Bragg Peaks
> for neutron users
ISSUE 15 | AUG 10

OPAL news

The OPAL Reactor and its cold neutron source returned to service on 8th May, and both have run to schedule with excellent reliability since then. In the last quarter (April-June), our four licensed thermal neutron beam instruments used 78% of the beam time from OPAL for user-program experiments. Including QUOKKA and PLATYPUS, our two licensed cold-neutron instruments, the overall utilisation rate for user-program experiments was 69%. Over the coming months, we expect this to increase to match the thermal instruments.

Major New Building Approved

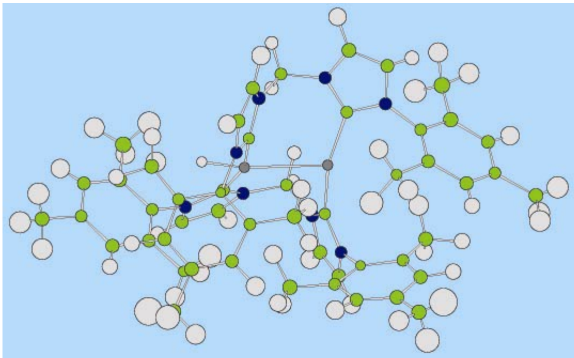
Main Entry (eastern) view of the approved Bragg Institute extension

In July, funding approval was given for a major new building extension for the Institute and its users. The new building complex is designed to hold up to 150 personnel, including users, long-term research visitors, and students or postdocs based at the Institute. This should be sufficient for a full suite of 18 neutron-beam instruments at the OPAL reactor in its present configuration, i.e. a single guide hall with all beam holes fully instrumented and utilised. At this point, we have 13 neutron beam instruments in operation, or under construction. The building will also accommodate all the laboratories, equipment and staff of the National Deuteration Facility, which will move from a number of other disparate locations on the ANSTO site. Our intent is that this physical co-location will lead to better service for those of our users who want to deuterate molecules and then perform small-angle neutron scattering and/or reflectometry at OPAL.

The funding decision follows approval on 24 June by the Public Works Committee of the Australian Parliament. Construction is expected to commence before the end of this year, with completion and occupancy early in 2012.

Around the instruments

Koala *(Laue diffractometer)*



The {μ-bis(NHC)}$_2$Pd$_2$H]$^+$ cation structure as determined by neutron Laue diffraction.

The first report of a molecular structure determined by single-crystal neutron diffraction using KOALA has been published in Angewandte Chemie. Titled "Reduction of a Chelating Bis(NHC)Pd(II) Complex to [{μ-bis(NHC)}$_2$Pd$_2$H]$^+$: A Terminal Hydride in a Binuclear Pd(I) Species Formed Under Catalytically Relevant Conditions", *Angew. Chem. Int. Edit.*, **49**(36), 6315-6318 (2010). The paper represents a large portion of the Master of Science project undertaken by Anung Riapanitra under the supervision of Dr Michael Gardiner, at the University of Tasmania.

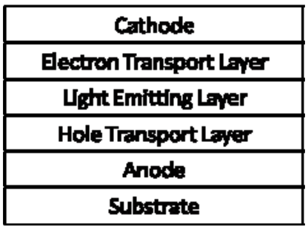
Two neutron-diffraction studies for the complex as crystallized from each of two different solvents are reported and the terminal nature of the hydridic hydrogen bonded to the palladium atom is clearly evident in each compound. The structure determined from data collected on KOALA (the other data collection was completed on VIVALDI at the ILL) is crystallographically disordered in solvent-containing regions and the hydride is distributed equally across two clearly defined sites. This material undergoes an intriguing phase change at lower temperature and will be the subject of further investigation.

Platypus *(reflectometer)* ***& National Deuteration Facility***

Mid-June saw our first experiment at OPAL using molecules purpose-synthesised in the Chemistry Laboratories of the National Deuteration Facility. Researchers from the

Centre for Organic Photonics and Electronics (University of Queensland) conducted an experiment using the PLATYPUS time-of-flight neutron reflectometer to study the structure of layered thin-films for Organic Light Emitting Diodes (OLEDs).

OLEDs have attracted interest for their superior performance compared to current display technologies. While tuning the colour emission of such devices is critical for their commercial viability, enhancing the efficiency and performance is also vital. OLEDs are generally composed of several organic layers deposited one on top of the other.

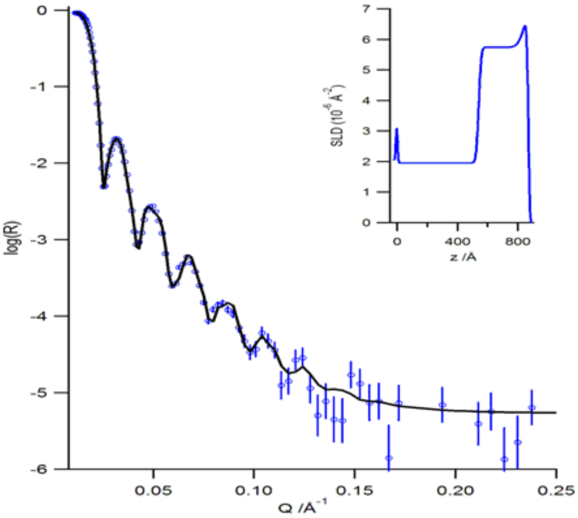


Layered structure of a typical OLED device.

In these technologies the thin-film morphology and interfacial interactions between different molecular layers are key aspects for a successful device.

In order to investigate the molecular interactions in these devices, we deuterated specific compounds to provide neutron scattering contrast between the different organic layers. Deuterated molecules for both the hole-transport and the electron-transport layers were produced at the National Deuteration Facility. A dendrimer-like, hole-transport molecule was custom synthesised from a base cyclic amine aromatic compound, that was pre-deuterated to 85% in large quantities using a Parr reactor. The electron-transport molecule (also a complex aromatic compound) was amenable to direct deuteration (to 70%) in the Parr reactor, without the need to develop a complex organic synthesis protocol from constituent reagents.

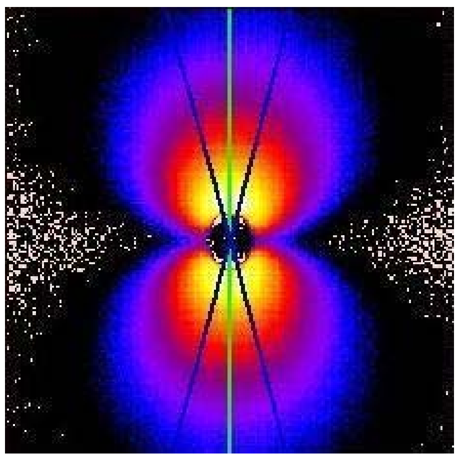
Combined with an *in-situ* spectrophotometer on the PLATYPUS sample stage, the Queensland team were able to use neutron reflectivity data to correlate device properties with the film's structure and thermal history following annealing.



Neutron reflectivity data from a multi-layer OLED device. The inset shows the refined scattering length density, with the region adjacent to the surface of the film comprised of deuterated molecules produced at the National Deuteration Facility.

Quokka *(SANS)*

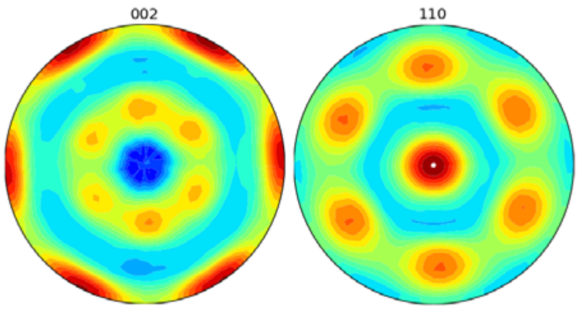
The first user experiment with polarised neutrons on QUOKKA was completed in May. The figure below shows the polarised SANS signal from pearlitic steel as measured by Elliot Gilbert and Vladimir Luzin in a 6-T horizontal magnetic field at 200 K, after subtracting spin down (flipper off) from spin up (flipper on) scattering.



A polarised SANS signal from pearlitic steel in a 6-T horizontal field as recorded on QUOKKA.

Wombat *(high-intensity powder diffractometer)*

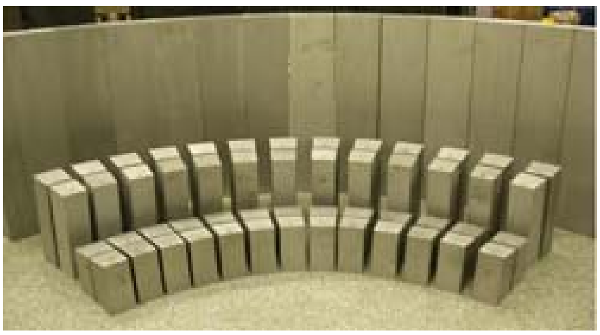
Klaus-Dieter Liss has re-joined the powder diffrection team to give user support on WOMBAT and ECHIDNA, after successful completion of an ANSTO Senior Research Fellowship: 'Modern Diffraction Methods project for the Investigation of Thermo-Mechanical Processes'. A major aim of the project was to develop *in-situ* time-resolved neutron measurements and to establish a texture measurement and evaluation facility, which is now available to users and is supported by the Institute.



Pole figure of structural nuclear material Zircaloy-4 after high-temperature heat treatment. (data evaluation: Saurabh Kabra)

Taipan *(thermal three-axis spectrometer)*

The beryllium blocks for the ARC-funded Molecular Spectroscopy option for our TAIPAN Thermal 3-Axis Spectrometer were recently inspected in the USA, and are currently being shipped to ANSTO. The polycrystalline beryllium acts as a low-energy filter to analyse the final neutron energy, after the scattering event at the sample.



The 52 blocks of beryllium that make up the TAIPAN low-energy neutron filter.

Sika *(cold three-axis spectrometer)*

SIKA has achieved its first milestone, in that the essential parts of the primary shielding have recently been installed at the reactor face on beam CG-4. This includes adaptation to the reactor face, movable shielding wedges and motion-control components. The next step is the integration of the motion-control components into the instrument control software.

The SIKA installation team.

12-T Vertical-Field Magnet

We have ordered a 12-T vertical-field magnet, similar to that available at the Berlin Neutron Scattering Centre (BENSC).

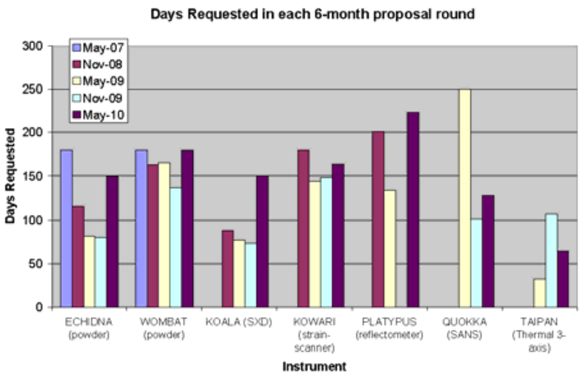
Also purchased from Oxford Instruments is a dilution-refrigerator insert which will enable users to attain sample temperatures down to 20 mK, either in conjunction with the magnet or within our standard ^{4}He cryostats. Both items are expected to be available to users in late 2011.

Left: *The Oxford Instruments dilution insert and;* ***Centre and Right:*** *The VM1 high-field symmetric magnet at BENSC.*

5th Proposal Round Summary

Our 5th proposal round closed with 195 proposals across 7 neutron beam instruments, and both Chemical and Bio-Deuteration at the National Deuteration Facility. Including existing approved programs and the mail-in system on ECHIDNA, 1062 beam days were requested across ECHIDNA, WOMBAT, KOALA, KOWARI, PLATYPUS, QUOKKA and TAIPAN.

Including strong demand through the National Science Council of Taiwan, roughly 27% of demand was from overseas (China, New Zealand, Singapore, UK, USA, Canada, and 9 other countries in Asia and Europe). 53% of demand was from Australian universities, DSTO and CSIRO, and 20% from ANSTO itself. Proposals were externally reviewed by up to 5 referees, with the final recommendations on allocation of beam time made by the Program Advisory Committee. Approved experiments will be run in the period October 2010 –March 2011.



Announcements

6th call for proposals – deadline 24 Oct 2010

The 2010-2 Round call for instrument time between April - September 2011 is now open for access to 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 **24 October**.

The Program Advisory Committee will meet to assess these proposals in February 2011.

ANSTO Bus Service Extended

ANSTO will continue to run its direct minibus service to and from Sutherland Railway Station until the end of 2010. While the timetable is unchanged, please note that

(1) The pick-up location at Sutherland Railway Station has changed, with pick up now from "Bus Stand, Ramp down from Railway Station";

(2) Cash is no longer accepted. Tickets are available from the Bragg Institute User Office, AINSE and the ANSTO Cafeteria.

Faces

Newcomers:

Mai Anh Burke, our new Laboratory Manager has pharmaceutical-industry sales and research experience in developing genetically modified mouse models for patients with skeletal muscle diseases and trialling potential therapies on these models.

Pezhman Khalili is an Electronics Technician in the Bragg Institute Data Acquisition Electronics group. Pezhman previously worked at an Australian Defence Force site in Sydney as an Electronics Technical officer.

Aravin Chellappah is providing engineering support as a drafting officer, with a background as a Mechanical Engineer and has experience as a CAD Designer–Drafter.

Chen Li recently joined the Institute as a drafting officer. He majored in Mechanical Engineering and has extensive experience as a Design Engineer.

Mike Weir recently completed a PhD at Sheffield University in the UK, before joining the Institute as a postdoctoral fellow funded by the Cooperative Research Centre for Polymers.

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