

# Crystallography at ANSTO's jewel, the OPAL reactor

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*Australian neutron scattering leapt into the 21st century with the start up of the OPAL reactor at ANSTO in 2006. The major part of the initial success has been in crystallography, carrying on the excellent tradition established since the late 1950s at the HIFAR reactor. The combination of state-of-the-art instrumentation, support facilities, expert scientific staff, and enthusiastic users of OPAL has yielded an impressive series of scientific results, as well as a fledgling industrial programme, and has trained numerous students who are now highly respected ambassadors for neutron scattering. Here we give an overview of highlights in crystallography that have come from the capabilities offered by and around OPAL, and hint at further developments in the field.*

## Introduction

The discipline of modern crystallography and the technique of X-ray diffraction were outlined by three of the great physicists of the early 20th century. In 2014 we are celebrating the UNESCO International Year of Crystallography [1] to mark the century that has passed since Max von Laue, William H. Bragg and William L. Bragg laid out the fundamentals of X-ray diffraction and its application to determination of crystal structure. In 1911, when von Laue first noted the diffraction spots from crystals the breadth and scope to which this technique would be applied could not have been imagined. 25 Nobel Prizes later, and the keys to secrets of life revealed in the structure of DNA, crystallography is still as strong a subject as ever, moving into its second century.

Over the last hundred years Australia has played a key role in the development of crystallography, and is now seen as a world leader in a number of diverse fields in the discipline. One of these fields is neutron diffraction, with focus at the OPAL<sup>1</sup> reactor (Figure 1) at ANSTO<sup>2</sup> and the Bragg Institute, the ANSTO research division that is primarily responsible for developing and operating the neutron-scattering capability around OPAL. But we are jumping ahead of ourselves. How did we get to this position?

## The formative years at HIFAR

As at many of the materials-testing reactors of the 1950s,

a subsidiary programme of neutron scattering also soon developed at HIFAR<sup>3</sup>, Australia's first research reactor (Figure 1), it too located on the Lucas Heights site. This programme was run by a small but dedicated team of scientists within the AAEC<sup>4</sup> (later replaced by ANSTO) with the interface to university researchers supported by an equally small team within AINSE<sup>5</sup>. Initial interest focussed on studies of nuclear-fuel materials, BeO and actinides in particular, mostly by single-crystal diffraction, which was seen as the technique of the future in the 1960s. The BeO work gave the first paper from HIFAR and was published in no less a journal than Nature [2].



**Figure 1: Australia's current research reactor, OPAL, in the background, with the first reactor, HIFAR, in inset.**

The second publication from HIFAR data (again in Nature!) described the joint X-ray and neutron refine-

<sup>1</sup> Open-Pool Australian Light-water reactor

<sup>2</sup> Australian Nuclear Science and Technology Organisation

<sup>3</sup> High-Flux Australian Reactor

<sup>4</sup> Australian Atomic Energy Commission

<sup>5</sup> Australian Institute of Nuclear Science and Engineering

ment of *p*-diphenylbenzene [3], remarkable in itself as presaging the X-N studies so prevalent a decade later, but also notable in that one of the authors was Hugo Rietveld, later famous as the developer of the Rietveld Method for refinement of powder diffraction patterns [4]. Rietveld was part-way through his PhD at the University of Western Australia, and would move on to Reactor Centrum Nederland at Petten in the Netherlands, where the materials of interest could only be prepared as powder samples, and the rest is history [5].

Powder diffraction did gradually develop in importance at HIFAR with application of the Rietveld Method and as the performance of the diffractometers improved. The High-Resolution Powder Diffractometer, HRPD [6], and later the Medium-Resolution Powder Diffractometer, MRPD [7], flourished when the numbers of detectors were increased (finally to 24 and 32 respectively), and were the most productive instruments by many measures when HIFAR shut down in 2007.

The long-wavelength polarised-neutron spectrometer LONGPOL [8] gave Australia a niche capability in the study of magnetic diffuse scattering, depolarisation, and other specialised magnetic phenomena, particularly in spin glasses [9].

Diffraction and crystallography underpin the majority of the ca. 750 neutron-scattering publications from HIFAR in its 50-year life. There were many forerunners of things to come amongst these publications and other events around HIFAR; we note in particular that the (first) one-day school in neutron diffraction organised by AINSE in 1970 attracted 81 attendees.

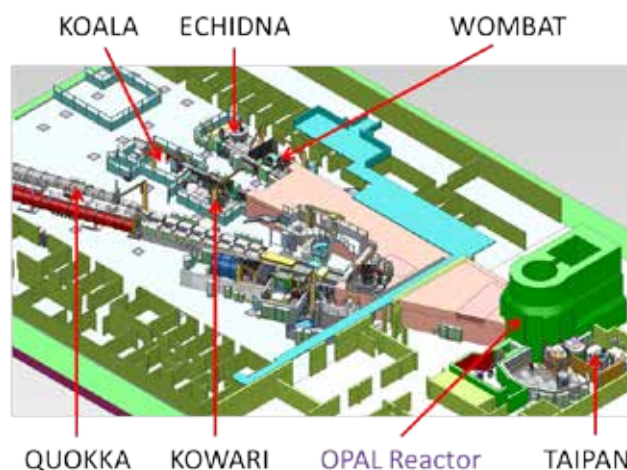
## “...by the 1990s it was clear that a modern research reactor would be necessary to restore Australia’s regional leadership in neutron scattering”

The team and instruments at HIFAR could not cover all scientific areas though, which led in the later decades of the last century to an increase in ‘suitcase science’ for many Australian neutron scatterers who sought beam time at the now considerably-more-powerful overseas facilities. This approach worked well for a select few, but by the 1990s it was clear that a modern research reactor would be necessary to restore Australia’s regional leadership in neutron scattering.

## OPAL, ANSTO’s jewel

ANSTO was given the go ahead in 1997 to build a modern 20 MW research reactor, later named OPAL, to replace the 10 MW HIFAR. Like HIFAR, OPAL is a multipurpose reactor<sup>6</sup>, but with the requirements of neutron scattering considered already in the design stage, and with state-of-the-art neutron optics, the increase in performance of the neutron-beam instruments over those at HIFAR is many times the simple factor of two in reactor power.

A series of workshops was held to choose the first suite of instruments, with the likely user bases closely consulted. The first instruments are generally to conventional designs using components proven elsewhere, but occasionally in unique assemblies. The budgets and schedules were tight, but all the instrument-construction projects have succeeded, and very well.



**Figure 2: Schematic layout around OPAL of the principal neutron-beam instruments used for crystallography.**

The HIFAR instruments mostly had technically specific names linked to the particular beam tubes, e.g. 4H1 for the instrument on the horizontal beam 4 inches in diameter on the 1st port, or 2TanA for the first (A) of the two on the shared end of the tangential beam tube 2 cm in diameter. This was all very well for the inner circle of neutron specialists of the day, but too obtuse for a good part of the wider mix of users of a national facility. Instead, the instruments on OPAL are named after (mostly) Australian fauna, usually with some physical relation to the capability of the instrument, and surprisingly memorable to frequent and infrequent users alike (Figure 2). After all, what is not to like about a WOMBAT?

<sup>6</sup> The principal activities at OPAL are:

- Production of medical and industrial isotopes
- Irradiation of silicon for the semiconductor industry
- Neutron activation analysis
- Neutron scattering

As befits a national facility, the science is largely driven by the external user programme, through a peer-review proposal system for access to the neutron-beam instruments. ANSTO's scientists obtain beam time via the same process. Certain scientific themes, where neutrons offer distinct advantages as a research tool, are showcased, principally via the Bragg Institute web pages [10]. These themes currently include energy materials, thermo-mechanical processes, magnetism, food science, biomolecules, and cultural heritage.

### Instruments and facilities for crystallography at OPAL

Most of the neutron-beam instruments use diffraction to some degree, but the following concentrate on crystallography:

- ECHIDNA – high-resolution powder diffractometer
- KOALA – single-crystal Laue diffractometer
- KOWARI – strain scanner
- WOMBAT – high-intensity powder diffractometer

A number of other instruments occasionally conduct diffraction experiments, such as the small-angle scattering instrument, QUOKKA, for the study of magnetic flux line lattices, and the three-axis spectrometer, TAIPAN, for characterisation of magnetic thin films or multilayers. A test Laue diffractometer, JOEY, can be used for single-crystal alignment.

### “researchers observed real-time structural changes in the graphite anode and ... cathode of a commercial Li-ion battery ..., the world's first *operando in situ* diffraction experiment on batteries.”

ECHIDNA was the first instrument to enter user operation, just after OPAL went critical in August 2006, and produced the first publication shortly thereafter [11]. This spearheaded a publication rate that puts ECHIDNA amongst the world's best neutron powder diffractometers, and in record time!

The high penetration power of neutrons facilitates use of bulky sample environments that offer quite extreme ranges of, e.g. temperature, magnetic field, and pressure, often in combination. The Bragg Institute sample-environment team works closely with the scientists to satisfy all demands, or to adapt equipment

brought by the users, wherever possible. In-house equipment includes cryostats, furnaces, dilution inserts, magnets, pressure cells, thermo-mechanical load frames, and gas-dosing devices.

A world-leading synthetic laboratory in its own right, the National Deuteration Facility (NDF) which is also part of the Bragg Institute, plays a key role in providing deuterated powder samples, notably for the demanding gas-absorption studies [12].

Some modelling support for data analysis is offered, primarily to get users started on modelling where this is appropriate [13]. First-principles energy calculations for identification of starting models for structure refinement, verification of crystal structures, choosing between different disordered models, and charge and spin densities are the main crystallographic applications.

The neutron diffraction techniques described below are also applicable to proprietary research on a fee-for-service basis, an access method that is proving to be increasingly attractive to several quite diverse companies and government research groups.

### Science themes

The diversity of the community that uses neutron scattering has resulted in a number of themes to the crystallographic research undertaken at OPAL.

### Energy materials

The high-intensity powder diffractometer, WOMBAT, has forged a strong reputation for undertaking complex *in situ* experiments. This is greatly facilitated by the large two-dimensional position-sensitive detector built by Brookhaven National Laboratory and one of only two of its kind in the world. A particular application of this capability has been in the study of battery materials, and a sizeable internal group and strong research programme has developed around this.

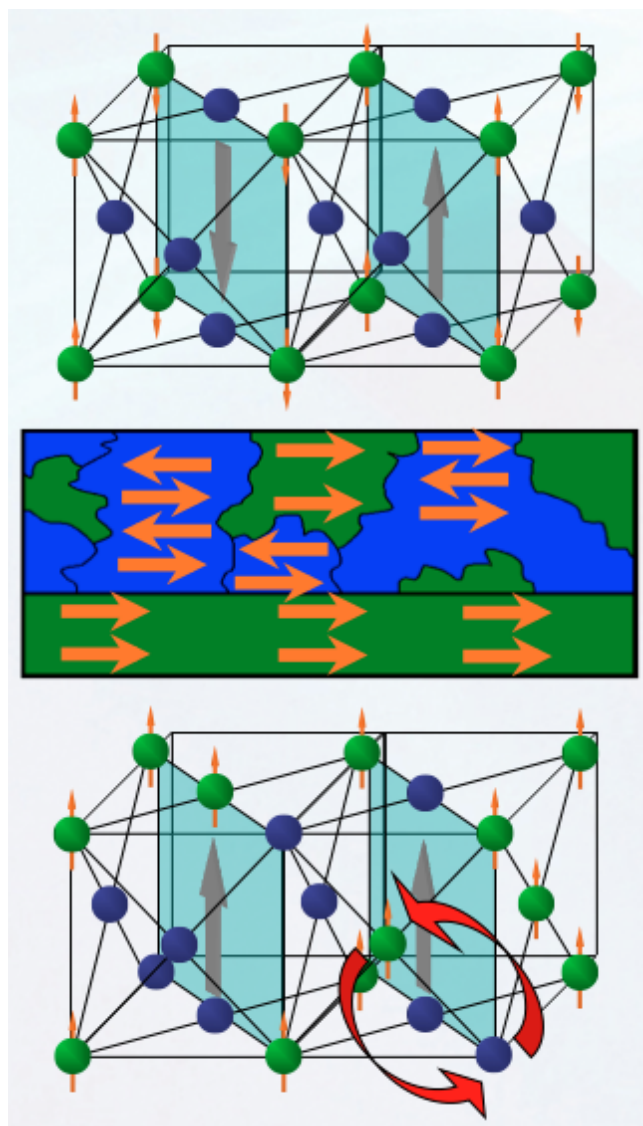
For instance, using WOMBAT, researchers observed real-time structural changes in the graphite anode and  $\text{LiFePO}_4$  cathode of a commercial Li-ion battery manufactured in Taiwan [14], the world's first *operando in situ* diffraction experiment on batteries. The researchers charted the position of the (002) reflection of the graphite anode during charging and discharging cycles. One observation of this study was that the reflection shifted to higher angles on discharge, indicating that the layers in the graphite were compressing. This behaviour was interpreted to result from the extraction of lithium ions during the discharge process. Understanding this behaviour and its impact on the anode and cathode materials is informing efforts to design more durable batteries.

## Magnetism

As an experimental tool for the study of magnetism at the atomic level, neutron scattering is without equal. The magnetic moment of the neutron can interact with the electronic magnetic moments of a crystalline material by diffraction to probe the magnetic structure and give both the location and orientation of the atomic spins.

In some cases it is the on-site expertise elsewhere at ANSTO that facilitates the science. This is particularly so for handling and collecting data from radioactive materials, a case in point being technetium oxides, for which little is known about the structure and properties due to the radioactivity and sparse abundance of all technetium isotopes. An experiment on  $\text{CaTcO}_3$  on ECHIDNA to follow the distortion of the known perovskite structure over a wide temperature range gave the surprising observation that this material is magnetically ordered to nearly 1000 K [15]. The researchers combined their results with *ab initio* modelling to find that the structure had a significantly more covalent type of bonding between the metal and oxygen atoms, which, it is believed, is what gives such a high magnetic-ordering temperature.

Artificially modulated magnetic structures, such as thin-film multilayers, heterostructures, and superlattices have become an important field in scientific research with numerous applications in the field of spintronics. Diffraction from such structures grown epitaxially can often be investigated using the three-axis spectrometer TAIPAN, by taking advantage of the crystal analyzer to reduce the inelastic background. Typically, the desired physical properties of such structures, for example exchange bias, are obtained by chemical modulation of different materials, which inevitably affects the behaviour of the system due to incommensurate growth, strain, and interface roughness. A new approach is to create a modulated antiferromagnetic (AFM)/ferromagnetic (FM) structure by modulation of chemical order in the same material [16]. By controlling the degree of chemical order through temperature modulation during growth, the authors could create a single-crystalline  $\text{FePt}_3$  film of homogeneous composition, but with alternating chemically ordered antiferromagnetic and chemically disordered ferromagnetic layers that resulted in a large exchange-bias effect. The nature of the antiferromagnetic ordering was found by diffraction on TAIPAN [16] (Figure 3).



**Figure 3: Chemical order in  $\text{FePt}_3$  leads to antiferromagnetism (AFM), chemical disorder to ferromagnetism (FM). Interfacing AFM and FM layers gives unique magnetic self-exchange bias [16].**

## Chemical crystallography

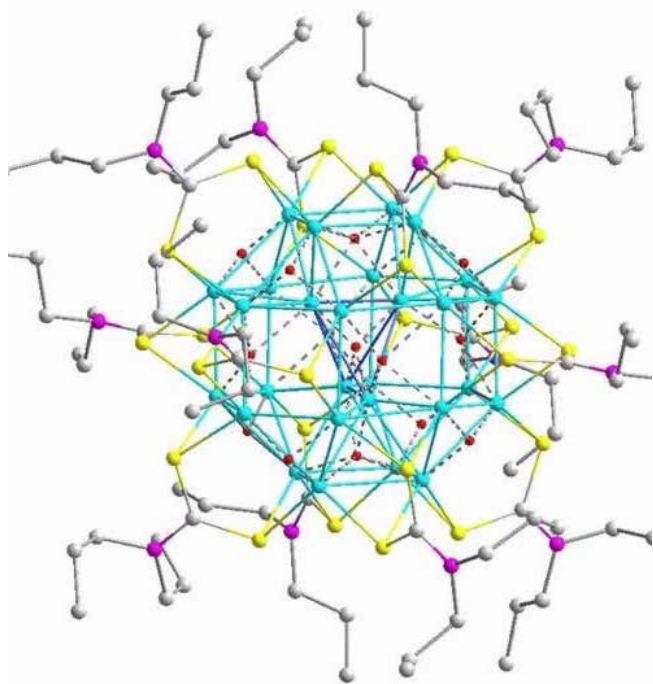
Despite having had a long and successful tradition of conventional single-detector four-circle instruments at HIFAR, ANSTO took the bold step to jump directly to the forefront of neutron single-crystal diffractometry with the dedicated Laue diffractometer, KOALA. The key component of modern neutron Laue instruments is a large solid-angle detector based on image plates, as on KOALA, or CCD detectors, as on JOEY.

Niche experiments for the neutron Laue technique include rapid crystallography to characterise phase transitions, crystal structures of very small samples typically  $0.1 \text{ mm}^3$  in volume which has opened up neutron diffraction to fields of chemical crystallography previously thought to be beyond reach, and volumetric surveys of

reciprocal space, particularly to identify or characterise new phases, aperiodic materials, and twinned crystals.

Chemical crystallography, especially hydrogen in the presence of considerably heavier atoms, hydrides, hydrates, hydrogen migration in co-crystals, and hydrogen bonding in all classes of materials, dominates on KOALA. A stunning example is the recent discovery and structural elucidation of an unprecedented 28-copper-atom, 15-hydride core [17] (Figure 4), in a molecule that provides a further clue to practical hydrogen storage.

WOMBAT with its large area electronic detector, may be better suited for some single-crystal experiments, especially those on larger crystals, with extreme sample environments, or when a monochromatic neutron beam is essential, such as for diffuse-scattering measurements. The study of structural disorder in ferroelectric  $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}$  is a fine example of the last application [18].



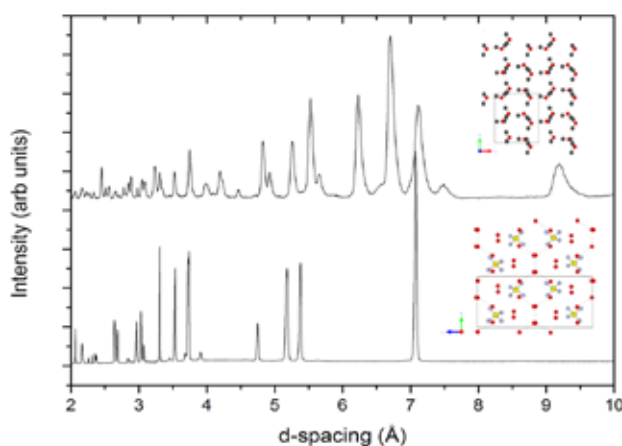
**Figure 4: The 28-copper-atom 15-hydride molecular core, surrounded by dithiocarbamate, elucidated by a single-crystal study on KOALA [17].**

### Earth and planetary science

A novel, world-first technique was used on the strain scanner KOWARI to investigate the deformation of ice dynamically (*in situ*) using neutron diffraction to determine the preferred orientation and strain. Laboratory-grown pure and ‘dirty’ samples of polycrystalline  $\text{D}_2\text{O}$  were shortened in the range from 5 to 40 % at variable temperatures and at three different constant deforma-

tion rates [19]. These observations have significant implications for our understanding of the flow properties of glaciers and ice sheets which commonly exhibit layers of ice mixtures.

More recently experiments upon ECHIDNA have been taken, literally, out of this world. Jupiter’s dramatic moon, Io, has volcanoes that eject ionized sulfur into space. These ionized particles become trapped in the magnetic field of Jupiter, and bombard the surfaces of Io’s sister ice moons, Europa, Ganymede, and Callisto, where it reacts with the surface ice to form sulfuric acid hydrates. Data collected in complement with X-ray data from the Powder Diffraction beamline at the Australian Synchrotron revealed a new phase of sulfuric acid hydrate, the first discovered in over a century [20] (Figure 5). This new material, sulfuric acid hexahydrate, is possibly abundant on the surface of the sister moons which may influence the myriad of geological features seen there.



**Figure 5: Complementary powder diffraction data for sulfuric acid hydrate from ECHIDNA (top pattern) and the Powder Diffraction beamline at the Australian Synchrotron (bottom pattern) [20]. Superimposed at right are the structures that can be refined from each pattern; the X-ray data yield very accurate sulfur and oxygen positions while the neutron data add the hydrogen (deuterium) positions.**

### Engineering materials

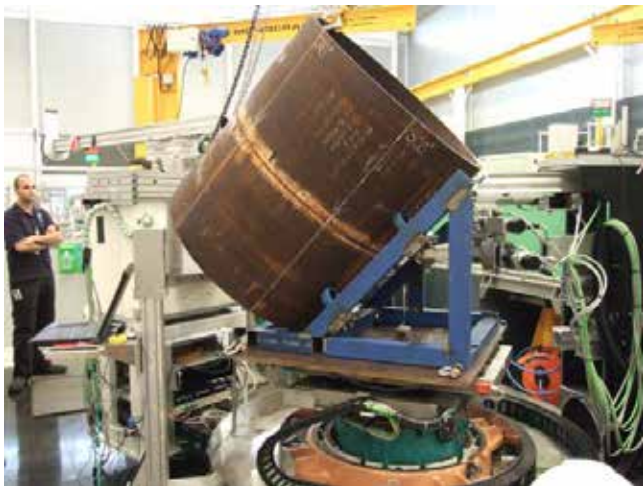
To the casual viewer the measurement of residual stress by strain scanning, as practised on KOWARI, only contains a light touch of crystallography in that the stresses are calculated from the changes in observed Bragg peak positions, giving effectively a lattice-level strain gauge. However the interpretation is underpinned by involved matrix relations between the choice of (reciprocal-space) scattering vectors and the real-space lattice, and by finely honed measurement precision.

The engineering problems tackled by strain scanning do have a regional aspect, with an emphasis on steel such

as rail components and gas pipes in Australia, as opposed to the dominance of problems involving aluminium and titanium in Europe and the USA, reflecting the local industries. The majority of studies on KOWARI have been on welds [21], claddings, and rail components [22] thus far, but interest in additive layer manufacturing, also known as 3D printing, is growing rapidly.

## **“...strain scanning ... with an emphasis on steel such as rail components and gas pipes ... as opposed to the dominance of problems involving aluminium and titanium in Europe and the USA”**

Because KOWARI has an unencumbered heavy-duty sample table and OPAL runs for ca. 300 days per year, users are prepared to travel halfway around the world to access the strain-scanning capabilities at the Bragg Institute. This was the case for a recent examination by TWI Ltd (UK) of welds in a section of a large-diameter natural-gas pipeline, which at 630 kg is to our knowledge the largest sample yet studied by neutron strain scanning world-wide (Figure 6).



**Figure 6: The section of a gas pipeline whose circumferential weld was examined on KOWARI. (Reproduced with permission of TWI Ltd (UK).)**

### **Cultural heritage**

A nascent research theme at the Bragg Institute is the application of neutron scattering to cultural heritage. This is likely to grow rapidly when our imaging instrument, DINGO, comes into user operation, but here we will concentrate on the crystallographic aspects.

Crystallography can play a key role in forensic investigations of materials that model those in the real artifacts, particularly under conditions that mimic in a controlled or accelerated fashion those endured by the artifacts. The non-destructive nature of neutrons coupled with the high penetration, often means that the artifact itself can be examined in its entirety. A topical example from HIFAR was the examination of the armour worn by bushranger Joe Byrne in the Kelly Gang's final encounter with the police in the Glenrowan siege in 1880 [23]. X-ray and neutron diffraction phase analysis and fluorescence elemental analysis led to the conclusion that the armour was manufactured after 1857 from good-quality rolled steel (similar to plough shares), most likely over a camp fire by an unskilled worker. The armour was also marked by bullets, which the study showed were not from the Glenrowan siege, but from after World War I!

Carrara marble is often used to face large buildings, but bowing and other degradation has been observed, particularly in climates different to the Genoan coast of Italy. Combined diffraction analysis on ECHIDNA and texture analysis and strain scanning on KOWARI showed that thermally induced stress resulting in micro-cracking is the likely cause of weathering and deterioration of the marble [24].

### **Concluding remarks**

These examples are just a selection of the many crystallographic highlights of the neutron-scattering programme at OPAL. A common element of the above is that it is the combination of state-of-the-art instrumentation, expert instrument scientists, and highly skilled support staff in sample environment, mechanics, electronics, and informatics that yields world-class outcomes.

## **“ANSTO is well on the way to achieving its commitment to make OPAL one of the top three research reactors for neutron scattering in the world”**

The range of crystallographic applications will inevitably increase and diversify as both the in-house expertise and the user base expand and develop. The current introduction of polarised-neutron capability via  $^3\text{He}$  spin filters on many of the instruments will see a dramatic growth in magnetism research. We are also

gauging local interest in protein crystallography, and membrane and fibre diffraction, which could lead to development of wide-angle diffraction capabilities using cold neutrons. Niche applications, especially those that also exploit other capabilities within ANSTO, including those at the Australian Synchrotron, will continue to appear, as evidenced by the technetium and planetary ice studies.

ANSTO is well on the way to achieving its commitment to make OPAL one of the top three research reactors for neutron scattering in the world.

## Acknowledgements

We gratefully acknowledge all the inspiration and hard work of the users and the instrument scientists that has led to the growing success at OPAL, a sampling of which has been presented here. We also thank Margaret Elcombe, one of the intrepid pioneer neutron scatterers at HIFAR, and Shane Kennedy, for their many insights into the exciting earlier times.

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**Professor Garry McIntyre** is the Research Leader for Hard Condensed Matter in the Bragg Institute at ANSTO. He received his PhD from the University of Melbourne in 1978 for work in X-ray diffractometry and mathematical crystallography. After post-doctoral positions in Uppsala and Edinburgh, he joined the Diffraction Group at the Institut Laue-Langevin (ILL) in Grenoble, France, where, over a 28-year period, he was instrument scientist at one time or another for most of the single-crystal diffractometers. He became an ILL Senior Fellow in 2005, has held a Visiting Professorship in Chemistry at the University of Durham since 2006, and became the first head of the ILL Graduate School in 2008. He moved to the Bragg Institute in 2010. His research interests focus on neutron scattering techniques, especially single-crystal diffractometry and the use of polarized-neutrons, diffraction physics, charge and spin density in molecular compounds, and structural chemistry.