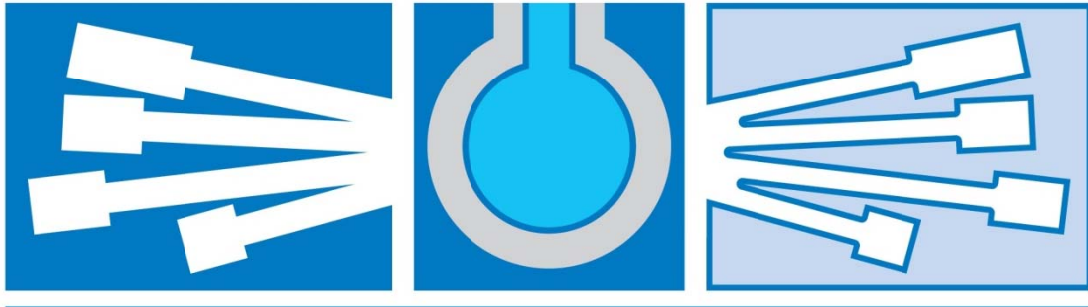
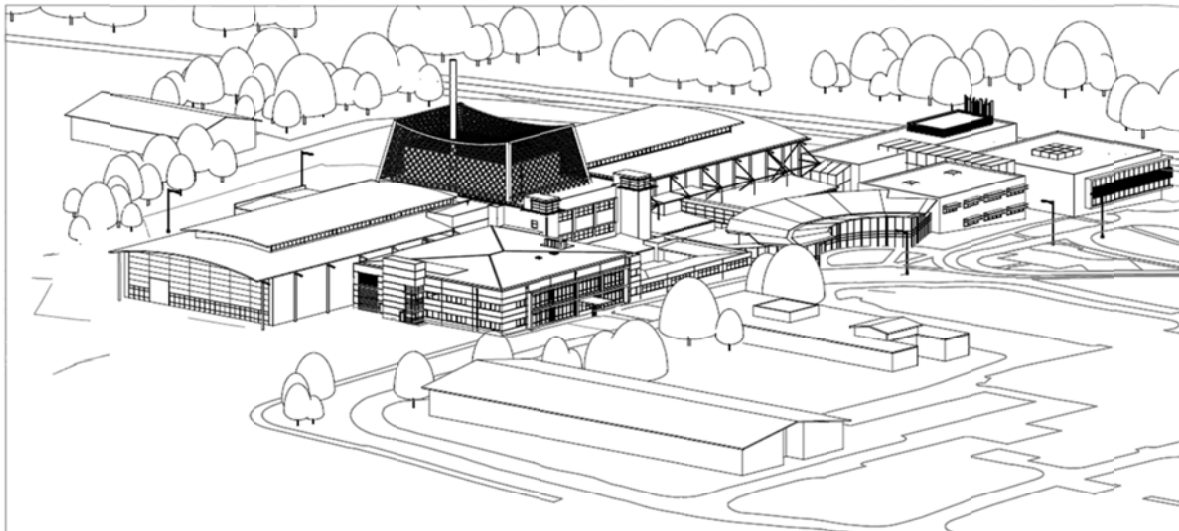




# Second Guide Hall for OPAL



Workshop  
16-18 April 2012, Sydney





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## EXECUTIVE SUMMARY

The importance of neutron scattering as a microscopic non-destructive characterization technique is well recognised around the world; new neutron sources (in China and Sweden) are under construction or are at an advanced stage of preparation, while a large number of major upgrades are underway elsewhere. Among the newest sources is the Australian OPAL research reactor which in its five years of operation has become a major component of Australian and Asian scientific infrastructure. Since the start of operations at OPAL, seven neutron scattering instruments of the highest quality have become available to the Australian scientific and engineering communities with another six nearing completion. This instrument suite, and the reactor's scope for medical and other isotope production, has created new communities working in biological and chemical structure, energy production and storage, engineering and materials science, and physics and technology. There is also the tangible benefit of international collaboration and exchange arrangements in the Asia – Oceania region and beyond. OPAL is now a major player in the world neutron scattering community.

ANSTO has begun a consideration of the medium- to long-term future of OPAL and its associated instruments. With exceptional foresight, OPAL was designed from the outset with the intention of adding a second guide hall viewing the existing thermal and cold neutron sources. This exciting possibility allows the installation of an additional set of up to 15 instruments. The Workshop on the Second Guide Hall for OPAL, held between 16 and 18 April 2012, gathered eighty national and twenty international experts to define the most promising science and technique developments in neutron science on a ten- to twenty-year horizon, the lead time for such developments. The workshop also sought to document emerging scientific and technical opportunities and to identify opportunities for new instruments that will maintain the pre-eminence of OPAL and its national and international use. To make the best use of the two guide halls, a further optimization of the cold source (or sources) will be required, particularly in regard to the detailed design and performance of the moderators; the recently established IAEA collaboration on this topic has full Australian participation. The possibility of installing a high-performance hot source for high neutron energy applications was also discussed.

The development of optics for neutron instruments has been rapid over the last decades. This has led to impressive gains in data acquisition rates and it is now possible to create entirely new types of neutron instrumentation. For example, one can now adapt the beam delivery system to the scientific requirements in a way that was previously impossible. Computer simulations and prototypes show that substantial improvements over the current generation of instruments. In addition, neutron optical devices can now deliver just those neutrons that are required for a particular application, leading to significant reductions in the experimental background. Thus the quality of the data will be greatly enhanced. This along with the large-volume cold neutron source at OPAL will allow a second guide hall to provide tailored neutron beams to a greater number and greater variety of instrument than is possible with the less flexible guide network that serves the current hall.

Self-assembled systems are present in everything from personal-care products to biological membranes. Neutrons are exquisitely sensitive to the presence and

locations of hydrogen, a major constituent of these materials. The second guide hall at OPAL offers the opportunity to construct an instrument that is optimized for these partially ordered systems allowing scientists to study self-assembly under external stimuli, such changing humidity and electric, magnetic and shear fields. In particular, the considerably higher net signal-to-noise possible with improvements in neutron focusing along with a wide neutron waveband and a large solid-angle detector, will enable measurements that were previously impossible. Moreover replacement of the hydrogen atoms by deuterium allows the characterisation of these structures in a way unmatched by other techniques. Thus the ability of the National Deuteration Facility to produce wholly or partially deuterated samples to be studied using a new specialised instrument housed in the second guide hall will provide Australia with an unprecedented capability to study and better control self-assembly, leapfrogging current inadequate structural probes available elsewhere. Such an instrument would also be used to for the structural characterisation of fibres, whether biological (e.g. cellulose, a potential feedstock for biofuels), or synthetic, such as Kevlar.

The development of more capable and more flexible neutron delivery systems will allow the ANSTO to develop instrumentation around a variety of equipment that can place the sample in extreme environments such as those experienced during industrial processes, or in the centres of the planets. One key area that would be enabled is the study of minerals and other materials under pressures comparable to those found within the earth while the minerals are being formed. This will provide new understanding of the structure and dynamics of the Earth's crust and upper mantle, knowledge that is crucial if we are to predict and mitigate natural disasters, reduce the impact of human activity on the environment and locate and exploit natural resources. Moreover, this capability will allow us to develop new materials and processes to address issues in energy, environment, and health. These materials can only be quickly and efficiently engineered if one can completely characterize complex and heterogeneous chemical systems, generally under real-world conditions, including extreme pressure.

Over the last few years, neutron imaging has emerged as an indispensable tool for a variety of new technologies such as fuel cells for automobiles. Unfortunately this technique has been limited by the best available resolution of 10  $\mu\text{m}$ . With a second guide hall and making full use of the advances in neutron optics, ANSTO would be able to build the world's first neutron microscope. The basic idea is to use a large band-pass cold polarised beam from the new second cold source with a sextupole magnetic lens system (which has similar properties to visible light microscope lenses), producing a magnified image on a large pixelated detector. With a long secondary flight path, possible with the second guide hall, a magnification factor of 50 will be attainable, allowing objects as small as 200 nm to be viewed. The specifications of this microscope are very well matched to the needs of Australian industry today; applications include the imaging of crack propagation, micro-porosity, and biological and polymer materials. In addition, this unique instrument will permit the visualisation of liquid layers of oil and water within sand and rocks, at the  $\mu\text{m}$  level, providing information of vital interest to the mining and oil industries. Future applications include carbon-fibre-reinforced polymers and other advanced composites. In addition such a neutron microscope is very well adapted to studies of nano-magnetic devices of critical importance to the communication and IT industries.

In short, this advanced microscope would be a world-leading characterisation tool, setting the agenda in the field of neutron microscopy.

Aside from these imperatives, strong cases were also made at the workshop for a positron source and associated beam lines for fundamental physics, and if major overseas funding is forthcoming, one or more experiments in fundamental neutron physics.

This workshop demonstrated that the idea of a second guide hall on the OPAL reactor was extremely well justified and timely, and is indeed an essential future step towards the full exploitation of this world-leading research infrastructure which supports Australian research and development, and in general, the Australian economy.

## INTRODUCTION

The OPAL Research Reactor was originally conceived as having a fifty-year life, cold- and hot-neutron sources, up to 18 neutron beam instruments on 6 neutron guides in a large guide hall. The facility was designed, from the beginning, in such a way as to allow a second guide hall and an eventual complement of 30 or more neutron beam instruments. In fact, such expansion has taken place at a number of leading neutron sources (particularly at the Institut Laue Langevin in Grenoble, France, and at NIST in Washington DC, in the USA), in conjunction with a second cold-neutron source in both cases. OPAL is the first reactor in the world to be designed from the outset with this upgrade path in mind, and ANSTO has made strenuous efforts to ensure that land and access has been kept free on the site of the second guide hall, whose location is completely determined by the beam-line penetrations into OPAL's reflector vessel and shielding.

OPAL presently has 7 operating instruments on 4 guides, while a fifth guide is presently under construction, with 2 instruments in commissioning and 4 under construction. All 7 initial instruments are oversubscribed, with usage approximately 50% from Australian universities, 20% from within ANSTO and 30% from overseas (including New Zealand). One of the new instruments is fully funded and staffed by the National Science Council of Taiwan, which provides roughly a third of the current overseas user base. Experience overseas indicates that scientific outputs scale with the number of operating beamlines and the number days the instruments are available. If Australia (and ANSTO) has the ambition for OPAL to produce science at a similar scale and level as the leading neutron sources, this can only occur if OPAL is fully instrumented – at present we have 20% to 25% of the coverage of our international competitors.

The decision to fund the construction of OPAL, with an initial 8 instruments, was made by the Australian government in 1997, and a contract was signed with the Argentinian company INVAP S.E. in mid-2000 for the reactor, a large modern cold source, 4 neutron guides (2 cold and 2 thermal) and the associated buildings including some labs and user cabins. Some desired scope was not taken up in the contract negotiations, in order to keep the project within the approved government funding: two guides, the hot-neutron source, an office building for ANSTO's staff and 10m of guide hall footprint were excluded from the contract. An office building sufficient for the first wave of 8 instruments was subsequently funded by ANSTO, and the Commonwealth's Super-Science Initiative funded one of the missing guides in 2009.

Construction of the initial suite of instruments was managed by ANSTO itself, with substantial input at all stages by the Australian science and engineering communities, along with expert overseas peers. The reactor went critical in 2006, and the first users and scientific paper arrived in 2007. The reactor and its cold source experienced significant teething problems until roughly one year ago, but all 7 initial instruments have been running flat out for users for the last year, and for the thermal instruments a number of years. The 6 additional instruments were selected via dialogue with our users and external advisors, including regular external review and involvement of community workshops, the Commonwealth's 2006 NCRIS process along with internal ANSTO brainstorming. Once all 13 instruments are operating, we still have a few clear and priorities, particularly a second neutron reflectometer, a time-of-flight

diffractometer, a cold-neutron single-crystal diffractometer, and extension of cold-neutron spectroscopy suite to higher energy resolutions.

The purpose of this workshop on 16-18 April 2012 is to think beyond this point, to look out 10 years ahead or so, and to assess the scientific and technological opportunities for the OPAL Reactor, to prioritise these if possible, and to start making the case for eventual capital and associated operational funding.

One obvious opportunity is to exploit the advances in neutron guide technology and neutron optics to tailor the incoming optical performance to the needs of particular instruments, which would then have significantly improved performance compared with those in the first guide hall, or indeed at other reactors around the world. The way OPAL was built, with the guides specified before the choice of instruments, and as part of the reactor facility itself, prevented this type of optimisation. But now we have an opportunity to do this, in a relatively unconstrained way.

Other obvious questions will be whether to install a second cold-neutron source, a graphite hot-neutron source or both, a positron source (as has been proposed independently by the Australian National University), and whether to try to pursue a major physics experiment to test the Standard Model of particle physics. It may not be possible to pursue all of these options, or indeed others that surface during the workshop, but we want to explore all such ideas and document them at the workshop.

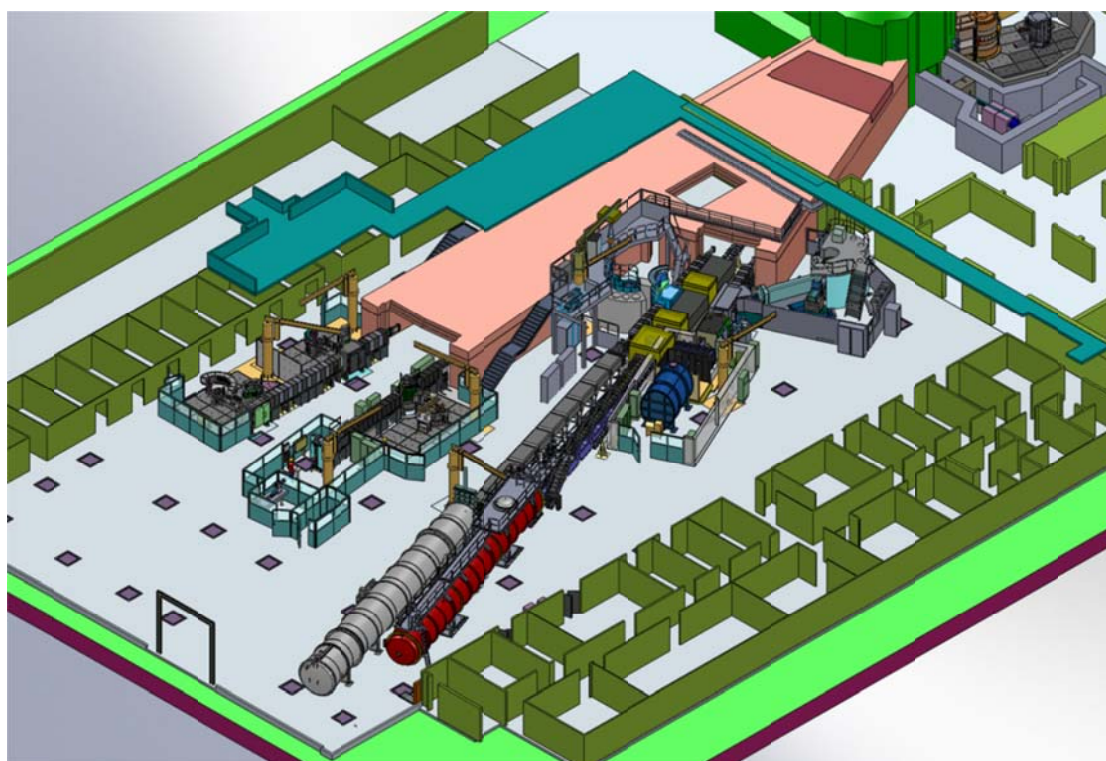


Fig. 1 Instrument configuration in OPAL's first Neutron Guide Hall, as it will be in mid-2013, with 13 operating instruments. The 4 thermal-beam diffractometers are at top-middle left, the 6 cold-guide instruments (including two long pinhole SANS instruments) are in the foreground, while 3 further instruments, one of which is not visible, are in the Reactor Beam Hall at the top right.

## MAGNETISM & SUPERCONDUCTIVITY

Science is in Australia's national interest - it impacts the development of human resources in developing the nation's future scientific leaders and underpins the technological basis for modern industry. The type of science discussed here is an important training ground for the next generation of scientists and technologists. Scientific and technological developments are keys to the future and to future prosperity. Economic and social studies have documented extensively that the income per capita for nations throughout the globe is directly correlated with investments in scientific research. Here we outline briefly the most challenging and important scientific directions to be followed using the high quality neutron beams available and in prospect for the Second Guide Hall at OPAL.

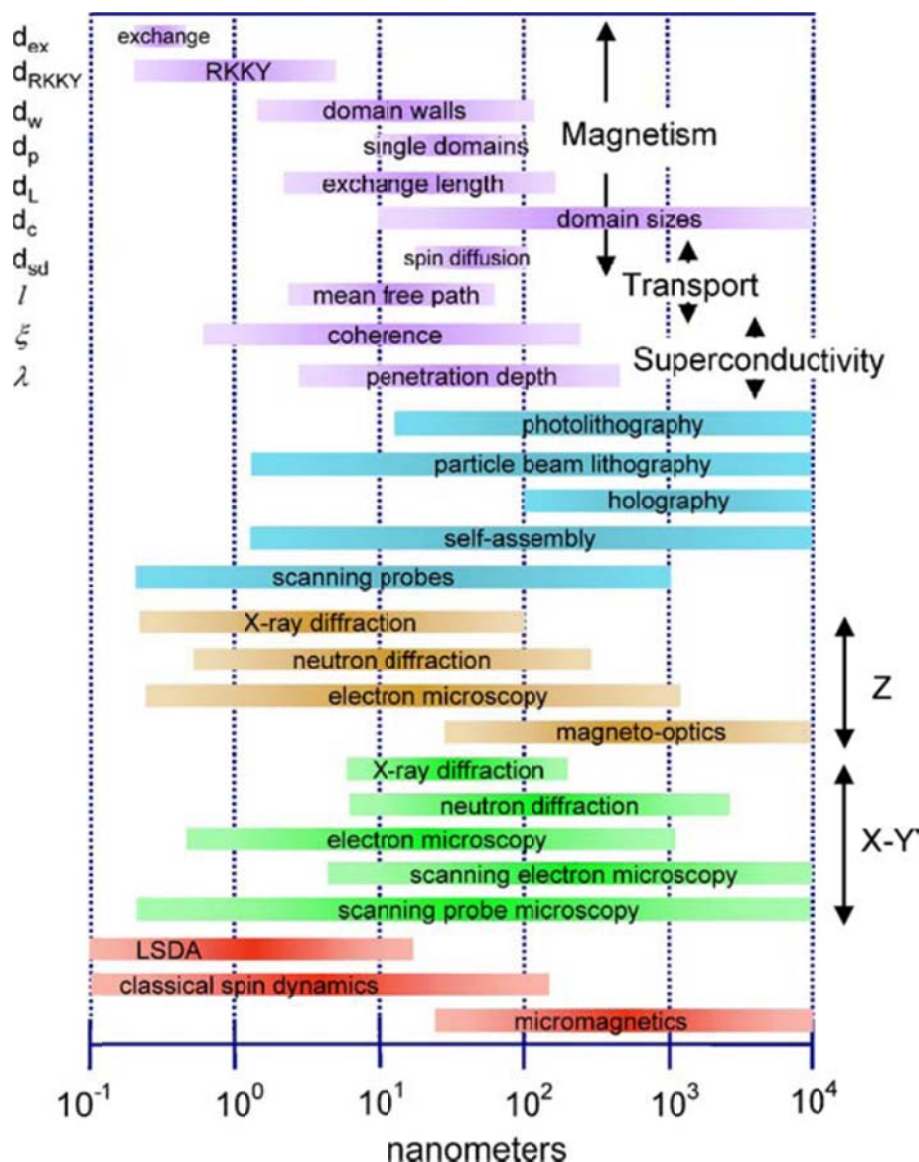


Fig. 2 The important length scales in the physics of magnetism and superconductivity and how these match with those of device manufacturing methods, neutron scattering and other important methods (courtesy of Ivan Schuller).



A second guide hall is necessary to enable the dramatically improved instrumentation required for the emerging science outlined below. The scope for new instrumentation is also reflected by the rapid growth experienced throughout the Asia-Oceania region.

### **Scientific Drivers**

Magnetism and superconductivity are key areas in modern science and technology and will continue to play crucial roles for the foreseeable future. Likewise, enhanced understanding and applications of technologies derived from magnetism and superconductivity have benefitted and will continue to benefit from neutron scattering studies. Modern condensed matter and materials physics are driven by pushing the limits of length scales into the nanometer scale and the limits of time scales below nanoseconds. The scientific drivers mentioned below attract attention in major research centers world-wide and their importance and significance cannot be overstated. The most important and challenging scientific directions include studies of functional/advanced materials, materials suitable for energy conversion, and - it is stated here as a worldwide priority - the quest for materials that can supersede the critical functions achieved with the increasingly sparse resource of rare earths elements.

In general terms the type of materials systems that are important are: nanostructured materials, low moment magnets, new hard magnets, high temperature superconductors, magnetic semiconductors and systems driving weak phenomena, functional materials, shape memory alloys, interfacial and surface magnetism and superconductivity, as well as materials close to instabilities and phase transitions. Investigations of disordered materials and frustrated magnetism and resolution of their behaviours are integral to complete understanding of modern and futuristic materials.

Two major fields of science which will be explored with the sophisticated suite of instruments accessible *via* a second neutron guide hall are *Quantum Matter* and *Nanoscience*. These topics are associated with nanophysics and nanomaterials, films, interfaces, heterostructures and involve the detection of weak magnetic signals. Such weak signals are manifest, for example, in the interplay between superconductivity and magnetism, and in multi-functional materials.

The relevant energy scales can be probed with thermal and cold neutrons. While there is no strong need for a hot source to address these issues, polarized neutrons and polarization analysis for both elastic and inelastic neutron scattering are very important.

External environments are crucially important for neutron scattering studies of *Quantum Matter*. In addition to scope for extended temperature studies, the key aids required for sample environment are pressure, magnetic field and electric field. The pressure range 3-10 GPa is desirable and feasible for inelastic scattering. However, leading capability would be provided by combined high-pressure and high-magnetic field capability. Here 3-10 GPa and up to 20 tesla is feasible in a 10 year time frame; a globally unique capability would be achieved with 100 GPa and 100 tesla (pulsed). Ability for *in situ* rotation of magnetic field is crucial. A competitive edge can be found with access to high-temperature-superconducting magnets which will eclipse

conventional low-temperature-superconductor systems in terms of cost, size, power consumption, stray field and ramp rate.

The use of extreme environments in neutron scattering is also very important for the geosciences and related mineral resources. Particular areas of interest are the change of iron valence under pressure as an indicator of subterranean conditions, and the search for mineral resources and lanthanoids using weak magnetism sensors.

While investigations of thin films are well established, the convergence of thin films with nanoscience is a novel emerging direction. The point is to push the magnetic sensitivity to the highest possible level, in other words this direction is to a large extent about detection of weak magnetic signals. Reflectometry and diffraction techniques are likely to be the most appropriate techniques.

Spintronics and current-induced spin polarization and spin polarization in semiconductor heterostructures are novel classes of phenomena related to this direction of research where magnetic effects in confined systems are addressed.

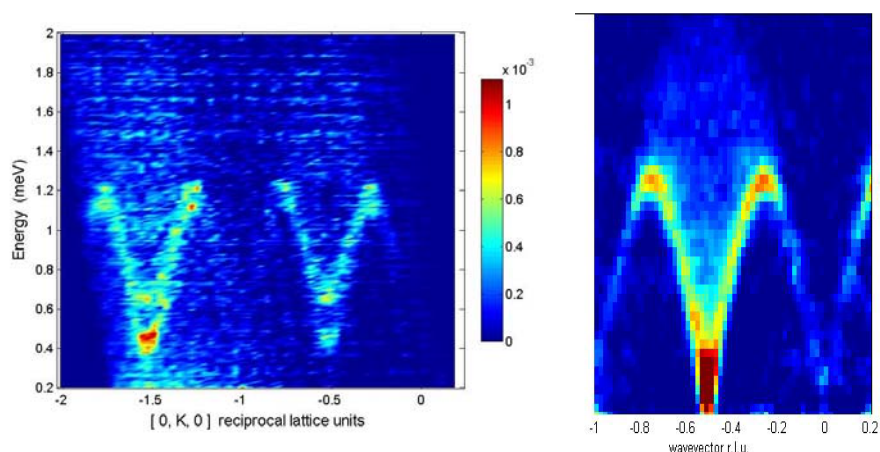


Fig. 3 High-resolution inelastic neutron scattering measurements (left) of the natural mineral Azurite show that there are two clear energy gaps in the spin wave spectrum at 60 mK. This indicates that the simple 1D Heisenberg spin-chain model (right) is not sufficient to describe this system, but that alternative theoretical models involving inter-chain coupling must be considered (from *Phys. Rev. B* **84** 184419 (2011)).

The field of one-dimensional (1D) quantum magnetism, i.e., studies on materials understood in terms of spins  $S = \frac{1}{2}$  or 1 which are coupled magnetically along only one crystallographic direction, has an impact on various topics of modern solid state physics. For instance, 1D quantum magnets allow studies of models and concepts relevant for understanding correlated electron materials. Various 1D and higher dimensional quantum magnets have shown interesting field-induced phenomena, among which Bose-Einstein condensation of triplons is a prominent example. In this situation, 1D systems can perfectly serve as a testing ground for new theoretical methods and techniques, like the use of conformal field theory or advanced numerical schemes, which can also be used to gain more insight into the underlying principles of quantum magnets in higher dimensions. Thus, neutron scattering data from 1D quantum magnets can be used to challenge new and emerging theories by rigorously testing new theoretical descriptions for low dimensional systems. Indeed, tests for

emerging theories in these challenging experimental fields are a major challenge for experimentalists.

The type of novel scientific phenomena which are central to understanding the behavior and application of the materials outlined above include: stimulated collective phenomena, magnetic proximity effect, collective phenomena in superconductors and magnets. Other important aspects are multiferroicity, dilute magnetism, magnetism in confined dimension - magnetic quantum dots, metal insulator and Mott transitions, low-dimensional magnetism, light and field induced magnetism and superconductivity, electronically driven inhomogeneities, spin injection, and exchange bias.

It is very important to realize that one issue which permeates modern science and technology is the unavoidable disorder present in all materials and devices of interest. In many cases such as exchange bias, superconductivity, magnetic semiconductors and hard magnets, disorder is not only present but may be at the heart of the science. Geometrical frustration is one such type of disorder in which nearest neighbor ions cannot reach an energetically favorable minimum in the ground state due to competing interactions. Instead, frustration can give rise to a degenerate manifold of ground states which lead to exotic states such as spin ice and spin liquid. Interestingly, further perturbations of frustrated systems can compound the inherent disorder leading to even more unusual phenomena. Thus, tackling the thorny issue of disorder and learning how to deal with it is essential with neutron scattering being the key tool to advance this aspect of matter.

**Materials preparation:** The range of methods employed in preparation of the types of materials outlined above includes crystal growth facilities, thin film preparation, nanofabrication, ion implantation among other sophisticated preparation methods. Aspects of materials preparation such as thin films and crystal growth are highly specialized activities. It is recognized that dedicated national crystal growth and characterization facilities are required to support work in these challenging fields of condensed matter science. As a specific example, there is a compelling case for Australia to address the lack of crystal growth facilities in collaboration with existing bodies such as the Australian National Fabrication Facility - it is proposed that a National Preparation Facility is established with access for users and staff available through a peer-reviewed proposal system.

### **Technological Drivers**

All of the above scientific drivers have direct impact on current and futuristic technologies in a wide range of fields via, for example, novel electronics, spintronics, superconducting magnets and hard magnets, data storage and functional materials. Areas of current and burgeoning interest include applications of high temperature superconductors and shape memory alloys. In addition to the long term benefits that cutting edge scientific research brings, there will be immediate benefits to local manufacturing and related industry. This will be driven, for example, by the need for quality design and construction of new high-tech, world leading, technically challenging instrumentation. The cutting edge instrumentation necessary to achieve the scientific targets illustrated above, will in turn drive a local support industry that is

able to compete worldwide - thereby opening new possibilities for technology exports.

### **Why Neutrons?**

Neutrons are the ideal tool to solve many of the important issues mentioned above. The reason for this is that neutrons provide straightforward, readily interpretable results which can be used to derive information directly regarding both the scientific issues and the materials systems. Neutrons provide structural information and critical parameters regarding disorder. It is perhaps not commonly recognised that in many cases (especially in magnetism) it is not straightforward to infer the magnetic structure or the superconducting properties from the physico-chemical structure. The spatial distribution of magnetic moments, especially at surfaces and interfaces, is of crucial importance both for the materials and for the phenomena mentioned above. Detecting time dependent phenomena, magnetic profiles and collective modes in novel, artificially structured materials will benefit greatly from the direct information which can be obtained from neutron measurements.

A particular challenge for neutrons – or rather the myriad of neutron scattering techniques and options that neutron science affords - is to help to understand how correlations between distant particles can lead to a wide variety of new properties in novel and functional materials. This will manifest itself by measuring not only the ordered or characterizing the disordered state, but also the excitations out of that state, a purpose for which neutrons are particularly suited. That these excitations can take on quasi-particle status is well known; this circumstance provides us an opportunity to evaluate fundamentally new behaviours on both the microscopic and macroscopic scale with neutrons.

A very significant aspect which this report addresses at large is the recognition that neutron scattering studies in the past have been associated primarily with the need for relatively large samples. This report demonstrates clearly that the new science to be explored can be matched by the sophisticated developments proposed for associated instrumentation and sample environments.

### **Instrumentation and Related Aspects**

We emphasize that sample environment is a crucial issue of enduring significance. In many cases, it is only through a high quality sample environment that it is possible to address key issues in the particular field of science. To ensure optimal benefits from the neutron beam science and its application to the scientific and technological drivers outlined above, it is vital that full attention is given to sample environment in parallel with the instrument developments in the Second Guide Hall. This will ensure that there are no limitations or impediments on the science and technology which can be pursued. The range of parameters to be defined depends crucially on the specific issues which will be pursued and also on the specific instruments which will be developed.

Important areas that will support the experimental investigations include: Monte-Carlo simulation of experiments; virtual experiments undertaken with actual

instrumental parameters; calculations undertaken, for example, by Density Functional Theory to connect experimental results with theoretical predictions.

Further scientific developments across many fields will be driven by extreme environments - such as are required for superconductivity and the earth sciences - and/or by the scope to extract very low signals with associated extremely low level background (required for example for diluted magnetic systems and nanosystems). These aspects require development of instruments beyond current limits of signal detectability and neutron beam size. Further advances will be achievable with instruments offering the following key aspects: high energy resolution, large detectors, neutron labeling, Larmor diffraction, spherical polarimetry (polarization transfer vector), polarization analysis and spin propagation analysis.

An exciting prospect is an instrument dedicated to exploration of magnetic properties. Besides high neutron flux, a dedicated spectroscopy instrument will employ polarized inelastic neutron scattering. Such a high quality instrument will be both a driver for science and an attractor for cutting edge research around the globe, particularly addressing issues in quantum matter.

A further exciting prospect is a dedicated diffractometer for thin films; such a dedicated instrument for polycrystalline thin films would be a world's first. In the same way a dedicated reflectometer suited to measure weak exotic local magnetism in heterostructures or nanostructures would provide an intense highly focused beam and a very small noise floor.

Quantum criticality that centres around the onset of magnetism where magnetic fluctuations are not properly understood will push the requirements of neutron scattering measurements of weak signals to the extreme. Enhancement of the crucial signal to noise ratio will allow the facilities proposed for a second guide hall to target studies of nanoscience at new levels of sensitivity – as low as a tenth part of the magnetic moment from a Fe monolayer. Novel and exotic phenomena under high pressure will lead to the discovery of new phenomena and ultimately new physics.

Simultaneous measurements involving a combination of optical properties and neutron scattering should also be addressed. Of particular significance is simultaneous magneto-optical Kerr effect and neutron reflection measurements on thin films.

All the above developments in instrumentation - especially the achievement of low background and sub-millimeter beams - will require advanced neutron optics of novel design.

## **Visions**

- To offer the world's best facility for science under extreme environments; this will both facilitate Australian science and attract high quality researchers from around the world.
- To establish a national materials preparation facility; this will be necessary both to ensure quality preparation facilities and conditions for the set of challenging materials to be prepared. In collaboration with the Australian National Fabrication Facility, this will enable the Australian science

community to ensure quality control of samples for investigation by the neutron beams at OPAL – a key resource for the nation.

- Dedicated studies of quantum matter and nanoscience require development of lock-in techniques to improve signal to noise ratio and to enable incorporation of additional experimental stimuli such as pump-probe experiments. Associated with these initiatives is the need for a dedicated instrument for nano-physics which enables investigations of different combination of materials while increasing neutron intensities in the sub-millimeter scale thus enabling enhanced investigations of materials under extreme conditions.

## **Recommendations**

**Sample Environment:** The unique sample environments identified above are essential for proper exploitation of these sophisticated materials and correspondingly require specialized personnel. Such high quality features combined with versatility would lead to a unique facility at ANSTO which would be attractive to users world wide. The particular facilities required are: *in-situ* rotatable magnetic fields, application of electric fields and currents, pressure. Flexibility is a key factor in these proposed initiatives – scientists need scope to be able to modify existing sample environments in response to the immediacy of experiential outputs.

**Expertise – A National Resource:** It is important to capitalize on the local technical experts in the various instrumentation areas in development of the neutron science to be carried out under this project. This will equally provide a national training ground for future science leaders.

**Neutron Beam Users and the Neutron User Community:** With a membership of over 320, ANBUG, the Australian Neutron Beam Users Group has expanded significantly since the advent of OPAL. It is crucial to maintain and further develop the local pool of clients that could benefit from and support the development of the instruments to be placed in Second Guide Hall. This expansion and outreach includes experts in Australia and in the Asia-Oceania region.

**Next-Generation Polarised-Neutron Instrument Design:** The imperatives for nano-structures in science and technology provide unique challenges - the sample size is limited, the magnetic density is small and the nature of the scattering is diffuse. Current conventional instruments are hard-pressed to meet these demands. The scientific imperatives call for focused new design of polarized neutron instruments to address the scattering characteristics of these important new types of materials.

**Instrumentation:** The above series of challenging scientific and technological drivers require a matching set of high quality instruments in order to allow these crucial advances to be achieved.

## COMPLEX AND HETEROGENEOUS CHEMICAL SYSTEMS - DYNAMICS AND STRUCTURE

To address issues in energy, environment, and health, on the global scale, novel materials and processes are called for. These can only be developed and engineered by being able to characterize completely complex and heterogeneous chemical systems, generally under real-world conditions. Neutrons are a central element of a gamut of characterization techniques, and Australia has a time-critical opportunity to be a global leader.

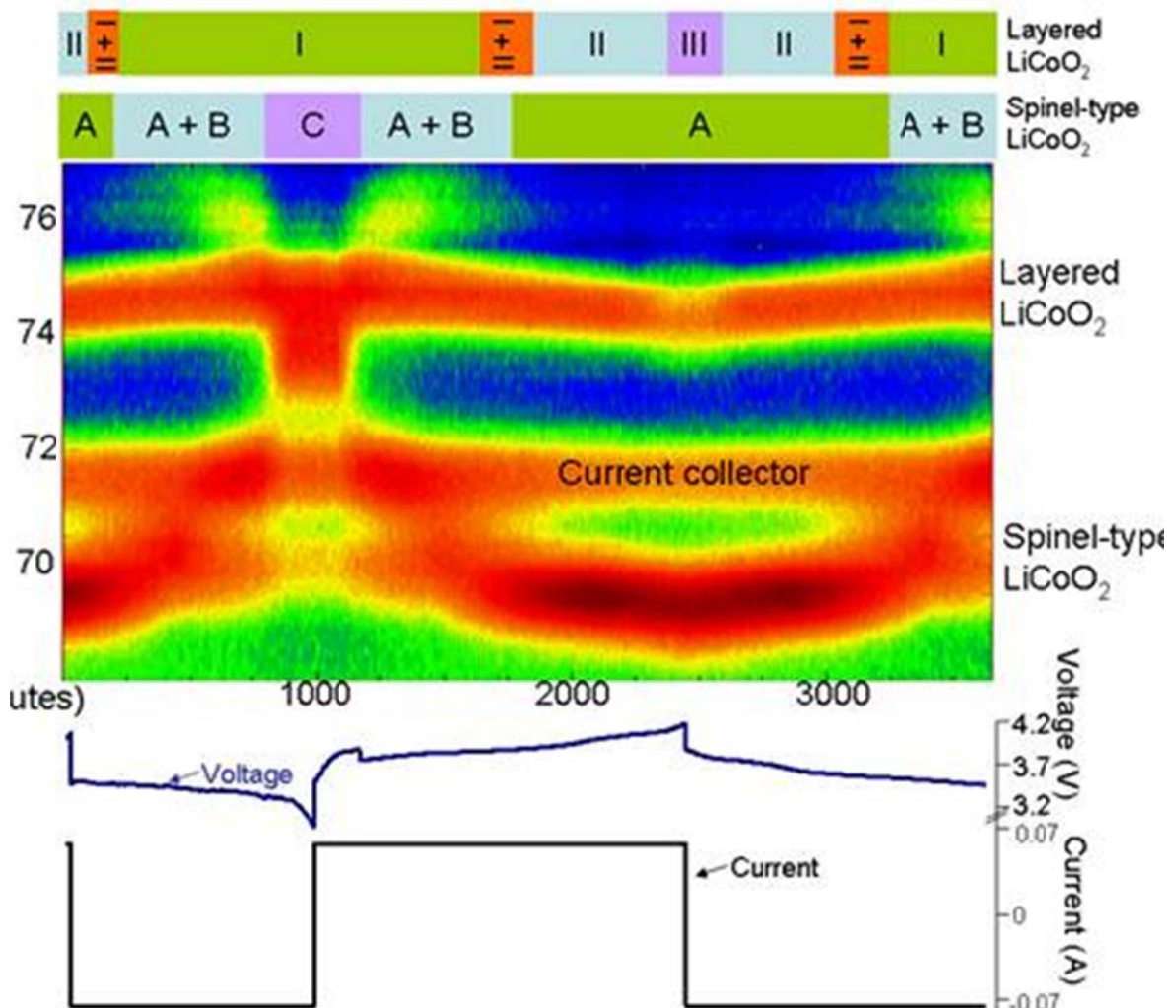


Fig. 4 Neutron diffraction can show how the various materials and components behave during electrochemical cycling in lithium batteries. (from N. Sharma, V. K. Peterson, M. M. Elcombe, M. Avdeev, A. J. Studer, N. Blagojevic, R. Yusoff, N. Kamarulzaman *Journal of Power Sources* **195**, 8258-8266 (2010).

### Research priorities

Central facilities provide opportunities for advanced materials characterization. This allows us to understand materials properties at an atomic level. Materials can be characterized *ex-situ* while complex materials processing has to be done *in-situ*. *Ex-situ* characterization can be done sequentially but *in-situ* characterization needs to be

done using multiple techniques simultaneously. Transformational advances are expected in a wide range of materials.

### Major scientific questions

- **Composites, metal- and polymer-based**  
Low-weight, long-life materials for the transport industry (aerospace & automotive)  
Biocompatible materials for the medical industry  
Enhanced strength and life time under extreme conditions for the mining industry (e.g. drills, pipes)
- **Supramolecular and large molecular structures**  
High volumetric and gravimetric storage materials for CO<sub>2</sub>, H<sub>2</sub>, and persistent chemical waste,  
Highly selective and efficient catalytic systems  
Highly selective and sensitive for rapid and reliable environmental and biological sensors
- **Structures in confinement**  
Drug delivery, agrochemical materials, catalysis and chemical processes, nuclear waste
- **Nanostructures - layered organic/inorganic materials, thin films**  
Catalysis, photonics and optical materials, sensors, photovoltaics,
- **Smart/ functional materials** for energy, health, environment and sensing ‘*the chemistry and physics of interfaces*’
- **Disorder, PDF in general, including magnetism**  
‘Real materials and systems engineering’
- **Molecular magnetism (driven by lanthanoids’ shortage, multifunctional)**  
Transportation and electronic devices
- **Earth sciences**  
We need to quantify the effect of water on rock stability, the properties of magmas, and the structure of amorphous Earth materials under the high pressures and temperatures found in the crust and upper mantle.
- **Advanced materials** are being incorporated into new products with shorter development times. Their wear characteristics require improved methodologies to meet this trend, for example carbon fibre polymer composite in aircraft components.
- **Gas hydrates**  
Formation of gas hydrates is a large problem in the oil industries with regard to pipe blockages. Understanding the structure and properties is essential to stop their formation. In addition there is extensive fundamental interest with regard to sequestration.
- **Geological materials**  
Dehydration of minerals in subduction zones leads to earthquakes. Partial melting of rocks in the mantle leads to volcanic activity. Understanding these processes is essential to being able to predict and mitigate them. This has particular relevance in the local seismic context e.g. Christchurch, New Zealand.
- **Solid-solid composites.**  
Energy storage and conversion devices such as batteries and fuel cells are composites of materials with related but distinct structures, dynamic and properties. The individual components are in general very well suited for study



by neutron scattering methods, but in order to understand and improve the performance of the ensemble we now need the ability to characterise them in situ across the solid-solid interfaces that provide, but also constrain, their functionality.

- **Fibres**

Fibres are important in many applications including reinforcement of composite structural materials, biomedical engineering, high-tensile ultra-light cables, etc. These need to be studied with 2-D diffraction techniques that require specialised detector geometries, sample environment and mounting systems.

## **Situation at OPAL**

Australia is currently well served in the investigation of static, generally ordered, structures, especially diffraction, with a number of world-class instruments. We are also potentially well served towards a small range of dynamics but there are clear absences in time range (very long time scales) and energies.

In addition to standard temperature and pressure STP conditions, the ability to vary the environment is critical. The major stimuli required include temperature, pressure, and gas environment, which generally need to be rapidly switched. OPAL has a limited number of suitable environmental cells, which needs to be enhanced considerably for a world-class user facility.

Major problems in Australia can be summarised as occurring in:

- Energy
- Health
- Environmental science including the minerals industry
- National security

In each of these areas, hydrogen plays a critical role and provides a continuing impetus for using neutrons. Hydrogen makes neutron scattering a natural choice but neutron scattering is not restricted to hydrogen, and the isotope dependence of neutron interactions provides additional exciting and novel opportunities. This is especially important for light elements – e.g. V-Cr cannot be easily distinguished by X-ray methods – the low energy of the edges makes anomalous dispersion extremely difficult. The hydrogen-deuterium contrast-variation method, in conjunction with neutron scattering, provides information unavailable by any other experimental method. Many materials in these areas are difficult to deuterate fully or partially and as such the study of real world problems will be enhanced by the ability to avoid this by separating incoherent from coherent scattering, a real challenge at present. Contemporary science is interested in multiple length and time scales.

### *International*

To address issues in energy, environment, and health, on the global scale, novel materials and processes are called for. These can only be developed and engineered by being able to characterise completely complex and heterogeneous chemical systems, generally under real-world conditions. Neutrons are a central element of a gamut of characterisation techniques, and Australia has the opportunity to be a global

leader. A clear example is to develop a regional excellence in understanding local structure and disorder via total scattering analysis, by providing monochromatic hot neutrons, a capability currently restricted to just three neutron-scattering centres, all in Europe. Australia's mining industry will gain independence and competitive advantage by the presence of a state-of-the-art neutron-based characterisation capability (currently 15% of Australia's energy production is used for aluminium smelting).

## Science Drivers

- ***In-situ* and time-resolved studies**
- ***Understanding complex systems under real conditions; functionality within relevant parameter space.***
- **Validation of experimental conditions and computational modelling. And optimisation of the synergy between experimental and theoretical techniques.**
- **Reactions – liquids; solids in liquids; fuel cells**  
Heterogeneous catalysis: key functionality is often at the interface or at phase boundaries and the need to determine the temporal evolution of such boundaries.
- **Catalysis gas-solid, liquid-solid, solid-solid**
- **Time-resolved structural and impulse experiments etc towards msec resolution**  
Couple the best of laboratory-based spectroscopy tools with in-beam structure determination to discover the dimensionality of dynamics (holistic approach).
- **Pump-probe spectroscopy.**  
Ability to monitor dynamics under the influence of external stimulus such as light, magnetic field etc,  
Pump-probe spectroscopy with both stimulus and monitoring.
- **Phase transitions at 'low' pressure (<3 Gpa) is currently our niche with e.g. light irradiation (small crystals but we need higher pressures)**  
Extremes of science occur at high pressures (and other reactive conditions). The ability to monitor physical and chemical processes at these extreme conditions will drive future science.
- **Radioactive samples**  
Understand functionality and improve processes for handling and transporting radioactive isotopes (actinides).  
Medical research such as damage to biological materials from ionising radiation.  
Mechanical properties such as defects caused by low-energy radiation damage.  
Access to actinide neutron resonances using hot neutrons.

## Instrumentation and Technique Development

### Desired Instruments

- Hot-source diffractometers for PDF and single crystal – Reactor building  
At 3000 K this will be the best in the world and allow new science working at resonances in addition to liquids and amorphous PDF work.
- Extreme Environment diffractometer – small focussed beam requires thermal neutrons. Can only be in second guide hall, due to space requirement.  
High pressure and high temperatures – Impact in earth science requires a dedicated instrument. Aim for 50 mm beam which will be the best in the world
- Multichopper spectrometer  
Multiple- $\lambda$  instrument. Critical to fill the energy gaps on the existing spectrometers. Important for low dimensional magnetism and disordered systems.
- Chemical crystallography diffractometer.  
Potentially the best in the world – in an area of Australian strength. Existing demand from the user community and offers the possibility to expand into biological science.
- Hot neutron time-of-flight spectrometer - Reactor building  
Necessary for the target energy and Q-range. This would be the first of kind at a reactor
- Polarised neutron diffractometer (hot) - Reactor building
- White-beam strain scanner with analyser crystal bank.  
There is a clear need to go beyond current strain-scanning single-peak methods to be able to extract whole-pattern and refinable information from complex samples and environment.

There is a need to aim for the hot source to operate up to 3000 K. The existing cold source provides good flux at 1.5 Å up to around 10 Å and this is optimal for instruments designed to address chemical problems.

### *Multitechniques (on the same beam):*

- Diffraction and Prompt  $\gamma$ -ray Activation Analysis (PGAA)
- PDF and spectroscopy, including with polarised neutrons
- Polarised neutrons to reduce incoherent scattering
- Contrast variation across neutron resonances ( $\Rightarrow$  hot source)
- Expanded length scale instrument – hot, thermal, cold

### *Sample environment:*

- Levitation furnaces, especially, but not only, for liquids
- Higher pressures, and improved medium-pressure (<3 GPa)
- Light irradiation, pump-probe experiments
- Gas-handling equipment
- Dynamic-nuclear polarisation
- Isotope substitution, not just H/D

### *Why is the Second Guide Hall necessary?*

- Provide capacity to fully utilise a unique national facility. Maximise return for the taxpayer. Increased capacity will attract global collaborations.
- More space, for operational flexibility, sample environment, safety, auxiliary laboratories. Separation of magnetic fields.

- Allow for multi-beam instruments and modern beam optics.
- Longer beams – focussing, microscope.
- Integrated climate control.

### **Recommendations**

The source, neutron delivery and instrument development must be conducted in parallel, and not as a sequential process. A group should be established to plan for this. This group should explore the opportunities presented by multi-vision instruments.

ANSTO should initiate projects looking at beam focusing and hot-source design in the short term.

Strengthen the sample environment group.

## MATERIALS ENGINEERING

The materials engineering community has, over the last decade or two, come to neutron scattering to use the currently available instrumentation. The future expansion of facilities at ANSTO offers further opportunity of engaging the materials engineering community to find the applications which are most pertinent. The next generation of instruments must be designed around these community requirements. While it is difficult, without consultation with industrial collaborators and a broader academic community, it is our belief that the field is heading towards the study of:

- *Process engineering* rather than static materials engineering, for example sintering of ceramics, nucleation and growth of powders, welding, and thermo-mechanical processing;
- *Complex sample analysis* including composites and materials with hierarchal structures;
- *Smart materials*, incorporating multiple functionalities, such as magnetism and ferroelectricity. Such materials require polarised neutron options as a key part part of the instrument design requirements.

This will require significant thought on the development and design of instruments, in order to accommodate increasingly complex samples and sample environments. The prospect exists, that upon further consultation, final instrument designs will be made based on the sample environment restrictions, rather than restricting these environments by the instrument design.

From an engineering perspective, the greatest opportunities will be in moving from sample-scale research to incorporating sample environments that represent small pilot plants, which more directly represent industrial and process engineering practices. This is a unique difference to current and future neutron and synchrotron instrumentation in Australia.

### Research Priorities

- Extreme environments (Radiation – Temperature – Pressure – Flow – Stress)
  - o Large in-situ sample environments which perhaps include small pilot plants to directly link to industry in a more useful way
    - Must have spatial resolution with 3D gauge volumes ranging from many  $\text{cm}^3$  down to less than  $0.1 \text{ mm}^3$
  - o Measurement of multiple scattering vector orientations simultaneously
    - This limits divergence of incident beam
  - o Small entrance and exit beam windows
  - o This would benefit from a bunker type setup to negate safety and containment concerns of operating such instrumentation in the regular guide hall space
- Structural complexity of materials of interest
  - o Engineering composites of varying length scales including highly hierarchal structures
  - o Complex sample geometries including very large components

- Must be capable of measuring an engineering component or full structure, not just a sample material
- Polarisation analysis required for smart magnetic materials

## **Opal Situation**

Current instrumentation,

- Kowari (great for strain scanning of single peaks in high symmetry materials)
  - Limits for complex sample geometry because of slit system. Upgrade to radial collimation may improve this.
  - Measures a single scattering vector at one time, thus make for very slow data collection and re-mounting required for 3D strain tensor solution. The re-mounting can be improved by robotic manipulation
- Wombat (hydrothermal synthesis, texture, temperature/phase studies)
  - Limitation is sample environment space
  - Restricted to have very large sample environment views to detector
  - Sample rotations required for full texture and strain analysis due to limited scattering vector collection
- Dingo
  - Large samples for industrial applications may still require scanning for full images
  - Resolution limited to 5 micron, can never get below 1 micron. Better resolution requires neutron microscope designs

## **International**

### ***Engineering Diffractometers***

Most recent major investment in neutron diffractometers for material engineering has been centred on energy-dispersive techniques at pulsed spallation neutron sources. To date, here is only one energy-dispersive strain scanner on a continuous source, POLDI at the Paul Scherrer Institute in Switzerland, but with only one detector and it is not an industrial-scale diffractometer. Since Australia will not have its own spallation neutron source in the foreseeable future, this presents the community with an opportunity to lead the world in this type of instrument development.

### ***Experimental Layout for Extreme Environments***

In some cases it may be necessary to build extra experimental end-stations outside the guide hall. This has long been the case at research reactors, and synchrotron sources have now also started to build large experimental end-stations outside the general institute containment (eg. JEEP at Diamond). We think this represents an opportunity to go to very extreme sample environments that are industrially relevant. Some large environments will need dedicated access separate to the regular guide hall, particularly where safety and containment issues exist.

## **Industrial Connection**

Engineering materials represent a strong motivation for the construction of improved instrumentation in a second guide hall at OPAL. There are already several industrial partners which assist in quantifying the societal impact of current neutron scattering operations. Identifying the potential to expand on these partnerships will enhance the community benefit and knowledge of ANSTO activities.

Potential exists for the creation of a larger industry/commercial group which can work directly with industry or through university linkages, CSIRO or along with ANSTO's Materials Institute. This perhaps needs to be somehow separated from the instrument scientist who may specialise in a single technique. Ideally an industry/commercial office should have broad knowledge covering all techniques.

In order to maximise this industrial impact it's important that potential customers are identified as soon as possible and their involvement made a critical part of the future expansion.

## **Instrumentation and Technique Development**

We conclude that the above community requirements could be addressed by 3 potential new instruments for future expansion into the second guide hall. These represent a dramatic improvement in the neutron scattering capabilities of Australia and provide the maximum complementarity with existing and future beamlines at the Australian Synchrotron.

## **Materials-Engineering Diffractometer**

The key requirements for this type of diffractometer include,

- Defined gauge volume down to sub mm sizes
- Small beams in (down to 0.1mm or smaller)
- Simultaneous sampling of multiple scattering vector orientations to the sample space
- Designs optimised for sample space and sample-environment versatility
- Maximum flux for time resolved *in-situ* measurements and small spatial resolution (optimised guides?)
- Instrument bunker located in a position to separate it as much as possible from the guide hall and other instruments
- Polarized-neutron option for magnetic scattering studies
- *In situ* SANS might form part of design to study kinetics of processes like synthesis reactions, grain nucleation and growth.
- Bragg edge transmission analysis for in-situ tomography or stress mapping.
- 

We believe there are three main options for achieving this:

1. A chopper type time-of-flight instrument
2. Double-crystal-energy-scanning monochromators with fixed position detectors
3. White incident beam with multi-analyser detector arms

Each of these options address the main scientific drivers, in particular the possibility of very large complex samples and sample environments. It is a requirement that such an instrument would be on an end-guide position.

Energy dispersive detection from a white-beam instrument represents a novel development opportunity in this area and would be world leading. Significant progress of the development of such instruments for residual-stress analysis which relate closely to this development have already been discussed in detail at the “Current state and future neutron stress diffractometers” workshop held by ANSTO in January 2012. Of particular interest is the section 5.2.2 on Long Term Developments<sup>1</sup>.

A typical layout for an engineering diffractometer in time of flight mode which allows a high degree of versatility in terms of sample environment access is shown below. It would be expected that full out of plane detector banks would also represent a significant advance for many of the engineering problems, however, this is coupled with increased restrictions on sample environments.

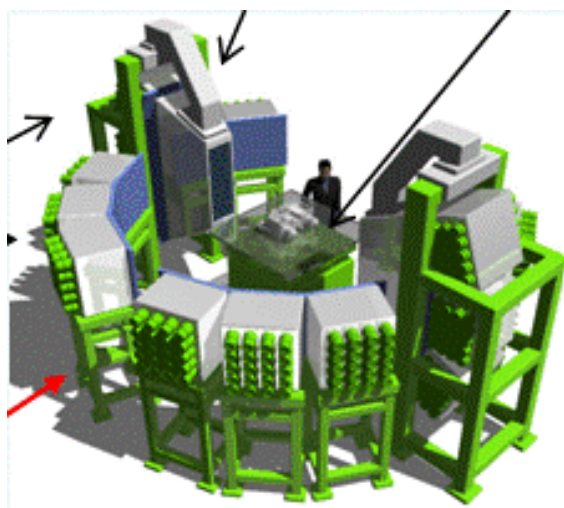


Figure 5. Example of time-of-flight instrument with large sample space for very complex environments.

### **Neutron microscope**

The current neutron imaging facility of Dingo (under development) will cover a significant portion of the required imaging for Materials Engineering which we have identified. The exception to this is in very high spatial resolution imaging which has impact particularly in the study of composites and hierarchal material structures. The requirements for this capability would best be addressed by a neutron microscope type instrument.

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<sup>1</sup> [http://www.ansto.gov.au/\\_data/assets/pdf\\_file/0020/52562/NSD\\_Workshop\\_Report\\_ANSTO\\_2012.pdf](http://www.ansto.gov.au/_data/assets/pdf_file/0020/52562/NSD_Workshop_Report_ANSTO_2012.pdf)



The main requirements are,

- Sub-micron resolution with preference for below 100nm
- Sub-micron resolution within larger specimens (current x-ray techniques in engineering are limited to small heavy materials)
  - o Selected volume (region of interest) tomography
- Micro-imaging using neutrons for complementary elemental contrast to x-ray sources
  - o Magnetic imaging

This instrument will require developments in magnetic lensing techniques. This will require a very long beamline to achieve the magnification values which open the prospect of investigation new materials engineering problems.

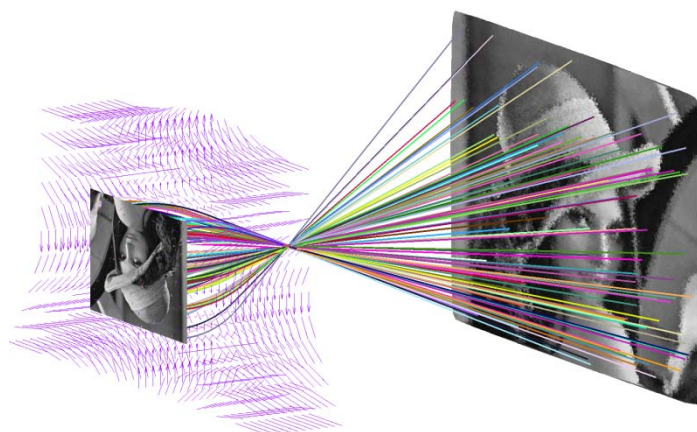


Figure 6. Simulated image with high and inhomogeneous neutron beam divergence.

### **Other Possible Instruments related to Materials Engineering** **High-Q scattering instruments for amorphous and nano-crystalline materials**

No doubt the pair distribution function (PDF) requirements of the Materials Engineering community cross over heavily with the Chemistry groups requirements for a hot source instrument with very large area detectors for faster data acquisition. This instrument will, however, have limited the sample environment versatility. The maximum Q-range available would have to be to at least  $30\text{\AA}^{-1}$  to make the investment worthwhile. For crystalline PDF this will still lag spallation sources significantly, however for liquids and amorphous materials it will be possible on such a source and would represent a significant improvement in the current instrumentation available to Australian scientists for this work.

### **Spin-Echo Imaging**

It has also been suggested at the workshop that there is potential for spin echo imaging giving 3D images without sample rotations with spatial resolution limits of approximately 10 microns. This option should also be investigated for 3D imaging of very large samples where regular tomographic studies are difficult.

### **Why the second guide hall?**

The major engineering diffractometer we are suggesting will not fit in the current guide hall. This limitation is due to size of the bunker required to house the sample environments of future industrial needs. It would need to be placed at an end-of-guide position which would allow for the greatest sample environment versatility.

For the neutron microscope if its pushed to the resolution limits of 100 nanometres or less. This will require specific vibration control for the sample environments which will need to be separate from the larger industrial components of the reactor and guide hall. This instrument would also likely need an end-of-guide position, however it would only use a small component of the incident beam and thus will not prevent other instruments of the same beam port.

A high-Q scattering instruments will require a position on the proposed hot source.

### **Source requirements**

The hot source does not offer much value for the described materials engineering diffractometer and neutron microscope. A second cold source however would present significant improvement for both of these. The hot source, however, is a requirement for the high Q-range diffraction experiments.

## SOFT MATTER

Soft matter systems are typically complex, hierarchical and pervasive across a wide range of fields from biology and health, food, nutrition and cosmetics, energy technologies, the environment, and a wide range of domestic and industrial processes. The complexity and multi-length scale nature of soft matter (ranging from sub-mm to essentially the atomic level) pose some of the key challenges to their study. With advances in fabrication of soft matter samples (including chemical and biological deuteration), neutron scattering techniques have become central in the study of the structure and function of complex systems.

Due to their complexity in structure and behaviour, the study of soft matter systems in artificial environments is far from ideal. This complexity relates to the temporal, spatial and energy domains. There is a need to concentrate on complex soft-matter systems in environments that are relevant to their production or use: for example systems that are evolving with time; systems under non-equilibrium conditions; heterogeneous or partially ordered samples. Hence there is a need for fast neutron scattering measurements, the ability to look at a wide range of length scales simultaneously, as well as the capacity to examine localized regions of the sample.

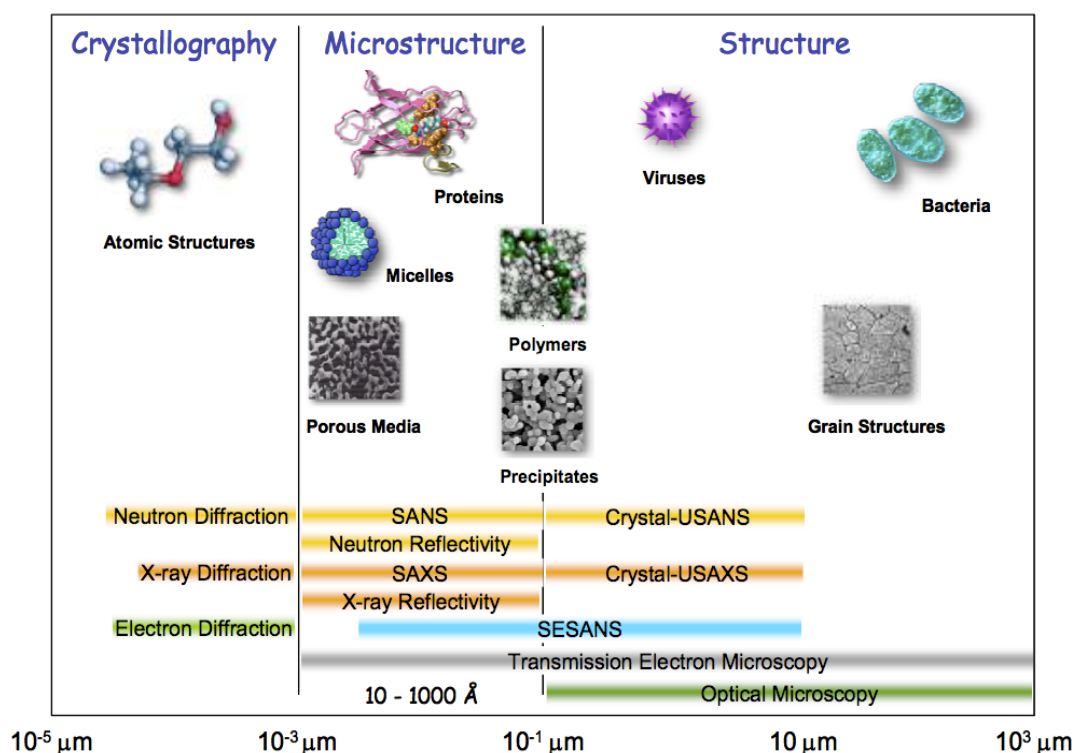


Fig. 7 How small-angle scattering and reflectivity measurements using neutrons and X-rays fit in with other methods, and at which length scales (courtesy of Jamie Schulz).

### Research priorities

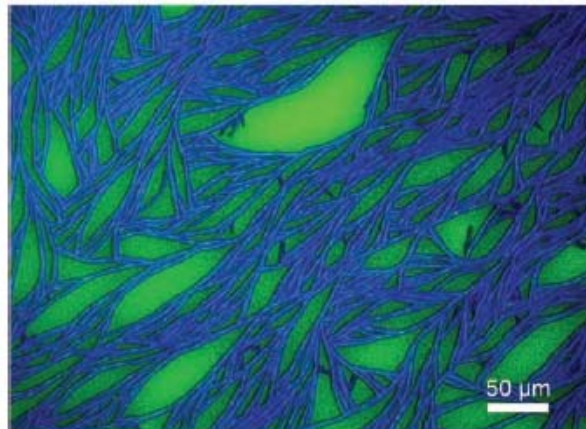
- Increasingly, there is a need to look at complex soft matter systems such as hierarchical structures, for example food systems, gels, complex biological systems, liquid crystals and polymers. In order to study these, the ability to measure over a wide range of length scales in a single measurement is essential.

- The ability to follow time-dependent processes over a range of time scales. Many of these processes occur much faster than currently accessible to the existing suite of neutron scattering instrumentation at OPAL. The ability to measure structural changes that occur over times of less than a second is needed.
- Soft matter systems are of broad technological importance. To understand structural changes occurring during processing, dedicated and tailored sample environments are required to enable in-situ, real-time studies. This is likely to be of significant interest to industry.
- To complement structural studies there is a need to understand the collective and individual motions of molecules or particles in a diverse range of complex soft matter systems.
- New developments should be aligned with the National Research Priorities. The breadth of soft matter research to be enhanced by developments in the second guide hall will address all of the National Research Priorities.

### Major Scientific Questions

#### *Optimisation of organic optoelectronics devices and molecular electronics*

Optoelectronic devices based on organic materials (conducting polymers, dendrimers, heterocyclic molecules, and self-assembled monolayers) are used in such applications as organic light emitting diodes (OLEDs) used in displays and lighting, organic photovoltaic solar cells (OPVs), and sensors for a range of materials including explosives.



**Fig. 8.** Luminescence microscopy image showing phase separation in the emissive layer of an organic light-emitting diode film after heating. The figure is a composite of two images taken at different excitation and emission wavelengths (blue–340 nm excitation, 370–400 nm capture; green–390 nm excitation, 495–550 nm capture) to discriminate between CBP (blue) and Ir(ppy)<sub>3</sub> (green) emission. Taken from: A. R. G. Smith, *et al.*, “Morphology and Stability of *Fac*-tris(2-phenylpyridyl)iridium(III) Blended Films: a Neutron Reflectometry Study”, *Advanced Functional Materials*, **21**, 2225-2231 (2011).

Typically these are layered, thin-film devices, where light adsorption or emission is controlled by the separation of electrical charge and is fundamentally determined by the nanostructures of the organic materials within the device. Understanding the nanoscale structure of such devices, as well as the movement of molecules (diffusion) between and within layers (Fig. 8) is crucial to improving their performance and

longevity. Understanding structures and processes at organic-inorganic interfaces are also vital in the development of next generation molecular electronics, chemical and biochemical sensors. Sophisticated sample environments will be required where device performance can be monitored simultaneously with neutron scattering measurements, and also allow for variation in temperature and ambient atmosphere.

*Development of soft matter systems for functional biomaterials and drug-delivery*

A host of soft matter systems have been developed as bio-functional coatings on medical and implantable devices, as scaffolds for tissue engineering, and as target directed controlled-release systems for drug delivery. Advances have also been made in specific contrast agents for advanced biomedical imaging techniques. Materials are as wide-ranging as their applications and include: polymers; plasma polymers and diamond-like films; nanoporous liquid-crystalline phases; polyelectrolyte capsules and coatings; peptide-based surfactants and other amphiphilic molecules; protein, enzyme and antibody decorated nanomaterials; and structures bio-engineered from E-coli derived proteins. Self-assembled soft materials such as complex multiphase polyphilic liquid crystals (Figure 2) offer huge potential for bio-compatible green materials, as well as engineered 100 Å-scale multiple chemical environments. It is becoming apparent that the structural complexity of liquid crystals can be comparable to that of conventional hard crystalline matter, with complex 3-dimensional lattices and (liquid) molecular arrangements within the unit cell. New methods in neutron scattering and deuterium labelling will be required to support research in this broad field that will continue to progress in conjunction with advances in biochemistry, molecular biology, medical science and nanotechnology.

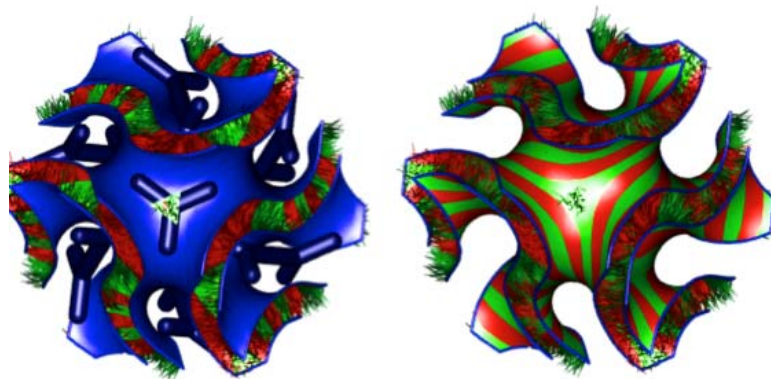


Figure 9. The exemplary structure shown here is proposed for Star-Polyphiles. It consists of two (blue) water networks, separated by a striped (red/green) hydrocarbon/fluorocarbon matrix (courtesy of Liliana de Campo).

*Studies of biological processes at the cellular membrane*

Biological processes that take place at the cellular membrane are central to all forms of life, yet knowledge of the structures of various cellular membranes and their functions in supporting biological processes remains scant. While being distinct from structural and molecular biology, soft materials currently play a central role in the development of biomimetic membranes. These model systems are used for investigating the behaviours of integral and membrane-associated proteins, the attack by enzymes and antimicrobials, and the function of receptors and other ligand

molecules. Development of superior, physiologically relevant membranes is a key challenge for soft matter researchers and with it comes also the possibility of exploring fundamental membrane structures based on phospholipids, glycoproteins, carbohydrates and cholesterol.

#### *Soft matter for energy technologies*

Soft matter systems are currently being widely used as key elements in materials for new non-fossil fuel based energy technologies. Metal-organic frameworks (MOFs) form the basis of technologies for optimised hydrogen storage matrices, platforms for efficient separation of natural and atmospheric gasses, and elements in carbon sequestration systems? Polymer electrolyte membrane (PEM) fuel cells are finding increasing utility in modern automotive transport, yet much remains to be understood at the molecular level about their function and optimisation. Organic ionic liquids (ILs) show promise both as green solvents as well as sophisticated electrolytes that can replace water in battery systems with a lower evaporation rate and larger electrochemical window. Neutron scattering techniques have both the capacity to explore the fundamental structure and dynamics of these materials, and most importantly to observe their function in devices associated with new energy technologies.

#### **Situation at OPAL**

- There will soon be two SANS instruments (QUOKKA and BILBY) and one USANS instrument (KOOKABURRA) at OPAL. No single instrument will cover a wide range of Q-space, which is seen as necessary for addressing the above research priorities.
- There is currently one time-of-flight, horizontal sample, multi-purpose neutron reflectometer (PLATYPUS). It is expected that an additional neutron reflectometer primarily for magnetic samples (vertical sample and mostly likely monochromatic) will be funded and built in the existing neutron guide hall within the next 5-10 years.
- The inelastic scattering instruments that are relevant to soft matter studies are the back-scattering instrument (EMU), and the PELICAN cold-neutron time-of-flight spectrometer. These instruments are currently under construction and will commence user operation in the 2013-2014 timeframe. However, the time-scales that are accessible on the present and future inelastic scattering instruments at OPAL are not continuous. Furthermore, the lowest energy resolution available, which is on EMU (1  $\mu\text{eV}$  or 2 ns) precludes the ability to study slow dynamical processes and molecular motions at the nano- and mesoscale level. Such processes include, but are not limited to molecular rheology of polymer melts, networks and rubbers, interface fluctuations in complex fluids, polyelectrolytes, transport in polymeric electrolytes and gel systems. In biophysics, it includes the molecular dynamics of proteins and membranes.
- Current OPAL instruments are multi-purpose and not optimized for specific applications. This was important in the early stages for building the community, but it is apparent that not all needs in soft matter are covered (e.g. separating dynamics and statics in SANS, wide-Q, sub-second kinetics, focusing optics etc.). In the second guide hall there is an opportunity to build instruments that are dedicated to meeting specific needs for a more mature neutron scattering community.

- The current suite of soft matter spectrometers are heavily oversubscribed and productive instruments.
- The National Deuteration Facility contributes isotopically-labelled chemical and biological materials that are essential for studies of complex soft matter systems.
- Complementary instruments such as X-ray reflectometry and Small-Angle X-ray Scattering are present at the facility and provide additional scattering contrast and provide important tools in sample characterisation and to aid in the interpretation of neutron data.

### **The International Context**

- There will be significant growth occurring worldwide in capacity and capability of neutron sources. Several major pulsed spallation sources will have come on line. Importantly, much of this growth is in our region with new sources in China, Japan and Korea. Much of this growth is driven by the need for greater capability in soft-matter research.
- Rapid development in complementary techniques for soft matter will continue to occur (NMR, synchrotron-based techniques, cryo-electron microscopy, scanning probe microscopies, molecular dynamics simulations, etc.) both nationally and internationally. There is a need to embrace and work with these complimentary techniques, while exploring areas where neutrons are particularly well-suited.

### **Science Drivers**

- Energy technologies associated with complex soft nanostructured systems, for example bulk hetero-junction organic solar cells. In these materials phase separation is a critical characteristic, and the length scales involved are well suited to neutron scattering measurements. Future display and lighting technologies will rely on flexible, low energy, organic materials.
- Sensors, such as polymer sensors for volatile organics, thin film biosensors, in which diffusion and the interaction between analytes and sensor materials needs to be understood.
- Studies of complex biological systems rely on characterisation of soft matter. Systems of importance include: cellular membranes, protein structural biology and the interactions between proteins, enzymes and materials such as DNA. Characterisation of equilibrium structures, non-equilibrium processes and studies of molecular dynamics will be essential. Development of more physiologically relevant model platforms will also be important for studies of complex multi-component systems such as cellular membranes.
- Fibre technology for new generation textiles. A better understanding of how the properties of natural fibres relate to their structures will help with advancing new applications as well as the development of new synthetic fibres and composite materials with multi-dimensional functionality.
- Food materials are complex soft-matter systems that interact with human physiology. The global challenge of feeding a growing population needs to be addressed by innovative approaches to understanding the preparation, processing and digestion of food. In addition, understanding mechanisms of breakdown (pH, enzymatic etc.) provide increasing drivers for research. Neutrons have an important part to play in these studies.

- Advanced pharmaceutical technology increasingly relies on targeted and controlled delivery and the incorporation of multiple functionalities within one structure. Colloidal, polymeric and other nanoscale systems provide an approach to achieve such an outcome, and are ideally suited for study by neutron scattering methods.
- The application of polymers to advanced materials of industrial relevance can be greatly assisted by neutron methods; both in terms of understanding fundamental polymer structures, as well as the impact of new processing technologies. Both polymer thin-film coatings and bulk polymer systems are of importance in modifying the structures and functional properties of numerous materials. Systems may include polymers made via conventional synthetic and processing means, as well as those produced from exotic precursors or via novel methods such as plasma polymerisation or ion-implantation techniques. Fundamental studies of polymer physics and chemistry are also of importance and include processes such as: nanoscale phase separation, surface de-wetting, sensing and conducting, chemical reactions and cross-linking, aging, degradation, and anti-biofouling.
- Hierarchical materials are organized, normally on more than one size scale and are pervasive in soft matter systems. There is a need to understand how structural changes occur, for example, during processing over the entire spatial range simultaneously, and how changes to structure on specific length scales influences function of the material. Neutron methods have traditionally been strongly used at the atomic and nanoscale to investigate such materials, but have relied on optical and other methods for characterisation of the larger order structures. This often means preparing distinctly different samples of a material (for example under high dilution), and complicates analysis where one may have to take into account phenomena such as molecular crowding and concentration effects.
- Despite wood being an ancient material it is able to achieve a breathtaking range of mechanical functioning with very limited range of cell wall polymers. The anisotropic arrangements of the long fibrous crystallites of cellulose are the key to this miracle of nature. The role of texture changes in the anisotropic hygro-expansive, and mechanical properties (particularly compressive loading) of wood is reasonably well understood for single wood fibres using x-ray fibre diffraction (see below). How wood cells function co-operatively in a solid piece of wood is less well understood, and is at the core of how tree trunks may bear massive loads yet still function as conduits for water and nutrients for the tree canopy. A suitable nanoscale-diffractometer would allow the characterisation of texture and cell wall shape changes under compressive loading and/or changing humidity conditions. Not only would this provide fresh insight into nature but also to provide inspiration for new materials.
- A number of green technologies have developed around the use of ionic liquids (ILs), low melting-point salts based on charged organic ion pairs. Ionic liquids have found widespread applications as strong solvents in industrial processes, in pharmaceuticals, as electrolytes, as a heat storage and transfer medium and due to their low vapour pressure has also been used in gas handling applications. Due to their capacity to be deuterated and their role in numerous nanoscale processes, ILs are extremely well suited to study by neutron scattering methods.



## **Instrumental and technique development**

The science drivers identified above require optimised flux, achieved by designing new instruments in conjunction with advanced neutron optics including an optimised cold neutron source, next generation neutron guides, focussing optics, etc. Advanced analysis and modelling techniques are integral to ensure that the maximum benefit is derived from the new instruments.

### *New instruments or capabilities*

- A neutron reflectometer with wide Q-range, optimized for fast measurements and small samples with variable resolution. While time-of-flight methods may be suitable to achieve this, use of a continuous white-beam source, focussed optics and energy resolving detection should be explored as a means to achieve this.
- The use of multiple incident beams in a reflectometry instrument will lead to a greater Q-range being achievable in a single measurement. The potential coupling of Larmor precession techniques should also be explored as a way of obtaining additional real-space information.
- Small-angle scattering options that should be explored to cover a wide Q-range in one shot and very fast measurements include a number of innovative technologies that are currently evolving. These include: A short instrument using polarized neutrons and magnetic sextupole lenses and a large-solid-area detector; Grazing incidence SANS; Multi-pinhole options.
- Both small-angle neutron scattering and neutron reflectometry implicitly assume that all scattering events are elastic. This is certainly not the case. Methods to incorporate energy discrimination should be investigated. It should be noted that newer methods designed to enhance time resolution as far as kinetics measurements are concerned, e.g. TISANE, are based on the same premise.
- Neutron spin echo spectroscopy is now a conventional method that is currently not available in the current or future instrumental suite. Such an instrument would extend dynamics capabilities into the temporal domain of relevance to soft condensed matter.
- There is no single instrument at OPAL optimised for medium angle studies in systems where there is long range order in nanoscale materials (e.g. liquid crystals, lipid multilayers, crystalline polymers and clays). The complexity of such materials can only be probed by diffraction experiments rather than the limited resolution of conventional small angle scattering. There are major challenges in the study of liquid crystalline materials (few Bragg reflections), large lattice parameters (requiring low angle diffraction) and the low contrast between distinct chemical species (necessitating amplification by selective deuteration). Construction of a dedicated SANS-diffractometer would strongly enhance Australia's expertise in studies of nanoscale crystalline materials

### **Why is the Second Guide Hall necessary?**

- The current instruments are multi-purpose by design and further improvement in capabilities will require instruments that are focussed on specific needs.
- The development of future spectrometers (especially Small Angle Scattering instruments) typically requires large footprints that are not available within the current neutron guide hall. The current guide hall is crowded and large instruments that are normally required for soft matter research cannot be accommodated.

Development of new “white-beam” instruments and other classes of spectrometer will require many more cold neutron guide positions, particularly end-of-guide positions. Only one cold neutron end-of-guide position is available in the current guide hall and has substantial space constraints that will limit its use.

## **UNDERSTANDING BIOLOGY AT THE MOLECULAR LEVEL – UNRAVELLING BIOLOGICAL COMPLEXITY**

The application of neutron scattering to biological systems offers several unique opportunities to improve our understanding of the structure and dynamics of biomolecules in action. Neutron scattering techniques are capable of probing the length and time scales that are important in biological processes such as membrane function and the interaction of proteins and drugs with these membranes. In addition, through the use of deuteration of molecules and molecular subunits, it facilitates the determination of internal structures and interactions between multiple biomolecules.

### **National Research Priorities**

Research that improves our understanding of structural biology and the dynamics of biological systems has direct impact on a number of Australian National Research Priorities, in particular “Promoting and Maintaining Good Health” and “Frontier Technologies for Building and Transforming Australian Industries”. In relation to the National Research Priority on Health, enhanced neutron scattering capabilities will increase our understanding of the molecular basis for:

- natural (“healthy”) biological processes
- causation of disease states
- early detection of disease markers and
- identification of therapeutic targets and treatment modalities.

For example, work on the proteins and complexes associated with neurodegenerative diseases such as Parkinson’s and Alzheimer’s Diseases will have a significant impact. Likewise, neutron-enabled research into how mutations associated with genetic diseases such as Type-II Diabetes influence the structure and function of proteins are critical for the resolution of health issues of national and international significance. Neutron based study of molecular events involved in phenomena such as the replication of DNA, and the function of systems which act to maintain good health (e.g. “Chaperone” proteins which nullify abnormal proteins in the body) not only offer increased understanding of the nature and causation of disease states but offer new targets for rational drug design for both cancer and degenerative diseases.

The understanding of protein and membrane structures, and their various interactions that will result from these capabilities will be a vital part in the development of “Breakthrough Science” particularly in the fields of medical therapeutics leading to a greater understanding of disease and the development of new and unique ways for treating infectious, inherited and lifestyle based diseases. This research will also enhance Australia’s existing research strengths in Frontier Technologies areas such as biotechnology and genomics/phenomics helping to develop opportunities in the treatment and detection of disease both of which address issues within the “Building and Transforming Australian Industries” research priorities. For example, increasing sophistication in the application of neutron reflectometry, combined with deuteration, will greatly advance the study the self-assembly of thin films which mimic cell membranes. This will enable the design and characterisation of biosensors produced by the sequential assembly of single molecular layers terminated by biomolecules with ‘sensing’ capabilities – such as antibodies or enzymes which bind target

molecules. Likewise, a recent advance in the use of biotechnology to produce polymer-modified recombinant proteins (PEG- terminated proteins that have improved stability and reduced kidney elimination) for potential use against cancer is benefiting from the ability of neutron scattering techniques to characterise molecular complexes.

In addition, research into agricultural and Australian native species biology will impact within the area of Safeguarding Australia from invasive diseases and pests and in helping to generate an environmentally sustainable Australia through transforming existing industries and sustainably using Australia's biodiversity.

### **Science Drivers** ~ *Major scientific questions*

*Structural biology* has characterised over 800,000 protein structures, but proportionally, certain classes of important proteins are under-represented in these structures. Proteins found in membranes are one such class, and are of importance because membrane proteins and membrane bound receptors account for ~30% of all mammalian proteins, but represent less than 1% of determined structures. They also represent the bulk of drug targets, as they are the first point of contact between a molecule and the cell. Likewise, glycoproteins represent 50% of all eukaryotic (including human) proteins but only represent 5% of all determined structures. They are proteins modified by the attachment of sugars to peptide side chains, which leads to alteration of the charge and manner by which they interact with other proteins and include membrane-bound and cytosolic proteins. The last class is protein complexes, which are of importance as biological systems are regulated by interacting molecules. There are numerous reasons why these proteins are under-represented, but foremost are:

- difficulty in crystallising proteins that have been removed from their native state (such as membrane proteins) requiring use of solution based X-ray and neutron techniques,
- inherent flexibility in many large proteins, glycoproteins or protein complexes, making them unsuitable for crystallography

Structural characterisation of such proteins is important for understanding genetic and degenerative disease. Nuclear Magnetic Resonance Spectroscopy (NMR), a solution based technique, has been used to address some proteins in these groups. However, this technique is unsuitable for large proteins. Being able to resolve this situation is critical to furthering of the scientific understanding of the molecular basis for good health and the causation of disease states, the identification of therapeutic targets, and the design of treatment methodologies. An instructive example is where neutron science has helped to understand the role of genetic mutations that underlie inherited forms of sudden cardiac arrest that affects otherwise healthy young adults (e.g. performance athletes). Using small-angle neutron scattering and deuterium labelling, the structure of a key assembly that forms between cardiac muscle proteins (cardiac myosin binding protein-C and actin) was determined, revealing a previously unidentified interaction that provided insight of the role of cardiac myosin binding protein C and how mutations in this protein may alter its function.

*Model membranes* - the phospholipid bilayer is the basic structure of most biological membranes. The structures of native membranes are highly complex, and consist of many hundreds of individual components, including lipids, sterols, sphingolipids, and proteins. The complexity of native membranes means that there is great interest in the study of simplified model membranes, which are more amenable to manipulation than real bilayers. Typically, thus far, the vast majority of models of cell membranes have been based on bilayers of simple phospholipids. These do not represent the complexity in composition, the correct surface charge, nor possess the same physical parameters in terms of flexibility and asymmetry of the bilayer. Work is progressing towards more realistic membrane models which aim to both reproduce some of the compositional complexity and the dynamic physical properties of the natural membrane. The development of these platforms will greatly increase the relevance of membrane research and by nature are ideal targets for neutron scattering applications. The demand for scattering investigations of these systems, which when combined with deuteration can give absolute compositional profiles through the membrane separating the contributions from water, phospholipid and protein, will increase well beyond the current and future capabilities of the first guide hall.

Phospholipid bilayer formulations can be targeted towards the organism of interest, which may for example be human cells, gram-negative bacteria, etc. For example, the development of new superdrugs requires the need for new approaches to killing gram-negative bacteria in particular. Anti-bacterial peptides show great promise in this regard. Neutron Reflection is an ideal method to determine how such peptides penetrate membranes and reveal general principles of attack. The example below shows an overview of the attack of a membrane by ColicinN (an anti-bacterial protein produced by *Escherichia Coli* to kill other *E. Coli*) bacteria. This illustrates, that a simple model system without the key membrane protein is unaffected by the ColicinN but when it is incorporated that not only does the ColicinN penetrate the membrane but its shape is altered significantly which is probably the key to its mechanism.

Membrane proteins are the targets of approximately 60% of all currently available drugs, yet there is very little structural information available regarding their mode of action. Producing model membranes with integral proteins incorporated opens up new areas of study. In particular the binding of ligands, antibodies to the external protein 'surface' offers potential for the determination of low resolution structural envelopes and mechanistic insight.

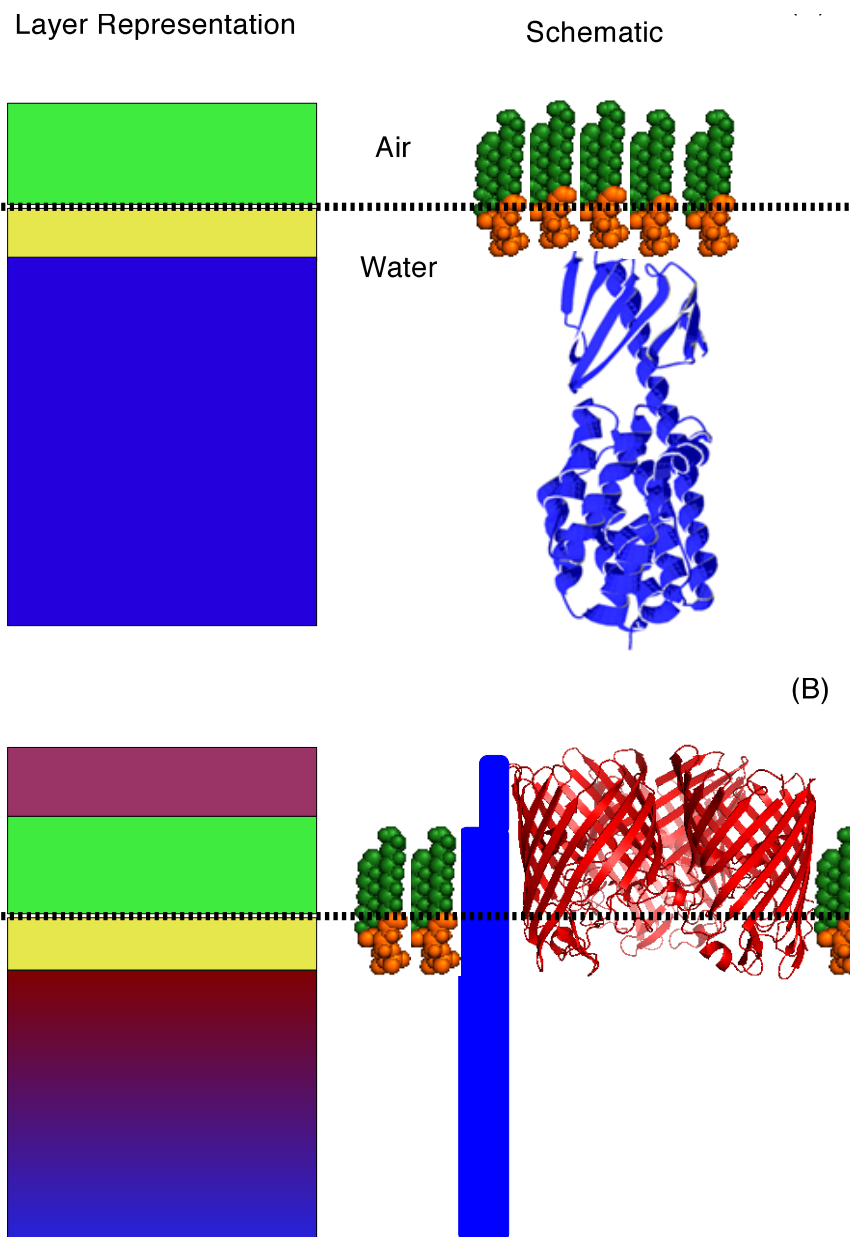


Figure 10. ColicinN – membrane interaction determined by presence of membrane protein. A) When introduced to a simple phospholipid membrane the ColicinN adsorbs underneath the membrane (i.e. outside the cell) with its crystal structure apparently retained. B) When the appropriate membrane protein is included in the simple model, the ColicinN penetrates the membrane with a significant change in shape.

*Biosensors* - The early detection of disease markers has the potential to enable early treatment intervention enabling lower cost and less invasive treatment options. Biosensors can also be applied to trace level detection of environmental pollutants. There has been a lot of functional testing/investigation of biosensors where impedance spectroscopy in particular has been used to monitor the activity of channels within membranes. There is, though, very limited structural information, especially when the sensor is 'active'. Neutron scattering through the application of reflectometry offers the potential to resolve the arrangement of the large multicomponent complexes that may form during sensor activation, see below. This offers the opportunity to rationally design the sensor surface for greatest efficiency.

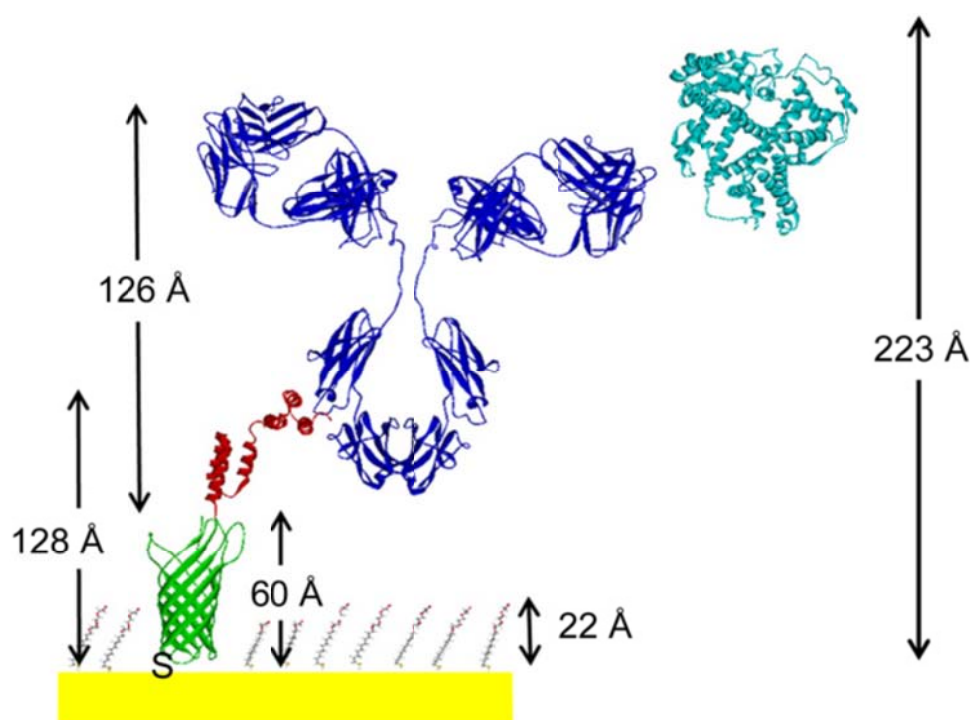


Figure 11. A cartoon representation of the structure of an antibody (IgG) based biosensor. The antibody was bound to a gold surface via an engineered membrane protein, with a standard anti-fouling molecule applied to the gold to prevent non-specific adsorption. Subsequently, Human Serum Albumin was bound from solution. Each step of this assembly process was defined *in situ* by neutron reflectometry.

Another major drive in structural biology is to move beyond the knowledge of a unique protein structure into understanding how these structures interact in a biological context. Although frequently represented as a static three dimensional structure, proteins are only functional if their structures are animated by dynamics, interconverting between many different sub-structures. It is increasingly recognised that to design effective drugs based on protein structures, their conformational flexibility must be taken into account. Protein dynamics extends over a wide range of time scales, from femtosecond to millisecond. Which motions are crucial for biological function, how the different timescales are related to one another are open questions in biology.

At present, neutron scattering enables the characterisation of protein dynamics in the picosecond to microsecond time regime. Extending the time-range to the microsecond would represent an important step in the biological scattering community, as this would enable the study of larger scale domain motions.

Characterising the complex hierarchy of protein dynamics will undoubtedly require the convergence of several techniques. Neutrons have an important role to play for several reasons:-

- the size constraints of NMR spectroscopy do not apply and larger systems, including complexes can be studied.
- the dynamics accessed by neutron scattering are directly comparable to those currently accessible by computational techniques.
- although water can be considered as a biomolecule in its own right, as the solvent of the majority of life's biological processes, relatively few techniques directly probe its dynamics. Neutron scattering enables the characterisation of water dynamics, from the hydration layer that surrounds bio-molecules to water in the whole cell

## **International**

We identified the following broad trends in biological scattering with neutrons:

- Large growth in the number of groups worldwide using neutron small-angle scattering and reflectometry to study bio-molecular interactions.
- Towards more complex realistic systems.
- Synchronising sample stimulation with data collection
- Importance of deuteration and selective deuterium-hydrogen labelling, applicable in several areas, most notably to disentangle protein subunits in complexes.
- Using focussed beams to enable smaller sample sizes.
- Increased use of inelastic neutron scattering techniques to probe protein dynamics

## **Situation at OPAL and What's Missing in Australia**

Current capabilities at OPAL supporting bioscience research mainly comprise small-angle neutron scattering (SANS) and neutron reflectometry. SANS, with subunit specific deuterium labelling and solvent contrast variation, is used to determine the component structure of complex biological molecules in physiological solutions. Neutron reflectometry reports on the structural makeup of molecular layers. Within the next two years there will be a time-of-flight spectrometer and back scattering spectrometer that will be used to report on molecular dynamics, a second SANS instrument and an ultra-small angle neutron scattering instrument. These instruments are augmented by the National Deuteration Facility, a suite of X-ray instruments, other auxiliary infrastructure for molecular and biophysical characterisation. Needs driving the construction of the 2<sup>nd</sup> Guide hall include both capacity and capability issues.

The small angle instruments currently in operation and construction are internationally competitive and expected to well serve the strong Australian structural



biology community. However, there is an apparent high, escalating demand for SANS and neutron reflectivity and these instruments are, on average, oversubscribed by a factor of 2.5 – 3.0 and increasing. Continued growth in this field would see the necessity for a further instrument of each type. The ability to work with smaller more intense beams would enable a set of experiments currently beyond the reach of current instruments. Extending the capability of neutron reflectometry with further instrumentation is crucial to enable the development and sophistication of the Australian biological community.

The current Guide Hall does not contain instrumentation supporting (a) neutron crystallography, (b) biological molecular dynamics on an appropriate time scale or (c) membrane diffraction. There are no instruments either in operation, or under construction in the southern hemisphere to perform macromolecular neutron crystallography. Neutron crystallography is valuable in the resolution of questions that can arise with X-ray crystal structures as to the position of key hydrogen atoms in biomolecules, particularly protein. In the past, this technique has not been particularly attractive to Australian researchers given the need to access appropriate instruments in the Northern hemisphere and to produce large protein crystals and subject them to long data collection times (weeks). The methodological constraints have been revolutionised by later generation instruments and the use of deuterated proteins which permits use of much smaller crystals for experiments lasting a few days.

Neutron scattering can enable the characterisation of protein dynamics in the picosecond to microsecond time regime. Instruments in operation, or under construction, in first guide hall only cover timescales up to 1 nanosecond and longer timescales are necessary to study biologically relevant dynamics. Domain motions in larger proteins or complexes on the millisecond timescale cannot be measured on the instruments currently under construction. These longer timescales are currently only accessible at few sources around the world. Extending the time-range to the microsecond by construction of a neutron-spin echo spectrometer would represent an important step in the Australian and regional biological scattering community, as this would enable the study of larger scale domain motions.

The important role of neutron diffraction in materials has been cemented by the penetrative and non-ionising nature of neutrons allowing non-destructive measurements in quite unusual sample environments, the sensitivity of neutrons to thermal motions and hydrogen bonding, and the opportunities for anisotropic studies. In biological materials, where mechanical functioning is influenced by crystal structure, alignment, texture and grain structure and these structural attributes are formed arrangements of polymers rather than atoms, the structures formed consequentially occur at large length-scales, and the role of thermal motions is quite different. Examples of these materials include silk and cellulose, materials which have been used since antiquity. A demand for new environmentally friendly materials drives quest to new applications, and the rise of biotechnology offers opportunities for new production methods. Neutron diffraction, and advances from the National Deuteration Facility in the production of deuterated biopolymers, would give novel insight into materials formed by these polymers.

Many biological systems contain order which is important in its biological context and eventual technological use on length scales that is not accessible by a single

instrument on our current instrumentation. In particular SANS instruments, while they may cover most of the required length-scales, are optimised for reconstructing shape of isolated biological molecules or complexes. Some examples of such systems may include thylakoid membranes and their potential to harvest light into electricity, ordered chitin phases in insect wings which are biophotonic devices and exotic non-lamellar bilayer phases which are found in cells under stress and very specialised mammalian sensory cells where there is an extremely high surface area and partitioning between two different phases. In the latter case the general physical properties of the system allow the control of complex physical and chemical processes which may be used to crystallise membrane proteins, design novel drug delivery systems and synthetic self-assembled systems which mimic useful life processes. These systems are all condensed soft-matter where knowledge about the periodic arrangements of many molecules acting co-operatively is critical. While x-ray scattering studies provide routine characterisation important gaps may be filled in by the use of molecular deuteration and medium angle neutron diffraction.

Currently the use of neutron based membrane diffraction enables higher resolution characterisation of the interaction of small to large molecules with model and real biological membranes than is possible with other techniques. There are two instruments in the world suitable to characterise simple one dimensional system – membrane bilayers. Examples of the use of such instruments include the interactions of peptides with membranes, characterisation of structure of the light powered ion pump in the bacterial purple membrane and the elucidation of the interactions of sugar molecules with membranes important in cryo- and anhydro- biology. These current instruments are limited in the range of length-scales they examine, and importantly because of the limited solid angle they cover, are best suited for the lamellar systems. The use of neutron based medium angle diffraction with a large solid angle enables science to examine more complex biological and biomimetic systems.

## **Instrumentation and technique development**

### **What's new?**

The major advances in instrumentation are related to: neutron guides, which make use of more efficient and tuneable neutron transport than current neutron guide technology; neutron optics, allowing the focusing of a neutron beam to a smaller size, facilitating the use of smaller samples; detector advances that will facilitate the high neutron count rates arising from smaller, more intense neutron beams. The enabling of techniques such as neutron spin echo spectroscopy will be the first of its kind in the Australasia region, answering fundamental questions regarding bio-macromolecular systems biology.

### **Why is the Second Guide Hall Necessary and Recommendations**

Research in the biological sciences, by its very nature, necessitates the use of diverse experimental techniques to probe often highly complex systems. As a source of cold neutrons, OPAL provides neutron scattering and spectroscopic techniques to advance the frontiers in biological research. The applications span fundamental, medical and health fields as well as primary industry, biotechnology nanotechnology, providing unique and otherwise inaccessible insights into systems biology and biological processes unobtainable using traditional non-neutron based approaches.

The section above highlights there are a number of capability and capacity issues that need to be met in order to optimise the contribution of neutron scattering at OPAL to the Bioscience community. This can be realised via the development of state-of-the-art facilities in the second neutron guide hall at OPAL. There is a unique opportunity to develop an integrated biological-user platform to service the needs of the biological user community across Australia and the Asia Pacific region as well as to capitalise on the Australian Government's already extant, and significant, scientific infrastructure investments at ANSTO and at the Australian Synchrotron (e.g., to complement the MX-crystallography, SAXS and infrared beam lines.)

There are four key instrument requirements to close the 'methodological loop', to meet the ever-increasing demand for neutron-based biological neutron research at OPAL and to meet the need for the ability to analyse smaller quantities of precious/difficult to produce biological material:

- **Neutron spin-echo spectroscopy** – for the analysis of biomacromolecular dynamics on timescales within the 'biomacromolecular regime' that are not accessible by time-of-flight or back-scattering techniques (e.g., for targeting disordered/flexible systems underpinning a number of neurodegenerative disorders, characterising domain motions in larger systems)
- **Neutron spin-echo reflectometry** – for the analysis of biomacromolecular deposition on non-ideal surfaces (e.g., fundamental membrane science, understanding fat deposition mechanisms and how to disrupt deposition on artificial arteries; biosensor development)
- **Neutron biomacromolecular diffraction** – 1D, 2D and 3D high-resolution studies for high-resolution atomic-level analysis (e.g., rational design of drugs and therapeutics).
- **Biological Small-angle neutron scattering** – for the analysis of biomacromolecular shapes including higher-order complexes and assemblies in solutions mimicking 'in situ' environments (e.g., identification of key molecular interfaces for drug targets; the controlled polymerization / depolymerization of biosynthetic materials for artificial tissue replacement; bone, skin, extracellular matrix, etc.)

The successful implementation of these techniques as applied to biological systems will depend on catering to the limitations that nearly all biological suffer from - material availability. The drive to work with smaller quantities or concentrations of difficult/expensive to produce molecules can potentially be met by hardware performance enhancements. This requires a sophisticated multi-factorial approach in the total concept design of the new OPAL guide hall and its instruments, incorporating:-

- A reliable and stable **cold source** for the generation of cold neutrons of wavelengths appropriate for biomacromolecular investigations.
- New generation **neutron guides** designed to reduce background noise.

- New generation **focussing optics** to increase neutron flux per unit beam area for focussing onto small sample environments.
- New generation **detectors** incorporating small pixel size, low background, and high count rates/response times.
- New generation **magnets and flippers** for neutron polarization based instruments (specifically for spin echo based techniques.)
- New **sample cell and sample-stage designs** for temperature, ionic strength and pH control and kinetic investigations (that become accessible if flux and signal-to-noise ratios are optimised.)
- Seamless cross-platform **sample-preparation techniques** (e.g., as serviced by developments at the NDF; yeast and mammalian expression systems); new user-driven data reduction, analysis and modelling **software/techniques** (designed in consultation with the user community.)

#### *Parallel Requirements*

A two-fold approach is required where neutron instrument technology advances the drive to do more with less material, ie enabling use of smaller sample size, and new systems are developed for production of the deuterium labelled form of these proteins. Small-angle neutron scattering coupled with advances in guide technology, optics and detector design will make currently unfeasible research possible, and opens up a range of new possibilities in biological research. This should be accompanied by the development of new (biotech-based) protein expression systems capable of producing sufficient quantities of deuterium labelled glycosylated proteins, and insoluble membrane proteins, to enable structure/function investigations. This requires the establishment of a cell culture facility for growth in heavy water, augmenting current capabilities at the National Deuteration Facility based at ANSTO.

#### **Leveraging the Australian Synchrotron Facility**

Much of the bioscience work undertaken currently at the Australian Synchrotron (X-ray crystallography, small-angle X-ray scattering, infra-red spectroscopy) would benefit strongly from complimentary structural information available from neutron scattering. But at present, neutron scattering is not feasible on many of these systems due to the requirement for large samples. A second guide hall implementing advances in neutron guides, optics and detector design would better leverage the Australian Government's investment in the Australian Synchrotron. As it would be expected that growth of interest in small-angle scattering will track with usage of the small-angle X-ray scattering beam line at the Australian Synchrotron, there will be an increasing number of researchers interested in the use of neutron scattering, creating ever increasing demand that will exceed the expected capacity of the current guide hall within the next decade.

## EARTH SCIENCES



Fig. 12 The Fimiston Open Pit is Australia's largest open-cut gold mine. It produces about 28 tonnes of gold per year, and is located off the Goldfields Highway on the south-east edge of Kalgoorlie, Western Australia. Original photograph taken by Brian Voon Yee Yap and downloaded from Wikipedia.

Increasing population is straining our ecosystem and putting the sustainability of life on Earth in doubt. As the population increases more resources are needed to support our way of life, people live in less viable places and the byproduct of human activity, pollution, increases. Earth Scientists work to provide a scientific basis for improved sustainability. An understanding of the structure, stratigraphy and chemical composition of the Earth's crust helps us to locate resources and to efficiently extract them. Understanding the forces in the crust and the natural processes on the surface of the Earth allows us to anticipate and possibly mitigate natural disasters such as earthquakes and volcanic eruptions. Understanding the impact on the environment of poor mineral extraction and waste disposal methods allows us to design more benign processes for the future and mitigate existing problems. Processes on the surface of the Earth are intimately linked to the structure and dynamics of the Earth's mantle. Understanding the solid Earth is an essential prerequisite to understanding and controlling processes at the surface.

Neutron scattering has an important role to play in this scientific process. Water and other light elements play a crucial role in controlling the structure and stability of minerals. For example, we believe that the dehydration of hydrous minerals in subduction zones leads to seismic activity. Understanding the role of water in rocks is essential for us to be able to understand the origins of Earthquakes and maybe

mitigate them in the future. Melting of rocks to form magmas leads to volcanic eruptions. Understanding the structure and dynamics of melts is an important step toward understanding the origins of volcanic eruptions and improving predictive methods. The first product formed when CO<sub>2</sub> is sequestered in rock formations under the ocean is amorphous calcium carbonate. We need to understand the long term properties of this material in order to validate this method of sequestration. The high degree of disorder, lightness of the elements and presence of water make this difficult using x-rays. Valuable minerals can be concentrated in the Earth hydrothermally. We need to understand this process to be better able to predict mineral location and improve extraction methods. Neutron scattering has a key role to play in all of these areas.

New tools are required to allow us to study Earth processes. We need to be able to study Earth materials at the pressure and temperatures of the upper mantle while controlling composition, volatile content and strain. Suitable multi-anvil high pressure-temperature devices exist but require high intensity, small beams of short wavelength neutrons which are currently not available. Developing a suitable neutron source, optics and detector system to enable this work will lead to major advances in our understanding of the Earth's structure and dynamics and directly contribute to improving the sustainability of life on Earth.

## Minerals in Earth's mantle

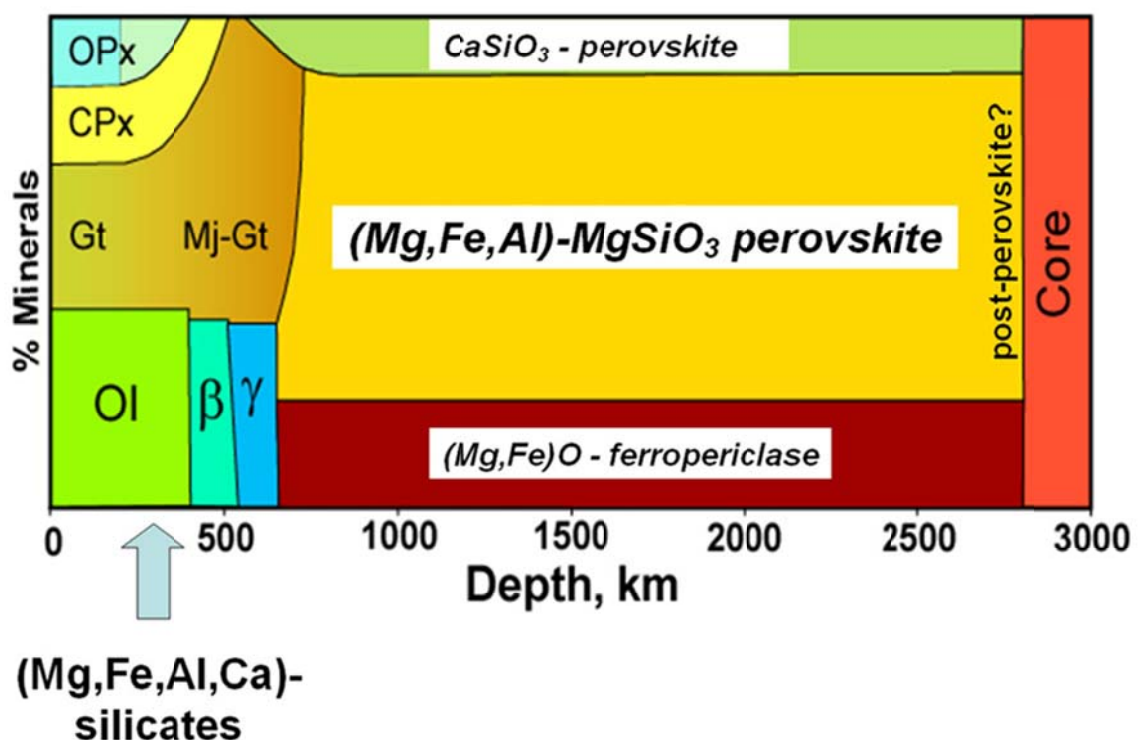


Fig. 13 The mineralogical composition of the Earth. The percentage composition of mineral phases is shown as a function of depth in the Earth. Ol denotes Olivine, Gt: garnet, CPx Clino-Pyroxene and OPx: Ortho-Pyroxene. Downloaded from the Salt Mash Image Library.

## **A REACTOR-BASED POSITRON BEAM FOR AUSTRALIA**

Positron experiments are a growing field of research, with applications to fundamental and biological research and materials analysis. Most activities throughout the world are currently based around radioactive isotope sources of positrons, predominantly  $^{22}\text{Na}$ . Most applications of positrons centre around their annihilation with their matter counterpart the electron, producing (typically) two gamma rays with energies of 511 keV, the rest mass energy of the electron/positron.

Positrons are used in biomedical science (Positron Emission Tomography) as a cancer and metabolic diagnostic, and in materials science as probe of open space and porosity in soft materials (such as polymers), defect distributions in metals (such as radiation damage in reactor pressure vessels) and semiconductors, and for atomic-scale surface studies. In atomic and molecular physics, understanding positron interactions with matter has been a goal for atomic and molecular physicists for decades, in addition new high intensity sources around the world are opening up possibilities for fundamental research into exotic quantum systems such as Ps (positronium – a bound state of a positron and an electron) and  $\text{Ps}^-$  (a positronium negative ion - made up of a positron bound to two electrons), their spectroscopy and interactions.

Currently there is a strong and growing community of researchers in Australia performing positron based research, based entirely around the use of  $^{22}\text{Na}$  isotopes as the source of positrons. These facilities service a cohort of approximately 15 research groups across the country in the areas of fundamental physics, bioscience and materials science. This number is increasing and we anticipate that it will grow to more than 50 research groups in the coming years. A significant component of this growth will be external users in the field of positron based materials analysis. In addition, there is strong engagement with the international research community in all these fields, with a similar number of groups interacting with the Australian community.

There is presently no positron source based at the OPAL reactor. However, a reactor based source has the potential for a substantial increase in the positron intensity compared to a radioisotope source (a factor of more than 100 is achievable), which consequently will increase the range (and accuracy) of the science and applications able to be undertaken. In some areas, this research will be a complement to the research already undertaken at the reactor, based around neutron scattering and other neutron techniques.

While the key driver of this initiative is the increase in positron flux, a further important consideration in support of a reactor based facility is the nature of the supply of  $^{22}\text{Na}$ , in sealed sources, for radioactive isotope based experiments. Currently there is a single world supplier of these sources and this presents a considerable risk.

### **Science drivers**

#### **Fundamental Science**

A broad case for fundamental science at the OPAL reactor is provided in a separate section (below) of this report. Here we present a more detailed overview of positron-

based fundamental studies that would be conducted at a reactor based positron facility. Currently, within the Australian positron community we have developed considerable expertise in the fundamental studies of positron interactions with single atoms and molecules (in the gas phase). The development of a new positron beam at OPAL will allow us to build on this existing core of activities and substantially increase both the quality and range of research in this area. High precision measurements of single positron scattering give us a strict test of quantum mechanical theories of particle interactions, and allow us to develop our understanding of the charge particle scattering problem. Some examples (by no means complete) of current areas of research which will be substantially enhanced by the availability of a more intense positron source include

- **Low-energy scattering benchmarks**

This incorporates the establishment of high precision cross section “standards”, which will provide a stringent test of the most advance theoretical calculations. They are also important for several of the subsequent applications of positrons in biomedical science.

- **Positron bound states**

Positrons are predicted to form bound states with some atoms and molecules, a novel quantum mechanical system which has been very difficult to target experimentally – partly due to the low flux of existing positron beam sources. The understanding and potential to manipulate such bound states would have profound implications for applications of positrons in materials and bioscience.

New areas of study which will be opened up by the availability of an intense positron source include

- **Cold positronium beams**

Controlled-energy positronium beams, particularly at low energies, have typically been very difficult to produce, but the few experiments that have been performed have found very interesting effects in positronium scattering from atoms, molecules and surfaces.

- **The study of  $\text{Ps}^-$**

$\text{Ps}^-$  is a bound state system comprising two electrons bound to a positron. As a three-body, charged-particle bound system, with all particles of the same mass, it provides an interesting test bed for fundamental quantum electron dynamics, including studies of the spectroscopy of such a system.

## **Materials Science**

Positrons can be used to address a range of materials research questions. Two of the more commonly used techniques, which would form the basis of research at a new positron beam facility, are outlined below. There are other positron based experiments that could also be incorporated to enhance a program of research in this area.

- **Positron-Annihilation Lifetime Spectroscopy (PALS)**

This technique is used to measure nano-scale free volume and defects in materials. Pulsed positron bunches are injected into materials at varying energies, where they thermalise and annihilate, resulting in the emission of two back-to-back 511keV



gamma rays. Before annihilation, the positrons diffuse to defect sites where they can be trapped and annihilate. The annihilation gammas are subsequently detected by fast scintillators, and the lifetime and intensity of the decay spectrum that are measured reflect the size and distribution of the open space in a material. PALS is applied to many different types of materials, from porous polymeric materials to silica, clays, semiconductors and metals. Control of the beam implantation energy allows for the control of the depth of penetration into the material, making it ideal for the study of layered materials and thin films.

A new PALS facility based on an intense positron source would provide significant new opportunities for this area of research. In particular, the possibility of focussing positrons to a sub-millimetre spot would allow the mapping of a sample in all three spatial dimensions, a potentially valuable tool for many applications.

- **Coincident Doppler Broadening Spectroscopy**

This technique, which involves the coincident detection and energy analysis of annihilation gamma rays, directly samples electron momentum distributions in the target material, allowing determination of electronic defect profiles. Again, a variable energy positron beam is injected into the sample where it thermalises, diffuses to defect sites, and annihilates. In this case, the energy of the annihilation gamma rays is analysed, to determine any Doppler shift from 511 keV, due to the momentum of the annihilating electron. As a result, it is extremely sensitive to local variations in electron distributions and can provide information about the chemical environment of the annihilation site. An example of such a measurement is shown in figure xx below.

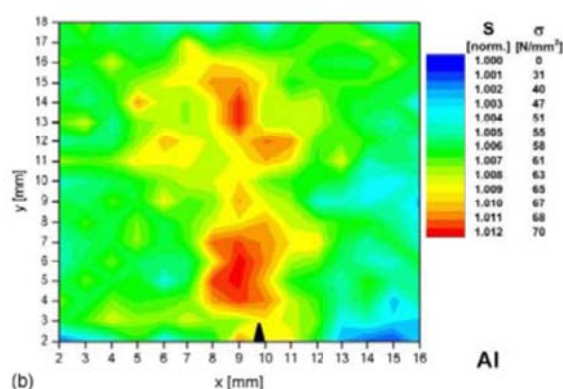


Fig. 14 Mapping of defects due to stress induced in an aluminium sample

- **Complementary neutron-based research**

There exists a high degree of complementarity in scientific applications of positron beam methods with neutron scattering. These are most obvious in structural studies of metallic and polymer based systems, where scattering methods such as neutron diffraction and small angle neutron scattering (SANS) are highly valued for their ability to provide the average atomic or molecular structure. However quite often, particularly in nanoscience, physical and chemical behaviour relates more to the local distributions that characterise departure from average. This is where positron methods can provide independent information on local order, particularly near surfaces. Such information is both valuable and complementary techniques such as neutron diffuse scattering and X-ray absorption spectroscopy.

## **Bioscience**

Positrons are a key component of Positron Emission Tomography (PET) – a widely used diagnostic for cancer. A PET scan involves the injection of a positron emitting radio-isotope into the body, usually complexed to a ‘carrier’ molecule that confers biological specificity. The carrier molecule selectively attaches to sites that are of concern (e.g., a tumour). A positron emitted at these sites with very high initial energy (~300 keV) must thermalise to energy below about 100 eV, before pairing with an electron and annihilating to produce two gamma rays. Gamma rays are imaged using sensitive detectors and sophisticated computer software, to give high-resolution images of the uptake site, facilitating diagnosis and treatment.

Although PET is a mature technology, little is known about the reactions of high-energy positrons as they thermalise in the body, or the rates for Ps formation prior to annihilation. By understanding these reactions we may revolutionize the role of PET in medical diagnostics and therapy. A key goal of research in this area is to conduct fundamental studies of the interactions of positrons with biological molecules, with a view to development of a superior dosimetry model for PET. Positron trajectories provide a view of thermalisation processes that could potentially underpin medical diagnostics and therapy.

- **Positron scattering from biological molecules**

Accurate cross section measurements for scattering of positrons from simple atoms to complex biomolecules can be being used as important, basic information for Monte Carlo models of positron transport in soft tissue.

- **Positron dose in liquids and soft matter**

By extracting an intense, controllable beam of positrons from the vacuum environment and injecting it into biological or liquid samples, it will be possible to compare dose calculations with experimental data. Such verification is critical to test the validity of dose and transport models and to improve our understanding of the underlying positron interactions with such systems.

## **Society and technology relevance**

There are clear and important examples of relevance of positron science to society and technological development. These are outlined in the science case above but in summary they impact on

- Materials science and the development of new and novel materials
- Bioscience and implications for a better understanding of the use and efficacy of positrons in PET diagnostics
- New instrumentation and techniques and their implications for breakthrough science and technology

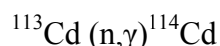
## **Instrumentation and technique development**

The positron community in Australia currently operates a number of radioisotope-based positron beam facilities. The two major beam line facilities based at the ANU are used for atomic, molecular and bioscience studies (low energy), and materials research (high energy). They both use 50 mCi <sup>22</sup>Na radioactive sources.

### Proposed Technology

An alternative production mechanism for positrons is pair production, whereby high-energy gamma rays are converted into electron-positron pairs upon impact with a heavy metal target. A useful means of producing high-energy gamma rays is via neutron absorption by an isotope such as  $^{113}\text{Cd}$ , which has an extremely large neutron absorption cross section.

Neutrons are produced in copious quantities in reactors such as OPAL and thus provide an efficient way of producing large numbers of positrons. In the following reaction:



more than 9 MeV is released in the form of gamma rays and, on average, 2-3 of these have energies in excess of 1.5 MeV. Absorption of these gammas by a platinum converter, or another refractory metal, produces positrons via pair production. Based on experience at the FRM-II reactor in Munich, we estimate that moderated positron fluxes of more than 100 times that of a high activity  $^{22}\text{Na}$  source could be produced at OPAL, with potential for even higher fluxes with improvements in technology. The design for the Munich source is shown in figure xx.

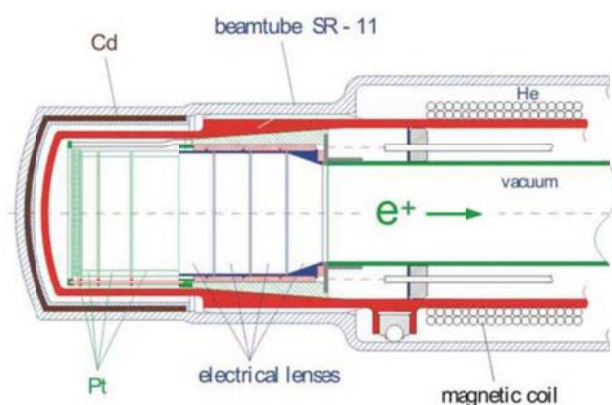


Figure 15: Schematic of the FRM-II positron source

In such an arrangement, the cadmium and platinum converters would be located inside the  $\text{D}_2\text{O}$  reflector vessel and the liberated positrons would be extracted and guided with electrostatic and magnetic fields beyond the biological shield of the reactor through a single beam line.

Primary factors driving the choice of source location at a research reactor include; thermal neutron flux ( $1-2 \times 10^{14} \text{ n/cm}^2/\text{s}$  is required), competition for the source location for other applications and source maintenance issues (such as stability of electromagnetic environment and replacement timelines). Installation of a converter using an enriched source of  $^{113}\text{Cd}$ , which is present only at the 12% level in natural Cd, would prolong the source lifetime to around 25 years.

### Potential Source Location

Several potential locations have been identified for such a source within the reactor. One possibility is to locate the source above the position currently allocated to a potential hot neutron source. Another possibility is to locate the positron source within one of the pneumatic tubes. Due to the ability to easily guide the positrons

with electric and magnetic fields, these locations can also be compatible with any other future developments for neutron beamlines within the reactor, without compromising the performance of either the positron or neutron facilities. Other suitable locations may also be possible.

### **The Instrument Facility**

While the family of research instruments that could be served by such a positron beamline is quite diverse, our choices would reflect the Australian research environment, so that for example fundamental studies, nano- and nuclear materials assessment and medical applications may take prominence.

We envisage 4-5 instruments being serviced in a switched nature by this beamline. A possible suite of experimental endstations may include:

- Positron Annihilation Lifetime Spectroscopy
- Coincident Doppler Broadening Spectroscopy
- Positronium Beams and Spectroscopy
- Atomic and Biomedical physics/chemistry
- A micro-focused positron beam

Efficient transport of positrons over relatively large distances (10's of metres) is possible, so that a positron instrument facility could be located at a position that is convenient for the overall development of the second Guide Hall, including for example, on a mezzanine floor. The footprint of the research facility is likely to cover an area of  $\sim 100 - 150 \text{ m}^2$ .

## **Nuclear/Particle/Astrophysics**

Measurements using cold and thermal neutrons address important scientific questions in nuclear physics, particle physics and astrophysics. Ongoing experiments search for new sources of time-reversal violation, test the electroweak theory through neutron decay and neutron weak interactions, provide important parameters for Big-Bang theory, and illustrate fundamental concepts in quantum mechanics. These experiments are now pursued at many neutron sources in North America, Europe, and Japan. Measurements using intense positron beams are useful for several investigations outside of condensed matter/materials science. Such a source has recently been commissioned at the FRM-II reactor in Munich. There is an existing active positron research community in Australia and we recommend the provision of special facilities to support this area of inquiry.

### **Scientific Opportunities:**

#### With neutrons:

Measurements of neutron electric dipole moment, neutron decay, neutron weak interactions, tests of quantum mechanics, etc. continue at various facilities, and we can guess that many of the scientific issues are likely to be resolved or addressed over the timescale of the next decade in many ongoing experiments. What can be done beyond this?

It is inevitable that new scientific questions will open on the timescale of a decade that cannot be anticipated. Our best guess now is that we expect new scientific opportunities in the next decade to more strongly emphasize questions whose roots lie mainly in cosmology/astrophysics. Examples of scientific opportunities which we feel are likely to still be interesting and unsolved in a decade include (but are not limited to):

- (1) Searches for weakly coupled forces of mesoscopic range from millimeters to microns (addresses predictions of string theories, ideas of compact extra dimensions in spacetime, symmetry breaking in weakly-coupled theories beyond Standard Model on a length scale associated with dark energy). In this case the potential advantage for ANSTO in this field can come from the availability of polarized neutrons coupled to a flexible policy to allow the possibility to use a scattering instrument for these purposes.
- (2) Search for baryon number violation through neutron-antineutron oscillations (addresses question of the baryon asymmetry of the universe, even a null result at achievable sensitivity has important cosmological implications). In this case the potential advantage of ANSTO would come from the green-field nature of the site (no existing intense neutron source has space for this experiment), the intensity of the cold neutron source, and the possibility to take advantage of the strong progress in supermirror neutron optics to extract more of the neutron phase space from the moderator. However it is clear that any such experiment would represent a major operation that would need significant international participation.

Brief scientific justifications for these ideas with more detail can be found at the end of this report (if required).

#### With positrons:

The advantage of a positron source at ANSTO comes from the very intense source strength possible coupled with the relatively small number of such intense sources worldwide. Such a source, based for example on the FRM-II design, can increase positron beam intensities available for research in Australia by two orders of magnitude and enable high-precision experiments of interest to tests of quantum electrodynamics (including positronium spectroscopy), precision tests of theories of three-body physics, new investigations in plasma physics, etc. in addition to their other numerous applications discussed in other sections of this report.

#### Source/Beam:

Intense cold neutron beams are needed for this area of physics. Slow neutrons allow longer observation times in an apparatus and can be manipulated more easily using neutron optical components and external fields, as often required for experiments which search for small asymmetries.

Apart from low neutron velocities, long observation times also imply longer flight paths i.e. long apparatus lengths. In this context, it is therefore desirable to preserve the possibility of a very long beam tube possibly extending to a hundred metres or more on the South side of OPAL.

Furthermore, typically experiments in this field require long measurement times (of order  $\sim 1$  year or more) and an often an end position on a guide.

Since the brightness of neutron sources are unlikely to increase, advances in neutron optics and polarization techniques are essential to make new experiments in nuclear/particle astrophysics possible. This technology is expected to continue its rapid improvements over the next decade and we will rely upon this advance to conduct new/better experiments in the future.

#### Instrumentation:

The searches for new weakly-coupled forces of nature with mesoscopic ranges can be conducted in principle using neutron scattering instruments with polarized neutrons. The question is whether or not the required amount of time for slightly nonstandard experiments of this type can be accommodated within the usual proposal system at a neutron scattering facility. ANSTO could possess an advantage relative to other facilities if it adopts flexibility in the consideration of such nonstandard uses of their polarized neutron scattering spectrometers.

Many experiments in the field of nuclear/particle/astrophysics with neutrons are highly sensitive to external magnetic fields. This is also an issue for spin-echo spectrometers. Some neutron facilities are starting to enforce stray magnetic field policies that require instruments to limit the magnitude of the magnetic fields that is allowed to extend into other instrument spaces. Adoption of such a policy at ANSTO

could be very important for preserving future instrumentation possibilities. Similarly, construction of instrument structures out of non-magnetic materials (e.g. aluminium instead of steel) should be given consideration.

### **Physics motivation to search for new weakly-coupled forces of nature using slow neutrons**

The possible existence of new weak forces of nature with ranges of mesoscopic scale (nanometers to millimeters) is attracting increased scientific attention. We still tell our students that there are four fundamental forces of nature: gravitation, electromagnetism, and the strong nuclear and weak subnuclear forces. However there is increasing suspicion that four may not be enough. Neither dark matter nor dark energy, hypothesized to pervade space in order to explain the apparent mass distributions of galaxies and the observed expansion of the universe, were anticipated by the current leading theories of matter and forces. These completely new sources of matter and energy, inferred from astrophysical observations and cosmological models, also call into question the long-term relevance of past intellectual and experimental strategies for discovering new fundamental interactions: perhaps physicists have been looking in the wrong places for new forces. Dimensional analysis applied to the mysterious dark energy of the universe seems to point to a length scale on the order of tens of microns, which corresponds to a regime in which we thought all was understood. New forces of nature must be very weak compared to the known forces at length scales above a millimeter, but they can be quite strong (at least compared to gravity) below this range.

Such possible new forces (especially those which couple to the spin of nucleons) are still poorly constrained by existing experiments. We propose to conduct sensitive searches for possible new forces that couple to the spin of neutrons. The same properties of neutrons which make them useful for probing condensed matter (coherent interaction with macroscopic amounts of matter, delicate manipulation of polarization, zero electric charge and low electric polarizability, access to a large dynamic range of length scales using scattering) also make them well-suited for searches for possible new spin-dependent interactions with nucleons in the regime of interest. The mathematical form of the possible interactions among protons, neutrons, and electrons with aligned spins and its possible dependence on spin, momentum, and distance are understood from general principles of relativity and quantum mechanics, but the strengths of such forces depend on theoretical details and can be very weak. Not all of the known particles feel all of the known forces and the same might be true for the new spin-dependent forces we propose to investigate. Most of the experiments which have been performed to search for such interactions are sensitive to force ranges  $\lambda > 1$  cm. Our goal is to search at much smaller distance ranges. Already reanalysis of past neutron measurements shows that they produce the best upper limits on possible new spin-independent interactions of nucleons at submicron distances. Constraints on spin-dependent interactions are much less stringent. These experiments could be conducted in principle using polarized neutron scattering spectrometers.

## The Physics of Neutron-Antineutron Oscillations

An observation of neutron-antineutron oscillations would constitute a discovery of fundamental importance for cosmology and particle physics. The direct experimental upper bound on the electric charge of the neutron is so stringent ( $q_n < 10^{-21}e$ ) that few physicists doubt that the neutron is electrically neutral, and no general principle of physics forbids an electrically neutral particle from transforming into its antiparticle. Such oscillations of electrically neutral particles into other states are no longer a surprising phenomenon. The observation of oscillations in these systems (neutrinos, Kaons, B mesons) continue to teach us about delicate aspects of physics (lepton number violation, CP/T violation, neutrino mass and mixing) which are not accessible using less sensitive techniques. It is therefore not unreasonable to expect that a search for oscillations in the neutron, a neutral baryon which is sufficiently long-lived to conduct a sensitive search, may uncover new processes in nature.

The search for neutron-antineutron oscillations addresses the question of the generation of the matter-antimatter asymmetry of the universe, one of the great mysteries of cosmology. A discovery of this process would prove that all nuclei are ultimately unstable. It would provide the first experimental evidence for baryon number violation, which is required to explain the observed baryon asymmetry of the universe (baryogenesis) according to inflationary cosmology, which sets B to zero in the very early universe. Since B and L are “accidental” symmetries at the perturbative level in the Standard Model there is no known fundamental reason why they should be conserved. Improved experimental bounds on B and L non-conservation will probe an energy scale corresponding to the electroweak phase transition in the early universe, a process which erases any B asymmetry generated earlier in time through thermally-activated nonperturbative electroweak gauge field configurations called sphalerons. Since this process violates B and L but conserves B-L, it introduces a fundamental division between possible baryogenesis mechanisms and makes most proposed modes for proton decay ineffective for baryogenesis. The changes required for  $n$ - $\bar{n}$  oscillations ( $\Delta B=2, \Delta L=0$ ) relates neutron-antineutron oscillations to neutrino-less double beta decay ( $\Delta B=0, \Delta L=2$ ) and the physics of B-L symmetry breaking and neutrino mass generation in several theories beyond the standard model which unify quarks and leptons, and its discovery would change completely our thinking of how forces might be unified at high energy scales. The experimental signature of antineutron annihilation in matter is spectacular enough that a “background free” experiment using free neutrons is possible, and a rigorous control experiment exists for any positive observation since the effect can be turned off by a very small change in the experiment’s ambient magnetic field. If no effect is seen at the sensitivities which can now be achieved experimentally we will at least strongly constrain (and possibly in combination with future experiments at the Large Hadron Collider and elsewhere eliminate) the possibility of B violation below the electroweak phase transition. By eliminating this possibility even a null experiment would make progress on a very fundamental question in cosmology and lend stronger support to the currently-popular theoretical scenario for generation of the baryon asymmetry (leptogenesis) which is the main intellectual motivation for large neutrino beam experiments for search for CP violation in neutrino oscillations. A null result would also set the most stringent constraint on the stability of nuclei.



The present direct limit on free neutron oscillation probability was established in 1991 in an experiment at the ILL using cold neutrons. This result has been marginally improved since that time by looking for antineutron conversion within the nuclei contained in large detectors designed primarily for neutrino observatories and proton decay and using theoretical calculations for antineutron interaction in nuclei. These indirect experimental techniques, however, have now reached an irreducibly background-limited regime from atmospheric neutrinos that now makes “discovery” through this technique very difficult, and also the theoretical calculation of antineutron conversion in nuclei may possess important uncertainties. Extensive developments in neutron optics over the last two decades now provide promising avenues to greatly improve upon the upper bound set at the ILL by a few orders of magnitude. Realizing these gains in sensitivity is impossible at existing neutron sources due to space constraints.

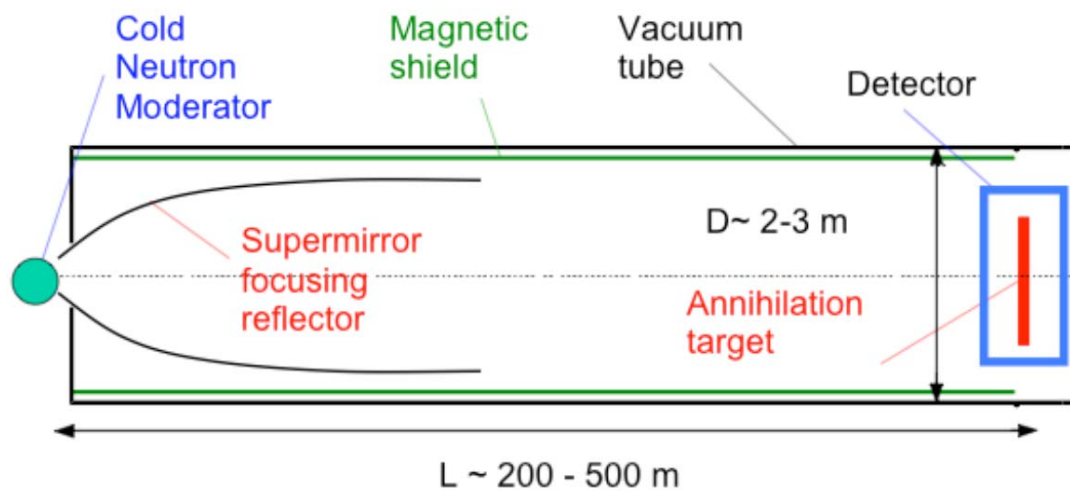


Fig. 16 Schematic of a possible experimental configuration for a new neutron-antineutron oscillation experiment at OPAL

In addition to these improvements in neutron hardware, recent theoretical work has increased the importance of the  $\Delta B=2$  channel for understanding baryogenesis. This work has shown that proton decay is not directly connected to baryogenesis and that any B asymmetry generated at the grand unification scale is likely to be erased at the electroweak phase transition. Many new theoretical ideas accommodate neutron-antineutron oscillations without proton decay. Rapid experimental advances in neutrino physics continue to support the strong theoretical suspicion that neutrinos are Majorana particles, which directly connects neutrino mass generation and neutron-antineutron oscillations in many quark-lepton unification models. Improvements in experimental constraints on supersymmetry from indirect experiments and now the LHC are starting to exert strong pressure on supersymmetry, thereby calling into question the relevance of much previous theoretical work on B violation. The theoretical landscape has therefore changed qualitatively since the previous experiment on neutron-antineutron oscillations.

## EDUCATION

Neutron scattering, science and technology is at the forefront of what is scientifically and technically feasible. Students, engineers and technicians who participate in neutron related activities will often be far ahead compared to their peers, because of the cutting-edge technology in use. This community should not only be proud to educate the next generation of university professors: nine out of ten of our students may end up in industry, banking or government jobs and their future impact on the economy will certainly be well above average.

ANSTO should consider making available a neutron beam for the use of tertiary students in Australia for education, as an undergraduate lab exercise (to measure Planck's constant, for example). History shows that many neutron instrument scientists gained their first knowledge of the field from an experience at the undergraduate level (for example in the late Cliff Schull's lab at the MIT reactor). The possibilities for such experiences at the student's home institution are becoming rarer with time, but it is not hard for Australian students to get to ANSTO. A simple measurement apparatus for such purposes could be implemented at ANSTO (perhaps as a movable setup, accommodating other instrument(s)).

## **HOT AND COLD SOURCES**

Hot and cold sources have been used throughout the world in research reactors to modify the neutron energy spectrum available in the reactor to higher or lower energies. The enhanced neutron spectra obtained allow access to a whole range of new experiments and solutions to new scientific and technological endeavours.

OPAL is a multipurpose research reactor with two thermal beams, two cold beams with a cold neutron source and a designated hot beam without a hot source (effectively another thermal beam). The design allows for a future hot source with provision for the installation and an existing dedicated hot beam with twin independent shutters for two reactor face instruments.

There are three reactor based hot sources in the world all situated in Europe. This means there is no access to hot neutrons in the Australasian region. Several cold neutron sources have been or are currently being commissioned in the Asia-Oceania region but the impact has so far been low compared to experience in Europe and the USA.

### **Hot source**

The initial planning and scoping for OPAL included the provision of a hot neutron source and hot beams. The hot neutron source was later forgone in preference to other facilities with the intention of acquiring funding in the future to complete the design, manufacture and installation of a hot source. The user demand for a hot source is even stronger today. Some areas of science and key questions should be listed here.

Since the initial considerations for a hot source, developments in engineered materials provide the opportunity to improve the expected performance using advanced insulating materials. The feasibility of reaching temperatures as high as 3000 K should be assessed as this would provide a performance edge compared to current hot neutron source capability and allow cutting edge experiments to be conducted at OPAL.

A hot neutron source would not require access to a second guide hall but is a natural addition to any future expansion of the OPAL Reactor. The hot source will allow access to a whole range of new scientific experiments and endeavours that will both complement and enhance the overall capabilities of the OPAL Reactor.



Fig. 16 Schematic diagram of the hot neutron source at FRM-II

### **Cold Source**

The existing cold neutron source at OPAL allows for the illumination of two large cold beam tubes. One of the beam tubes provides cold neutrons to the existing neutron guide hall and associated instruments while the other beam tube to an instrument at the reactor face. A second guide hall would allow the design, construction and installation of many more cold instruments feeding off the second beam tube. Such an investment deserves careful consideration to ensure the cold source feeding these instruments is optimised to provide both the maximum flux and ideal spectrum.

The existing cold source vessel is due to be replaced following 10 years of full power operation because of radiation induced embrittlement. Such a requirement presents an opportunity to improve the design and performance of the cold source. An improved cold source providing enhanced performance to match the requirements of the science and instruments planned for the second guide hall and indeed those in the existing guide hall should be considered as part of the second guide hall expansion. Performance improvement techniques currently under investigation such as directionally focused moderators, nano-crystalline diamond coatings and optimised moderators should be considered as part of the design process. The large volume available for the cold source allows detailed geometry optimisation to tailor the cold neutron spectrum specifically for each of the beam tubes and with advance neutron optics perhaps for individual guides. This approach of optimised cold source-neutron

optics-instrument design should be the basis of all work associated with the second guide hall expansion.

## NEUTRON GUIDES AND OPTICS

Instruments should be built around the anticipated sample environment to guarantee an optimized illumination of the sample with neutrons. The future research in guide hall 2 is expected to concentrate on the investigation of small samples, samples under extreme conditions, *in-situ* measurements using complementary techniques, time dependent phenomena in hard- and soft-condensed-matter physics. In particular, instruments will be used for geoscience where the samples are exposed to extremely high pressure and temperature.

### **Situation at OPAL**

In the first guide hall, conventional beam lines are installed on curved neutron guides, one of which at 300mm high is possibly the largest in any reactor in the world. While the institute has some internal expertise in making use of neutron optics to optimize the instruments, it is presently constrained by headcount in this area. In order to properly adapt the existing instruments and the new instruments to be designed for guide hall, it is necessary to build up internal expertise by creating a neutron optics group. Due to the healthy situation on the market of supermirror guides, polarizing equipment we do not advise ANSTO to build up its own production capabilities. However, it is important to establish good connections to international research institutes and companies active in this field. It is important to be able to fabricate optical devices on the basis of mirrors and other components from companies or from research institutes. The method of investigating real samples of real materials under real conditions and in real time will be of societal importance for Australia. Moreover, the development of advanced equipment for the experiments may lead to technology transfer to high-tech companies to local industry.

### **International situation:**

The existing continuous sources in the Asia-Pacific region provide a significantly lower flux than OPAL. Moreover, they are designed for conventional investigations and based on the current neutron technology. J-PARC will be another state of the art modern facility. However, due to the pulsed structure of the beams it is complementary to OPAL. Therefore, OPAL can take a leading role in the Asian-pacific region. This leading role will be amplified if a 2nd guide hall is realized, relying on the most advanced neutron scattering techniques and functionalized as stated above. This statement is even true in a world-wide context.

### **Science drivers:**

#### *Major scientific questions*

The future developments in hard condensed matter will focus on the development of functional materials, i.e. materials that combine various degrees of freedom like magnetism, ferroelectricity, stress and strain etc. These tasks can be achieved either by using bulk materials or by combining various materials in the form of artificial structure, like multilayers where functionality can be induced at the interfaces.

Another important development will concentrate on energy research, i.e. extraction, storage, transport, and conversion of energy. Many of these investigations have to be conducted while the process is happening.

Another important area is biology and soft condensed matter, where the samples are often so small that they cannot be investigated by present means. A major challenge is

the investigation of the dynamics. Advanced neutron optics will allow the investigation of ongoing processes in-situ.

#### *Societal and technological development*

The installation of a 2<sup>nd</sup> guide hall at OPAL will foster the technology transfer from other countries to Australia. The fabrication of advanced equipment will strengthen the position of the Australian industry on the world-wide market. It has been repeatedly proven that research centers of excellence attract high-Tech companies in the close surroundings of the facility. Examples are the ILL in Grenoble, the Atom egg in Garching and the synchrotron and neutron facilities in Sweden.

#### **Instrumentation and technique development**

##### *What is new?*

The 2<sup>nd</sup> guide hall at OPAL will allow performing experiments in geoscience, condensed and soft matter physics under realistic conditions. The proposed instruments will be, for the first time, be fully optimized from the source to the sample and built around the sample environment.

##### *How does it address the science drivers?*

It is proposed to transport the neutrons in the 2<sup>nd</sup> guide hall from the cold source to the sample by means of the last generation of elliptic neutron guides that have the advantage of deliver only neutron beams of the required size and phase space that is relevant for the experiment. This way, the background in the guide hall and as produced by the sample environment is minimized. This leads to a much better signal to noise ration and to reduced costs for shielding. It gives, in addition, more flexibility in the arrangement of the instruments and sample environment.

To be more specific, we propose to build specialized beam lines for high pressure studies which are adapted for various beam lines and sample sizes. For example, it is envisaged to build a beam line for i) 10 mm samples for extreme pressures above 100 GPa for studies in Geoscience, for ii) 100 mm samples for the study of quantum phase transitions exceeding 10 GPa and for iii) 1 mm sized samples for low pressure studies using elastic and inelastic neutron scattering. Here the neutrons will be delivered by means of a low cost, straight or elliptic neutron guide to a small monochromator and focused on the sample using parabolic guides. Due to the small beam cross sections, the shielding requirements are small. Therefore, these suite of instrument will be very compact and cost effective.

For reflectometry, we propose to build reflectometers for hard- and soft-condensed-matter using ideas similar to the Selene<sup>2</sup> concept recently developed and realised at PSI and being considered for ESS. The major feature of this instrument is the definition of the beam size and the divergence of the neutron beam far away from the sample. Therefore, essentially zero background is expected. Moreover, only the sample is illuminated, thus boosting the signal to noise ration. In addition, a flux gain of a factor of 100 is expected compared to the traditional designs. For small angle neutron scattering from small samples, a similar concept for two-dimensional beam optics may be applied using Montel optics.

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<sup>2</sup> [http://kur.web.psi.ch/amor/selene/selene\\_report.pdf](http://kur.web.psi.ch/amor/selene/selene_report.pdf)

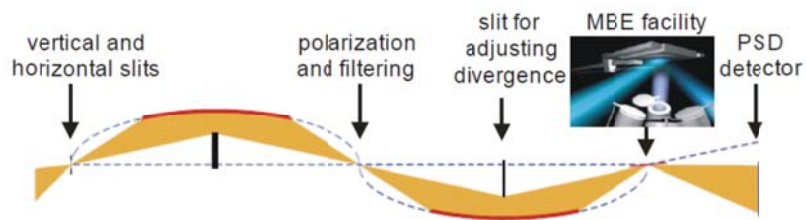


Fig. 17 Schematic of a beam line for in-situ reflectometry during the growth of multilayers using the combination of the SELENE<sup>3</sup> concept with MBE or PLD. The definition of the beam size and the divergence at the sample position are conducted far away from the sample (2-4 meters) guaranteeing a very low background.

*Why is the second guide hall necessary?*

The 1<sup>st</sup> guide hall at OPAL is based and optimized on current technology and supposed to serve the present needs of the universities in Australia. The 2<sup>nd</sup> guide hall will expand into areas in which neutron scattering was not able to be performed. It will allow to investigate small samples a domain presently occupied by synchrotron light sources, which are inherently weakly sensitive to magnetism and light elements, and cases where deep penetration of the radiation and radiation damage is important. Extreme conditions require building the instrument around the sample environment. This is complementary to the more general purpose of the instruments in the 1<sup>st</sup> guide hall. Moreover this new class of experiments will be complicated and will require much longer beam times. The set-up times will also be increased. Ultimately, an extremely low background is required.

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<sup>3</sup> J. Stahn, T. Panzner, U. Filges, C. Marcelot, and P. Böni, *Nucl. Instrum. Methods A* **634**, S12-S16 (2011).



## POLARIZED NEUTRONS AND LARMOR LABELING

There are two main drives for using polarized neutrons in materials science studies:

(1) Polarization analysis separates spin-dependent from non-spin-dependent events when a beam of polarized neutrons is sent through a sample. The most common use is to separate magnetic scattering from nuclear scattering in the studies of magnetism. In soft matter and biological material studies, the technique is used to reduce the spin-incoherent scattering background from hydrogen-rich materials. Polarized neutron imaging is used to observe mesoscopic and macroscopic magnetic field configurations (e.g. magnetic domains, trapped magnetic fields in superconductors).

(2) Larmor labeling methods use the spin-precession characteristics of polarized neutrons in magnetic fields to allow either energy or momentum changes of neutrons during scattering to be measured with high accuracy beyond conventional methods. This technique is used in studying the dynamics and structures of soft-matter, molecular biology or magnetism. Below we give a snap-shot of the fields, where both polarized neutrons and Larmor labeling including Neutron Spin Echo methods are or will be important.

**Magnetism:** This is the traditional field of polarized neutron scattering where polarization analysis (longitudinal<sup>4</sup>, XYZ<sup>5</sup> or spherical polarimetry<sup>6,7</sup>) provides information about magnetic moments associated with unpaired electron spins in a sample. While polarization analysis has seen wide-spread applications, in this field the potential of Neutron Spin Echo (NSE) spectroscopy<sup>8</sup> has not been fully exploited yet, partly due to the small samples available. Furthermore, the emerging techniques of Larmor diffraction<sup>9</sup> and Spin-Echo Scattering Angle Measurements (SESAME)<sup>10,11</sup> have the potential to shed new light on magnetic phase transitions, the role of stress and strain and the coupling of structural and magnetic degrees of freedom. The following cursory review sees a good number of “hot topics” in which polarization analysis and NSE techniques are or can be instrumental:

- Superconductivity
- Magnetic proximity effects
- Quantum magnetism
- Low-dimensional magnetism
- Novel magnetic systems such as spin ice and spin liquids

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<sup>4</sup>R.M. Moon, T Riste, W.C. Koehler, Phys. Rev. 181 (1969) 920 R.M. Moon, T Riste, W.C. Koehler, Phys. Rev. 181 (1969) 920

<sup>5</sup> A.P. Murani and F. Mezei in F. Mezei (ed.), Neutron Spin Echo, Lecture Notes in Physics Series, Vol. 128 (Springer, Heidelberg, 1980) p. 104

<sup>6</sup> F. Tasset, Physica **B 156 & 157** (1989) 627 and F. Tasset et al., Physica **B 267-268**, 69 (1999).

<sup>7</sup> M. Janoschek et al., Physica **B 397** (2007) 125

<sup>8</sup> F. Mezei in F. Mezei (ed.), Neutron Spin Echo, Lecture Notes in Physics Series, Vol. 128 (Springer, Heidelberg, 1980) p. 3 and in “Neutron spin echo spectroscopy”, Lecture Notes in Physics Series, Vol. 601, ed.: F. Mezei, C. Pappas, Th. Gutberlet (Springer, Heidelberg, 2003) p. 1

<sup>9</sup> M. T. Rekveldt, T. Keller and R. Golub, Europhys. Lett., **54** (2001) 342

<sup>10</sup> R. Pynn in Neutron Spin Echo, Lecture Notes in Physics Series, Vol. 128 (Springer, Heidelberg, 1980) p. 159

<sup>11</sup> M. T. Rekveldt, NIMA **114** (1996) 366 and W.G. Bouwman et al., Journal of Applied Crystallography **33** (2000) 767

- Molecular magnets
- Magnetic functional materials such as multiferroics, materials for spintronics and magnetocaloric materials
- Nanomagnetism, magnetic nanoparticles (including drug delivery)
- Magnetic thin films, multilayers, and patterned surfaces that usually associate with spintronics materials

**Soft matter and life sciences:** Polarization analysis has been used for separating coherent and spin incoherent scattering, in e.g. hydrogen containing materials. It has the potential to improve the signal/noise ratio for structural studies such as SANS, diffuse scattering or protein crystallography. In addition, polarization analysis makes it possible to separate coherent from incoherent dynamics in one experiment and on the same sample by e.g. time-of-flight spectroscopy.

In soft matter and biology, where the relevant length and timescales reach from sub-Angstrom and picoseconds to nanometers and several tens of nanoseconds and beyond, Neutron Spin Echo (NSE) spectroscopy is the only method, which can measure the slow motions on several ten nanosecond timescales. NSE spectrometers are particularly powerful in the small angle neutron scattering region. A NSE spectrometer would complement the existing inelastic instrument suite at ANSTO and serve the soft matter and biology community in Australia and South-East Asia.

Structural studies of food relevant materials, colloids etc. will benefit from high resolution Spin-Echo SANS (SESANS), which allows correlations to be measured directly in real space. The high penetration power of neutrons might also allow in-situ measurements simulating industrial processing conditions.

**Imaging** State-of-the-art high-resolution polarized neutron imaging also in combination with spherical polarimetry (3D depolarization) setup<sup>12</sup>, or mini-Cryopad<sup>13</sup>) can resolve magnetic inhomogeneities and magnetic domains<sup>14</sup> and has the potential to become a valuable tool in nanomagnetism. The combination of imaging with spin-echo techniques may open up possibilities for direct 3D imaging without using tomography techniques<sup>15</sup>.

## SITUATION AT OPAL

Australia has a long tradition on polarized neutrons because there was a dedicated polarized neutron instrument, LONGPOL<sup>16</sup>, at HIFAR. Consequently among the staff of ANSTO there is a critical mass of expertise and interest in using polarized neutrons.

Presently polarized neutrons are implemented at the reflectometer (supermirror polarizer and analyzer) and SANS (supermirror polarizing cavity). A <sup>3</sup>He polarising station is on the way from the Institute Laue Langevin (ILL) in Grenoble, France to

<sup>12</sup> M. T. Rekveldt, *Le Journal de Physique Colloques* **32-C1** (1971) 579

<sup>13</sup> R. Pynn, private communication

<sup>14</sup> I. Manke et al., *Nature Communications*, **1** (2010) 125

<sup>15</sup> W.T. Lee, "Spin Echo Imaging" in *Neutron Imaging and Applications*, H. Bilheux, R.L. McGreevy, I. Anderson, ed., Springer-Verlag (2008).

<sup>16</sup> S.J. Campbell et al., *J. Phys. E: Sci. Instrum.* **7** (1974) 195 and N Ahmed et al., *J. Phys. E: Sci. Instrum.* **7** (1974) 199

ANSTO. Work is underway to implement polarized  $^3\text{He}$  based polarizers and analyzers on three spectrometers (time-of-flight and triple-axis), diffractometer, SANS (analyzer) and reflectometer (for analyzing off-specular scattering). Additional implementations on existing diffractometers and new instruments being constructed (imaging, SANS and back-scattering spectrometer) will bring polarization analysis to virtually all instruments. The newly commissioned time-of-flight spectrometer also has a supermirror polarizer. In addition, the new 12-Tesla high field magnet is available for use with polarized neutrons.

It appears likely that ANSTO will gain considerable experiences with conventional polarization analysis (mainly longitudinal) over the next few years and may therefore be in a good position to exploit more advanced options in the context of a new guide hall. Several of these options, such as dedicated polarized neutron instrument, NSE or SESAME instruments, cannot be accommodated in the existing guide hall due to lack of space.

Presently there is no instrument using Larmor labeling technique at ANSTO, which leaves a void in the coverage of energy/time scale to study dynamics important for soft matter, molecular biology and magnetism. Without a remedy that may come with new instruments in a new guide hall, this might further hamper the adoption of new techniques such as Larmor diffraction, phonon focusing, 3D polarimetry with NSE, SESAME techniques that expand the use of neutron scattering in new topical fields that will benefit from these techniques.

## NATIONAL AND INTERNATIONAL ENVIRONMENT

At present, polarization analysis and Larmor-labeling techniques have seen a more wide-spread use in facilities in Europe and the US. Europeans and in particular the ILL have been leading in many instances in applying polarized neutrons in the study of new scientific topics and in developing new polarized neutron techniques. The first NSE spectrometer<sup>17</sup> was built at the ILL by Hayter and Mezei in the 1970s and the world's most advanced NSE instrument, capable of reaching Fourier times of  $\sim 1$  microsecond is also located at the ILL, in the second ILL guide hall<sup>18</sup>. Cryopad was invented at ILL by Tasset<sup>4</sup>, who also built the first polarized  $^3\text{He}$  filling station<sup>19</sup>. The first neutron resonance spin echo instrument (NRSE) was built at the LLB in collaboration with the TU Munich<sup>20</sup>, the first NRSE-TAS was realized in Berlin<sup>21</sup> and SESANS was developed at Delft<sup>9</sup>. In the US, NIST has polarization analysis capabilities in its diffractometer, reflectometer, SANS, and spectrometers and also a NSE spectrometer. The construction of the SNS has seen a second NSE spectrometer in the US and helps the environment to support an on-going development of polarized  $^3\text{He}$  based neutron polarizers and analyzers. There is a large and active research community that uses polarization analysis in Europe. The research community in

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<sup>17</sup> J.B. Hayter in F. Mezei (ed.), *Neutron Spin Echo*, Lecture Notes in Physics Series, Vol. 128 (Springer, Heidelberg, 1980) p. 53 and P.A. Dagleish, J.B. Hayter and F. Mezei, in F. Mezei (ed.), *Neutron Spin Echo*, Lecture Notes in Physics Series, Vol. 128 (Springer, Heidelberg, 1980) p. 66

<sup>18</sup> P. Schleger et al., *Physica B* **241-243** (1998) 164

<sup>19</sup> F. Tasset, *Proceedings of the International Workshop on Polarized He-3 Beams and Gas Targets and Their Applications*, Oppenheim, Germany (2002)

<sup>20</sup> M. Koeppel et al., *Physica*, **B266**, 75 (1999)

<sup>21</sup> T. Keller et al., *Neutron News* **6** (1995) 16-17

using Larmor labeling technique are mainly in Europe couple with the fact that these instruments are mainly located in Europe.

In Oceanic and Asian regions, the facilities that may become the centers for polarized neutron works are ANSTO's OPAL and the new facility J-PARC in Japan. In Japan, the neutron scattering facility IRR-3 has polarized neutron capabilities, a Cryopad and a NSE instrument. In addition Japanese groups are active in developing MIEZE-type instrumentation<sup>22</sup>. Polarization analysis and Larmor labeling instrumentation are integrated part of the J-PARC instrument suite to support the Japanese research community.

In Australia, as we mentioned above, ANSTO has a long tradition of using polarized neutrons in research. Many universities in Australia have past and present research works in magnetism that uses polarized neutrons. In the Oceanic and Asian regions, there is also an on-going collaboration between ANSTO and researchers in Taiwan, mainland China, and Southeast-Asian countries such as Singapore. With the addition of polarization-analysis capabilities in more instruments, it is foreseeable that the Australian research community using polarized neutrons, as well as international collaborations, will expand in the coming years.

There is a largely untapped potential in using Larmor labeling techniques for research both in Australia and in other countries in the region. Soft matter and biology researchers in Australia have long been using ANSTO's instruments and would welcome the use of polarized neutrons if these prove to be beneficial in suppressing the spin incoherent background from hydrogen. The same community would likely see the potential for their research in Larmor-labeling techniques. Larmor methods are complicated to set up, and for this reason dedicated user support is vital to ensure scientific viability. The experience in Europe and the US is that a group of dedicated researchers and instrument scientists alike to bring about the critical mass in interest and know-how is of crucial importance. Often the difference between success and failure, in particular with these complex instruments, lies in whether instrument scientists are active and evangelical about the technique or not. It is possible that there can be a critical mass in the research community that grows with the number of Larmor labeling instruments available in the region,

## **INSTRUMENTATION AND TECHNIQUE DEVELOPMENT WHAT'S NEW AND HOW DOES IT ADDRESS SCIENCE DRIVERS?**

The use of polarized neutrons is an active field of instrumental research and developments, benefiting from advances in neutron optics as well as from new methods of using polarized neutrons. It is not yet clear how far these developments will go.

SESANS has already shown its ability to measure pair correlation functions over very large distance scales (from ~10 nm to 20 microns) with strongly scattering samples (which means shorter experiments and a greater potential for time-dependent measurements and interrogation of different parts of a single sample). We expect

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<sup>22</sup> Y Kawabata et al., *Physica B* **385-386** (2006) 1122

similar advances in SERGIS<sup>23</sup> measurement of diffuse scattering from surfaces, allowing access to lateral structures of interfaces. It has been shown that SESAME can be used to discriminate between specular and diffuse reflection, thereby allowing specular measurements to be made on rough or wavy samples. Such samples may be of more scientific interest those deposited on the canonical silicon substrates. Because SESAME (i.e. both SESANS and SERGIS) can use neutron beams with divergence of 2 degrees or more, there is a potential to exploit new optical components to focus neutrons on very small samples and to make measurements with good momentum resolution. Larmor diffraction, a mere curiosity some years ago, is now being used fairly routinely to measure changes in crystal lattice parameters with an unprecedented accuracy, better than that achievable with synchrotron X-rays. Given the level of precision that can be achieved, one can easily imagine that new phenomena will be discovered and that, for example, the role of lattice strain in nanomagnetism will be explored in detail. Recent experiments have shown that it is possible to combine NSE with Cryopad<sup>24</sup> or high magnetic fields applied to a sample<sup>25</sup>. At least two groups are now developing simple technologies for making SANS and reflectometry measurements in combination with polarimetry (using a so-called mini-cryopad). These developments may well open up new research areas in nanomagnetism. Recently, the combination of NRSE with triple-axis spectroscopy opened up new areas of condensed matter physics: e.g. measurements by Keimer's group using phonon focusing have shown remarkable correlations between Kohn anomalies and superconducting gaps in conventional superconductors<sup>26</sup>. So far, the development of polarization techniques for TOF applications is in its infancy and as more work is done to address this area one can imagine that new technologies will emerge.

New materials in magnetism are emerging rapidly. The current trend of these materials especially nanostructures pose a unique challenge: The sample size is limited, the magnetic density can be small, the magnetic scattering is often diffuse or with length scales that can be on the high end for SANS and low end for diffractometers. Current instrument can be hard-pressed to meet the demands for a good measurement. Focused new design of polarised neutron instruments would be needed to address this challenge.

## **WHY IS THE SECOND GUIDE HALL NECESSARY?**

As mentioned above, it will be impossible to fully exploit the potential offered by polarized neutrons within the existing guide hall. There simply are not enough beams and, in several cases, the existing instruments cannot be easily reconfigured to use polarized neutrons. This implies that, without a second guide hall, ANSTO will have to forego some of the most topical areas of research such as investigation of nanomagnetism (which will likely be required for new generations of computing and communications technology) and studies of complex fluids (such as polymers and colloids) under conditions that are more relevant to industrial processes than the carefully designed experiments on model systems that are performed today.

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<sup>23</sup> G.P. Felcher et al., Proceedings of SPIE **4785** (2002) 164

<sup>24</sup> C. Pappas, E. Lelievre-Berna et al., Phys. Rev. Lett. **102** (2009) 197202

<sup>25</sup> E. M. Forgan et al., Phys. Rev. Lett. **85** (2000) 3488-

<sup>26</sup> P. Aynajian, et al. Science **319** (2008) 1509

It will also be important in future to configure instruments to avoid magnetic cross talk. One class of experiments will surely require the application of ever larger magnetic fields to samples, while sophisticated Larmor precession techniques are extremely sensitive to small remnant fields and even more effected if such fields change with time. The unavoidable conclusion is that experiments of the two types will need to be separated spatially, almost requiring the addition of a second guide hall.

To summarize, the committee recognizes that the second guide hall will offer the possibility to become a major international player at several topical fields involving polarized neutrons. The example of the ILL, however, shows that success very much depends on the human factor. The recommendation is to build a critical mass of enthusiastic and highly motivated young scientists, who will be able to do exciting new science while developing novel neutron instrumentation techniques with polarized neutrons.

## APPENDIX 1 – List of Attendees

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**APPENDIX 2 – Instruments suggested during the workshop**  
 (E = Executive Summary; M = Magnetism & Superconductivity; C = Chemistry;  
 ε = Materials Engineering; S = Soft Matter; B = Biology)

<b>Instrument</b>	<b>Source</b>	<b>Science Interest</b>
<b>Membrane Diffractometer</b>	<b>Cold</b>	<b>E, C, B</b>
<b>High-Pressure Diffractometer</b>	<b>Thermal</b>	<b>E, C</b>
<b>Neutron Microscope</b>	<b>Cold</b>	<b>E</b>
<b>Thin-film Diffractometer</b>	<b>Thermal</b>	<b>M</b>
<b>PDF Diffractometer</b>	<b>Hot</b>	<b>C, ε</b>
<b>Single-Crystal Diffractometer</b>	<b>Hot</b>	<b>C</b>
<b>Multi-Chopper Spectrometer</b>	<b>Cold</b>	<b>C, M</b>
<b>Hot Time-of-Flight Spectrometer</b>	<b>Hot</b>	<b>C</b>
<b>3-D Reciprocal Space Mapper</b>	<b>Hot</b>	<b>M</b>
<b>Polarised Diffractometer</b>	<b>Hot</b>	<b>C</b>
<b>White-beam strain scanner</b>	<b>Thermal</b>	<b>C, ε</b>
<b>Materials Engineering Diffractometer</b>	<b>Thermal</b>	<b>ε</b>
<b>Spin-Echo Imaging</b>	<b>Cold</b>	<b>ε</b>
<b>Wide-Q Fast Reflectometer</b>	<b>Cold</b>	<b>S</b>
<b>Single-Shot SANS</b>	<b>Cold</b>	<b>S</b>
<b>Compact high-resolution SANS</b>	<b>Cold</b>	<b>S</b>
<b>Spin-Echo Reflectometer</b>	<b>Cold</b>	<b>B</b>
<b>Biomacromolecular Diffractometer</b>	<b>Cold</b>	<b>B</b>
<b>Spin-echo spectrometer</b>	<b>Cold</b>	<b>S,B</b>

<b>Multiple techniques</b>	<b>Science Interest</b>
<b>Neutrons + optical spectroscopy</b>	<b>M</b>
<b>Reflectometry + MOKE<sup>27</sup></b>	<b>M</b>
<b>Diffraction + PGAA<sup>28</sup></b>	<b>C</b>

<sup>27</sup> Magneto-optical Kerr Effect

<sup>28</sup> Prompt  $\gamma$ -Ray Activation Analysis

## APPENDIX 3 – Program

<b>Monday 16 April</b>	AINSE Theatre, Lucas Heights
8.30 – 9.00	Registration & Coffee
<b>Chair:</b>	Richard Newbury ( <i>UNSW</i> )
9.00	Welcome by Adi Paterson ( <i>ANSTO CEO</i> )
	Welcome by Brendan Kennedy ( <i>AINSE and ANBUG</i> )
9.15 – 9.45	<b>Introduction and Charge to the Workshop</b> Rob Robinson ( <i>ANSTO</i> )
9.45 – 10.15	<b>Magnetism</b> Ivan Schuller ( <i>University of California San Diego</i> )
10.15 – 10.45	<b>Superconductivity</b> Jeff Tallon ( <i>MacDiarmid Institute, New Zealand</i> )
10.45 – 11.00	Coffee
<b>Chair:</b>	Tom Vogt ( <i>University of South Carolina</i> )
11.00 – 11.30	<b>Energy Materials</b> Vanessa Peterson ( <i>ANSTO</i> )
11.30 – 12.00	<b>Earth Sciences</b> Simon Clark ( <i>Lawrence Berkeley Lab.</i> )
12.00 – 12.30	<b>Fundamental Physics</b> Mike Snow ( <i>Indiana University</i> )
12.30 – 12.35	Group Photograph
12.35 – 13.30	lunch
<b>Chair:</b>	Patrick Hartley ( <i>CSIRO</i> )
13.30 – 14.00	<b>Polymers</b> Toshiji Kanaya ( <i>Kyoto University</i> )
14.00 – 14.30	<b>Biology and Deuteration</b> Jill Trewhella ( <i>University of Sydney</i> )
14.30 – 15.00	<b>Soft Matter</b> Duncan McGillivray ( <i>University of Auckland</i> )
15.00 – 15.15	tea
<b>Chair:</b>	Shane Kennedy ( <i>ANSTO</i> )
15.15 – 15.45	<b>Materials Engineering</b> Klaus-Dieter Liss ( <i>ANSTO</i> )
15.45 – 16.15	<b>Science with Positrons</b> Christoph Hugenschmidt ( <i>Technical University of Munich</i> )
16.15 – 16.45	<b>Present and Future Cold and Hot Source Possibilities in the OPAL Reactor</b> Greg Storr ( <i>ANSTO</i> )
16.45 – 17.15	<b>Neutron Guides and Optics</b> Peter Boni ( <i>Technical University of Munich</i> )
17.15 – 17.30	<b>Summary of the Day</b> Rob Robinson ( <i>ANSTO</i> ) & Chris Ling ( <i>ANBUG</i> )
18.00 for 18.30	<b>Dinner at the ANSTO Cafeteria</b> After-Dinner Speech by John White ( <i>Australian National University</i> )

<b>Tuesday 17 April</b>	OPAL Auditorium, B83
8.30 – 9.00	Registration & Coffee
<b>Chair:</b>	Mike James ( <i>ANSTO</i> )
9.00 – 10.00	<b>Short specific proposals for new instruments</b> (5-10 mins each)
10.00 – 12.00	<b>Parallel Workshop Sessions on Scientific Opportunities</b> (spokesperson):  <b>Biology</b> (Andrew Whitten, University of Queensland) <b>Chemistry</b> (Brendan Kennedy, Sydney U.) <b>Magnetism &amp; Superconductivity</b> (Oleg Sushkov, UNSW) <b>Materials Engineering</b> (Mark Hoffmann, UNSW) <b>Soft Matter</b> (Ian Gentle, University of Queensland) <b>Fundamental Physics</b> (Tony Klein, University of Melbourne) <b>Central Oversight Group</b> (TBD)
12.00 – 12.30	Report back to full Group (5 minutes each)
12.30 – 13.30	lunch
	<b>Parallel Workshop Sessions on Technology Opportunities</b> (spokesperson):  <b>Inelastic Neutron Scattering</b> (John Stride, UNSW) <b>Diffraction</b> (Garry McIntyre, ANSTO) <b>SANS &amp; Reflectometry</b> (Ian Gentle, University of Queensland) <b>Fundamental Physics</b> (Mike Snow, Indiana University) <b>Positrons</b> (James Sullivan, Australian National University) <b>Imaging</b> (Ulf Garbe, ANSTO) <b>Guides &amp; Optics</b> (Peter Böni, Technical University of Munich) <b>Polarised Neutrons</b> (Catherine Pappas, Technical University of Delft; Roger Pynn, Indiana University) <b>Cold and Hot Sources</b> (George Braoudakis, ANSTO) <b>Other Methods (e.g. PGAA)</b> <b>Central Oversight Group</b> (TBD)
16.00 – 17.00	Report back to full Group (5 minutes each)
18.00 for 18.30	<b>Dinner with Australian Wine Tasting</b> (Mike James) <b>at the ANSTO Cafeteria</b> After-Dinner Speech by Tony Klein ( <i>University of Melbourne</i> )

<b>Wednesday 18 April</b>	OPAL Auditorium, B83
8.30 – 9.00	Registration & Coffee
9.00 – 9.10	<b>Plenary Session</b>
9.10 – 12.00	<p><b>Further Parallel Workshop Sessions on Scientific &amp; Technological Opportunities</b> – including Report Writing (spokesperson):</p> <p><b>Biology</b> (Andrew Whitten, University of Queensland)  <b>Chemistry</b> (Brendan Kennedy, Sydney U.)  <b>Magnetism &amp; Superconductivity</b> (Oleg Sushkov, UNSW)  <b>Materials Engineering</b> (Mark Hoffmann, UNSW)  <b>Soft Matter</b> (Ian Gentle, University of Queensland)  <b>Fundamental Physics</b> (Tony Klein, University of Melbourne)  <b>Inelastic Neutron Scattering</b> (John Stride, UNSW)  <b>Diffraction</b> (Garry McIntyre, ANSTO)  <b>SANS &amp; Reflectometry</b> (Ian Gentle, University of Queensland)  <b>Fundamental Physics</b> (Mike Snow, Indiana University)  <b>Positrons</b> (Steve Buckman, Australian National University)  <b>Imaging</b> (Ulf Garbe, ANSTO)  <b>Guides &amp; Optics</b> (Peter Böni, Technical University of Munich)  <b>Polarised Neutrons</b> (Catherine Pappas, Technical University of Delft;  Roger Pynn, Indiana University)  <b>Cold and Hot Sources</b> (George Braoudakis, ANSTO)  <b>Other Methods (e.g. PGAA)</b>  <b>Central Oversight Group (TBD)</b></p>
12.00 – 13.00	lunch
13.00 – 15.00	<p><b>Report Writing</b> (spokesperson):</p> <p><b>Biology</b> (Andrew Whitten, University of Queensland)  <b>Chemistry</b> (Brendan Kennedy, Sydney U.)  <b>Magnetism &amp; Superconductivity</b> (Oleg Sushkov, UNSW)  <b>Materials Engineering</b> (Mark Hoffmann, UNSW)  <b>Soft Matter</b> (Ian Gentle, University of Queensland)  <b>Fundamental Physics</b> (Tony Klein, University of Melbourne)  <b>Inelastic Neutron Scattering</b> (John Stride, UNSW)  <b>Diffraction</b> (Garry McIntyre, ANSTO)  <b>SANS &amp; Reflectometry</b> (Ian Gentle, University of Queensland)  <b>Fundamental Physics</b> (Mike Snow, Indiana University)  <b>Positrons</b> (Steve Buckman, Australian National University)  <b>Imaging</b> (Ulf Garbe, ANSTO)  <b>Guides &amp; Optics</b> (Peter Böni, Technical University of Munich)  <b>Polarised Neutrons</b> (Catherine Pappas, Technical University of Delft;  Roger Pynn, Indiana University)  <b>Cold and Hot Sources</b> (George Braoudakis, ANSTO)  <b>Other Methods (e.g. PGAA)</b>  <b>Central Oversight Group (TBD)</b></p>
15.00 – 16.45	<b>Full Formal Report back to Complete Group</b> (20 minutes each)
16.45 – 17.00	<p><b>Summary of the Workshop</b> by Panel:  John White (Australian National University)  Bill Stirling (CEA-France)  Dan Neumann (NIST)  Greg Storr (ANSTO)</p>

# APPENDIX 4 – Notes from After-Dinner Speech by John White, 16 April 2012

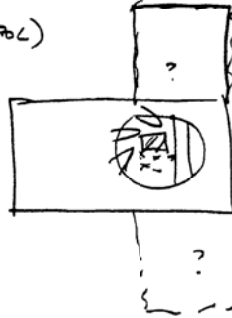
27.11.97 at I.L.L. met  
Present OBJECT ① To discuss the new HIFAR reactor with members of I.L.L. and to examine options for the instrumentation which might affect the reactor design and cost.  
 ② To discuss the new jobs of head of the neutron scattering group.

Present Andrew Wildes (ex LONGPOL)

Alan Hewat

Garry McIntyre

Sax Mason



no want (Michael Walsh) an ANSTO engineer on 1 year secondment to Alan Hewat to carry forward design & construction of a 10cm neutron detector for DA.

## Matters discussed:

- Core configuration & fuel (20% Eu), purpose of reactor, audience need, need for internationally attractive neutron facilities, flexible building site and reactor penetration.
- JWW "devil's advocate" points:
  - Through hole. G.M. has experience of Rido.
  - Thermal guide do we want them? Certainly now has a multilayer guide to do INIS reaction. Works well. Guides have changed a lot in last 5 years - will do so in next. Leo b/g in Hall a great advantage of new guide can get to  $\lambda = 1 \text{ \AA}$  - seems possible. AH would now build powder diffraction guide not in hall.
  - Cold source should be optimum - approachable from two sides or two bundles for future expansion.
  - Hot source. AH "devil's advocate" position is to have one! not other way around. M. Lehman says break even for present source is 0.7  $\text{\AA}$  against thermal. ILL source 2000  $\text{\AA}$  (most probably), instruments would not beat ILL. Why not have best in front. No p<sub>n</sub> at new reactor.
  - Electronics, Thermal 3 axis near reactor optimised like ORPHEE - always needed (AW). Spin echo - codulation may kill intensity. ? value. LONGPOL would need rebuilt. Backscattering possible.
  - SANS & reflectometry a must at least level of instrumentation - will remain valuable.
  - 4 circle diffractometer at reactor face. Like replacement of D2.
  - Access highly important.
  - 90% neutron relaxation from filters. They really work. Separation of neutron component can be done intrinsically (AW).
  - JWW asked all for 1/2 page on the various cannot they make. Would see it gets to the table.

Saw M. Lehman. He notified here works well. view at end of thermal guide.  
 Ian Anderson.

JWW → C. TUNIZ

9/12/97

- \* I raised the question of a through tube both with the Australian group and subsequently with the reactor chief at Grenoble. Gary McIntyre has experience with the through hole at the Riso reactor as I mentioned when I was at the advisory committee in November. From the point of view of safety Dr Bauer said that there were no additional problems raised by a through hole. The safety considerations were essentially the same as having two horizontal holes looking at a single cold source. This is a matter that should be taken up in more detail with Bauer as it may provide great flexibility in the future for the reactor as a neutron beam source.
- \* Thermal guides. You will remember that I was acting as devil's advocate in our consultative meeting in November. It now looks as if super mirror guides with a critical angle twice that for nickel can be routinely produced both at the ILL and at the Neutron Scattering Centre in Wurenlingen, Switzerland (Dr P. Hoghoj). This means that thermal guide tubes can now conduct neutron wavelengths as short as about one angstrom to external instruments and this makes them worthwhile. The point that was made by Shane Kennedy about the lower background in the guide hall is therefore a telling point for instrument design. I asked Dr Hewatt if he would make an analysis of the background of ILL near the reactor and away from it so that we could have some actual data on these points. Alan Hewatt confirmed that he would now choose to build a powder instrument in the guide hall rather than in the reactor hall. This was a point that I raised in November a "litmus test" of the value of thermal guide tubes.
- \* Neutron optics is an extremely important area. It relates to the thermal guide tube point made above but also to the way in which neutrons will be used in the immediate and long distant future. A medium flux reactor such as that proposed for the Lucas Heights site can be made very powerful by the appropriate use of neutron optics. These involve the use of multi layer mirrors, multi layer bending, band pass filters etc. The technology is advancing very quickly and the leaders are once again in Switzerland and Dr Ian Anderson at the ILL. I think it would be desirable to invite Dr Anderson to Australia in January to give a presentation of modern neutron optics methods. This might radically change some of the instrument conceptions that people are working on at the moment and later.
- \* Cold source. It was agreed in the meeting with the Australians, and also in the discussions with the Directors, that an optimum arrangement would be to have a large cold source approachable from two sides so as to allow for future expansion of the neutron area. One side only could be used in the initial setup of the instruments so as to stay within the proposed budget.
- \* Hot source. Alan Hewatt said that the "devils advocate" position is to have one, not the other way around! The value of a hot source is very much to be doubted. In discussions with Dr M. Lehmann (who is one of the foremost diffractionists at ILL and who has been chiefly responsible for work on hot source instruments) I discovered that the present Grenoble hot source has a break even point of 0.7 angstroms. That means to say that for wavelengths longer than this a thermal beam from the reactor is still better than a hot source beam. I was able to gather some documents from the ILL on the performance of their hot source which currently works at 2000°C. There was much discussion with the Australian group and also with others on whether one needed to go to a hot source in a medium flux reactor. Anything less than a 2000°C source would not be worthwhile. There exist studies at the ILL for hot sources of variable temperature and for temperatures above 2000°C. Some of the documentation is attached.
- \* The group suggested that there will always be the need for a three axis spectrometer near the reactor. This instrument should be optimised like the instrument on ORPHEE. There is doubt about whether spin echo and such very high resolution instruments would be worthwhile because of the extreme collimation needed to make them work. This needs to be investigated further. It was also commented that Longpol at Hifar would certainly need to be rebuilt if it were to be transferred to the new reactor. Back scattering spectrometers were certainly a possibility.
- \* Sans and reflectometry were certainly a must and will remain valuable for the foreseeable future. The best of instrumentation should be achieved.

## Appendix 5 - Acronyms

ANBUG	Australian Neutron Beam Users Group
ANU	Australian National University
ESS	European Spallation Source, Lund, Sweden
FRM-II	Forschungs Reaktor München, Germany
IAEA	International Atomic Energy Agency
ILL	Institut Laue Langevin, Grenoble, France
IR	Infra-red
JEEP	Joint Engineering and Environmental Processing Beamline, Diamond Synchrotron, UK
J-PARC	Japan Proton Accelerator Research Complex, Tokai, Japan
MBE	Molecular Beam Epitaxy
MIEZE	Modulated Intensity by Zero Effort
MIT	Massachusetts Institute of Technology
NCRIS	National Collaborative Research Infrastructure Strategy
NDF	National Deuteration Facility
NIST	National Institute of Standards and Technology, USA
NMR	Nuclear Magnetic Resonance
NRSE	Neutron Resonance Spin Echo
NSE	Neutron Spin Echo
PALS	Positron Annihilation Lifetime Spectroscopy
PDF	Pair Distribution Function
PET	Positron Emission Tomography
PGAA	Prompt $\gamma$ -ray Activation Analysis
PLD	Pulsed Laser Deposition
POLDI	Pulse Overlap time-of-flight Diffractometer, Paul Scherrer Institute, Switzerland
PSD	Position-Sensitive Detector
PSI	Paul Scherrer Institute, Switzerland
SANS	Small-Angle Neutron Scattering
SAXS	Small-Angle X-ray Scattering
SERGIS	Spin-Echo Resolved Grazing Incidence Scattering
SESAME	Spin-Echo Scattering Angle Measurements
SESANS	Spin-Echo Small-Angle Neutron Scattering