Bragg Peaks
> for neutron users
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OPAL news

OPAL continues to run extremely well, with >95% reliability in the last quarter. In fact OPAL ran for a total of 300 days in 2015, far in excess of any of the other high-performance neutron sources around the world, whether reactors or spallation sources. In addition, in January 2016, we benefitted from the first Thursday-night reactor restart (as opposed to a weekend restart) at OPAL, and there are three more such restarts scheduled for 2016. This will make life much easier for both users and staff and will lead to higher utilisation of the 300 days per annum that OPAL operates.

Please give us your feedback, via https://neutron.ansto.gov.au/Bragg/proposal/Questionnaire.jsp to let us know if this improves things for you.

Bragg Institute news

BILBY, the new time-of-flight SANS instrument (red), situated in OPAL's Neutron Guide Hall.

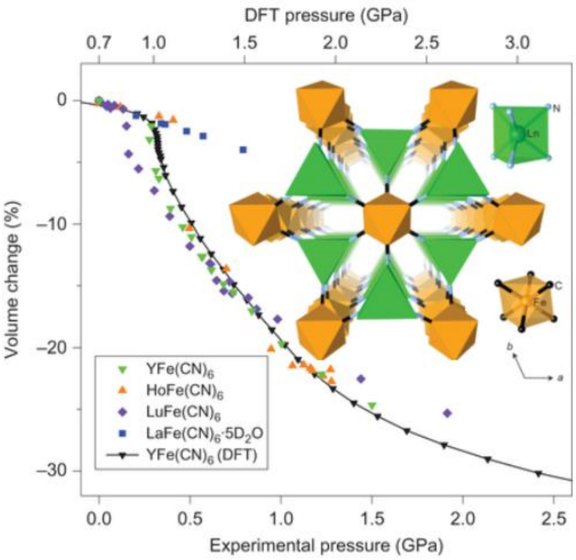
In early December, the Australian Radiation Protection and Nuclear Safety Agency gave approval to commence user operations on the new BILBY time-of-flight small-angle neutron scattering instrument. User experiments approved in the 2016-1 Neutron Round have been scheduled, including some transfers of proposals to QUOKKA, and proposals are welcome in the 2016-2 Neutron Round, with a proposal deadline of 15 March 2016.

The licencing of BILBY brings the number of operating neutron beam instruments at OPAL up to twelve.

The operating licence application for our 13th instrument, the EMU backscattering spectrometer is about to be submitted to ARPANSA, with the expectation that the licence will be awarded within the next quarter.

Around the instruments

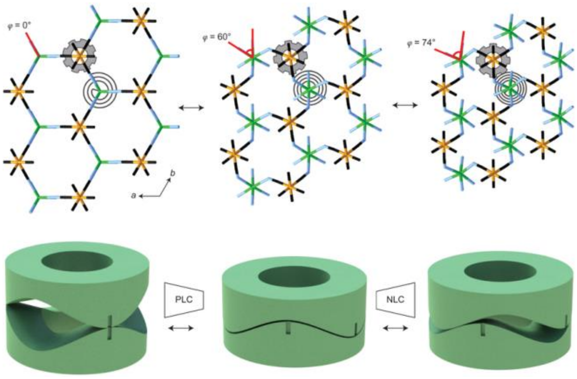
WOMBAT (high-intensity powder diffraction)



Large pressure-induced compressibility of the anhydrous $LnFe(CN)_6$ materials is evident from both neutron powder diffraction and calculations. Inset: the hexagonal structure of $LnFe(CN)_6$, consisting of alternating LnN_6 trigonal prisms (green) and FeC_6 octahedra (orange). The C (black) and N (blue) atoms of the cyanide bridges are also shown.

An article just published in *Nature Chemistry*, from the University of Sydney and the Institute demonstrates the extreme compressibility of hexagonal $LnFe(CN)_6$ frameworks (Ln = Ho, Lu or Y), which exhibit one of the largest known pressure responses for any crystalline material.

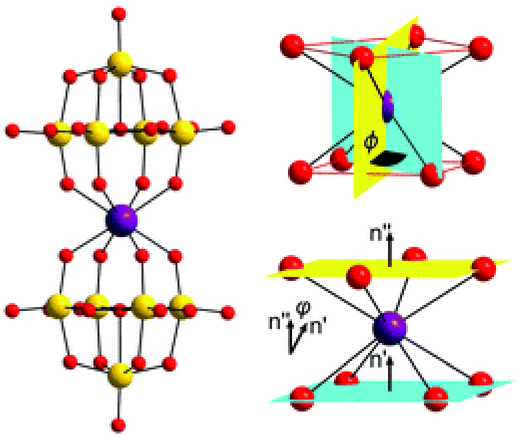
Using a combination of *in-situ* high-pressure powder diffraction on WOMBAT and *ab-initio* density functional theory calculations, the mechanism for this high compressibility was determined. The compression of $YFe(CN)_6$ progresses via a complex mechanism involving dramatic structural distortion whereby the LnN_6 units act like torsion springs synchronised by rigid $Fe(CN)_6$ units performing the role of gears. The materials also show significant negative linear compressibility via a cam-like behaviour. The torsional mechanism is fundamentally distinct from the deformation mechanisms prevalent in other flexible solids and relies on competition between locally unstable metal coordination geometries and the constraints of the framework connectivity, a discovery that has implications for the strategic design of new materials with exceptional mechanical properties.



Top: *A projection of the structure, showing how the torsion-spring-like YN_6 units twist from trigonal prismatic geometry at ambient pressure and back toward the same geometry at higher pressures. The twisting is accompanied by rotation of the rigid gear-like $Fe(CN)_6$ units.* ***Bottom:*** *Illustration of the cam-like behaviour of the YN_6 unit, which as it twists gives rise to positive linear compessibility (PLC - contraction with increasing pressure) followed by negarive linear compressibility (NLC expansion with increasing pressure) along the c axis.*

DOI: [10.1038/nchem.2431](https://doi.org/10.1038/nchem.2431)

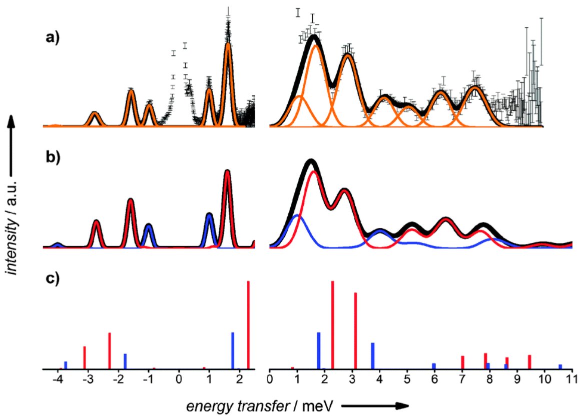
PELICAN (cold-neutron time-of-flight spectrometer)



Molecular structure (left) and representations of the two distortion angles of the Tb coordination (right) for the $[Tb(W_5O_{18})_2]^{9-}$ polyanion in ***Tb****; atom colour code: W (yellow), O (red) and Tb (violet).*

The first paper on a magnetic system, from our cold-neutron time-of-flight spectrometer PELICAN, has been accepted for publication *by [ChemComm](#)*.

Ab-initio calculations using the well-established CASSCF/RASSI computational strategy to interpret the high-quality inelastic neutron scattering spectra from [PELICAN](#) have allowed the assignment of the INS spectra to two distinct co-crystallised polymorphic phases of $Na_9[Tb(W_5O_{18})_2]$ (**Tb**); **Tb-a** and **Tb-b**; a terbium-containing single-molecule magnet analogue in the family $Na_9[Ln(W_5O_{18})_2]$, in which Ln = lanthanide or rare earth.

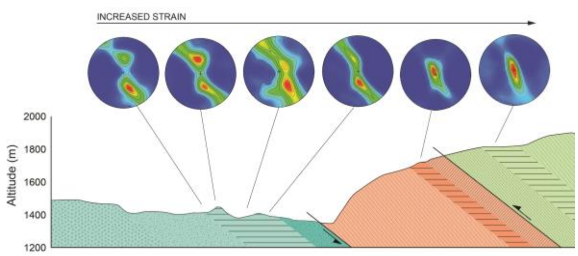


Inelastic neutron scattering spectra of ***TbD*** *at λ_i = 4.74 (left) and λ = 2.37 Å (right) at 30 K. (a) Experimental spectra with Gaussian fitting (orange) and convolution of individual peak contributions (black). (b) Simulated INS spectra of the two present polymorphic phases* ***Tb-a*** *(red),* ***Tb-b*** *(blue) and combination (black) using the set of optimised crystal-field parameters. (c) Theoretical spectra arising from transition probabilities calculated from CASSCF/RASSI results for Tb-a (red) and Tb-b (blue). A 70:30 molar ratio of Tb-a : Tb-b is assumed for (b) and (c).*

The combined experimental-theoretical approach sheds new light on the sensitivity of the electronic structure of the Tb(III) ground states to small structural distortions from axial symmetry, thus revealing the subtle relationship between molecular geometry and magnetic properties of the two isostructural species that comprise the sample. This work, a collaboration between the University of Melbourne, Monash University, RMIT and ANSTO, also has important implications for future surface deposition of single-molecule magnets.

DOI: [10.1039/C5CC07541F](https://doi.org/10.1039/C5CC07541F)

KOWARI (strain scanner)



The anatomy of Himalayan Main Central Thrust shear zone has been explored via strain texture measurements on KOWARI. Quartz (c-axis) textures from a section of the shear zone in north-west India are shown. Textures with strong cluster distributions towards the higher altitudes indicate an increase in strain magnitude

Shear zones are narrow zones of intense shearing inside the Earth's crust, and are key elements in controlling the architecture and evolution of tectonically active regions. In the Himalayas, several shear zones have displaced large crustal blocks and ultimately controlled the formation of the world's highest mountain range. At present, we lack an understanding of how these shear zones develop, and how they control mountain-building processes. However, analysis of strain textures inside rocks is providing some exciting advances in our knowledge of shear zone 'anatomy'.

A team from Monash University and the Institute has been using the KOWARI strain scanner to gain insights into the development of rock textures from a major Himalayan crustal shear zone: the Main Central Thrust. Data obtained on KOWARI demonstrates the formation of strong textures within quartz, suggesting a substantial increase in strain magnitude towards the shear zone core. The data suggests that this shear zone is at least 6km in thickness, and likely facilitated high degrees of tectonic movement. This project has yielded the clearest and highest quality textural data of Himalayan rocks to date, and their role in answering questions about Himalayan evolution will become very important.

News

Sculptures of the Braggs unveiled in Adelaide, South Australia

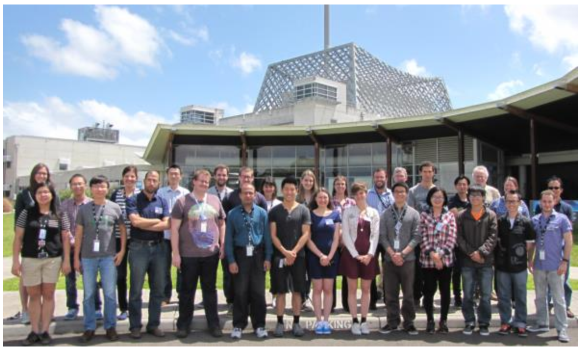
The Bragg Institute is named in honour of William Henry and William Lawrence Bragg, Australia's first Nobel Prize winners who were awarded the 1915 Nobel Prize in Physics for the discovery and development of X-ray crystallography.

The busts of father and son team William Henry and William Lawrence Bragg with W.H. Bragg's granddaughter Lady Lucy Adrian, W.L. Bragg's grandson Andrew Bragg, and the Honourable Hiew Van Le AO, Governor of South Australia.

A bronze bust of William Henry Bragg was officially unveiled on 2nd December 2015 by the Governor of South Australia, the Honourable Hiew Van Le AO, on North Terrace in central Adelaide and is positioned next to that of his son Lawrence Bragg.

A second copy of the bust has been presented to the Institute and now stands on display in our foyer.

ANSTO-AINSE Inelastic Neutron School held at OPAL, 22-27 November 2015



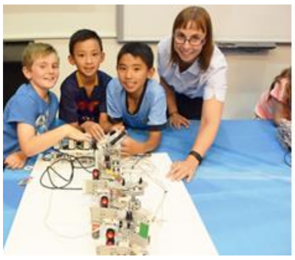
Delegates of the Inelastic Neutron School in front of the OPAL research reactor.

During a one-week intensive study course covering theory, practical sessions and data analysis, 21 students and early-career researchers from Australia and Taiwan engaged with our instrument scientists, engineers and technicians to operate our four neutron spectrometers; Taipan, Pelican, Sika and Emu; analyse the resultant datasets and present the findings to their peers.

Delegate feedback on the new-format neutron school was extremely positive, recognising that learning experiences such as this are crucial in developing skills that can be used at neutron sources around the world.

Thank you to all attendees and those who participated in developing the school content

Students Build Their Own Instrument Models




A team of budding young scientists put their summer holidays to good use, building their very own versions of the TAIPAN and WOMBAT instruments – out of LEGO® with the assistance of Macquarie Innovations Centre at Macquarie University and our instrument scientists Kirrily Rule and Helen Maynard-Casely.

The models will be used by visiting school groups to explain the operation of the instruments, which both have movable sections that recreate the monochromator, sample and analyser/detector.

Announcements

15 March 2016 Proposal deadline (2016-2 Round)

The 2016-2 Proposal Round is open for beam time between July and December 2016 and access to 12 neutron-beam instruments (ECHIDNA, WOMBAT, KOALA, KOWARI, TAIPAN, SIKA, PELICAN, BILBY, QUOKKA, KOOKABURRA, PLATYPUS and DINGO), along with chemical- and bio-deuteration, our two X-ray instruments and the new Physical Properties Measurement System. Proposals should be submitted online by 15 March 2016 via https://neutron.ansto.gov.au

New Faces

Arrivals

Carla Raymond has just begun a Masters of Research with an archaeological focus at Macquarie University. She is spending several months at ANSTO with Joseph Bevitt gaining practical skills on the operation of the DINGO instrument, and visualisation of tomographic data with the aim of imaging Egyptian artefacts.

Jessica Heinemann is member of the ANSTO Graduate Program and currently on a four month rotation at the Bragg Institute, job shadowing Jamie Schulz. Her background is in Biomolecular Science and Science Communication Outreach. Following the completion of her term with the Institute, Jessica will return to the ANSTO Discovery Centre.

Justine Wheeler is a Summer vacation student, completing a Masters of Research with Macquarie University. Working with Richard Mole and Helen Maynard-Casely, Justine will be collecting data using both WOMBAT and PELICAN to examine the changes in magnetic structure and spin-state transitions of iron-carbide at depth.

We welcome Steven Cornet, who joins the Institute as a 2-month guest researcher from from Wageningen University. He is conducting research into the assembly behaviour of organogelators. This Master thesis project is in collaboration with Elliot Gilbert and Marta Martinez-Sanz.

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