

Physical Chemistry Chemical Physics **12** 3102-3107 (2010)

L Smrcok, D Tunega, A Ramirez-Cuesta, A Ivanov and J Valuchova

The combined inelastic neutron sattering(INS) and solid-state DFT study of hydrogen-atoms dynamics in kaolinite-dimethylsulfoxide intercate

2010 Clays and Clay Minerals **58** 52-61 (2010)

L Smrcok, D Tunega, AJ Ramirez-Cuesta and E Scholtzova

The combined inelastic neutron scattering and solid state DFT study of hydrogen atoms dynamics in a highly ordered kaolinite

Physics and Chemistry of Minerals **37** 8 571-579 (2010)

T Smyth, A Perfumo, R Marchant, I Banat, M Chen, R Thomas, J Penfold, P Stevenson and N Parry

Directed microbial biosynthesis of deuterated biosurfactants and potential future application to other bioactive molecules

Applied Microbiology and Biotechnology **87** 1347-1354 (2010)

A Soper, J Teixeira and T Head-Gordon

Is ambient water inhomogeneous on the nanometer-length scale?

Proceedings of the National Academy of Sciences **107** (2010)

G Srinivas, A Lovell, N Skipper, S Bennington, Z Kurban and R Smith

Ammonia absorption in calcium graphite intercalation compound: in situ neutron diffraction, Raman spectroscopy and magnetisation

Physical Chemistry Chemical Physics **12** 6253-6259 (2010)

A Stadler

Dynamics in biological systems as seen by QENS

Z Phys Chem **224** 201-214 (2010)

U Staub, Y Bodenthin, C Piamonteze, M Garcia-Fernandez, V Scagnoli, M Garganourakis, S Koohpayeh, D Fort and S Lovesey

Parity- and time-odd atomic multipoles in magnetoelectric $GaFeO_3$ as seen via soft X-ray Bragg diffraction

Physical Review B **80** (2009)

T Stevenson, TP Comyn, A Daoud-Aladine and AJ Bell

Change in periodicity of the incommensurate magnetic order towards commensurate order in bismuth ferrite lead titanate

Journal of Magnetism and Magnetic Materials **322** 22 L64-L67 (2010)

C Stock, W Buyers, K Rule, J Chung, R Liang, D Bonn and W Hardy

Magnetic field resonantly enhanced free spins in heavily underdoped $YBa_2Cu_3O_{6+x}$

Physical Review B **79** (2009)

C Stock, R Cowley, J Taylor and S Bennington

High-energy neutron scattering from hydrogen using a direct geometry spectrometer

Physical Review B **81** (2010)

W Suder and S Williams

Neutron diffraction residual stress measurements in key-hole laser formed weldments

Journal of Physics: Conference Series (2009)

I Swainson, C Stock, P Gehring, G Xu, K Hirota, Y Qiu, H Luo, X Zhao, J-F Li and D Viehland

Soft phonon columns on the edge of the Brillouin zone in the relaxor $PbMg_{1/3}Nb_{2/3}O_3$

Physical Review B **79** (2009)

R Tabor, J Eastoe, P Dowding, I Grillo and S Rogers

Bidisperse colloids: nanoparticles and microemulsions in coexistence

Journal of Colloid and Interface Science **344** 447-450 (2010)

Y Tanaka, S Collins, S Lovesey, M Matsumami, T Moriwaki and S Shin

Determination of the absolute chirality of tellurium using resonant diffraction with circularly polarised X-rays

Journal of Physics Condensed Matter **22** (2010)

L Thomas, N Blagden, M Gutmann, A Kallay, A Parkin, C Seaton and C Wilson

Tuning proton behavior in a ternary molecular complex

Crystal Growth & Design **10** 2770-2774 (2010)

L Thomas, A Florence and C Wilson

Hydrogen atom behaviour imaged in a short intramolecular hydrogen bond using the combined approach of X-ray and neutron diffraction

New Journal of Chemistry **33** 2486-2490 (2009)

I Todorov, DY Chung, H Claus, KE Gray, QA Li, J Schleuter, T Bakas, AP Douvalis, M Gutmann and MG Kanatzidis

Selective substitution of Cr in $CaFe_4As_3$ and its effect on the spin density wave

Chemistry of Materials **22** 17 4996-5002 (2010)

K Tomiyasu, H Kageyama, C Lee, M Whangbo, Y Tsujimoto, K Yoshimura, J Taylor, A Llobet, F Trouw, K Kakurai and K Yamada

Magnetic excitations in infinite-layer antiferromagnetic insulator

Journal of the Physical Society of Japan **79** (2010)

J Tomkinson

Comment on: 'FTIR and FTRaman spectra, assignments, ab initio HF and DFT analysis of 4-nitrotoluene' by S Ramalingam et al., Spectrochemica Acta A 75 (2010) 1308-1314

Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy **75** 4 1377-1379 (2010)

J Tomkinson, S Parker and D Lennon

No evidence for Evans holes in the ABC vibrational structure of KH_2AsO_4

The Journal of Chemical Physics **133** (2010)

V Tran, A Hillier and D Adroja

Reply to 'Comment on "Muon-spin-rotation study of the superconducting properties of Mo_3Sb_7"'

Physical Review B **82** (2010)

V Tran, A Hillier, D Adroja, Z Bukowski and W Millier

Evidence for a spin pseudogap in the normal state of superconducting Mo_3Sb_7

Journal of Physics Condensed Matter **21** 485701 (2009)

A Tremsin, J McPhate, W Kockelmann, J Vallerga, O Siegmund and W Feller

Energy-resolving neutron transmission radiography at the ISIS pulsed spallation source with a high-resolution neutron counting detector

IEEE Transactions on Nuclear Science **56** 2931-2937 (2009)

K Trickett, H Brice, O Myakonkaya, J Eastoe, S Rogers, R Heenan and I Grillo

Microemulsion-based organogels containing inorganic nanoparticles

Soft Matter **6** 1291-1296 (2010)

K Trickett, D Xing, J Eastoe, R Enick, A Mohamed, M Hollamby, S Cummings, S Rogers and R Heenan

Hydrocarbon metallosurfactants for CO_2

Langmuir **26** 4732-4737 (2010)

K Trickett, D Xing, R Enick, J Eastoe, M Hollamby, K Mutch, S Rogers, R Heenan and D Steytler

Rod-Like Micelles Thicken CO_2

Langmuir **26** 83-88 (2010)

I Tucker, J Penfold, R Thomas, C Dong, S Golding, C Gibson and I Grillo

Surface and solution properties of anionic/nonionic surfactant mixtures of alkylbenzene sulfonate and triethyleneglycol decyl ether

Langmuir **26** 10614-10626 (2010)

I Tucker, J Petkov, J Penfold and R Thomas

Adsorption of nonionic and mixed nonionic/cationic surfactants onto hydrophilic and hydrophobic cellulose thin films

Langmuir **26** 8036-8048 (2010)

C Utfeld, J Laverock, T Haynes, S Dugdale, J Duffy, M Butchers, J Taylor, S Giblin, J Analytis, J Chu, I Fisher, M Itou and Y Sakurai

Bulk electronic structure of optimally doped $Ba(Fe_{1-x}Cox)_2As_2$

Physical Review B **81** (2010)

B Varga, F Migliardo, E Takacs, B Vertessy, S Magazu and M Telling

Study of solvent-protein coupling effects by neutron scattering

Journal of Biological Physics **36** 207-220 (2010)

PD Vaz, MM Nolasco, F Gil, PJA Ribeiro-Claro and J Tomikinson

Hydrogen-bond dynamics of C-H ... O Interactions: the chloroform ... acetone case

Chemistry-a European Journal **16** 30 9010-9017 (2010)

C Vecchini, M Poienar, F Damay, O Adamopoulos, A Daoud-Aladine, A Lappas, JM Perez-Mato, LC Chapon and C Martin

Magnetoelastic coupling in the frustrated antiferromagnetic triangular lattice $CuMnO_2$

Physical Review B **82** 9 (2010)

M de Vries, J Stewart, P Deen, J Piatek, G Nilsen, H Ronnow and A Harrison

Scale-free antiferromagnetic fluctuations in the s=1/2 Kagome antiferromagnet

Herbertsmithite Physical Review Letters **103** (2009)

MD Vries-Melein, D Visser, J Mulder, L Megens, S Imberti, W Kockelmann and H Kars

Mesopotamian hematite seals in a new light

6th International Congress on the Archaeology of the Ancient Near East 2008 (2009)

H Walker, R Ewings, F Fabrizi, D Mannix, C Mazzoli, S Wilkins, L Paoloasini, D Prabhakaran, A Boothroyd and D McMorrow

X-ray resonant scattering study of the magnetic phase diagram of multiferroic $TbMnO_3$

Journal of Physics Condensed Matter **404** 3264-3266 (2009)

A Walters, T Perring, J-S Caux, A Savici, G Gu, C-C Lee, W Ku and I Zaliznyak

Effect of covalent bonding on magnetism and the missing neutron intensity in copper oxide compounds

Nature Physics **5** 867-872 (2009)

L Wang, R Tabor, J Eastoe, X Li, R Heenan and J Dong

Formation and stability of nanoemulsions with mixed ionic-nonionic surfactants

Physical Chemistry Chemical Physics **11** 9772-9778 (2009)

G Weber, J Essex and C Neylon

Probing the microscopic flexibility of DNA from melting temperatures

Nature Physics **5** 769-773 (2009)

H Wei, W Kockelmann, E Godfrey, D Scott and W Xiaohong

Non-destructive phase analysis of Song Dynasty iron coins by TOF neutron diffraction

Acta Scientiarum Naturalium Universitatis Pekinensis **46** 245-250 (2010)

E Weidner, I Shabalin, M Telling, C Jewell, D Gregory and D Ross

Pressure-dependent deuterium reaction pathways in the LiND system

Physical Chemistry Chemical Physics **12** 2089-2097 (2010)

T Willers, Z Hu, N Hollmann, P Koerner, J Gegner, T Burnus, H Fujiwara, A Tanaka, D Schmitz, H Hsieh, H-Lin, C Chen, E Bauer, J Sarrao, E Goremychkin, M Koza, L Tjeng and A Severing

Crystal-field and Kondo-scale investigations of CeMIn5 (M=Co, Ir, and Rh): a combined X-ray absorption and inelastic neutron scattering study

Physical Review B **81** (2010)

R Wimpory, A Paradowska and K Nikbin

Residual stress measurements in large scale component sections

Materials Science Forum **652** 321-327 (2010)

C Wu, G Wu, Z Xiong, W David, K Ryan, M Jones, P Edwards, H Chu and P Chen

Stepwise phase transition in the formation of lithium amidoborane

Inorganic Chemistry **49** 4319-4323 (2010)

G Xu, G Gu, M Hücker, B Fauqué, T Perring, L Regnault and J Tranquada

Testing the itinerancy of spin dynamics in superconducting $Bi_2Sr_2CaCu_2O_8$

Nature **5** 642-646 (2009)

Y Yan, I Telepeni, S Yang, X Lin, W Kockelmann, A Dailly, A Blake, W Lewis, G Walker, D Allan, S Barnett, N Champness and M Schroder

Metal-organic polyhedral frameworks: high H_2 adsorption capacities and neutron powder diffraction studies

Journal of the American Chemical Society **132** 4092 (2010)

G Yang, Z Jiang, H Shi, M Jones, T Xiao, P Edwards and Z Yan

Study on the photocatalysis of F-S co-doped TiO_2 prepared using solvothermal method

Applied Catalysis B Environmental **96** 458-465 (2010)

C Yin, G Li, W Kockelmann, F Liao, J Attfield and J Lin

Frustrated and unfrustrated magnetic orders in the 10H Perovskite $Ba_5Sb_{1-x}Mn_{4+x}O_{15-\delta}$

Chemistry of Materials **22** 3269-3276 (2010)

C Yin, G Li, W Kockelmann, J Lin and J Attfield

Charge transfer and a magnetic crossover in hexagonal $BaRu_{1-x}Mn_xO_3$ perovskites

Physical Review B **80** (2009)

M Zaberchik, K Chashka, L Patlgan, A Maniv, C Baines, P King and A Kanigel

A Possible evidence of a two-gap structure for the Cu_xTiSe_2 superconductor

Physical Review B **81** 220505 (2010)

P Zaleski, K Szymanski, J Przewoznik, K Recko, S Cottrell and L Dobrzynski

Cr_3Si doped by Co studied by muon spin relaxation and scanning electron microscopy techniques

Journal of Alloys and Compounds **498** 5-12 (2010)

A Zeidler, J Drewitt, P Salmon, A Barnes, W Crichton, S Klotz, H Fischer, C Benmore, S Ramos and A Hannon

Establishing the structure of GeS_2 at high pressures and temperatures: a combined approach using X-ray and neutron diffraction

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

B Zhang, M Kurmoo, T Mori, Y Zhang, F Pratt and D Zhu

Polymorphism in Hybrid Organic-Inorganic Bilayered Magnetic Conductors (BEDT-TTF)$_3$((FeCl$_4$)-Cl-III)$_2$, BEDT-TTF = bis(ethylenedithio) tetrathiafulvalene

Crystal Growth & Design **10** 782-789 (2010)

J Zhang, E Kisi, D Riley, M Styles and A Paradowska

Single crystal elastic constants of the MAX phase Ti_3AlC_2 determined by neutron diffraction

Materials Science Forum 638-642 2417-2422 (2010)

S Zhang, E Godfrey, B Abbey, P Xu, Y Tomota, D Liljedahl, O Zanellato, M Fitzpatrick, J Kelleher, S Siano, J Santisteban and A Korsunsky

Materials structure and strain analysis using time-of-flight neutron diffraction

World Congress on Engineering 2009, Vols I and II 1412-1419 (2009)

S Zhang, E Godfrey, W Kockelmann, A Paradowska, M Bull, B Abbey, A Korsunsky, P Xu, Y Tomota, D Liljedahl, O Zanellato, M Fitzpatrick, M Daymond, R Toda, R Holt, J Kelleher, S Siano and J Santisteban

Materials engineering: high-tech composites to ancient metals

Materials Today **12** 78-84 (2009)

S Zhang, S Hainsworth and E Oliver

Temperature dependence of low cycle fatique behaviour in extruded

5th International Conference on Mechanical Stress Evaluation by Neutron and Synchrotron Radiation (2009)

S Zhang, W Kockelmann, A Paradowska, J James, G Burca and L Chapon

IMAT: an maging and engineering facility for ISIS TS-II

5th International Conference on Mechanical Stress Evaluation by Neutron and Synchrotron Radiation (2009)

S-Y Zhang and J Kelleher

Engin-X: neutrons for materials engineering

MECA SENS V (2009)

H Zhou, Y Jo, J Carpino, G Munoz, C Wiebe, J Cheng, F Rivadulla and D Adroja

Orbital fluctuations in the S=1/2 Mott insulator Sr_2VO_4

Physical Review B 81 (2010)

3 April 2009

Nigel J Mason
(The Open University)

Synchrotron radiation – a perfect mimic of starlight?

21 April 2009

Matthias Vojta
(University of Köln)

Lattice symmetry breaking in cuprate superconductors: how stripy is the pseudogap?

28 April 2009

Simon Phillips
(Research Complex, Harwell)

Cleaving the Holliday junction: how the synchrotron gave us an insight into the molecular mechanism of inheritance

12 May 2009

Chris Hooley
(University of St. Andrews)

A simple theory of the Invar effect in iron-nickel alloys

19 May 2009

Julia Yeomans
(University of Oxford)

Drops on micropatterned surfaces: how butterflies stay dry

26 May 2009

Roberto Car
(Princeton University)

Spectral signatures of short range order in condensed water phases

2 June 2009

Jonathan Doye
(University of Oxford)

Exploring the dynamics of self-assembly and crystallization in coarse-grained models of patchy colloids, proteins and DNA

9 June 2009

Pavlos Lagoudakis
(University of Southampton)

Nanoscale and hybrid optoelectronics

11 June 2009

Paul Chaikin
(New York University)

Experimental geometry with colloids and candies

23 June 2009

Yuri VTaran
(Joint Institute for Nuclear Research, Dubna)

Time of flight neutron stress analysis of fatigue degradation and martensitic transformation of austenitic steel AISI 321 under uni- and biaxial cycling loading

26 June 2009

Dr Alke Meents
(DESY, Hamburg)

Origin and temperature dependence of radiation damage in biological samples

30 June 2009

Professor Jeffery Tallon
(MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand)

Exotic or conventional – the physics of High-T_c superconductors

7 July 2009

Martin Rotter
(University of Oxford)

Going beyond the dipole approximation to improve the refinement of magnetic structures by neutron diffraction

10 July 2009

Dr Chris Jacobsen
(Stony Brook University)

X-ray microscopy: where is it at, and where might it go?

15 July 2009

Bob Cywinski
(University of Huddersfield)

Can thorium save the planet?

21 July 2009

Mark de Vries
(University of St. Andrews)

Scale-free antiferromagnetic fluctuations in the S=1/2 kagome antiferromagnet herbertsmithite – two interpretations and their implications

10 August 2009

R. Mukhopadhyay
(Bhabha Atomic Research Center, Mumbai)

Molecular motions in confined geometry

15 September 2009

Young Jun Chang
(Lawrence Berkeley National Laboratory, California)

Electronic properties of $SrTiO_3$: effects of the structural phase transition and interface doping

25 September 2009

Prof Dr Helmut Dosch
(DESY, Hamburg)

Grand challenges for megafacilities

6 October 2009

Markus Garst
(University of Köln)

Thermal expansion and magnetostriction close to quantum criticality

21 October 2009

Ulrich Roessler
(Leibniz Institute, Dresden)

Skyrmions in chiral magnets

10 November 2009

Patrick Soukiassian
(Paris-South University, Orsay)

Amazing nano-objects and nanochemistry at semiconductor surfaces and interfaces

17 November 2009

Anne de Visser
(University of Amsterdam)

Superconducting ferromagnets

19 January 2010

Pierre Toledano
(Universite de Picardie, Amiens)

Landau approach to phase transitions: rigorous results

26 January 2010

Dr Ilya Eremin
(Max-Planck-Institut)

Superconductivity and metallic spin density wave in iron-based superconductors

28 January 2010

Pierre Toledano
(Universite de Picardie, Amiens)

Landau theory of multiferroic materials

9 February 2010

Christoph Salzmann
(University of Oxford)

Ice XV and other forms of solid water

16 February 2010

Feliciano Giustino
(University of Oxford)

Electron-phonon interaction in copper oxides and iron pnictides

23 February 2010

Dr Kostya Trachenko
(Queen Mary University of London)

Understanding liquids and glass transition on the basis of elastic waves

2 March 2010

Dr Matthew Krzystyniak
(University of Oxford)

Neutron Compton scattering as a probe of proton micro-dynamics in condensed matter systems and molecules

9 March 2010

Dr Moritz Hoesch
(Diamond Light Source)

Giant Kohn Anomaly and the phase transition in charge-density-wave $ZrTe_3$

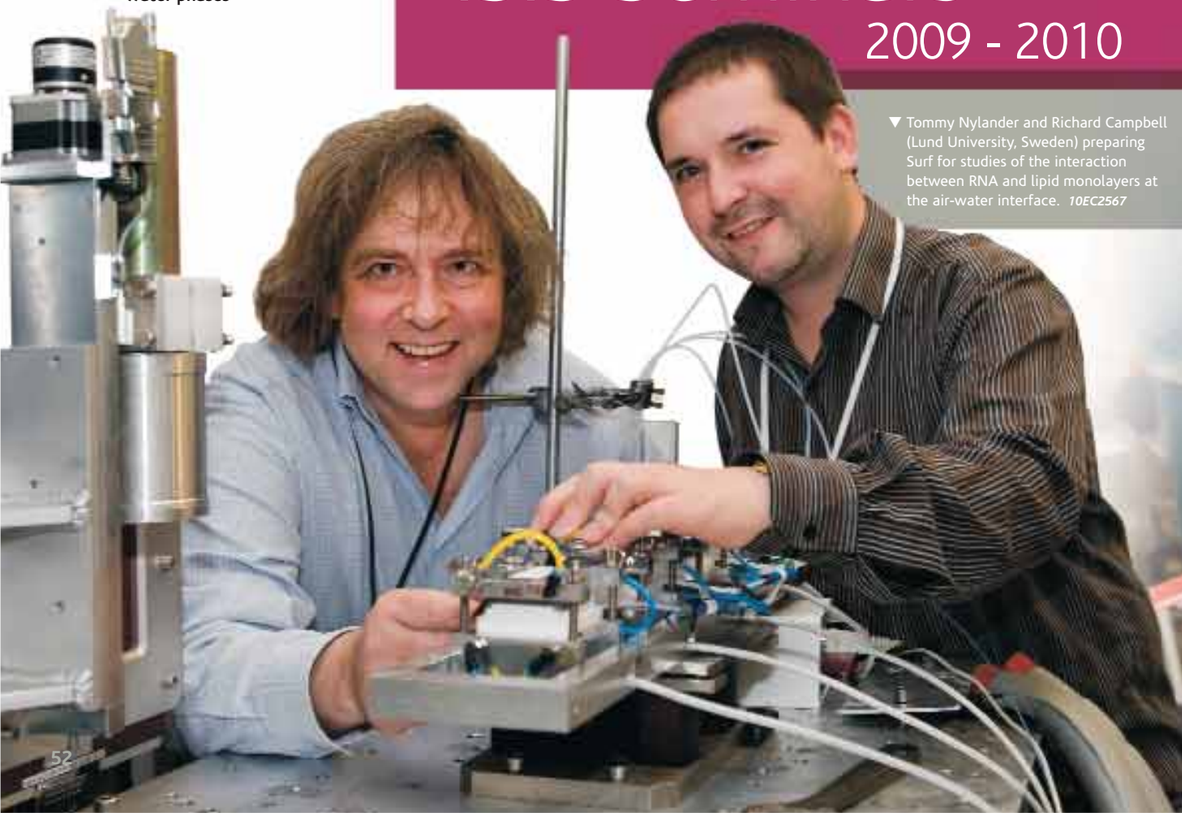
16 March 2010

Dr Donna C. Arnold
(University of Kent)

Perovskite and perovskite related ferroelectric and multiferroic materials

▼ Dominic Fortes (UCL) preparing to study high-pressure polymorphs of hydrates of relevance to the interior of icy bodies in the outer solar system on Pearl. *10EC2517*

ISIS Seminars
2009 - 2010



▼ Tommy Nylander and Richard Campbell (Lund University, Sweden) preparing Surf for studies of the interaction between RNA and lipid monolayers at the air-water interface. *10EC2567*

▼ Isabel Franke (Oxford University) using the new muon instrument HiFi to decouple the spin fluctuations with high magnetic fields in the geometrically frustrated antiferromagnetic garnet $Gd_3Ga_5O_{12}$. *10EC2546*

ISIS in facts and figures

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

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

Chair		D Lennon	University of Glasgow
IUG1	**Crystallography**	D Gregory P Lightfood	University of Glasgow University of St Andrews
IUG2	**Liquids & Amorphous**	J Holbrety B Webber	Queen's University Belfast University of Kent
IUG3	**Large Scale Structures**	A Zarbaksh J Lakey	Queen Mary College, London University of Newcastle
IUG4	**Excitations**	A Boothroyd P Mitchell	University of Oxford University of Manchester
IUG5	**Molecular Spectroscopy**	F Kargl D Lennon	University of Wales – Aberystwyth University of Glasgow
IUG6	**Muons**	S Kilcoyne T Lancaster	University of Salford University of Oxford
IUG7	**Engineering**	G Swallowe M Fitzpatrick	Loughborough University The Open University

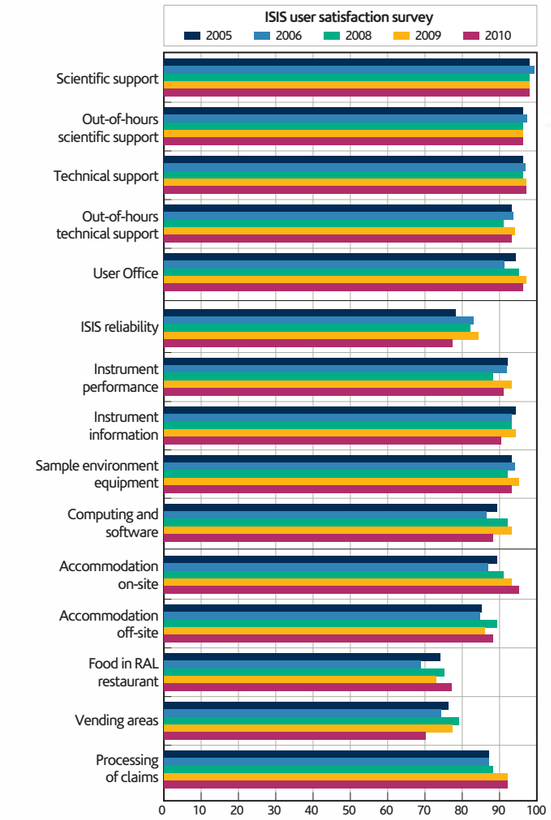
AD Taylor	Director ISIS
U Steigenberger	ISS Division Head
ZA Bowden	IEO Division Head
D Greenfield	II Division Head
RL McGreevy	IDM Division Head
PJC King	Oversight of ISIS User Programme
R Browning	ISIS User Programme Manager

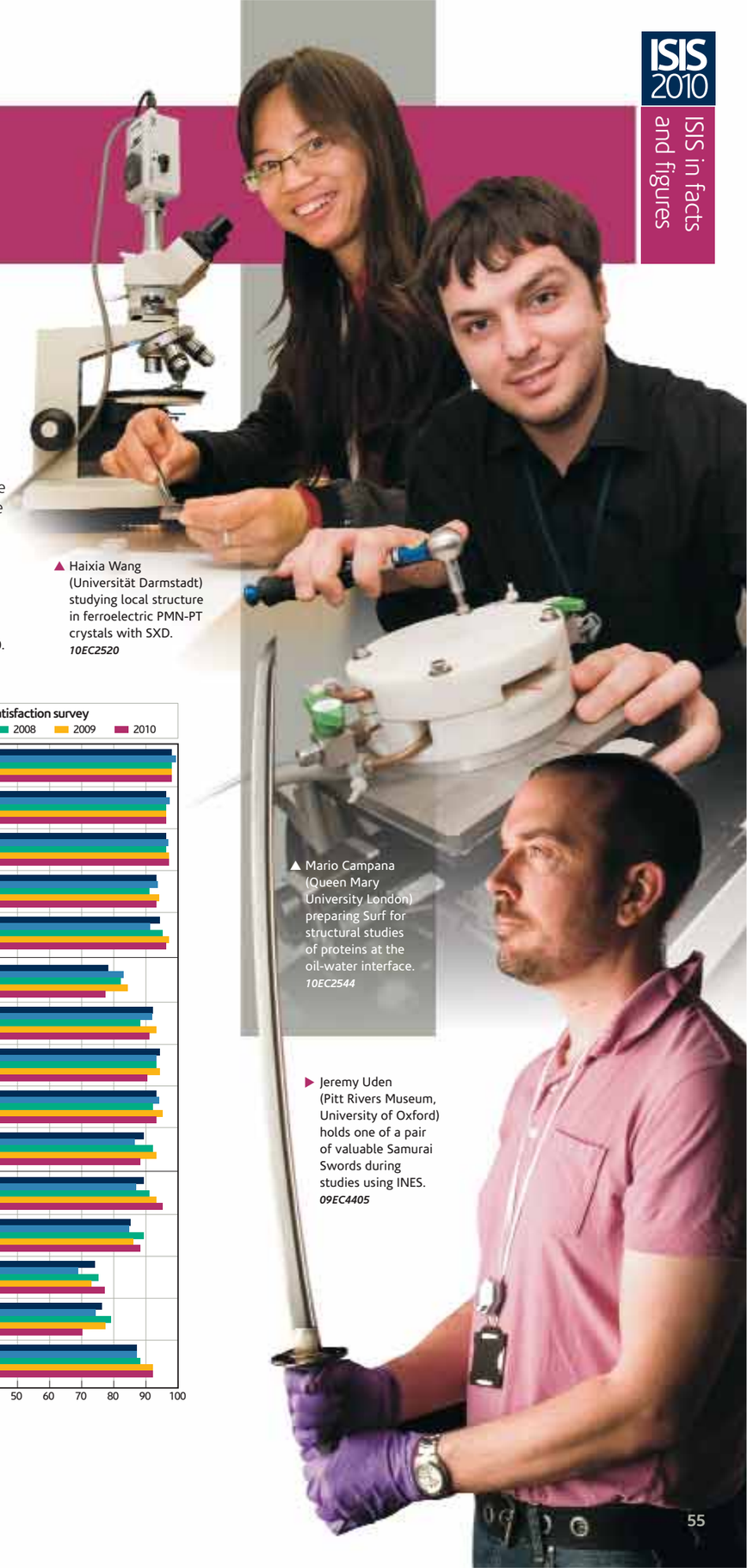
▲ ISIS User Committee Membership for June 2010. The IUC exists to represent the user community on all aspects of facility operation.

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 from 2005 to 2010.





▲ Haixia Wang (Universität Darmstadt) studying local structure in ferroelectric PMN-PT crystals with SXD. ***10EC2520***

▲ Mario Campana (Queen Mary University London) preparing Surf for structural studies of proteins at the oil-water interface. ***10EC2544***

▶ Jeremy Uden (Pitt Rivers Museum, University of Oxford) holds one of a pair of valuable Samurai Swords during studies using INES. ***09EC4405***

Beam statistics
2009-2010

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

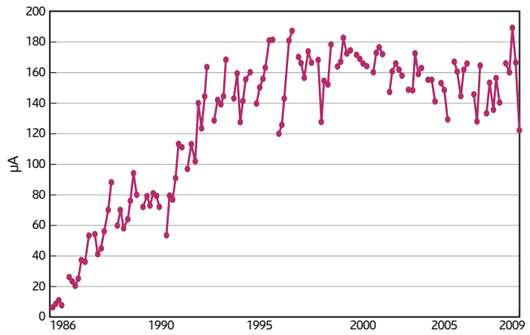
The tables below give beam statistics for the individual cycles in the year 2009-2010, together with year-on-year statistics for ISIS performance.

Cycle	09/1	09/2	09/3	09/4	09/5
	19 May – 25 June 09	7 July – 13 Aug 09	22 Sept – 22 Oct 09	24 Nov – 20 Dec 09	16 Feb – 25 Mar 10
Beam on Target 1 (hr)	714	681	381	770	491
Total Beam Current (μA-hr)	148255	141197	81718	165403	93170
Average Beam Current for beam on Target 1 (μA)	171.7	174.2	171.9	174.7	176.7

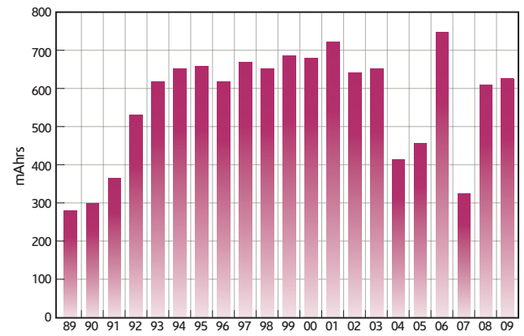
▲ ISIS operational statistics for year 2009-2010.

Year	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009
Total Scheduled Days	168	168	168	156	165	106	134	196	92	163	156
Total Time on Target (days)	153	154	158	144	152	96	107	174	74	144	126
Total Integrated Current (mA-hrs)	687	687	725	612	647	409	459	749	326	612	630
Average Beam Current (for beam on target) (μA)	187	186	192	178	177	177	178	179	183	177	179

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



▲ Average ISIS average beam current per cycle.



▲ The ISIS integrated beam current over the last twenty years.

▶ Samantha Ford (Durham University) preparing SXD to study pressure effects on proton migration 3,5-pyridinedicarboxylic acid. ***10EC2552***

ISIS

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