Neutron Scattering Group
RS•C & Institute of Physics
NSG

Newsletter

IN THIS ISSUE | News | Spotlight | Conference Reports | Prizes | What's on | Contact

No: 2 – March 2005

News

FUTURE ACCESS TO NEUTRON FACILITIES: A STRATEGY FOR THE UK

The Council for the Central Laboratory of the Research Councils (CCLRC) has been asked by the Minister for Science and Innovation, Lord Sainsbury, to lead a review entitled "Future Access to Neutron Facilities: A Strategy for the UK". This is a unique opportunity for you to influence future Government science policy - we need and welcome your input to this review.

The following website

http://www.neutrons.cclrc.ac.uk/

has been established to provide the focus for the consultation exercise. It describes the remit of the review and answers many key questions. Registering on this website will ensure you are kept informed on the consultation process and its developing conclusions. To participate you must register here

http://www.neutrons.cclrc.ac.uk/Activity/Register

By relying on e-mail mailing lists you may receive more than one copy of this message - please accept our apologies if this is the case. The initial duplication reflects our desire to ensure that the consultation process is fully inclusive.

The CCLRC, http://www.cclrc.ac.uk/, operates major science facilities and manages access to complementary international facilities on behalf of the UK science and engineering community. These include the ISIS neutron spallation source at the Rutherford Appleton Laboratory, Chilton, UK and the ILL at Grenoble, France.

Spotlight

Andrew S. Wills

NSG - Willis prizewinner 2004

The Neutron Scattering Group of The Institute of Physics and the Faraday Division of the Royal Society of Chemistry have established a Prize for outstanding neutron scattering science. The prize is named in honour of the founding chairman of the Neutron Scattering Group, Professor B T M Willis NMUM which was held at Warwick June 2004.

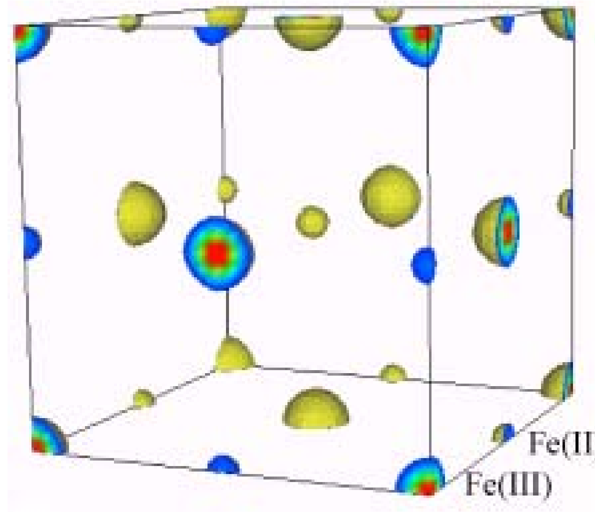
Magnetism provides a wonderful stage within which to explore many concepts that are core to our understanding of condensed matter. It also provides one of the most pertinent probes of bonding in both chemical and biological systems. Neutron scattering, particularly with *polarised* neutrons, gives us information about where the unpaired electrons that give rise to magnetic moments are, and in which direction their associated fields lie. As these electrons are also involved in catalytic or REDOX mechanisms, the study of magnetism can help us understand the bonding changes that take place during these reactions. My interests in magnetism centres on the role that neutron scattering has to play in developing this science.

In terms of condensed mater physics, experiments that characterise the location of and density of magnetisation by using polarised neutron diffractometer have helped unravel the chemical bonding in a wide range of materials, *e.g.* superconductors and molecular ferromagnets. Developing the science to a wide range of chemical and biological problems is difficult as these rarely crystallise as the single crystals required for the current instruments, such as D3 at the ILL. In order to open up these areas of science, we are working to develop the studies of magnetisation densities from powder samples using the state-of-the-art ^{3}He spin filters being developed at the ILL and ISIS. The goal is to enable the determination of where unpaired electrons are localised in a wide range of systems just as we refine the chemical structure of powders. Our first results from a test experiment last year show the promise of the technique with the observation of $0.05\mu_B$, that is to say approximately 1/20th of an unpaired electron, being observed on the Ni of YNi_3.

Below a characteristic temperature the periodicity of crystalline materials typically causes the magnetic moments to order into symmetric arrangements- magnetic structures. Historically, workers in magnetism quickly found that structures were being observed that could not be described within the conventional space groups used by crystallographers and new types of symmetry needed to be developed. The most general symmetry descriptions are based on representational theory which was developed by Bertaut in the 1960s. According to the theory, symmetry types are characterised by the forms of the different representations and the way that they propagate through the crystal structure. In this description the limitations of the crystallographic space groups become clear- they correspond to the simple symmetries which are described by representation matrices that are of order one. In a three-dimensional crystalline solid, representations can be up to order 6 and higher order symmetry types are possible that cannot be well described by space groups. Today, crystallography is going through an expansion, just as magnetism did, that is driven by the need to describe complex incommensurate structures that cannot/do not fit into the space group definition. This is being done using so-called super space groups. The lessons that have been learnt by magnetism and the closeness of the analogy between magnetic symmetry and crystal symmetry suggests that more complex structures are possible that cannot be described even within this extended formalism and that eventually the higher-order symmetries of representational theory will have to be invoked. One of my interests is in developing the use of representational theory in magnetism as a framework for facilitating the refinement of magnetic structures and understanding the details of the Hamiltonian that lead to their formation. Our application of these ideas to many different types of problem has demonstrated the wonderful types of complex structure that are possible and acts as premonition for the exciting developments that crystallography will have in the years to come.

When complex ordering does happen an experimentalist is often faced with more questions than answers. Simple neutron scattering measurements may not provide the answer as much information is not transferred by the dipolar interaction between neutrons and magnetic moments. For these systems the maximum amount of information that can be taken from an experiment is required- this is provided by Spherical Neutron Polarisation analysis as realised in the CRYOPAD. CRYOPAD allows the changes to the neutron polarisation that are induced by scattering from the sample to be completely characterised and so provides access to the ultimate experimental 'fingerprint' of a magnetic structure. In the case of CuB_2O_4, which is important to fundamental physics because it features an unusual magnetic soliton lattice, this information allowed us to determine that the low-temperature incommensurate magnetic structure was in fact a helix and not a sine wave. An observation that is important in understanding the physics of this material.

Continuing the theme of magnetic order, one of the questions that has captivated condensed matter for many years, and myself for several, is what happens when conventional order is frustrated so the moments do not freeze into ordered arrays. What other types of magnetic order are possible? Our work on model frustrated systems has revealed strange glass-like magnetic states- the 'topological spin glass' state of $(H_3O)Fe_3(SO_4)_2(OH)_6$ or the partially ordered phases of $Gd_2Ti_2O_7$. Again, neutron scattering provides the most useful incisive tools and by using a combination of unpolarised and polarised neutrons we have been able to characterise both the static and the unconventional fluctuations in these systems.



MaxEnt reconstruction of the magnetisation map in a powder sample of Prussian Blue. Large density corresponds to Fe(III), and the small to the first observation of a ferromagnetic component at the Fe(II).

To conclude, I do not think that any experimentalist could fail to be excited by the developments that are being facilitated by the continuing upgrades being made to our neutron scattering resources. The improvement to the quality of the data that these changes are allowing is, in turn, causing us to re-examine the types of experiment that can be performed and indeed the frameworks that we use to understand the results. This, in a sense, is a challenge that new neutron technologies are making to experimentalists, and I look forward to being frustrated by!

• **Dr. Andrew S. Wills**, Royal Society University Research Fellow, Dept. of Chemistry, Christopher Ingold Laboratories, University College London, 20 Gordon Street, London, WC1H 0AJ, UK.
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Conference Report

'Neutron scattering from Biological Systems'

Meeting: 13th-14th December 2004, Abingdon, UK

In association with the Neutron Scattering Group, this year's autumn meeting on 'Neutron Scattering from Biological Systems', organised by the BCA Physical Crystallography Group was hosted at Cosener's House, Abingdon in Oxfordshire.

The meeting gave an outline of the contribution of neutrons to biology, for example small-angle neutron scattering (SANS) and reflectometry from systems such as enzymes, amyloids, and membranes, proteins absorbed on surfaces, drug delivery vehicles, and biosensors. There was also a talk on neutron protein crystallography and neutron fiber diffraction. A total of nine talks were given in specific topics. As a beginner in X-ray protein crystallography with the intention of doing neutron protein crystallography in the future, I found the talks given by Peter Timmins and Matthew Blakely exceptionally useful. Peter was the first speaker, talking about 'The structure of Troponin from skeletal muscle' and how combining SAXS, SANS and X-ray protein crystallography provided information on the actinmyosin interface and also on the conformation and flexibility of the myosin heads in the relaxed state and the active state, with the aid of its regulation by two proteins, tropomyosin and troponin. This function was better understood having solved the X-ray structures of the proteins, with the identification of the Ca^{2+} binding site.
Matthew Blakeley with his talk titled 'Recent Results from LAD1' talked about three structures solved using neutron protein crystallography. The work done on 'The 15-K neutron structure of saccharidefree concanavalin A' was very interesting, as this new technique of freezing a large crystal to a very low temperature (15K) without cracking, then collecting data that revealed twice as much water (as D_20) molecules (including disordered water molecules) with respect to the room temperature structure. The overall B-factor was also reduced and this was shown by the enhanced definition of the nuclear density (2FoFc). Jayne Lawrence presented the other talk of particular interest to me; 'Neutron Reflectometry studies on DNA-Membrane interaction'. It was about gene therapy to becoming a practical method for treating genetic disorders using an efficient means of delivering DNA to target cells. Zwitterionic phospholipids (DMPC, DSPC) could be used as DNA vectors, and this interaction was enhanced by addition of Ca^{2+}. Neutron reflectivity was used to determine the existence and extent of such interactions, examining the effects of DNA, in the presence and absence of calcium, on a monolayer formed at the air-water interface by the zwitterionic phospholipids. Tim Wess talked about the crystallinity of collagen, which could form micro fibrils, and how SANS could be used to work out fibril dynamics and interchangeable water molecules. There were also a lot of other interesting talks, but challenging too. The common point taken from the meeting was that neutron scattering from biological systems provided contrast variation, which enabled one to contrast out parts of a complex system, for example the nucleic acid from the lipids, or the protein from the muscle fibres. A specific major point for protein crystallographers is that the scattering of deuterium is approximately the same as carbon, nitrogen and oxygen. I believe this meeting was a very good learning experience.

Helal Ahmed
School of Chemistry, Brunswick Street, The University of Manchester, Manchester M13 9PL

I really enjoyed a talk by Jayne Lawrence on 'Neutron Reflectivity Studies on DNA-Membrane Interactions' for the application of gene drug delivery vectors. It was also interesting and beneficial to learn about instrument and target station developments at both RAL and ISIS. At the meeting I presented a poster entitled 'Segregation enhanced in an aqueous alcohol system by cooling and compression'. This poster session gave me an opportunity to explain my research interests to a wide audience and hear their views. I very much enjoyed attending this meeting and am thankful for the generous student bursary which allowed me to do so.

Lorna Dougan
University of Edinburgh
Institute of Structural & Molecular Biology
The Molecular and Optical Science group

Nien-Jen also attended the meeting and presented a poster on his work '*Neutron scattering experiment in elucidation of membrane aggregation mechanism*'

Nien-Jen Hu
University of Edinburgh
Institute of Structural & Molecular Biology

Prize

Neutron Scattering Group – Willis prize

The Neutron Scattering Group of the Institute of Physics and the Royal Society of Chemistry intends to award the next Willis prize at the NMUM in 2005. Nominations for the prize should be forwarded to Professor Don McK. Paul by **31st May 2005**.

D.M.Paul@warwick.ac.uk

Guidelines for the B T M Willis Prize:
(http://www.isis.rl.ac.uk/NSG/)

Bursaries

Student bursaries

to attend
ICNS 2005 in Sydney, Australia
27th November to 2nd December 2005

The Institute of Physics and the Faraday Division of the Royal Society of Chemistry
Neutron Scattering Group

The Neutron Scattering Group is pleased to offer a number of student bursaries to assist with the costs of attending the ICNS 2005 meeting in Sydney. This is an international forum for the presentation and discussion of recent developments in neutron sources, the techniques of neutron scattering and their application to physics, chemistry, biology, materials science and industry.

Details of the meeting and the registration form can be found at:

http://www.icns2005.org/announce.html

Up to five bursaries of £200.00 will be available on a competitive basis. Applications should be submitted to the chairman (D.M.Paul@warwick.ac.uk) by the end of May 2005.Applications should take the form of a letter of introduction from the student, outlining their background and the contribution they expect to make. Each application should also be supported by a letter of reference from the student's supervisor.

Successful applicants are expected to acknowledge the support of the Neutron Scattering Group in their presentation, and on their return, provide the Neutron Scattering Group committee with a short written report on their contribution and the meeting of 200 words or half a page of A4.

Eligibility: Applicants are expected to be student members of the Institute of Physics or the Royal Society of Chemistry, and also to be a member of the Neutron Scattering Group (or be in the process of joining). A maximum of two bursaries can be awarded to a given student in the course of their PhD studies, and, in general, no applicant is eligible to receive more than one bursary in any academic year.

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What's on

"Magnetism, Neutrons and High-Pressure"
[Neutron Scattering Group]

Edinburgh

1-2 September 2005

Please contact: Dr Konstantin Kamenev
K.Kamenev@ed.ac.uk
Tel: +44(0)131 651 7232

Neutrons and X-rays as probes of Condensed matter a celebration of the work of Professor Roger Cowley

Oxford

June 30th – July 1st, 2006

Please contact: Dr J P Goff
jpgoff@liv.ac.uk
Tel: +44(0) 151 794 3418

Contact

Editor: A. Zarbakhsh, Queen Mary, University of London.

Contributions for the next issue:

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To join the neutron scattering Group, please visit either:

the Institute of Physics
http://physics.iop.org/IOP/Member/

the Royal Society of Chemistry
http://www.rsc.org/members/join.htm

NSG home page
http://www.isis.rl.ac.uk/NSG

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