## Blue Mountains Workshop on
# Future Opportunities in Neutron Scattering

### Hydro-Majestic Hotel, Medlow Bath, NSW, Australia
### 2-4 December 2005

A group of 28 international experts and Australian research leaders met in the Blue Mountains between 2 and 4 December 2005 to discuss the question "*What would you do in the next 15 years, if you were in our shoes, with a brand-new 20-MW reactor, and 9 funded instruments?*" The workshop was held immediately following the ICNS2005, the International Conference on Neutron Scattering. The attendees came from ten leading overseas neutron laboratories, regional collaborators in Taiwan and Japan, the Australian user community, and from ANSTO (see Appendix 3). All those who have advocated specific beam-line capabilities for the second wave of instruments at OPAL, in recent years, were also invited.

The international experts were of the opinion that the Bragg Institute has made good progress in construction of a large suite of state-of-the art instruments. They cautioned that all stakeholders should recognise that ANSTO is attempting to bring on a large number of instruments on a very aggressive schedule. ANSTO has also recognised the need for standardisation and user friendliness, including good instrument control and data acquisition systems. There is good evidence that Australia's instrument selection process has worked well so far, and that together the Beam Instruments Advisory Group and ANSTO have made good decisions on the first wave of instruments.

A series of recommendations were made as in the following pages. **The two major recommendations were**:

1. to allow sufficient time for shakedown and commissioning of the instruments;
2. to have an on-going capital-improvement programme at the level of 1 - 2 instruments per year.


Back row: Tom Holden, Thom Mason, Wen-Hsien Li, Roger Pynn, Feri Mezei, Garry McIntyre, John Thornton
Middle row: Klaus-Dieter Liss, Mike James, Andrzej Radlinski, Darren Goossens, Stewart Campbell, Ian Gentle, John Stride
Front row: Roland Gähler, Shane Kennedy, Margaret Elcombe, Kazu Kakurai, Chris Ling, Elliot Gilbert, Jill Trewhella, Rob Robinson, Craig Buckley, Mike Fitzsimmons, Winfried Petry, Greg Warr
Not included in photograph: Brendan Kennedy, Tony Klein.

**Recommendations:**

- The experience of the international community is that the user programme will benefit from a thorough shakedown period. In the initial phase, ANSTO should plan for half of the beamtime to be spent on instrument shakedown, during the scientific commissioning period.
    - Instruments should only be moved from scientific commissioning into user programme in a manner consistent with the availability of resources to service users.
    - User operations should be planned to ensure high reliability including provision for requisite maintenance.
    - Scientific success will depend on the early availability, reliability and support for a complete suite of sample environments.

- A sustained capital improvement programme is recommended at the level of 1 - 2 new instruments per year, or equivalent in sample environment apparatus and/or instrument upgrades.
    - For the near future, higher priority should be given to making existing instruments work well , rather than development of new ones.
    - The choice of new (second-wave) instrumentation should not be driven solely be existing user demands, but should also seek to develop new communities and opportunities.
    - The Bragg Institute will need to balance running the first-wave instruments with the growth of new capability and new fields, in order to achieve and maintain an internationally competitive position.
    - Careful consideration and substantial investment will be needed to ensure the availability of a full suite of sample environment equipment, on which scientific productivity will depend strongly.

- Many good ideas on new instrumentation were presented at the workshop (see Appendix 1); the eventual choices should be matched to Australian scientific environment, along with the opportunity to develop niche opportunities, while conforming to available resources.

- Biology is ripe for the development of high-impact neutron scattering applications and the strong biology community in Australia could capitalize very effectively on the neutron scattering capabilities currently under development at OPAL, especially SANS and reflectometry, as well as on potential future developments in high-resolution crystallography and inelastic or quasielestic instrumentation. Appendix 2 summarizes the discussions of the group on the opportunities and strategies for biological neutron scattering at ANSTO.

- Outreach – there is an opportunity for Australia to play a larger role in international collaborative science and the exchange of students - ANSTO may wish to consider establishing an educational program, including rotating lectureships, summer schools, conferences jointly with the synchrotron, international exchange programmes, student fellowships, joint appointments, etc., in order to make major scientific impact and attract the best scientific talent. An effort should also be made to get scattering incorporated into university curricula.

- Joint neutron / synchrotron activities should be encouraged, to maximise the combined scientific impact from neutrons and X-rays.

- A development test-bed / technical beamline should be constructed, for instrument development, training personnel, component testing, and educational purposes.
    - Resources should be made available for one or two major development activities, so that the Bragg Institute is the "place to go to" for something technical. The institute should trade for or buy everything else.

- ANSTO's reward system should be aligned with its objectives (i.e. a mix of service, collaboration and in-house science)
    - A successful user program relies on the excellence of the Institute's staff and the in-house research.
    - Users should be intimately involved in the operation of the instruments
    - Rewards could include promotions, prizes, merit increases for improving instrument operation; recognition and encouragement of collaboration and in-house science, etc.;
    - It is a precondition for a dynamic user operation for the scientists to have their own active scientific programs.

- Access and living conditions for users should be organised to make ANSTO an attractive destination for researchers. Experience at other facilities has shown that amenities such as transportation, lodging and restaurant/café facilities, administration, and an environment conducive to scientific discussion and informal interactions are important to the success of a user operation.

- The Bragg Institute should capitalise on the strengths of the Australian scientific community in developing programmes at ANSTO.
    - This will involve finding a definitive niche, in addition to the broader service role.

- The computational infrastructure must be matched to the data-rate needs of the instruments. Success is bound up with the ability to do adequate computation, and there will be a need for high-power computation, for real-time real-space, modelling and visualisation, during the experiment(s).

- There must be strong interaction between nuclear and scientific responsibilities on an almost daily basis.

- In the immediate term, ANSTO should develop a coherent communications plan to ensure that key stakeholders have accurate and timely information about OPAL, especially during its start-up phase. Key messages might be: world-class science responsive to Australia's research priorities; nuclear science for medicine, industry and energy; successful construction project – on-time, on-budget and safe.

## Appendix 1: Specific 2nd-Wave Instrument Opportunities for OPAL, discussed at the workshop.

### Ultra Small-Angle Scattering (USANS) – Andrzej Radlinski

The case to build a USANS instrument goes back over four years. The working group was formed in December of 2001 at the SANS workshop and a presentation was made to BIAG in February 2003. A recent survey of the domestic community indicated that this instrument has the greatest number of potential users / strongest support of ten surveyed instruments. There is a genuine desire on the part of the existing USANS community to see this instrument realised and some degree of impatience given the lengthy period of time that this instrument has been proposed. The majority of potential users are already using SANS; this group is both the largest from the ANBUG membership (33%) and has the largest IAT.

Applications of the techniques are as diverse as SANS and USANS extends the study of objects to tens of microns. There is a large and active local community with recent examples including ferrofluid emulsions (Greg Warr); inorganic polymers (Craig Buckley); structure of oil bearing rocks and adsorption of greenhouse gases in coal (Andrzej Radlinski), cement (Terry Sabine, Bill Bertram, Laurie Aldridge) and polymer phase segregation (Elliot Gilbert) with experiments having been conducted at NIST, ILL and GKSS.

### 4-Circle Single-Crystal Diffractometer - Chris Ling & Garry McIntyre

The single-crystal diffractometer in the initial suite of instruments (KOALA) will use the quasi-Laue method to achieve extremely high speeds during volumetric surveys of reciprocal space, satisfying the principal needs of the chemical crystallography community. However, the quasi-Laue method is not well suited for certain specific needs of the physics and materials science communities, which include high structural and magnetic precision, complex sample environments, diffuse scattering data (short-range order), parametric examination (P, T, H) of individual reflections, and texture analysis. A monochromatic 4-circle instrument, in a role complementary to that of KOALA, would satisfy these needs and give OPAL a truly comprehensive suite of single-crystal capabilities.

### High-Resolution Inelastic Scattering - Winfried Petry & Rob Robinson

Soft matter physics (including polymers, complex fluids and biology) is strongly related to relaxations and fluctuations, which extend from times below phonon excitations to infinity. Inelastic and quasielastic neutron scattering with high-energy resolution is well suited to address these relaxations. Amongst these, spin-echo spectroscopy has the best resolution and appropriate real-space range. It is also necessary to bridge the 1-100 μeV energy gap between the spin-echo range and that covered by the (funded) crystal-monochromator time-of-flight spectrometer. This is best done with a multi-disk chopper direct-geometry spectrometer. From the Australian perspective, this approach is very well suited for biological problems.

### Neutron Imaging, Radiography and Tomography – Klaus-Dieter Liss & Shane Kennedy

The unique scattering- and absorption properties of neutrons as compared to X-rays allow investigating hydrogen-containing bodies such as plants, moisture, hydrated oxides, oil and polymer in machine parts, future high-tech materials, geological ores, archaeological items, biological and medical systems. Phase contrast methods using pin-hole geometries will have to be investigated and compared with other imaging solutions.

Experience in Europe and North America suggests that the case for a radiography beam-line could not be built on revenue generation alone. It was suggested that commercial activities may constitute ~30 % of beam time. The benefit to ANSTO would most likely come through engagement of a broader applied research community, which could be expected to cross-link with the neutron scattering program (particularly with residual stress and SANS experiments), and may eventually lead to engagement of industrial users.

There may be a case for placing a radiography station on a cold neutron beam (rather than thermal neutron beam), to access different Bragg edges and enhanced contrast variation.

**Magnetism Beam Line - Shane Kennedy**

A 5 Tesla horizontal split-pair cryomagnet is currently being designed in collaboration between Bragg Institute and HTS-100 (a New Zealand based magnet manufacturer). Funding for the construction of this device is being sought from the New Zealand government. New Zealand may also contribute to the funding and development of a 15 Tesla split-pair magnet. Experience in Europe has shown that great care must be taken to shield neutron-spin-echo spectrometers from high field magnets.

The expertise exists within the National Central University in Taiwan to pursue $^{3}$He polarization technology. This presents an opportunity for collaborative development of a range of $^{3}$He polarizing cells for the OPAL neutron beam facilities.

It seems improbable that a case for a 25 Tesla beamline could be made at this stage, however such facilities are planned in Europe and in USA and the OPAL neutron guide hall has been designed to accommodate such a device.

**Grazing Incidence Diffraction and GISANS – Klaus-Dieter Liss**

Modern solid state research including magnetic, electronic and biological membrane systems is focused on nanometer sized structures often in epitaxial or self-arranged layers. Extended investigation methods for strain, disorder, correlations, order etc. are required. Neutron scattering methods can examine the properties of anno particles in one and two dimensions. Both being surface sensitive, GISANS will probe correlations on a nanometer scale in all three dimensions while Grazing Incidence Diffraction (GID) will probe for atomic scale effects like lateral strain in quantum dots or lateral magnetic order in one layer.

**Deuteration Facilities**

ANSTO should ensure that high-quality deuterated chemicals are available for users. They should establish a deuteration laboratory, equip and staff this facility to ensure that routine and custom materials are available.

- Deuterated biomolecules (proteins etc…)
- Deuterated solvents ($D_2O$, organic solvents…)

- Deuterated organic molecules (monomers, surfactants, phospholipids etc…)
- Replacement of hydrogen in inorganic materials
- Deuteration of protein crystals

Such a facility should be established with wide consultation with the user community as well as with other such international facilities.

**Hot Source – Craig Buckley, John Stride & Garry McIntyre**

There was strong support for the installation of a hot source at OPAL to support both elastic and inelastic instruments. This is a potential niche area for ANSTO. Other regional and US reactor sources are not planning one. It would be first outside of Europe.

In particular, there was support for:
- A liquids and amorphous diffractometer to enable PDF analysis.
- An inelastic instrument over the energy range 5-250 meV, that would for example be useful in the study of hydrogen dynamics.

A hot time-of-flight instrument would provide for a large community in physics, chemistry and materials science (dispersive excitations, densities of states, spectroscopy, hydrogen in metals, PDF analysis, elastic/inelastic structure factors, amorphous materials, single/polycrystals). There is a desire for a wide-angle detection capability, not an IN1-Be-filter type. Such an instrument would be unique in world and would benefit regional users as access to spallation source instruments will remain limited.

**Sample Environments**

Expressions were voiced from all present that good, reliable, well supported sample environments were essential.

- The users should not be expected to waste time messing about with them.
- A sample environment device is only used well if there is a local responsible who is interested in using it.
- Current (eg Orange) cryostats are not designed to dissipate 4W of power from sample which can occur with the development of combination in-situ experiments (eg low temperature, polarised light and neutrons).
- European and Japanese centres are currently changing to “liquid free” cryogenics. This provides higher reliability and lower maintenance costs, but demands a higher initial investment.
- High magnetic fields
- High pressure anvils
- Development of new in-situ experiments require new sample environment cells
    - Thermo-mechanical processing
    - uniaxial deformation processes
    - shear stress
    - forging machine
    - fast real time experiments at high temperatures
- Accurate measurement of sample conditions.
- Couple SANS with other techniques - eg spectroscopy.

**Possible enhancements of current instruments**

- More efficient detectors with better resolution are being developed all the time and we should take advantage of this. Possibly learn from X-ray science.
- The current instruments were initiated 4 years ago and technology has progressed since then. Continual improvements to these instruments is necessary to keep at the forefront. This would keep the current expertise (engineers, technicians, programmers ) in-house until needed for new instruments.
- If the background levels do not reach expectations then additional shielding will be required.
- Explore the possibilities of special shaped guides (twists S-shaped, focussing). Aim to split guides early and develop more end positions
- Specific enhancements were:
  - Load frame for the strain scanner
  - $^{3}He$ technology for polarisation into big detectors
  - More options on TAS - polarisation, more detectors, more environments.

## Appendix 2: Biological Neutron Scattering - Jill Trewhella

Biology is ripe for the development of high-impact neutron scattering applications and the strong biology community in Australia could capitalize very effectively on the neutron scattering capabilities currently under development at OPAL, especially SANS and reflectometry, as well as on potential future developments in high-resolution crystallography and inelastic or quasielestic instrumentation. Full development of this community of users should be viewed as a long-term goal as the systems of interest are very complex, and require significant investment in sample production and data interpretation. Realization of the potential will thus depend upon demonstrating success with shorter-term milestones.

For the SANS and reflectometry instruments already under construction, there is an active international community of biological users that can help seed the build up of a vital Australian user group by producing some early high-impact results using the OPAL instruments. SANS is the ideal technique for probing the structures of protein complexes and assemblies, critical for understanding bio-molecular machines and communication in bio-molecular networks. Reflectometry provides insights into biological membranes and the proteins embedded in them.

An essential underpinning for success will be providing a high-quality experience for the first users. This high-quality experience means not only a good neutron instrument, but knowledgeable and available scientific and technical staff to ensure data acquisition and analysis goes smoothly, a quality support laboratory for sample handling, and adequate software tools for data reduction, analysis and interpretation. Biologists are very interested in real-space interpretation, and so computational tools to enable real-time, real-space analysis, perhaps in combination with data from other non-neutron techniques, would be a very big attraction for the community.

Two areas of high interest in biology that would require additional instrumentation are high-resolution structure and protein dynamics.

More than half the users at synchrotron facilities are protein crystallographers looking for atomic-level detail in their structures, and the developing Australian community will have a similar profile in this respect. The recent success of the neutron protein crystallography instrument at Los Alamos has attracted the US protein crystallography community's strong interest because it is a high-quality instrument and neutrons can uniquely provide accurate information on the positions of hydrogen atoms, that are key to understanding enzyme mechanisms and fundamental questions about solvent interactions. *A specialist panel should be assembled to evaluate the potential for neutron protein crystallography at OPAL*. If this capability could be developed at OPAL, it would provide an important window of opportunity for developing a strategic partnership with the already strong and very active biological synchrotron user community in Australia.

The most highly cited biological neutron scattering paper from the ILL is an inelastic-scattering study of protein dynamics, and there is a community of Australian researchers interested in this area. This group should be re-engaged in developing plans for future inelastic/quasielastic scattering instrumentation. There was a strong view among many that this could be a frontier area in which real breakthrough science is possible.

To date, biological neutron scattering has been pursued by a relatively specialized group of experimenters, and the long term success of OPAL will be to attract the “main stream” structural-biology community. Two important strategies for achieving this will be to tap into the naturally developing interest in what can be done in the current frontiers of biology with this new Australian neutron capability, and to work with the developing synchrotron user community to build upon the overlapping expertise, and take advantage of the complementarities between x-rays and neutrons. Key to both of these strategies will be strong collaborations with the universities, especially in the molecular and microbial bioscience departments where the modern biotechnology expertise to make samples optimized for specific neutron scattering experiments exits. In this context it will be important for students in these departments to learn about neutron and x-ray scattering techniques and applications in their curriculum. Financial support to get students to OPAL for training sessions and for experiments will be a valuable investment.

**Summary recommendations:**

Engage the Australian biology community as users of SANS and reflectometry and in planning for future instrumentation for crystallography and inelastic/quasielastic capabilities.

Provide the biology users with the resources needed for a high-quality experience at OPAL.

Develop strategic partnerships with the universities, especially where there is biology and sample-preparation expertise, and get neutron and x-ray scattering modules into the curricula.

Engage the synchrotron bio-user community by developing complementary capabilities and leverage the strong high-resolution structure community that are already strong proponents for the synchrotron sources.

## Appendix 3: List of attendees

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