Institute and OPAL news

In the first quarter of 2013, the OPAL reactor itself has operated with very good reliability and predictability. The thermal-neutron instruments returned to service during March, and all were ready for external users in April, according to schedule. It was a tremendous achievement to install the new cold guide CG-2, and also to replace a total of 72m of existing guides during the 5-month shutdown of OPAL’s Neutron Guide Hall. Congratulations to the large team of people both within the Institute, and across all of ANSTO, who made all of this possible – the work was all completed ahead of schedule and without incident.

In addition, the cold-neutron instruments QUOKKA and PELICAN have been running, albeit with substantially reduced flux, with thermal neutrons, as we await the return of cold neutrons from OPAL, this is now expected to occur in August 2013.

Around the instruments

EMU (backscattering spectrometer)

In late April, EMU’s stainless-steel vacuum vessel was delivered to the Institute and installed in its position in the Neutron Guide Hall, on the CG-3 guide. EMU is designed to allow cold-neutron spectroscopy down to the 1-microvolt energy range, opening up a range of studies in the diffusion of hydrogen and water in biological and chemical systems, or tunnelling of methyl or ammonium groups within molecules.

The National Deuteration Facility continues to provide custom-synthesised deuterated materials to the national and international science communities, in order to perform advanced characterisation studies previously hindered by the lack of relevant deuterated compounds.

Diocdeacyldimethylammonium chloride (DOAC) is a widely used cationic surfactant in textile softeners and hair conditioner in our daily life and is usually mixed with various surfactants, such as alcohols, to improve its functionality. Molecular-level studies of DOAC mixed with alcohols that could reveal the relationship between the thermodynamic behaviour, phase separation, and molecular packing are still quite limited. The molecular structure for each component in a mixed monolayer is difficult to analyse independently by spectroscopic methods, and thus to date the lateral interaction in the mixed monolayer is not yet well understood at the molecular level. Such information is very important in both fundamental studies of biomembranes and in applications of novel detergent systems.

In a joint collaboration with the Hokkaido University-Catalysis Research Centre in Japan, we sought to investigate the structure and lateral interactions of mixed monolayers of DOAC and a neutral surfactant of stearyl alcohol (SA) using sum frequency generation spectroscopy (SFG). The aims of the study were (i) to understand the physicochemical properties of mixtures of a cationic and a neutral surfactant at air/water and air/solid interfaces; (ii) to understand the relationship between the structure and interaction of lipid molecules with charged head
groups in membranes on a molecular level; and (iii) to enable control of the functionality of the membranes by a suitable mixing process. SFG is a second-order non-linear optical technique which is particularly useful in surface science due to its high selectivity and sensitivity. In this study, SFG spectroscopy together with deuteration allowed quantification of molecular order and condensation within DOAC and stearyl alcohol. To avoid the spectral interference in the C−H stretching region for DOAC and SA molecules, the deuterated analogue of SA, perdeuterated stearyl alcohol-d37 (dSA), was synthesized and used in the study. SFG observations demonstrated that molecular packing and conformational ordering of DOAC molecules are substantially improved by mixing with dSA. This study was part of a visiting fellowship awarded by the Japan Society for the Promotion of Science to Dr Tamim Darwish in 2010 and the work has recently been published in *Langmuir*. ([http://pubs.acs.org/doi/abs/10.1021/la400143k](http://pubs.acs.org/doi/abs/10.1021/la400143k))

**Kowari** (strain scanner)

Erich Kisi and Chris Wensrich (*The University of Newcastle*), Vladimir Luzin (*ANSTO*) and Oliver Kirstein (*ESS*) have applied the neutron diffraction strain scanning method to the problem of the stress distribution in granular materials under a consolidating pressure. Strains measured in axial, radial, circumferential and an oblique direction using the neutron strain scanning diffractometer KOWARI at ANSTO give the full stress tensor as a function of position. The theory underlying the method has been developed [1] and applied to Cu [2,3], zirconia and Fe [4,5] particles within various dies, see Figure.

![Axial stress in Fe powder under 160 MPa consolidating pressure in a converging die.](image1.png)

Granular materials, extremely important in food production, minerals extraction, pharmaceuticals and powder metallurgy, can be poured like a liquid and yet can support static shear stresses like a solid. Due to a locally and macroscopically inhomogeneous nature, algebraic constitutive models are difficult to develop. Continuum (finite element) or individual particle (discrete element) numerical models are being widely explored. However, there were previously no methods for their experimental validation.

**Pelican** (*time-of-flight spectrometer*),

Inelastic neutron scattering spectrum from water using an incident neutron energy of 3.74 meV.

Our PELICAN time-of-flight spectrometer has recently recommenced “hot commissioning”, following the 5-month shutdown of OPAL’s Neutron Guide Hall, and receipt of regulatory permission to run with thermal neutrons, rather than cold neutrons.

Initially the choppers were removed from the instrument and a sample diffraction pattern was obtained from a Si standard, while in late April we successfully measured our first diffraction pattern from a sheet of polyethylene using an incident neutron energy of 3.74 meV.

Since obtaining the above results, we have also obtained the QENS spectrum of water at room temperature with the same instrument configuration; the elastic line is at 0.0 meV and the other scattering in both neutron energy loss and neutron energy gain, on either side of the elastic signal is essentially from the vibrational density of states in the sample. The self-diffusion constant estimated from the quasielastic width of these raw data was 1.9 x 10⁻⁹ m²s⁻¹, compared with the literature value (Singwi and Sjölander *Phys. Rev.* 119, 863-871 (1960)).
Taiwan Team welcomes new Leader

The National Science Council of Taiwan’s ANSTO-based neutron scattering group welcomed their new group leader Jason Gardner in April. Jason is a staff member at their synchrotron and comes to us with over 15 years experience at the NIST Center for Neutron Research in the USA and Chalk River National Laboratories in Canada. Jason got his PhD at Warwick University under the supervision of Don McKenzie Paul and overlapped with Rob Robinson at Los Alamos during one of his postdocs. Jason’s science interests are in exotic low temperature magnetic materials and have been based around pyrochlore magnets for the past 15 years. Jason will also run a low temperature, high field laboratory in Taiwan.

Helping our friends from China

Xiaolong Liu, an instrument scientist on the texture diffractometer at the Neutron Scattering Lab, China Institute of Atomic Energy (CIAE) arrived at the Institute in March for six months of training with instrument scientist Vladimir Luzin on our KOWARI strain scanner. Xiaolong’s visit is organised and sponsored by the International Atomic Energy Agency, through a Technical Cooperation project.

Pole figures obtained for an Al/Mg composite using KOWARI:

As part of this training and a collaborative research project between Harbin Institute of Technology, the CIAE and the Bragg Institute, a series of experiments are in progress to study texture in a series of Al/Mg composites in 50/50 combination produced by accumulative roll bonding (ARB). ARB is a form of severe plastic deformation designed to fabricate ultrafine grained, bulky metallic materials with excellent mechanical qualities and can be used to join dissimilar metals to produce laminated structures with alternating layers of different metals. In the case of Al/Mg composites, the good formability and high strength of aluminium and the low density and high damping capacity of magnesium are coupled. The overall performance of the composite is influenced by the microstructure (dislocation density, grain size and grain orientation), which is rather complex and shaped by the interplay of many different factors of the ARB process (rolling temperature, rolling cycles, annealing temperature and time).
The wide coverage of the KOWARI detector has enabled the simultaneous measurement of multiple pole figures, with 3 Al and 6 Mg pole figures obtained for each sample.

Over the coming months, Xialong will be analysing data obtained using KOWARI and correlating the results of texture measurements with damping performance measurements to enhance their understanding of the ARB process.

**Bragg Institute Celebrates its First Ten Years**

To celebrate the first ten years of the Bragg Institute, ANSTO has released a commemorative report that includes a compilation of the achievements of the Institute, told by the people who were involved in developing the Institute from its beginnings. A PDF of the report is available [here](#). Hard copies are available upon request from the User Office.

**Announcements**

The 2014-1 Proposal Round is open for beam time between January and June 2013 and access to all neutron-beam instruments. Proposals should be submitted online by **15 Sept 2013** via [https://neutron.ansto.gov.au](https://neutron.ansto.gov.au). Given the uncertainties about the return to cold neutron service from OPAL, only thermal-neutron and NDF proposals can be submitted in this round.

**ANSTO-AINSE Neutron School, 12 – 16 August 2013**

Neutron techniques across all thermal instruments at OPAL (ECHIDNA, KOALA, KOWARI, TAIPAN and WOMBAT) will be covered in the school, to be held at ANSTO (Sydney), 12 – 16 Aug 2013. Candidates will participate in tailored experiments to further enhance their understanding of the relevant techniques, attend lectures and spend significant time analysing data.

**Applicants should submit an abstract, before 14th June, outlining their scientific interests with relation to neutron scattering. The template can be downloaded [here](#).**

**New Faces**

**Arrivals**

Eliza Barker has recently joined the Bragg Institute User Office as a trainee administration assistant. Eliza recently completed her HSC studies at Kirrawee High School.

Stanley Lee joins the Sample Environment Team as part of the 2013 ANSTO Graduate Program. He has completed a combined Mechanical (Biomedical) Engineering / Law degree at the University of Sydney.

**Departures**

In April, Chen Li, Aravin Chellappah and Tony Lam have ANSTO to further their careers. The Institute wishes them the best in their new endeavours!

Best wishes also to Warren Brown who has moved from the Institute to ANSTO Health in order to work on Molybdenum-99 operations.

**Contact us**

Bragg Institute User Office, Building 87, ANSTO Locked Bag 2001, Kirrawee DC NSW 2232, Australia  
T +61 2 9717 7232, F +61 2 9717 3606  
E bragg-user-office@ansto.gov.au  