

OPAL news

At the time of writing, the OPAL Reactor and its cold neutron source are both running well, after a return to service from a long shutdown on 14th December 2009. During the shutdown, problems with the cold neutron source cryogenic system were resolved, and major work (in the form of applying some sealing clamps) was performed to stem the seepage of light water into the heavy-water reflector vessel. While the latter has no safety consequences, and has a minimal effect on the neutron beam program, it has substantial cost implications for the operation of OPAL.

The emphasis at OPAL will now be on achieving higher reliability, in terms of running to the published schedule. At the time of writing a total of 24 papers have been published using data from OPAL, with a further 6 papers submitted (to our knowledge).

Bragg Institute News

We have recently approved the scope, budget and estimated schedule for (1) a suite of Sample-Environment apparatus, including a new cryomagnet/dilution refrigerator combination, a high-end gas-handling system, and various pieces of supporting equipment; and (2) DINGO, a new purpose-built Neutron Radiography/Tomography/Imaging Station to be installed on beam HB2 in OPAL's Reactor Beam Hall. The sample-environment subproject is led by Paolo Imperia, while DINGO is led by Ulf Garbe. These are two of the five key elements in the \$37M Neutron Beam Expansion Project announced in the Australian Government's May 12th Budget Statement. We are also in the process of erecting an additional temporary building to house up to 25 staff working on the NBI-2 Project.

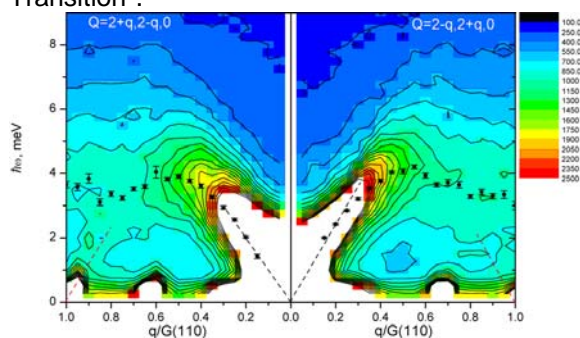
Around the instruments

Taipan (*thermal 3-axis spectrometer*)

The first paper from TAIPAN has been accepted for publication in *J. Phys. Soc. Japan*. This paper resulted from an inelastic neutron scattering experiment on the $\text{Cu}_{1.85}\text{Se}$ superionic conductor performed as part of commissioning tests on TAIPAN. The data covered a wider q -range and were measured with higher accuracy than previous work. By comparing the experimental phonon dispersion curves with

lattice dynamics calculations using density functional theory, the force-constant matrix was obtained from first principles.

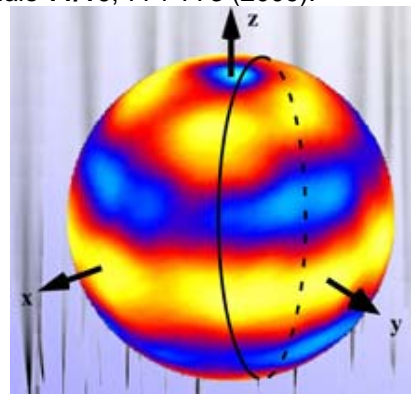
The full title and reference is: S. A. Danilkin, M. Yethiraj and G. J. Kearley, "Phonon Dispersion in Superionic Copper Selenide - Observation of Soft Phonon Modes in Superionic Phase Transition".



Measured transverse acoustic phonons in the fast ionic conductor $\text{Cu}_{1.85}\text{Se}$.

Kowari (*strain scanner*)

Research using neutron and X-ray diffraction (on our KOWARI strain scanner, along with synchrotron radiation at the European Synchrotron Radiation Facility) has been featured on the cover of the October edition of *Advanced Engineering Materials*. The work, on time-dependent texture measurements on the age-old problem of plastic deformation in copper, was done by Kun Yan, Klaus-Dieter Liss, Ulf Garbe and Oliver Kirstein in the Institute, along with other authors at ESRF and the U. of Wollongong. The full reference is K. Yan, K.-D. Liss, U. Garbe, J. Daniels, O. Kirstein, H. Li and R. Dippenaar: "From single grains to texture", *Advanced Engineering Materials* **11/10**, 771-773 (2009).



Colour coded intensity distribution on the 111 Debye-Scherrer ring plotted against azimuthal angle and time respectively along the horizontal and vertical axis.

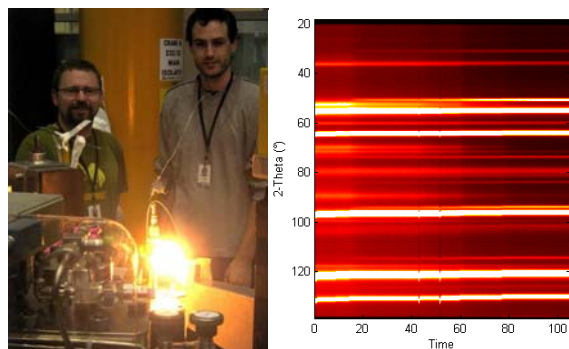
Wombat (high-intensity powder diffractometer)

Drew Sheppard, Mark Paskevicius and Craig Buckley from Curtin University of Technology have been using WOMBAT to investigate the potential of MgH_2 as a low-weight, high-capacity hydrogen-storage material for use in on-board vehicle fuel replacement systems.

The adsorption of H_2 by Mg and the generation of MgH_2 is highly endothermic and does not occur at room temperature. The thermodynamics of this reaction are made more favourable by the addition of Si to the reaction pathway, allowing H_2 sorption to occur at temperatures and pressures more conducive to vehicular storage:



Unfortunately, this modification kinetically hinders the regeneration of H_2 below 200 °C. By implementing a high pressure gas cell and a series of adjacent heat lamps to heat the sample stepwise to 350 °C over 48 h, *in-situ* neutron diffraction patterns were obtained during the decomposition of MgD_2 in the presence of Si. The kinetics of MgD_2 decomposition and the crystallite sizes of MgD_2 , Si, and Mg_2Si determined from the diffraction data are of vital importance in explaining the nature of the extreme kinetic barrier that restricts D_2 sorption. Once understood, further modifications to the system are envisaged that will improve the viability of MgH_2 as a hydrogen-storage medium.

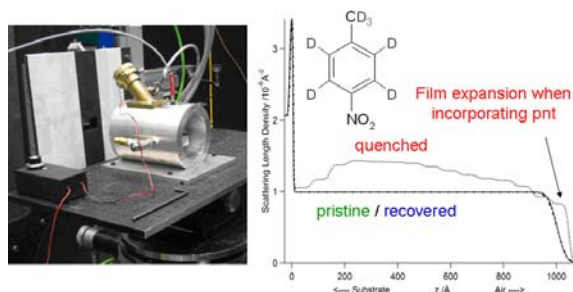


Left: Mark Paskevicius (left) and Drew Sheppard (right) using gas-loading equipment and heating lamps on WOMBAT; Right, *in-situ* powder diffraction pattern illustrating the decomposition of MgD_2 .

Platypus (Reflectometer)

PLATYPUS re-entered the User Program in December with experiments both at solid and free-liquid surfaces conducted thus far. A busy year for 2010 is envisaged with more than 35 different user experiments planned over the next 7 months.

The most recent PLATYPUS data to be published (Cavaye *et al.*, Langmuir, 2009) is highly topical, and relates to the *in-situ* study of explosive sensing using thin dendrimer films in concert with fluorescence spectroscopy. Using PLATYPUS, the team led by Prof. Paul Burn from the University of Queensland, showed that the sensing process takes place in seconds and was fully reversible. Moreover, using a deuterated explosive analogue (d-para-nitrotoluene) we were able to observe the nanoscale distribution of the explosive within the dendrimer film; as well as demonstrate very high sensing efficiency, with the photoluminescence of more than 3 dendrimer molecules quenched by a single para-nitrotoluene molecule. Substantial interest has already been generated by this work following recent presentations at international scientific meetings in Korea and Singapore.



Neutron reflectometry and *in-situ* fluorescence spectroscopy

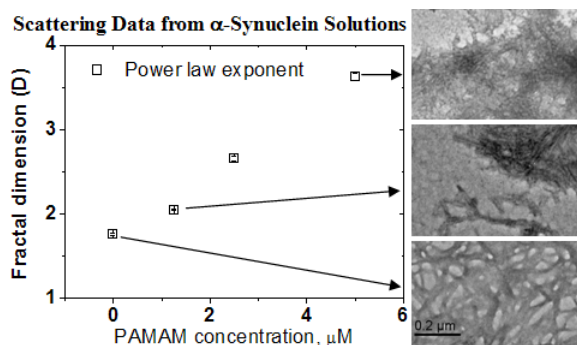
SLD profiles of before and during sensing of p-nitrotoluene. The pristine state can be recovered by blowing with nitrogen gas.

National Deuteration Facility (Bio- and chemical deuteration)

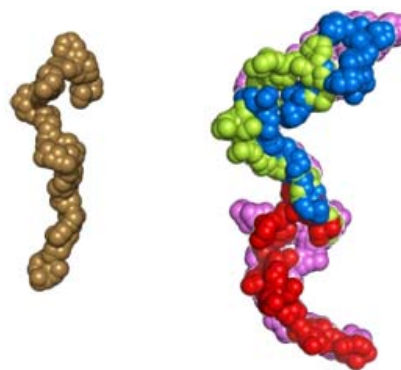
Research on the Parkinson's disease related protein, α -synuclein, is aimed at understanding folding pathways of this protein. α -Synuclein undergoes self-association into amyloid-like fibrils through a number of not yet fully characterized oligomeric species.

In 2008-9, Agata Rekas and Seok Il Yun of the National Deuteration Facility investigated the interaction of α -synuclein with a man-made highly branched, polymer, known as "PAMAM dendrimer". They found that the dendrimer

inhibits or even reverses this abnormal self-association of α -synuclein, and thus might be a starting point in the development of better treatments for Parkinson's disease, which affects around one in 250 Australians. With scientists at Materials Engineering, they used an electron microscope to observe the concentration-dependent effects of the dendrimer and verified the results with SANS at the NIST Center for Neutron Research, which showed a change in the shape of α -synuclein aggregates. The future research on this project aims at finding a precise localisation for PAMAM molecules on amyloid fibrils before their disaggregation occurs, and will use SANS and USANS techniques with contrast variation.



Another aspect of the involvement of α -synuclein in Parkinson's disease is its interaction with the neurotransmitter dopamine, present in healthy neurons and depleted in Parkinson's affected brain tissue. Based on previous research which showed that dopamine inhibits formation of α -synuclein fibrils, Agata Rekas, Robert Knott and Anna Sokolova, in collaboration with scientists at Melbourne University, used SAXS and *ab-initio* modelling algorithms to investigate the shape of α -synuclein oligomers formed in the presence of dopamine. This study aims at finding the mechanism of interaction of dopamine with α -synuclein and thus specifying its protective role against α -synuclein fibrillation. They found that dopamine-induced α -synuclein trimers are composed of laterally-oriented partially-overlapping protein molecules which show more defined secondary structure elements and a more consistent shape model than α -synuclein monomers. In the future, we plan to employ deuteration and neutron contrast to study these molecular interactions in more detail using QUOKKA.



Monomer

Trimer

The α -synuclein monomer (left) and α -synuclein trimer (right) structures.

Announcements

5th call for proposals – deadline 7 May 2010

The next (2010-2) call for proposals for instrument time Sep 2010 to Feb 2011 is for all 7 initial neutron-beam instruments (powder diffraction, SANS, reflectometry, strain scanning, single-crystal diffraction, triple-axis) and the National Deuteration Facility (bio- and chemical deuteration).

Proposals for neutron-beam instruments and the National Deuteration Facility should be submitted via our online proposal system <https://neutron.ansto.gov.au> by **May 7**.

Proposals will be reviewed in May/June and the Programme Advisory Committee will meet to assess these proposals in July 2010.

Neutrons and Food Workshop, Nov. 2010

The Institute was successful in gaining \$24k of external funding from the Department of Innovation, Industry, Science and Research, under its International Science Linkages Program, for a workshop "Neutrons and Food: Addressing the challenges of food science in an evolving global environment using novel methods". The workshop will run 1 – 3 November 2010 in Sydney, in partnership with the European Union's NMI-3 *Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy*, which has also provided funding support. We expect 70-80 attendees from Australia and around the world.

For more details, please contact Elliot Gilbert Elliot.Gilbert@ansto.gov.au.

Faces

Visitors:



Dr. Zin Tun, Principal Research Officer with the Canadian Neutron Beam Centre in Chalk River spent a 2-month sabbatical with us in December and January. Zin conducted a number of in-situ electrochemical experiments using our PLATYPUS reflectometer, and also helped

with our magnetic powder diffraction program on WOMBAT

Newcomers:

Anton Le Brun is a new post-doc in the National Deuteration Facility. He is investigating biomolecules and biological membranes. Before joining ANSTO he worked at the Diamond Light Source where he commissioned a high-throughput protein crystallography beamline.



Saurabh Kabra is a new post-doc in the Thermo-Mechanical Processes team developing materials for extreme environments. He has used the neutron diffraction beamlines at Los Alamos National Laboratory (SMARTS & HIPPO) to study the mechanical behaviour of such materials.



Hal Lee leads the Institute's ^3He Polarisation Project. The project will bring polarised ^3He -based neutron polarisers and analysers to the Institute's instruments. Hal arrives from the Spallation Neutron Source at Oak Ridge National Laboratory.



Paris Constantine is a Project Engineer/Group Leader providing project-engineering support to our \$60M portfolio of instrument construction projects. His experience includes defence and commercial research and development roles, working on aerospace, sonar and radar systems.



James Taylor is a new post-doc in structural biology working with Bill Hamilton and Jill Trehwella. He arrives from the University of Portsmouth, UK where he investigated Type I bacterial restriction-modification systems using SANS at the ILL.



Jorden Lickiss is a Trainee administrative assistant within the Bragg Institute User Office. Jorden recently completed her HSC studies at Oak Flats High School.



Departures:

Paul Hathaway led our Data Analysis Team, and has moved on to become Software Engineer / Scientist at the Diamond Light Source, near Oxford, in the UK.



Roland Bircher recently completed his post-doc with us in molecular and molecular-network magnetic materials.



Lewis Ryan has completed his Year-in-Industry studies under the supervision of Klaus-Dieter Liss. He has returned to Canberra to study medicine.

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