

OPAL news

Since July 1st, the OPAL Reactor has run well, with an overall availability of 87% and a reliability of 84% (as measured against the original published schedule). However, we continue to experience major difficulties with the out-of-pile systems for the cold neutron source, and have only run with cold neutrons for 6 days in the last 3 months. At the time of writing there is no estimate for a return to cold-neutron service. We also continue to labour under an inflexible fuel management strategy, which has led to far more schedule changes than anyone desires.

Despite these difficulties, our four diffractometers (ECHIDNA, WOMBAT, KOWARI and KOALA) have used 90% of the available beam days, with KOALA the only instrument using less than 95%. User experiments have comprised 62% of the available reactor days on these 4 diffractometers, with the proportion as high as 78% on WOMBAT.

Bragg Institute News

In the Australian Government's latest budget, it was announced that ANSTO will receive \$37 million of new capital funding for new guides and instrumentation at OPAL. Following this, a two-day scoping workshop was held at the Institute on 27-28 August, with 80 researchers from Australia and overseas (below) to discuss both the scientific justification and project implementation.



As a result of this meeting, a report was published on the 2nd SANS instrument (Goanna or Bilby), a Back-scattering Spectrometer (Emu), a Neutron Radiography, Tomography and Imaging Station (Dingo). The workshop also came up with a prioritised list of sample-environment apparatus. The report is available

from the Bragg Institute's website: http://www.ansto.gov.au/data/assets/pdf_file/0008/43793/Scoping_Workshop_Report_final_a.pdf.

Helping Out Our Canadian Friends

In the week of 6 October, we hosted Profs. Dominic Ryan (McGill University, Montreal) and Sean Cadogan (University of Manitoba) for experiments on our ECHIDNA high-resolution powder diffractometer on "the O(II) to O(I) structural transition in $Gd_5(Si,Ge)_4$ ". This is part of our effort to assist the Canadian neutron community while the NRU Reactor at Chalk River is shut down. Prof. Ryan is President of the Canadian Institute of Neutron Scattering, their user society. Interestingly, Prof. Ryan also gave a seminar at the Institute on "Why can't you use thermal neutrons to study gadolinium-based materials?"



Profs. Sean Cadogan (left) and Dominic Ryan (right) with instrument scientist Max Avdeev.

First Joint Paper from OPAL and Australian Synchrotron

The first refereed article featuring data from both the Australian Synchrotron (in Melbourne) and the OPAL Research Reactor (here in Sydney) has been accepted for publication in the *Journal of Solid State Chemistry*. The work was performed on the ECHIDNA high-resolution powder diffractometer at OPAL and the Powder Diffraction Beamline at the Australian Synchrotron, by researchers from The University of Sydney and staff of the two facilities.

The full reference is "Structural Studies of Ba_2LaIrO_6 - New Light on an Old Problem", Q. Zhou, B. J. Kennedy, M. Avdeev, L. Giachini and J. A. Kimpton, *J. Solid State Chem.* 182 (2009) 3195-3200.

Around the instruments

Sika (cold three-axis spectrometer)

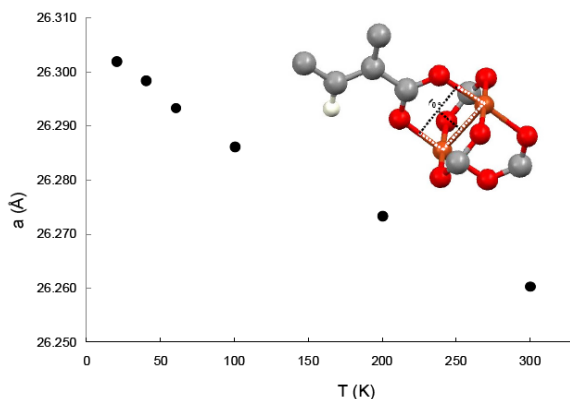
We are in the process of installing the Sika dance floor (supporting plates shown below). When completed, the dance floor will comprise 50m² of highly polished black granite on which the instruments will move around on high-precision air pads under computer control. Sika, the 9th neutron beam instrument at the OPAL reactor, is an \$8M project funded by the National Science Council of Taiwan, and managed by the National Central University.



Echidna (high resolution powder diffractometer)

Work led by Vanessa Peterson on the study of Cu₃(btc)₂, where btc = 1,3,5-benzene tricarboxylate, a material that contracts, as shown below, when heated has been accepted for publication in the prestigious chemistry journal *Angewandte Chemie*.

This work has revealed two new vibrational mechanisms for negative thermal expansion (NTE) in Metal-Organic Frameworks: the first instance where 3- rather than 2-connecting bridges contribute to NTE; and expands the known means by which such properties can be introduced into novel materials.



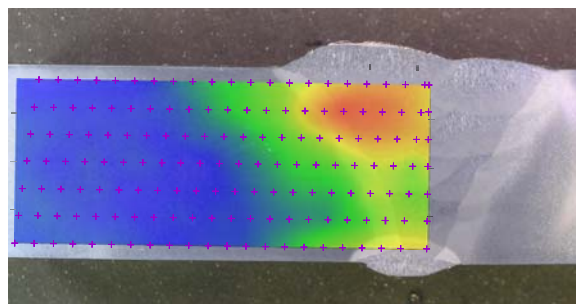
Density-functional theory and molecular dynamics calculations were performed at ANSTO, along with neutron powder diffraction on the ECHIDNA powder diffractometer, while inelastic neutron scattering data were taken on the TOSCA and NEAT spectrometers at ISIS (UK) and the Berlin Neutron Scattering Centre (Germany). This work also forms part of a broader collaboration between the Institute and Cameron Kepert's group at The University of Sydney.

Kowari (strain scanner)

ANSTO scientists, as part of a 15 member Consortium, have been awarded a major grant through the Australian Government's Industry Cooperative Innovation Program to develop a weld with the lowest as-welded residual stress.

Excessive residual stress is a major concern in the production of alumina from bauxite by the Bayer refining process in which exposure of welded steel plant components to large quantities of sodium hydroxide results in Caustic Stress Corrosion Cracking.

Kowari has been successfully used to record the 3-dimensional weld internal structures and stress map features in steel with a stress accuracy of 10 MPa and spatial resolution of 2 mm. As Kowari can achieve these stress scans non-destructively it is being used to optimise welding methods, thus avoiding the need for expensive and time-consuming post-weld heat treatment of welded steel plant components.

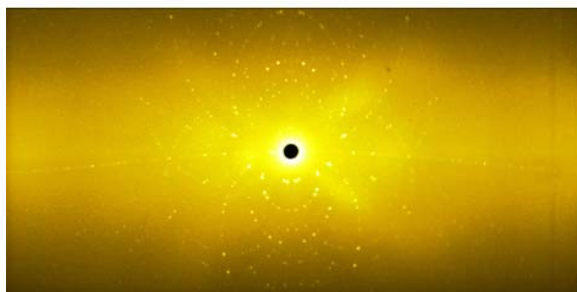
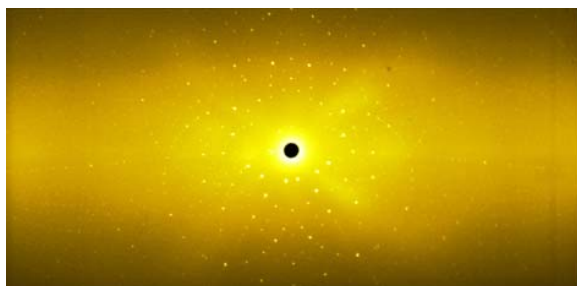


The image above illustrates the longitudinal stress component map (min. -120 MPa, max. 600 MPa) overlaying the cross-section of a weld. Plate thickness, vertical dimension, is 20 mm.

Koala (Laue diffractometer)

Dr Michael Gardiner of the University of Tasmania undertakes research in organometallic chemistry which has applications in catalysis, synthesis and materials. His first proposal for neutron beam-time on KOALA sought to establish whether a material prepared by M.Sc. student Anung Riapanitra contains an hydridic ligand. We are also tackling the question whether the two structures determined via X-ray diffraction for this material are actually distinct structures and whether the material is polymorphic.

Neutron diffraction images were collected at 150K (top) and 100K (bottom) demonstrating that a change of structure to one with a unit cell of doubled volume occurs on cooling. The reversibility of this phase change was demonstrated by cycling between the two temperatures with no apparent loss of crystallinity thus demonstrating that the two structures correspond to different phases of a single chemical compound. Data collection on the higher temperature phase has been completed and the results are being prepared for publication. Further experiments are envisaged to probe the specifics of the transformation to the low temperature phase.



Spot the difference: One material, two different diffraction patterns, a case of a polymorphic catalyst.

Announcements

2012 Small-Angle Scattering Conference



Following a vote of the delegates at SAS 2009 in Oxford, we have been successful in a competition to bring SAS 2012, the 2012 International Conference on Small-Angle Scattering, to Sydney. The bid was led by Elliot Gilbert, on behalf of the Australian and New Zealand small-angle communities (with explicit involvement from the Australian Synchrotron, CSIRO and 6 universities). Tentative dates are for 11-15 November 2012.

New ANSTO Bus Service

ANSTO is pleased to announce a regular and direct mini-bus service between ANSTO and Sutherland railway station. This is intended primarily for users and visitors coming to ANSTO. This service will be run as a trial until 18 April 2010, with possible extension.



The mini-bus stops at Sutherland (Bus Bay 1, East Parade), ANSTO motel and ANSTO reception/security. The cost is \$5 per single trip (no concessions).

The timetable is available at http://www.ansto.gov.au/data/assets/pdf_file/0/011/44120/Bus_timetable_factsheet.pdf.

4th Call for Proposals at OPAL

The 4th call for proposals is open and includes all 7 initial instruments (powder diffraction, SANS, reflectometry, strain scanning, single-crystal diffraction, triple axis). The National Deuteration Facility is offering biodeuteration of molecules such as proteins, nucleic acids and biopolymers, and for the first time, partly deuterated or perdeuterated organic molecules through chemical deuteration. Investigators seeking chemical deuteration should contact either Paramjit.Bansal@ansto.gov.au or Tamim.Darwish@ansto.gov.au. Please contact Peter.Holden@ansto.gov.au for biodeuteration.

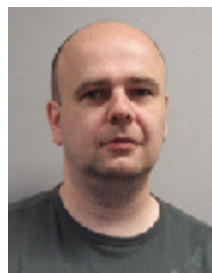
All proposals are to be submitted via the Online Proposal System <https://neutron.ansto.gov.au/> by **November 27**.

Proposal review will take place in December and January, with the Program Advisory Committee meeting in early February. The first experiments in this round are likely to be scheduled in April 2010.

Faces

Newcomers:

Paolo Imperia is Project Leader Sample Environments as part of the \$37M NBI-2 Project. Paolo was senior scientist at the University of Hamburg and soft X-ray beam line scientist at the BESSY II synchrotron, Berlin.



Ulf Garbe, is Project Leader of the Neutron Radiography / Tomography / Imaging station, also part of the NBI-2 Project. Ulf was responsible for the texture application on Kowari and Wombat at OPAL and also at the FRM II reactor (Munich).

Anna Sokolova has accepted the role of scientist for the 2nd SANS that will be constructed as part of NBI-2. Anna was previously a post-doctoral researcher within our food-science project.



Tai Nguyen is newly arrived as a mechanical support technician in the Neutron Guide Hall. Tai's most recent posts were with Pacific Brands and Unilever.

Neeraj Sharma, PhD USyd, is a postdoctoral research fellow in the energy related materials project. He will be using neutron scattering techniques to optimise (mainly Li⁺ ion) battery performance.



Paul Judge joined us as a mechanical support technician in the Neutron Guide Hall. Paul has an extensive technical experience developed within the pharmaceutical manufacturing industry.

Joseph Bevitt recently joined us as Scientific Coordinator. Prior to joining us, Joseph implemented the Excellence in Research Australia (ERA) initiative at The University of Sydney and was coordinator of the NSW Synchrotron Consortium.



Departures:

Having replaced Herma Buttner as Acting Scientific Coordinator, Richard Garrett will be supporting ANSTO's Executive Team. The Institute wishes Richard all the best in his new role.

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