Report on:

“Scoping Workshop on New Guides, Instruments and Sample-Environment Apparatus at OPAL”

Lucas Heights, 27-28 August 2009
Executive Summary

On 27-28 August 2009, around 80 researchers from Australia and overseas gathered at the Bragg Institute, to discuss the scientific justification and project implementation of the $37M Neutron Beam Expansion Project at the OPAL Reactor. The project builds on the previous successful Neutron Beam Instruments Project (2000-2007), which funded the original suite of 8 instruments, along with 2 subsequent instruments funded in other ways, and features a new split cold neutron guide (CG-2) with two end positions, three new instruments (a second small-angle neutron scattering machine, a high-resolution back-scattering spectrometer and a neutron radiography/tomography/imaging station) along with a substantial suite of sample-environment apparatus. Attendees included representatives of 8 leading Australian universities, 2 CSIRO divisions, 3 ANSTO Institutes, New Zealand and 8 leading overseas neutron laboratories in the USA and Europe.

The case for a second SANS machine rests on the overwhelming interest and demand from the domestic community in soft matter, structural biology, materials science, magnetism and superconductivity. A machine is proposed which will complement Quokka, but with options to reach both lower and higher Q, and a much narrower incident wavelength resolution. A time-of-flight option would also open up short time kinetic studies. Most likely the machine will only need a $^{58}$Ni guide, and it can be located directly adjacent to Quokka.

The back-scattering spectrometer will open up spectroscopic studies at lower energies (longer times) and longer length scales than on the Pelican time-of-flight spectrometer, substantially enlarging the energy range that can be accessed at OPAL. There are some real choices to be made, between (a) the classical-style machine (like IN16), (b) a phase-space-transforming machine (as at NIST or FRM-II), and (c) an inverted geometry time-of-flight machine. The choice is strongly coupled to guide options, and in the next few months, ANSTO should examine and assess all three guide-instrument combinations. It is clear that the classical-style instrument is the only option that can fit into the existing guide hall without significant changes to the existing guide network and instrument layout.

Neutron Radiography/Imaging/Tomography at OPAL will open up the study of engineering, cultural-heritage, fossils, energy extraction and other technologies in which one wants to see hydrogenous materials like water, oils or plastics inside metallic or ceramic objects. The preferred location will be in OPAL’s Reactor Beam Hall on HB-1 or HB-2, and ANSTO should give immediate attention to the issues regarding the overall length of the machine and the effect of its footprint on access to Sika, Taipan and the access hatches in the floor and ceiling. The machine will have extremely high intensity, and will likely give ANSTO the opportunity to excel in dynamic imaging with neutrons.

Regarding sample-environment apparatus, the workshop came up with a prioritised list of magnets, cryogenic devices, furnaces, pressure cells, stress rigs and so on. As for the guides and optics, various options were discussed, along with the risks that the project will face, particularly in managing schedule. But the ultimate choices depend very strongly on the needs of the SANS and backscattering instruments.
In the spirit of the existing naming convention at OPAL, the following names were suggested for the three new instruments: Goanna (2nd SANS), Emu (Backscattering) and Dingo (Radiography).

**GOANNA – The 2nd SANS Instrument at OPAL**

The science case for SANS as a tool for understanding nanostructured materials is well-established. The current SANS instrument, *Quokka*, was over subscribed 4:1 in its first ever call for proposals, attesting to the demand for “workhorse” SANS for the Australian and regional user community. Even after clearing the expected backlog from the current user community, the growth in user number is expected to maintain very high demand. In considering the needs for a second SANS instrument, this demand is a starting point.

A new instrument should also accommodate future science needs in understanding the structure of both natural and synthetic nanostructured materials, which the workshop participants have identified as:

1. **Widening the accessible size range through wider q range, particularly to larger length scales (lower q).** In many applications, a wider dynamic q range is desirable. That is, gathering data over a wide q range obtainable in a single measurement.

Many emerging areas of study include systems that exhibit structure on multiple lengths scales, or are hierarchically structured. Examples include biological materials such as mother-of-pearl, in which the hierarchical structure is not understood at the molecular level, collagen and a wide range of biomacromolecular complexes and extra-cellular matrices. Emulsions may be comprised of nanostructured dispersed or continuous phases such as lamellar phases or microemulsions, or colloidal nanoparticles in either phase or at the interface. At the other end of the scale, nanostructured materials containing ionic liquids as a component need to consider the molecular organization of the solvent.

In order to study such systems, a combination of techniques such as USANS and SANS, SANS and WANS, SAXS/WAXS, or scattering + imaging are currently utilized. This is becoming a serious limitation in that sample preparation for these techniques may not be the same, or reproducible, and reliable investigation of time-dependent behaviour on multiple length scales is virtually impossible.

![Figure 1. Biology on several length-scales: example of collagen. From P. Fratzl, *Cur Op in Coll and Int Science* 8 (2003) 32-39.](image)
2. **Fast data acquisition in order to track kinetic changes in the structure of a sample as a result of chemical or physical changes.**

Many chemical and physical changes that occur in nanostructured systems span multiple length scales. Polymerisation in colloidal amphiphilic systems – e.g. emulsion, miniemulsion, microemulsion and dispersion polymerisation – is very widely used in industry, and may involve the formation and growth of large structures at the expense of small ones. As these techniques become increasingly sophisticated in the control of particle morphology and nanostructure, *in-situ* kinetic tracking of structural evolution will become an increasingly important tool, into which SANS can provide unique mechanistic insights. The advantages of time-of-flight SANS are that the whole small-angle scattering pattern is collected in each time pulse interval allowing both short exposures (for strong scatters and synchronised data acquisition with externally applied stimuli.

The dynamic development of structure under shear, strain or magnetic fields an area of potential expansion in the future.

Current SANS instrumentation typically allows time-resolved studies to be undertaken only over a limited Q range and with slow time-slices, especially at the lowest accessible Q. This can be significantly improved by (i) increasing beam cross section and sample area (ii) lower wavelength resolution, and (ii) use of multiple detectors to capture more than one Q-range. All of this occurs at some cost in resolution, but significantly increases versatility and could be optimized for a variety of applications.

3. **High spatial (δq) resolution to study highly-ordered systems displaying e.g. crystalline or liquid-crystalline order.**

![Figure 2. Flux line lattices of V₃Si measured at ORNL, typical example where excellent spatial resolution (δq) is needed in SANS geometry. From M. Yethiraj *et al.* (1999) *Phys. Rev. Lett.* **82**, 5112](image-url)
There are numerous examples of systems which are highly ordered on one or more of the length scales of interest, and the wavelength resolution of conventional SANS instruments is a serious limitation in understanding such structures. Examples include, identifying phase structure or phase transitions in dispersions of lyotropic phases (e.g. cubosomes, hexosomes) within thick or otherwise x-ray opaque systems, or ordering of colloidal nanoparticles within lyotropic phases. Systems may also undergo ordering transitions dynamically such as under flow, or during chemical reactions. Flux line lattices in superconductors require high spatial resolution.

The new SANS instrument also needs to exist within the suite of neutron beam instrumentation offered at Opal, allowing materials structural characterization over the widest possible range of conditions and length scales as shown in the Table below.

<table>
<thead>
<tr>
<th>Instrument</th>
<th>$q_{\text{min}}$ (Å$^{-1}$)</th>
<th>$q_{\text{max}}$ (Å$^{-1}$)</th>
<th>$D_{\text{min}}$ (Å)</th>
<th>$D_{\text{max}}$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quokka (SANS)</td>
<td>0.0008</td>
<td>1.0</td>
<td>6</td>
<td>7 000</td>
</tr>
<tr>
<td>Kookaburra (USANS)</td>
<td>0.00002</td>
<td>0.005</td>
<td>1 200</td>
<td>300 000</td>
</tr>
<tr>
<td>“Dingo” (neutron imaging)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Goanna</td>
<td>0.0002</td>
<td>1.5</td>
<td>4</td>
<td>30 000</td>
</tr>
</tbody>
</table>

Our objective is to develop an instrument that can operate as a workhorse SANS to meet current community demands, but with the versatility to respond to the growing demand for the three capabilities described above. The instrument will also ‘close the gap’ in Q-range between QUOKKA and Kookaburra.

A chopped beam operating in time-of-flight mode offers advantages for capturing a very wide Q range in a single instrument configuration, increasing the maximum Q to 1.5 Å$^{-1}$ or more. Time-of-flight detection will also allow improved control over spatial resolution by electronic control of time-binning. A high dynamic Q range is enhanced by the use of multiple detectors.

In order to expand the lowest accessible Q, the collimation system should include a slit collimated vSANS configuration as a “drop-in” option, allowing access as low as 4 x 10$^{-4}$ Å$^{-1}$ for 20m sample-to-detector distance. This will allow high beam flux to be used optimally at low Q.

TECHNICAL ASPECTS

Performance Requirements:

Compared to Quokka:

Increased dynamic Q range by factor of 25 (Ability to perform kinetic measurements)
Higher wavelength resolution (at least 2%)
Lower $Q_{\text{min}}$ (at least 2 x 10$^{-4}$ Å$^{-1}$) to overlap with USANS (Kookaburra)
Greater $Q_{\text{max}}$ (at least 2 Å$^{-1}$)
Higher maximum detector count-rate (at least factor of 30)
The above performance requirements can be achieved by the following:

- Time-of-flight disk chopper design
  - Dynamic Q range benefits
- Use of additional high performance / high resolution detectors viz.
  - High resolution (lowest Q) using e.g. DENEX 250CN
  - 2 x 4 movable panel $^3$He multi-tube detectors (each tube of 8 mm diameter x 1 m high)
    - Each panel = 48 tubes either vertically or horizontally mounted
  - Benefits from greater reliability and significantly higher countrates (ca. 100 kHz ORDELA versus ca. 3 MHz per panel)
    - Benefits of greater $Q_{\text{max}}$
- Incorporate movable x-y slit optics into collimation system
  - Improvement in $Q_{\text{min}}$ and overlap with USANS
- 40 m long instrument to access minimum Q
- Incorporate double bounce monochromator into optics to enhance wavelength resolution (down to 2%) as alternative to velocity selector
- Preferable to utilise 200 mm x 50 mm guide cross-section for slit option but is achievable with 50 mm square cross-section
- The use of ballistic guide near sample to increase intensity in slit mode should be considered in simulations as further approach to maximise flux at sample position for faster kinetics studies using more conservative $Q_{\text{min}}$ values (e.g. 0.01 Å$^{-1}$)
  - This would benefit a range of communities including biology for the study of even weakly scattering samples where resolution can be relaxed.
- External detector vessel rail system to accommodate range of sample environments while minimising air scatter (e.g. sample area variable from 0.5 to 2 m without use of expensive gate valve on detector vessel – saving $200K)
- Capacity to incorporate multiple converging pinhole optics

**Budget Estimate**

Detectors:
- 4 x 2 x 48 $^3$He tube detectors plus electronics $2800k$
- DENEX 250CN $200k$

Detector Vessel
- Stainless steel or aluminium (2.5 m) $1300k$
- Rail system for variable sample area $100k$

Sample Area
- 6 degrees of freedom (e.g. AZ Systemes as per Quokka)$300k$

Collimation System
- $^{58}$Ni (to be simulated) 20 m movable guide system plus vacuum vessel including translation tables $1500k$
- Lenses and prism optics $30k$
- Ballistic guide (to be simulated) $100k$
- Double-bounce monochromators $100k$
Bunker
- ASTRIUM velocity selector (8 – 21% resolution) $300k
- Four disk-chopper system (time-of-flight) $500k
- Maximum wavelength cut-off mirror $30k
- Shielding $200k

Electronics and Safety Interlock System $200k

Personnel Costs (12 person years) $1000k

Total $8400k
The principal focus of the “Backscattering Spectrometer Work Group” was to establish the scientific case for a high-energy-resolution inelastic neutron spectrometer as well as to explore different technical options that could be implemented at OPAL within the “Neutron Beam Instruments Project 2” (NBIP – 2).

The purpose of the workshop was to:

- Inform Australian research organisations and universities of the capabilities of high-energy-resolution cold-neutron spectroscopy.

- Promote the use of neutron spectroscopy in order to study phenomena related to quasi-elastic phenomena (QENS) such as:
  - Proton diffusion in metals and oxides
  - Relaxation processes in polymers
  - Self-diffusion in metals and alloys
  - Diffusion processes in liquids
  - Ion diffusion through membranes
  - Diffusive motions in biological systems (proteins, membranes, DNA, cells…)

- Inelastic phenomena, such as:
  - Tunneling spectroscopy in molecular crystals
  - Hyperfine splittings

- Elastic phenomena, such as
  - the study of dynamical transitions in biological systems.

- Identify the future needs and opportunities in this field of research, including those in the study of emerging alternative energy systems, such as new battery and fuel-cell materials.

- Present options for a high-energy-resolution backscattering spectrometer at OPAL and receive feedback on these options.

- Identify equipment that is needed for such type of instrument.

There are important benefits to Australia in building a high-resolution inelastic neutron scattering instrument and the availability of such an instrument will create a pool of experts who may tap into the pool of expertise that is already available at other world-class facilities such as NIST, the ILL or FRM-II. The turn around time for Australian users will be greatly reduced as there is no such instrument available
locally at the present. From an educational perspective a world-class instrument will build expertise in Australia and will almost certainly help to attract graduates.

1. Scientific case and justification for a backscattering spectrometer at OPAL

Many topical issues in spectroscopy require access to long time scales and therefore need high energy resolution. Furthermore time scales of complex systems (e.g. soft matter, biological samples glass forming systems) are stretched over a very wide time or frequency range. Neutron backscattering can access a time scale of several nanoseconds, which is not possible with conventional neutron spectroscopy using time-of-flight or 3-axis techniques. Technically this is possible by using perfect crystals at a Bragg angle of 90° to prepare a monochromatic incident beam and to analyse the scattered neutrons simultaneously over a large solid angle. Thus neutron backscattering is of utmost importance for 'extending our view' onto the dynamics of many complex materials which are in the focus of today’s topical issues.

The proposed instrument is foreseen to be a high-performance, high-resolution instrument adapted to spectroscopic measurements and the scientific case reflects that. Provision of a high-resolution spectrometer at the Bragg Institute will perfectly augment the available infrastructure, most notably the Pelican time-of-flight instrument, by extending the energy scale for motions down to the µeV range, or ns timescales. Various scientific areas are highlighted below; the first four, the core science (biology, chemistry, physics and materials science), are considered to be areas in which users could be attracted immediately. The last three areas, potential science (geo-sciences, environmental sciences and cultural heritage), are thought to be areas of potential growth within the Australian context:

2. Core science and applications

Biology

With the completion of the Human Genome Project in 2003 (about 25,000 genes), biologists are faced with an overwhelming number of new systems that need to be studied at the molecular and atomic levels. Each gene is responsible for making a different protein, which in turn directs and controls a specific process in a cell – for example, enabling a particular chemical reaction to occur using enzyme, or allowing selected atoms or molecules to pass through a cell membrane. The underlying mechanisms are often extremely subtle, and involve complex assemblies of large molecules arranged in precise three-dimensional shapes that move and interact in intricate ways. The exploration of this burgeoning field of molecular biophysics is making huge progress. Teams of scientists around the world are analysing key structures such as proteins, RNA, DNA and cell membranes. To understand fully their biological roles also requires elucidating their dynamics and interactions, in particular in relation to surrounding water molecules which play a significant role in mediating biochemical behaviour.
Inelastic neutron scattering is a tool that is extremely well suited to explore this world at a nanoscale level and a powerful technique to probe the dynamics of biological macromolecules and water. Experiments can be performed close to physiological conditions or under extreme conditions such as high and low temperature. In addition, neutrons can penetrate deeply into a biological sample without damaging it. Finally, hydrogen can be substituted with deuterium isotope to label and therefore highlight different sample components.

The pressure to improve the current structural dynamic biology techniques and methodologies is high, and a number of developments are ongoing at neutron research facilities all around the world. This proposed instrument will allow the Australian biology community to have dynamic data to support a better understanding of mechanisms and functions involved in life sciences, often for molecules that are drug targets or have important pharmacological or technological applications. Neutron backscattering spectrometers are largely used to probe for example, the dynamics of natural membranes and lipids, the dynamics of proteins in interaction with drugs, protein complexed with RNA or membrane, biological systems under extreme environmental conditions (temperature, salinity …) and dynamics of macromolecular water. Recent achievements include oriented membrane investigations, experiments using high pressure, and molecular dynamics measurements in live cells. Understanding biological molecules in their absolute physiological environments is crucial and a big challenge. In the last few years in vivo studies started using the backscattering technique. Experiments were performed with living cells to explore the dynamical properties of macromolecules and water molecules in this crowded and complex environment. Is the cell interior a gel or colloidal-like structure? What is the dynamic state of cytoplasmic water? What are the in vivo molecular dynamic adaptation mechanisms to extreme conditions of temperature, pressure, salinity, or radiation? What are the in vivo proteome interactions with drugs? Answering these questions will certainly open up a new chapter of molecular biophysics.

Chemistry

The application of neutron backscattering techniques to elucidation of dynamic systems in chemistry will find wide application in the existing potential user base across academic chemistry, engineering and materials science in Australia. The particular strength of neutron backscattering lies in its probing of the energetics and dynamics of light atoms – most especially hydrogen. Such questions are not readily addressed by other methods. The ability to locate the position of hydrogen atoms in supramolecular and molecular systems and probe the characteristics of the range of binding sites available will enhance understanding of current materials and provide the understanding from which targeted modifications for particular uses can flow. In catalytic systems the manner in which substrates interact with the catalyst, are transformed and then released with the catalyst reverting to its starting state can all be probed by backscattering with the information gained being strongly complementary to that obtained from laboratory based methods.

The applicability of backscattering methods to potential catalyst systems is also well demonstrated. Again, materials for the “hydrogen economy” are a considerable driving force, but efforts are not restricted to this area. There are numerous highly-regarded research groups located in a range of institutions across Australia
undertaking studies of potentially catalytic materials. Several of these are already actively engaged in the use of neutron diffraction methods for initial compound characterization – most particularly in the crystallographic determination of the presence or absence of hydride. The availability of backscattering to characterize the proposed catalytic activity of these materials represents a major enhancement of local capability and could be expected to be in high demand for this use as soon as it is commissioned.

In order to understand and predict the interplay between supramolecular-bond and macroscopic properties, backscattering spectroscopy presents itself as a desirable tool for investigating the presence of supramolecular bonds and their fluctuations (bond breaking/forming). Specifically materials may be studied in either switched state (phase), achieved either through the external stimulus for the material, or environmental stimuli such as temperature or cosolvent for example. In a self-assembled state –with most bonds formed– this approach brings bond fluctuation rates into the frequency range accessible to backscattering spectroscopy. In the fully disordered state –with most bonds broken– backscattering allows one to looking for dynamical heterogeneities, i.e. signatures of a fraction of the realizing supramolecular linkages. Because backscattering achieves simultaneous sensitivity to frequencies and length scales, such experiments complement the characterization opportunities offered by more classical techniques such as NMR or SANS. The materials concerned with such experiments stem from synthesis approaches pioneered by J.-M. Lehn (France) in the eighties and E. Meijer (the Netherlands) in the nineties, and others, as far as hydrogen-bonded materials. There is now tremendous activity in this field, a recent highlight being the class of self-healing materials proposed by L. Leibler (France). There are also experimental opportunities for illuminating the solvent-phase formation mechanisms of coordination polymers –2D and 3D crystalline networks, with excellent groups in Australia being led by R. Robson (U. Melbourne), C. Kepert (U. Sydney) and S. Batten (Monash U.).

Polymer dynamics is one of the major field in backscattering spectrometry and with the continuously expanding field of polymer applications, the potential of scientific challenges that can be addressed is growing significantly. The advancements in the capabilities of functionalised polymers have not only improved existing polymer applications like industrial and consumer plastics and polymer blends, but has also created completely new applications. In nanotechnology one can see the development of highly functionalised polymer systems to encapsulate pharmaceutical products (drug delivery systems), tuning of hydrophilic/hydrophobic interactions and isolation of internal/external functions in dendrimers, templating polymers and meso-porous polymer systems or polymer blends and polymers with filler materials. Polymers can be synthesized for specific applications like fuel cell membranes, battery electrolytes/electrodes or electronic applications like plastic LEDs or polymer solar cells. A lot of research is aimed at improving the industrial applications of thin polymer foils or polymer film coating as corrosion or wear protection. The research groups that develop functionalised polymer systems have gathered a suite of instrumentation to characterize their systems; techniques for macroscopic characterisation like DSC, modulated DTA and rheology. Often microscopic techniques are required to understand the functioning of polymers on a molecular length and time scale. Research groups apply techniques like NMR, dynamic light scattering or dielectric spectroscopy. In all these fields basic understanding of local
polymer dynamics as a function of parameters like temperature, pressure, pH etc. is essential, which ultimately should lead to better products. Often model systems are prepared with the aim of carrying out high-resolution spectroscopy and comparing the results with theories or MD-simulations. The synergy of computer simulations and backscattering experiments is of increasing importance for the above mentioned complex polymer systems.

In order to achieve the appropriate sensitivity of neutron backscattering spectroscopy to the most labile and/or strongly-interacting functional groups, these studies will rely on cooperation with the National Deuteration Facility.

**Physics**

Materials with high ionic conductivity are of great technological interest in energy storage and conversion and in environmental monitoring. Some important applications of solid-state ionicics are batteries, fuel cells and sensors. Increasing demand for microbatteries led to the development of high-energy-density and long-life-cycle rechargeable lithium batteries. However the Li-ion conductivity is rather low and ways to lift it up are under investigation for both cathode materials and solid state electrolytes. In this respect the quasielastic neutron scattering studies of new Li battery materials are important because they give direct information about diffusion and mobility of ions. High energy resolution is essential for this type of research. Backscattering instruments are therefore well suited as they provide energy resolutions in the range of $\leq 1$ eV.

Other important materials are proton conductors related to the field of protonics with implications for the ‘hydrogen economy’. In these systems QENS studies help to reveal the mechanism of fast jump processes. Solid polymer electrolytes like PEO/LiClO$_4$ (polyethylene oxide) are under extensive study using neutron backscattering spectroscopy. They have a rich phase behaviour that depends on the temperature, lithium concentration, thermal history, and anion identity. QENS studies give information about PEO mobility in different phases.

**Materials science**

So-called modern materials are increasingly relevant in all walks of life as more exacting demands are made upon producers of consumer goods. The revolution in mobile communication and portable computing has been due in a large part to new materials becoming increasingly available – such as high density polymer electrolytes, liquid crystals of use in full-colour displays and organic photovoltaics, high-performance battery materials and functional polymers. Previously conservative engineering fields such as the automotive and aviation industries are increasingly embracing composite materials in a bid primarily to drive down fuel consumption, but also by providing increased functionality such as shape retention components. Nanotechnology is a potential area of growth for Emu, in tandem with its sister instrument, Pelican, and one in which the Australian community has existing expertise. Nanostructures of many types, tubes, rods, wires, ribbons, etc., are currently being produced by a range of techniques and require careful characterization before finding potential technological applications. Emu will be very relevant in determining the precise nature and dynamics in these structures, whilst also being
very sensitive to the presence of entrapped impurities, such as small molecules. With
the depletion of petroleum reserves predicted to become a major concern for
worldwide commerce within 20 to 30 years, hydrogen storage technologies are
paramount for the delivery of the hydrogen economy. Current limitations concern the
containment of the gas either by physi-sorption, chemical absorption, under specific
conditions of pressure and temperature. Emu will be an ideal instrument to study the
adsorption or chemical uptake of hydrogen, whilst the physical properties of
lightweight porous materials could be studied under a range of conditions of
temperature and pressure.

Potential Science

Geo-sciences

The study of the earth’s natural processes is of fundamental importance to life on
earth. The range of subjects, from mineralogy of the crust through to the properties of
the earth’s mantle, are relatively unexplored areas for neutron scattering. This is
despite the advantages of the technique (use of bulky ancillaries to obtain extreme
temperatures and pressures, etc.) and given the degree of Australian expertise in at
least some of these fields. The inherent advantages of the technique of access to high
pressures and temperatures is considered a definite advantage for the study of the geo-
sciences, and the instrument may well service studies into the level of hydration of
minerals, water leaching of rocks and the sequestration of gases as in clathrate-type
materials.

Environmental sciences

The science of our environments, whether it be large-scale urban developments,
sparingly populated tundra or marine ecosystems are intrinsically tied into our
continued well-being. Understanding the delicate interplay of the many contributing
factors is non-trivial, requiring the input from many fields of science and high degree
of computer modeling. Australia has world-renowned research groups investigating
issues such as global climate, urban pollution and oceanography and these provide an
ideal basis for developing this type of research on Emu. Aerosols of different types
can be central to health problems in highly polluted areas and large-scale weather
patterns – could the sensitivity of Emu be put to use investigating these relatively low-
density states? Water usage and depletion of aquifers is also an acute Australian
problem that may see some applications on Emu – intercalated water in clays and
soils, geological hydration.

Cultural heritage

Australia is home to the oldest continuous civilization on earth and has an incredibly
diverse cultural heritage. The non-destructive analysis of artefacts by neutron
scattering techniques can lead to new insights into fabrication techniques and uses
whilst preserving the objects for posterity. Dyestuffs and pigments have been widely
used in the indigenous populations of Australasia. A problem for many curators and
librarians is that of water diffusion into, or degradation of, components of cultural
objects. This may manifest itself as embrittlement of paper, the flaking of paints, etc., and clearly, those effects related to levels of hydration, may be suited to the spectroscopic instruments Pelican and Emu at the Bragg Institute.

3. Instrumental considerations

Options for a Backscattering Spectrometer at OPAL

The design of backscattering spectrometers has advanced considerably since the first demonstration experiment at Munich. Present spectrometers boast large analyzers (>20% of 4π sr), advanced neutron optics, choppers, crystals mounted on choppers and Doppler drives, etc. The design of new backscattering instrument is thus a complex undertaking. The backscattering breakout group identified four basic possibilities for such an instrument at ANSTO. The design is complicated by the space limitations on the proposed new guide CG2. The four possibilities will be referred to as:

1. the “classic” design best realized by the IN16 spectrometer at the ILL;
2. the “PST” design of the NIST Backscattering spectrometer and SPHERES at FRM-II;
3. the “hybrid” design of the new IN16B instrument being built at the ILL; and
4. the time-of-flight option like the BASIS instrument at the SNS and the DNA instrument being constructed at J-PARC.

In the following we discuss the advantages and disadvantages of each of these possibilities and how these characteristics affect the type of science that the instrument will best address.

The Classic Design

Figure 3. Schematic Diagram of the IN16B Back-scattering Spectrometer (courtesy of ILL)
The single most important element that characterizes the “classic” design is the extraction of the beam from the guide through the use of a graphite deflector. The primary advantages of this configuration are that additional instruments can be placed downstream of the backscattering spectrometer (probably not a major consideration at OPAL) and that the detectors are placed far from the high neutron fluence present in the guide thereby enhancing the signal-to-noise on the instrument. This makes it ideal for studying Li diffusion, of importance for optimizing Li-ion batteries. In addition, since there are actually two deflectors, the incident wavelength is changed by “simply” translating the spectrometer along the guide.

The main disadvantages of this design (at least as realized in IN16) are that the dynamic range (in energy) is limited by the narrow wavelength band reflected out of the guide and the mismatch in the Q-resolution between the primary and secondary spectrometer which results in a lower monochromatic neutron current. These can be alleviated to at least some extent through the use of modern neutron optics which can increase the beam divergence that is transported to the instrument and the energy band deflected out of the beam. However the degree of these improvements is not clear. The Bragg Institute should investigate the degree to which the primary spectrometer of IN16 can be improved through the use of high-\(m\) supermirrors and focusing Bragg optics. It is also important to note that in our opinion, the “classic” design is the only possibility that is likely to fit inside the current OPAL guide hall without the use of a bender or an elevated guide.

**The Phase-Space Transform (PST) Design**

The effectiveness of the “classic” design is limited in that the monochromator system has historically supplied a beam with insufficient divergence to take full advantage of the large angular acceptance of the analyzer system. One way to alleviate this problem is the phase-space transform (PST) first proposed by Bert Alefeld in 1984. In this method, neutrons diffract from mosaic crystals mounted on a rapidly rotating chopper that accepts a broad energy range and converts it into a broad angular divergence. In other words the beam goes from “white” to “wide”. This feature has been incorporated into the backscattering spectrometers both at NIST and at the FRM-II.

![Figure 4. Schematic diagram of a Phase-Space Transform Design (courtesy of FRM-II).](image)
This design results in the highest flux on the sample and the widest possible dynamic range that one can attain with a Doppler drive for varying the incident neutron energy. This provides the highest scientific throughput. The primary disadvantage of this design is that the guide ends near the detectors, thus the signal to noise ratio is relatively high. If a PST-type design is chosen, the Bragg Institute must employ all possible means to suppress background. Effective methods employed at NIST and FRM-II include filters and velocity selectors which limit the wavelength spread and a background suppression chopper which limits the time neutrons are present. These methods all reduce the number of unwanted neutrons present at the end of the guide and thus the background.

Changing wavelengths is also a bit more problematic as the instrument must rotate (around the PST) to change angles and the flux gain arising from the PST is not as high for shorter wavelengths. Thus, if the PST design is adopted, the Bragg Institute should carefully consider whether or not to provide multiple wavelengths.

**The Hybrid Design**

It is possible to design the instrument so that the instrument can operate in either the classic mode or the PST. The user can then collect data in a low background mode for those problems that require the best possible signal-to-noise. On the other hand one can use the PST for those problems that benefit from the highest count rate. This is the design adopted for the new backscattering instrument IN16B at the ILL. A changeover between different configurations will nevertheless be a major intervention of 1-2 days.

**The Time-of-Flight design**

The best energy resolution that the Pelican instrument will achieve is \( \approx 60 \, \mu \text{eV} \) giving rise to a gap in the spectrometer accessible energy range when Pelican is combined with any of the three previous instrument design options. This would be an issue for systems including biological materials and polymers that have dynamics covering a wide range of time scales. The time-of-flight design option as realized at the SNS would naturally cover this range. This would require a chopper system to create a pulsed white beam followed by a long flight path. Additional choppers would be needed to prevent frame overlap. The required length of this flight path or the rather short neutron pulses that would be required mean that such an instrument would have a slightly relaxed resolution of perhaps 5 \( \mu \text{eV} \). In addition, the need to chop the beam means that this design provides the lowest count rate at the elastic line of any of the design options.
Figure 5. Schematic Diagram of a time-of-flight Back-Scattering Spectrometer (courtesy of Eugene Mamotov, Oak Ridge National Laboratory).

Summary Table

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Resolution</th>
<th>Dynamic Range</th>
<th>Count Rate</th>
<th>Signal-to-noise</th>
</tr>
</thead>
<tbody>
<tr>
<td>IN16</td>
<td>&lt; 1 eV</td>
<td>&lt; 30 eV</td>
<td>1/2 High</td>
<td>Good</td>
</tr>
<tr>
<td>Spheres</td>
<td>&lt; 1 eV</td>
<td>&gt; 30 eV</td>
<td>High</td>
<td>1/2 Good</td>
</tr>
<tr>
<td>BaSiS</td>
<td>5 eV</td>
<td>200 eV</td>
<td>Low</td>
<td>Best</td>
</tr>
</tbody>
</table>

General instrument components needed

Whatever instrument layout will be considered, there are several components which are in common and have to be considered.

Primary guide

A bent primary guide is not recommended due to the high losses induced. Furthermore this solution would allow for a single wavelength only. Placing the instrument on a mezzanine seems inadvisable. The whole instrument including its vacuum chamber will probably weigh 20-30 tons. The Doppler drive may introduce vibrations. S-shaped guides are not advisable and an inclined instrument will impose risks in operation. The guide divergence has to be matched to the mosaic of the PST and a sufficiently large divergence is needed to guarantee the 31µeV energy transfer.
after PST-effect.

**Doppler drive**

It is strongly recommended to buy a commercial Linear Motor Doppler drive from AEROLAS (unique producer; costs ~300k€). The same drives are running at FRMII and ILL (IN16B) for 3 and 2 years, respectively, without major problems. The energy transfer range for Si(111) will be 31µeV with this drive and within limits different velocity profiles and amplitudes (< ± 75mm) can be used. It should be noted that the increased energy transfer is achieved by a large amplitude of displacement, which increases optical errors (slight degradation of energy resolution).

![Image](image_url)

**Figure 6. The Linear Motor Doppler Drive for IN16B at ILL (courtesy of AEROLAS).**

**Chopper or PST**

A slower running chopper as on IN16 avoids the need to enclose the graphite deflectors in a cassette and thus windows (IN16: ~75 m s⁻¹). An IN16-type chopper allows for improvement by using better graphite crystals (minor engineering input). If a PST is selected the first choice required is between two designs: a disc with 2 windows (IN16B) which is more compact (R~35cm) but introduces higher crystal acceleration, or - a disc with 3 windows (HFBS, SPHERES), which is bigger (R~60cm), but has reduced crystal acceleration. Larger discs make a larger shadow on the analysers. All discs would probably run at about 250 m s⁻¹, which according to recent calculations, seems to be the optimum speed. In all cases the crystals have to be packed in cassettes. The horizontal crystal inclination within the cassettes, and the intrinsic and effective mosaic of the crystals, must be optimized for the primary guide divergence. All PST solutions need important engineering input (even if copied) for layout and testing.

**Secondary spectrometer housing**

Clearly a vacuum chamber would be desirable to minimize gas/air scattering and therefore the background. At NIST the background decreases by a factor of 3 when pumping the secondary spectrometer. On the other hand a vacuum vessel significantly reduces the flexibility of the spectrometer as well as access to the sample area. The vessel size may become critical if in addition to Si(111) other analyser configurations are to be used. Stability calculations are needed (important engineering input for layout + calculations). Attention must be paid to ensure that the
analyser alignment is not disturbed by the deformation of the scattering chamber due to the vacuum. Alternatively an Argon gas chamber can be built, which similarly restricts flexibility (long flushing times), but is less demanding regarding chamber size (SPHERES) and engineering issues. Introducing flight boxes is the most flexible solution, but leaves air gaps around the sample area and introduces windows (4 neutron passages - IN16).

Analysers

First a choice of the analyser crystals has to be made:

Si(111) single crystals are certainly the first option, and it is recommended to have two sets of these:

- undeformed crystals (for ~ 0.4µeV energy resolution) and
- deformed Si(111) crystal setup (resolution can be tweaked by choosing the appropriate thickness of crystals as $\frac{E}{E} \sim 2 \frac{d}{d} = 0.88 \frac{t}{R}$)

If two sets are realised then the deformed crystal setup should be optimized for a resolution near 1µeV or slightly higher (d~0.8-1mm). This guarantees complementarity of both setups and increases the intensity of the deformed crystal setup. If only one analyser setup is desired then the choice of the SPHERES crystal thickness is probably near optimum (~0.65µeV).

Access to large Q-values requires using Si(311) crystals (Q~3.7Å⁻¹): If this option is realised it would immediately rule out the bent guide solution which allows for only one wavelength. The thickness of Si(311) should be chosen to give an energy resolution in the range of 4-6 µeV and provide a sufficiently large dynamic range. Attention should be paid that the chopper/PST can rotate fast enough to allow Si(311) neutrons returning from the monochromator to pass.

Detectors

Probably a multidetector array with vertical space sensitivity would be of interest (e.g. new IN16B development).

Diffraction detector

A simultaneous diffraction detector should be considered. User demand for this feature at IN16 is very high.
DINGO – The Neutron Radiography, Tomography and Imaging Station at OPAL

Why build a neutron imaging facility?

Neutron Imaging has seen a rebirth after the introduction of electronic imaging detectors (mostly CCD cameras) in the early 1990s. Electronic imaging processing allows for image normalization for the beam profile, contrast enhancement and region of interest imaging as well as computed tomography. It is a powerful tool for non-destructive testing and evaluation, with properties complementary to X-rays: Most metals can be penetrated easily, while the hydrogen content of all organic materials can be detected with high sensitivity even through thick metal walls of machine parts and others.

For problems that cannot be solved with X-rays, there is a high probability that they can be solved with neutron imaging. Applications are in industry, non-destructive testing, archaeology, biology, geology and fundamental research.

Currently, there is only one neutron imaging facility in the Southern hemisphere, in South Africa. The best facilities in the Northern hemisphere (FRM-II, PSI, HMI, NIST) are fully booked, even overbooked by scientific and industrial applications, so there will definitely be uses for an Australian facility once it has become known to the Academic and industrial world.

Imaging methods

Currently applied imaging methods are:

Neutron Radiography:
simple shadow imaging like X-ray exposure.

Neutron Computed Tomography:
Collection of many different angular views of a sample through 180 or 360 degree to reconstruct a three-dimensional image

Phase Contrast Imaging or Diffraction Enhanced Imaging:
The use of a very small pinhole plus long flight tube generates a beam with lateral coherence, which allows to use diffraction effects for edge enhancement. This technique allows for sensitive examination of e.g. Aluminium foams, and can even distinguish an interface between two different Aluminium alloys. Works best with long wavelengths, i.e. cold neutrons.

Stroboscopic Imaging:
The use of a cooled CCD camera with image intensifier allows for the examination of periodic processes with high time resolution. The image intensifier is used as a fast shutter that is repeatedly triggered on identical time windows of the periodic process in the ms range until sufficient intensity has been accumulated on the detector for a good image.
Example: Running car engine.
Energy Scans and Bragg-Edge Imaging:
The use of a double crystal monochromator allows for energy scans, though with a drastically reduced intensity. Many materials, esp. cast metals, build crystalline phases with a certain lattice constant. If the wavelength of the incoming neutrons becomes greater than that lattice constant, there will be no more coherent (Bragg) scattering, which leads to increased transmission of the neutron beam. Latest Experiments show that it will be possible even to detect stress and strain with sensitive energy scans. Most Bragg edges lie in the energy range of cold neutrons.

Magnetic imaging:
The most recent research is done with polarized neutrons, and depolarisation measurements of the beam. $^3$He cells are used as polarisers and analysers. Measurements are performed on magnetic fields, and on Quantum Phase Transitions in crystals between the paramagnetic and ferromagnetic state. A monochromatic beam in the cold energy range is required.

High-resolution imaging:
Recent research with ultra-thin scintillation screens has reached spatial resolutions between 20 and 30 micrometers. The available neutron flux on this length scale is very small. To obtain reasonable contrast on this small scale, the higher interaction probability of cold neutrons is suited best.

Thermal or cold neutrons?
While thermal neutrons have a slightly higher penetration capability, cold neutrons are to be preferred for most applications due to increased interaction probability, longer wavelengths for diffraction effects, and the possibility of Bragg Edge Scans which can be performed only with cold neutrons. Should a combination of neutron optical elements (neutron guides etc.) plus flight tube be used, then cold neutrons provide a larger reflection angle, leading to larger beam spread.

Neutron guide or flight tube?
Early neutron radiography installations for film suffered from bad and blurred image quality: it is only in the last two decades that resolution has not been limited by the available detection system, but rather by poor beam collimation. Today’s electronic detectors, with their increased sensitivity, allow one to sacrifice neutron flux in order to obtain higher image resolution.
The measure for beam collimation is expressed as the ratio of the distance L between the sample and the diaphragm (smallest diameter) of the initial collimator and the diameter D of that diaphragm.

Typical early film installations worked on collimation ratios of 30 to 50, whereas the minimum collimation of the new ANTARES facility at FRM-II can be selected as 400 or 800.

An installation on a beam tube without any neutron optical devices has the big advantage that the beam collimation is only determined by the geometrical properties of collimator and flight path, and is independent of the wavelength. By exchangeable apertures, the collimation and beam intensity can be optimised for each application.

A neutron guide will destroy the initial collimation by its multiple reflections. A typical Nickel coated guide has, directly at its exit, a collimation of about 70 for cold and 115 for thermal neutrons. (Schi95) A supermirror guide will decrease the available collimation inverse proportional to its m-value.

The collimation of a neutron guide setup can be increased by adding a circular diaphragm to the end of the guide (sacrificing a major part of the available neutron flux) plus a long flight tube. In sufficient distance, the geometrically defined collimation will apply.

Such an installation exists at the former Hahn-Meitner-Institut, now Helmholtz-Zentrum, Berlin.

The initial neutron guide causes further problems.

The following pinhole effectively creates a pinhole camera that will image the incoming neutron guide to the sample position. The smaller the diaphragm, the clearer will be the structure of the neutron guide, including all joints between segments, which results in a vertical stripe structure. Should the intensity variation between the stripes become greater than 20-30% of the maximum intensity, beam normalisation may become impossible, and thus computed tomography will no longer be possible.

If the incoming guide is curved, which applies to most neutron guides, the spectrum will be inhomogeneous, shifted towards higher energies at the outside of the curvature due to garland reflections. This can be partly compensated by a long straight section of neutron guide after the curved section.

Assuming that the pinhole at the end of the neutron guide is in the order of 2 cm, the maximum (energy-dependent) reflection angle of the supermirror guide will cause the beam to spread on its consecutive flight path. For each wavelength, the spread angle will be $2 \times m \times 0.1 \degree \times$ wavelength(A).

For a cold spectrum with its centre at 3.5 A, a m=2 super mirror guide, and 10 m flight path (resulting in $L/D=500$), the available beam diameter will be in the order of 26 cm. For a thermal spectrum with its centre at 1.8 A, it will be only 14 cm.

But in reality, there is a different beam spread for each wavelength, meaning that a homogeneous spectrum is available only in the centre part of the beam, with the average wavelength shifting to larger values with the radius from the centre beam axis. A spatially inhomogeneous spectrum will deliver inhomogeneous attenuation values even for homogeneous materials, making quantitative techniques like computed tomography more difficult, and less sensitive to small variations.

If a flight tube without neutron optical devices is installed, the beam will only be defined by the geometry of source area, collimator and flight tube, with no energy-dependent effects.
The beam diameter will be defined the diameter and position of the diaphragm, or the smallest diameter of the collimator system. If the ratio of the sample-to-diaphragm distance \( L \) to the diaphragm diameter \( D \) is kept constant, then the neutron flux in the centre of the beam does not depend on the position of the diaphragm related to the source, but the diameter of the beam does. In case of a flight tube installation, the smallest diameter of the collimator should be placed just outside of the biological shielding, where additional smaller diaphragms can be exchanged to provide variable \( L/D \) ratios. The flux at the sample position \( \Phi_s \) can then be derived from the flux at the diaphragm \( \Phi_d \) as \( \Phi_s = \Phi_d / (4L/D)^2 \).

At the ANSTO experimental hall, the flux is given as \( 3.6 \times 10^{10} \text{n/cm}^2/\text{s} \) (for wavelength > 0.9 Å). We can then calculate the expected flux for the sample position for different collimation ratios as:

\[
\begin{align*}
\Phi_s (L/D=200) &= 5.6 \times 10^8 \text{n/cm}^2/\text{s} \\
\Phi_s (L/D=400) &= 1.4 \times 10^8 \text{n/cm}^2/\text{s} \\
\Phi_s (L/D=500) &= 9.0 \times 10^7 \text{n/cm}^2/\text{s} \\
\Phi_s (L/D=800) &= 3.5 \times 10^7 \text{n/cm}^2/\text{s} 
\end{align*}
\]

This flux – although thermal, compared to cold – is even higher than the flux at the ANTARES facility of FRM II at Technische Universität München, Germany, which provides

\[
\begin{align*}
\Phi_s (L/D=400) &= 1.0 \times 10^8 \text{n/cm}^2/\text{s} \\
\Phi_s (L/D=800) &= 2.6 \times 10^7 \text{n/cm}^2/\text{s} 
\end{align*}
\]

To calculate the useable beam diameter, we must look at the possible geometry in more detail.

Between the reactor face and the back wall, there is about 10.6 m space. The imaging facility needs a blockhouse with about 75 cm wall thickness. The crane does not reach to the back wall, so the back wall must be moved into place by air cushions, which need about 0.5 m space behind the wall. The inside wall will be 1.25 m from the back wall of the experimental hall. Considering the space for the detector, the sample position will be at least about 0.85 meters from the back wall, and thus 8.5 meters from the reactor face. (The reactor face is about 4.3 meters from the beginning of the beam tube nozzle. ) A collimator and shutter wheel is suggested at the outside of the reactor wall, putting the smallest diameter \( D \) at roughly 0.5 meters from the reactor face. The available \( L \) is thus about 8 meters.

This gives us the diameter \( D \) for the appropriate collimation ratios:

\[
\begin{align*}
D (L/D=200) &= 4.0 \text{ cm} \\
D (L/D=400) &= 2.0 \text{ cm} \\
D (L/D=500) &= 1.6 \text{ cm} \\
D (L/D=800) &= 1.0 \text{ cm} 
\end{align*}
\]

Let \( D_0 \) be the diameter of the beam tube nozzle, \( D \) the diameter of the diaphragm, \( D_s \) the diameter of the fully illuminated beam at the sample position, and \( D_u \) the diameter
of the penumbra region, and $L_0$ the length between beam tube nozzle and diaphragm, $L_1$ the length between diaphragm and the sample position.

Then we get

$$D_s = \frac{L_1}{L_0} (D_0 - D) - D$$

and

$$D_u = \frac{L_1}{L_0} (D_0 + D) - D$$

With $L_0 = 5.0$ m, $L_1 = 8.0$ m and $D_0 = 0.2$ m (vertical) and $D_0 = 0.14$ m (horizontal, limited by the beam channel, and assuming a square source area at the beam nozzle of 20 x 20 cm$^2$)

we get vertically

$$D_s (L/D=200) = 21.6 \text{ cm}$$
$$D_s (L/D=400) = 26.8 \text{ cm}$$
$$D_s (L/D=500) = 27.8 \text{ cm}$$
$$D_s (L/D=800) = 29.4 \text{ cm}$$

and horizontally

$$D_s (L/D=200) = 12.0 \text{ cm}$$
$$D_s (L/D=400) = 17.2 \text{ cm}$$
$$D_s (L/D=500) = 18.2 \text{ cm}$$
$$D_s (L/D=800) = 19.8 \text{ cm}$$

The penumbra region extends even further, giving the area where the intensity drops down to zero.

We get vertically

$$D_u (L/D=200) = 34.4 \text{ cm}$$
$$D_u (L/D=400) = 33.2 \text{ cm}$$
$$D_u (L/D=500) = 33.0 \text{ cm}$$
$$D_u (L/D=800) = 32.6 \text{ cm}$$

and horizontally

$$D_u (L/D=200) = 24.8 \text{ cm}$$
$$D_u (L/D=400) = 23.6 \text{ cm}$$
$$D_u (L/D=500) = 23.4 \text{ cm}$$
$$D_u (L/D=800) = 23.0 \text{ cm}$$
**Draft project plan and schedule:**

**Year 1:**
1. develop collaboration between FRM II and OPAL to gain efficiencies based on the newly designed ANTARES II.
2. Instrument advisory team (IAT): proposed members
   B. Schillinger, E. Calzada, P. Vontobel, E. Lehmann, M. Hoffmann, R. Lewis, L. Edwards, B. Harrison, F. Bartsch
   Propose 6, 12, 24, 36 month schedule
3. Conceptual design of shielding and instrument in the reactor beam hall RBH for PCG and IAT approval
4. on approval detailed shielding design and design review by MC calculations
5. design of instrument optics and components layout (internal or external pinhole)
6. immediate purchase of CCD camera package, scintillation screens, CMOS camera, test and development server and software package
7. factory acceptance testing of detector systems
8. define list of motion control requirements
9. define safety interlock system for hot beam line and SAC approval

**Year 2:**
10. final design review and preliminary regulatory review
11. detailed specification and tender review
12. purchasing and procurement of remaining instrument components
13. manufacturing and delivering instrument and shielding components
14. factory acceptance testing of sample stage and beam optics
15. software development
16. develop user community and collaboration

**Year 3:**
17. continue manufacturing and delivering instrument and shielding components
18. software testing
19. installation
20. cold commissioning of individual components

**Year 4:**
21. continue installation
22. radiation surveys and licence approval
23. hot instrument commissioning
21 friendly users experiments

**List of key components:**
1. Shielding walls and roof
2. detector systems (standard CCD and high speed CMOS)
3. high res and high efficiency scintillation screen
4. motion control system (24 axis)
5. safety interlock system
6. pinhole and aperture infrastructure
7. beam optics
8. sample stage (rotation and translation)
9. fast shutter
10. selector wheel for pinholes (phase contrast)
11. selector wheel for crystal filters (sapphire and Bi, Be)
12. instrument cabin
13. data acquisition rack and servers
14. DAE, SICS and DAV software

Project risks:
1. cost: minimal (based on existing design at FRM II)
2. schedule: minimal (based on existing design at FRM II)
3. performance: subject to instrument location (RBH HB1/2 low, NGH TG-1 high)
Sample-Environment Apparatus

Sample environment is a key area in a user facility: it serves a number of very different instruments with systems able to immerse samples in low or high magnetic fields, to expose them to different gas at different pressures, with very accurate temperature, humidity, pressure, vacuum controls and so on. The environment can be determined by a gas flow, a magnetic field, an applied electric field, pressure or a combination of them at a range of temperatures from few milliKelvin to thousand of degree Celsius. Controls and cabling can reach a high level of complexity and the standardization of procedures and systems has been the best practice in leading institutions worldwide in order to minimize potentially catastrophic errors and lost of precious measuring time.

In determining the top priorities and the future research trends, consultation with the local users’ community and with leading researchers overseas is of paramount importance. The present necessities for instruments need to be addressed and future trends need to be anticipated allowing performing critical scientific experiments in a timely manner.

Two breakout sessions for the sample environment were held, as part of the workshop. These sessions have been in charge to address the future necessities for sample environment and to specify which instruments should be acquired under the frame of the NBP-2 program. The key questions to be addressed are what sort of equipment is needed, what magnets and relative specifications. It has been required to prioritize the items list and to identify the pieces of equipment that will offer unique scientific opportunities at ANSTO taking into account the recent investment in 3He. Furthermore, it has been asked to provide a realistic budget and a schedule estimates taking into account the experience and lessons learned in previous similar projects.

This document summarizes the results of the lively and engaging discussions during the sample environment sessions. Under the NBIP-2 program we propose 16 items for investment, as listed and indexed with their priorities in the table at the end.

A review of the necessities of the local user community was undertaken in July 2009 and a first list of requested instruments was presented and discussed during this workshop. Around 25 key users attended the sample environment sessions so we believe the final resulting list well represents the needs of the user community. The exception to this was the soft condensed matter group, who were unfortunately underrepresented due to conflicting breakout sessions. The list of necessary equipment has been developed taking into consideration not only the general necessities of the Institute, but also necessary consideration has been given to specific instruments that can give unique science opportunities to the Bragg Institute and could represent an exceptional step forward for the Australian scientific community.

- Cryogenic and Magnets

For cryogenics equipment we recommend an investment of $2 280 000. With the proposed 12T asymmetric vertical magnet and dilution fridge inserts (>50 mK) the Bragg Institute will compete favourably with the key US and European institutions. This magnet is quite similar to a recent ILL and ISIS purchase and thus there is a relatively low risk of a delay in the commissioning date. A cryopol (cryogenic
polariser, ILL design) is the key device to exploit the recently ordered \(^3\)He polarisation system and we recommend that one to be purchased. This will open a new field of science on the powder diffractometers (i.e., magnetisation distributions in molecular magnets, nano-scale samples, etc). We also recommend the purchase of a low-cost vector magnet (horizontal + vertical) to create a niche in the area of magnetic neutron scattering. Besides adding flexibility it allows for magnetic field at arbitrary angle with respect to the scattering vector, which is of use for investigations of complex magnetic structures, including multiferroic materials.

- **High Temperature**
The acquisition of high temperature equipment is necessary in order to complement the presently existing ILL type vacuum furnace and to expand the range of science available on the new in-situ reaction chamber (ISRC). An innovative levitation furnace design is currently under development within the framework of the European NMI3 project. It should be available in 3 years time, therefore inside the timeframe of the NBIP-2 program. The acquisition of such an instrument will greatly improve the ability to assess materials at higher temperatures and it will have an important impact on current research about high temperature innovative materials.

- **Pressure and gas control**
There is a relatively low amount of high pressure equipment currently available at the Bragg Institute. For this reason it is considered important to investment in this field starting from standard basic equipment like pressure clamps, continuously loaded cells and compression rigs.
In order to comply with the upring demand of gas absorption community (eg neutrons for the hydrogen economy) we propose a major investment in gas handling systems with automated controlled mixing, gas flow and adsorption options.

- **Basics**
Beam time is currently being lost due to a lack of existing basic infrastructure. Thus a significant investment is required in standardized equipment including pumping, thermometry, temperature control, leak testing. This equipment should conform to other institutions overseas. On one side this will simplify the experimental work for national and international users and on the other hand it will allow following the best practice trends already present in overseas leading institutions.

- **Soft Matter**
A priority list of equipment for the soft condensed matter group should be developed at a later date with the key scientists.

- **Time schedule**
The estimated completion time for most of these purchases is ~18 months. However we estimate up to ~36 months for 3 customised, but prototyped items (12T magnet, Cryopol and levitation furnace).

- **Final Recommendations**
Based on the experience of the HMI and ILL sample environment managers it is essential that at least 2 technicians be brought on board to commission this new list of equipment as it arrives at the Bragg Institute in order to have it immediately available for the users. In the longer term the aim is to strengthen the sample environment team.
and to ensure reliable operation over a long time span of this very specialized equipment.

The discussion group strongly agreed with the following 2 recommendations:

R1: A helium gas recovery system, including liquefying system must be implemented at the Bragg Institute in order to comply with environmental requirements & reducing long term operational costs.

R2: A sample preparation and characterisation laboratory, to the best international standards, is required for users to obtain the maximum output from the neutron scattering experiments. This will also assist researchers from regional universities who do not have access to such facilities to better prepare for experiments at the Bragg and other Australian large scale facilities.

**- Investment List**

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Cost</th>
<th>Priority</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basics (controllers, tubing, pumps, thermometry etc.)</td>
<td>$500,000</td>
<td>1</td>
</tr>
<tr>
<td>12T asym magnet + 50mK dil insert</td>
<td>$1,500,000</td>
<td>1</td>
</tr>
<tr>
<td>1T vector field magnet (hor. / vert.)</td>
<td>$200,000</td>
<td>2</td>
</tr>
<tr>
<td>Cryopol</td>
<td>$300,000</td>
<td>1</td>
</tr>
<tr>
<td>1 Orange cryostat</td>
<td>$80,000</td>
<td>2</td>
</tr>
<tr>
<td>2 Closed cycle cryostat</td>
<td>$200,000</td>
<td>1</td>
</tr>
<tr>
<td>Pressure clamps</td>
<td>$150,000</td>
<td>1</td>
</tr>
<tr>
<td>Continuously loaded cells</td>
<td>$250,000</td>
<td>2</td>
</tr>
<tr>
<td>Compression rigs</td>
<td>$400,000</td>
<td>3</td>
</tr>
<tr>
<td>Furnace for Euler cradle</td>
<td>$100,000</td>
<td>1</td>
</tr>
<tr>
<td>3 inserts for ISRC</td>
<td>$150,000</td>
<td>1</td>
</tr>
<tr>
<td>Levitation furnace (aerodynamic)</td>
<td>$300,000</td>
<td>3</td>
</tr>
<tr>
<td>Gas handling systems for mixing</td>
<td>$100,000</td>
<td>1</td>
</tr>
<tr>
<td>Gas handling systems for adsorption</td>
<td>$500,000</td>
<td>1</td>
</tr>
<tr>
<td>Soft matter equipment</td>
<td>$250,000</td>
<td>1</td>
</tr>
<tr>
<td>Labor, commissioning, etc (8 p.y.)</td>
<td>$800,000</td>
<td>1</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>$5,780,000</strong></td>
<td></td>
</tr>
</tbody>
</table>

**SAMPLE ENVIRONMENT AND LABORATORY FACILITIES for Small-Angle Scattering**

1. The instrument that has been proposed will be capable of measurements over a wide range of momentum transfer and, because of its time-of-flight capability, will be capable of observing the whole Q range selected in short periods of
time. The scattering power of the sample will be the limiting factor on the choice of the time buckets selected for kinetic experiments. The design process should illustrate the options available for users in both Q range and time scale.

2. For these types of experiments not only is it essential to have freshly prepared materials (bio systems) but it is also necessary to avoid tedium in the operation of the instrument by ensuring that command files can be used to control not only DAC but also parameters of ancillary apparatus such as sample conditions and timing of external changes imposed upon the sample.

3. The instrument as proposed will be capable of performing a wide variety of chemical, bio, and engineering related experiments. The working group thus considered that the provision of electronically controlled peripheral systems was essential to take full value from the choice of instrument that is being made. The possibilities of the very high dynamic Q range, the variable wavelength resolution from 2% to 14%, the increased intensity at Q and the projected min Q of 0.0001 Å⁻¹ offer great scope in these experiments.

4. For routine exploratory work sample changers (variable temp) capable of holding both Banjo cells and rectangular Helmer cells are required. The importance of the rectangular cells relates to the option of using a fine rectangular slit and the DENEX high resolution detector to go to a Q_min of 2*10⁻⁴ Å⁻¹. We considered this option very important for extending the exploratory work of the instrument and as a complement to Quokka.

5. In relation to time-dependent experiments, we propose several costly pieces of equipment:

*Stop flow apparatus.*
For experiments involve chemical reactions, biological systems, such as proteins and DNA, protein-nanoparticle interactions, kinetic of association is important. Measurement of this phenomena is function of variables such as pH, salt content, and concentration will give small angle scattering unique insight into mechanism.

*Anton-Parr Rheometer;* there is strong track record in Australia of self chemistry, polymer and colloid science. This instrument which allows *in-situ* measurement of small angle scattering from colloid components as function of contrast as a running medium and conditions of controlled shear has been shown to provide fundamental insight into the relation of macroscopic properties to microscopic and nano structure. For this work, it is essential that rheometer be controllable electronically with this spectrometer by recommended file. It must also be capable of simultaneously measurement the real and
imaginary parts of shear response of the colloid system as function of temperature. Additional feature needed in the instrument for some of applications is ability to synthesize the dispersion in-situ while small-angle scattering is being observed.

Temperature jumper apparatus; For experiments requiring observation of rapid reaction and also to observe the temperature dependence of system such as described about for stopped flow, a dedicated temperature jumper system will be required.

Cryo fumes; A number of solid states chemical reactions need to be followed as extensive temperature ranges using contrast variation in isotopic mixture, small angle scattering is available to fast quench of reaction of high temperature to isolate intermediate

Pressure cell; many biological reactions have large volume changes due to changes, for example, in protein conformation. These reactions can be studied effectively by changing the external pressure which influences both the reaction rate (through the volume of activation) and also the reaction outcomes through the volume change in the reaction. For this reason we propose that a pressure cell be built for the small angle instrument.

Laboratory facilities and technical support
Research in soft matter has not such a great need for very costly ancillary apparatus (dilution refrigerators, high field magnets etc…) as does work in ‘hard matter’. What is most essential is the provision of separate chemical and biological laboratories at which there is technical help for doing chemical and biological synthesis on the site. World’s best practice in this respect provides scrupulously clean glassware and manipulative instruments, readily available for researchers when they arrive at the facility. This then allows the preparative processes needed and the quick set-up of experiments to exploit the neutron scattering apparatus to maximum effect.

Typical apparatus needed for biological preparations are centrifuges, chromatography, protein and nucleic acid purification, dynamic light scattering (to check aggregation) and UV-visible spectrometers for amino acid estimation.

On the chemical side it is essential to have dry box facilities vacuum furnaces and vacuum systems, which will allow the manipulation in glass and transfer into sample containers of air sensitive materials. We consider these ancillary components of the use of the spectrometer as important as the necessary devices required for hard matter research. It is also the view of this group that there should be some in-house development of such devices; the success of the in-house designed Rapid Heat Quench Cell is a key example of this. A key matter in all of these developments is the recruitment of able technical and in
some cases scientific capacity capable of accepting the frequent and continuous requests of the user community. An approximate cost-estimation of these requirements including some which will overlap with requests from the hard-matter community (electro-magnet, gas adsorption apparatus and Instron) is given in the list below:

- Electromagnet $200k
- 20 position sample changer as per Quokka $50k
- VSANS sample changer (30 mm – 75 mm height) $50k
- 10-position thermostatted sample changer $50k
- Gas adsorption system $500k
- Temperature bath $15k
- Tensile tester (Instron) $200k
- Anton-Paar Rheometer $300k
- Pressure cell $300k
- Cryofurnace $500k
- Stopped flow $250k
- Temperature-jump cell $200k
- Humidity chamber $100k
Guides and Optics

**Questions posed to other workshop groups**

1. What should the guide deliver to the instruments in terms of
   - Flux?
   - Wavelength range?
   - Divergence?
2. What should the benchmark be for each instrument?

**Timeline**

Concepts should be decided and locked around March 2010. Guide orders should be placed around June 2010, but allow collaborative tweaking of the design.

**Important Timing Issues**

Big instrument work should be planned to coincide with in-pile work and shut-down (end 2011 / early 2012 but flexible). All cold guides will be shut down longer than this for installation of integrated shielding. Existing in-pile guide should be replaced during CG2 installation. At this point an improved design should be considered, for example elliptic nose, shared funnel splitters etc. Existing operations should not disturbed (platypus stays where it is if possible). MCNP simulations should be performed to better understand current source performance.

**Shielding Issues**

We need to understand how the new guide affects radiation at the bunker and improve CG shielding significantly. It appears that with 2 guides we are close to the limit, and with a 50% increase in radiation levels new shielding will undoubtedly be required. Primary and secondary shutters will need reworking, because the current design & mechanisms could be improved.

**Concepts**

A number of options for the guides have been qualitatively examined. Traditional SANS (straight m=1) and elliptic guides have been discussed. In terms of backscattering (BSS) there are several variations including two locations for benders to separate the beam from the SANS beam, before and after platypus, or raising the BSS onto a mezzanine using a vertical separation of the guides. The bender option is attractive because it would create another possible end position for a reflectometer and/or test beam. If the losses of the bender are significant then the mezzanine may prove attractive, but this requires further study. In particular, the arrangement of shielding and foundations for the mezzanine may be a complication.

**Risk Analysis**

1. Risk of guide implosion, mitigated by using steel vacuum housing instead of evacuated guides.
2. Risk of borated glass too close to the moderator causing early failure, mitigate by sodium float glass or, even closer, aluminium substrate guides.

3. Schedule risk of starting too late, mitigate by hiring fast and buying scientists’ time at their current facilities; holding a workshop early summer; meeting (possibly in NIST) with Dan Neumann; contacting vendors early about capacity and budget estimates; providing financial incentives for early delivery of guides (and penalties for late delivery); using a laser tracker for tracking all objects in hall for somewhat parallel construction.

4. Budget risk related to extra guide requirements, e.g. design fixed for in-hall instruments which later need outside-hall position, or major changes. Such a large change late in the process are unlikely because of the large cost.
## Appendix: Workshop participants

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<tr>
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## Appendix: Workshop Program

### 27-28th August 2009
OPAL Auditorium, Building 83, ANSTO, New Illawarra Road, Menai, NSW, 2234

### Thursday, 27th of August 2009

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<td>9.00</td>
<td>Opening and Welcome</td>
<td>Adi Paterson, ANSTO</td>
<td>John White, ANU</td>
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<td>9.05</td>
<td>An Overview of Opportunities and Experience so far at OPAL</td>
<td>Rob Robinson, ANSTO</td>
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<td>9.30</td>
<td>Charge to the Workshop</td>
<td>Rob Robinson, ANSTO</td>
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<tr>
<td>9.35</td>
<td>What we have promised the Commonwealth</td>
<td>Frank Klose, ANSTO</td>
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<tr>
<td>10:00</td>
<td>Coffee</td>
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<tr>
<td>11:00</td>
<td>Scientific Opportunities with a Back-Scattering Instrument at OPAL</td>
<td>Bernhard Frick, ILL</td>
<td></td>
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<tr>
<td>11:30</td>
<td>Scientific Opportunities with Neutron Radiography/Tomography/Imaging at OPAL</td>
<td>Burkhard Schillinger, FRM-II</td>
<td>Lyndon Edwards, ANSTO</td>
</tr>
<tr>
<td>12.00</td>
<td>Scientific Opportunities with Advanced Sample Environments</td>
<td>Michael Meissner, Helholtz-Zentrum Berlin</td>
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<tr>
<td>12.30</td>
<td>Lunch</td>
<td></td>
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<tr>
<td>13.30</td>
<td>Five minutes for each interested attendee</td>
<td>Rob Robinson, ANSTO</td>
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<tr>
<td>14.30</td>
<td>Guide Options for CG2 at OPAL</td>
<td>Shane Kennedy</td>
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<tr>
<td>15.00</td>
<td>Afternoon Tea and Workshop photo</td>
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<tr>
<td>15:30</td>
<td>Parallel Sessions (Scientific &amp; Technical): SANS (secretary – Elliot Gilbert) BSS (secretary – Oliver Kirstein) Radiography (secretary – Ulf Garbe) Sample Env. (secretary – Scott Olsen) Guides (Secretary – Frank Klose)</td>
<td>Greg Warr</td>
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<td></td>
<td></td>
<td>Dan Neumann</td>
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<td></td>
<td></td>
<td>Peter Vontobel</td>
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<td></td>
<td></td>
<td>Eddy Lelievre-Berna</td>
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<td></td>
<td></td>
<td>Phil Bentley</td>
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</tr>
<tr>
<td>17.30-18.00</td>
<td>Report back to main session</td>
<td></td>
<td>Dan Neumann, NIST</td>
</tr>
<tr>
<td>18.30</td>
<td>Dinner</td>
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</table>

### Thursday Evening

3-Course Dinner in the ANSTO Cafeteria
**Friday, 28th of August 2009**

<table>
<thead>
<tr>
<th>Time</th>
<th>Presentation</th>
<th>Presenter</th>
<th>Chair</th>
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</thead>
<tbody>
<tr>
<td>9:00</td>
<td><strong>Welcome Back</strong></td>
<td></td>
<td>Shane Kennedy, ANSTO</td>
</tr>
<tr>
<td>9:05</td>
<td>Options for Back-Scattering at OPAL</td>
<td>Dan Neumann, NIST</td>
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<tr>
<td>9:25</td>
<td>Options for Sample Environments at OPAL</td>
<td>Eddy Lelievre-Berna, ILL</td>
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<tr>
<td>9:45</td>
<td>Options for Radiography at OPAL</td>
<td>Peter Vontobel, PSI</td>
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<tr>
<td>10:05</td>
<td>Options for SANS at OPAL</td>
<td>John Barker, NIST</td>
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</tr>
<tr>
<td>10:30</td>
<td><strong>Coffee</strong></td>
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<tr>
<td>11:00</td>
<td>Break into Parallel Sessions (Technical):</td>
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<tr>
<td></td>
<td>SANS (secretary – Elliot Gilbert) BSS</td>
<td></td>
<td>Greg Warr</td>
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<tr>
<td></td>
<td>(secretary – Oliver Kirstein)</td>
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<td>Dan Neumann</td>
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<tr>
<td></td>
<td>Radiography (secretary – Ulf Garbe)</td>
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<td>Burkhard</td>
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<tr>
<td></td>
<td>Sample Env. (sec. – Scott Olsen)</td>
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<td>Schillinger</td>
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<tr>
<td></td>
<td>Guides (secretary – Frank Klose)</td>
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<td>Michael Meissner</td>
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<td></td>
<td>Phil Bentley</td>
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<tr>
<td>12:00</td>
<td><strong>Lunch</strong></td>
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<tr>
<td>12:30</td>
<td>Charge for writing Workshop Report</td>
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<tr>
<td>13:30</td>
<td>Write Report</td>
<td>Dan Neumann, NIST</td>
<td>Rob Robinson, ANSTO</td>
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<tr>
<td>16.00</td>
<td>Workshop Summary and Close</td>
<td>Greg Warr</td>
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<td></td>
<td></td>
<td>Ulf Garbe</td>
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<td></td>
<td></td>
<td>Michael Meissner</td>
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<td></td>
<td>Frank Klose</td>
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Appendix: The Emu

The Emu is a large flightless bird native to Australia. Emus stand 1.5 to 2 metres tall, and on average weigh 36 kilograms. They have 3 toes, and long legs which allows them to run extremely fast. In this species, the female is larger than the male. Emu's feed on grass, leaves and small insects. They live all over Australia in grasslands.

The female lays up to 20 eggs, which are large and are soft dark green in colour. These eggs are often prized not only by humans for decoration pieces, but by animals as a food source. The male incubates the eggs for a period of 7-8 weeks, and does not leave the nest for this period. When the eggs hatch, the male emu looks after the hatchlings for another six months.

- **Amazing Fact:** The Emu is the world's third largest bird. The Ostrich and the Cassowary take the top positions.
- **Animal Facts:** The nest of an Emu can be up to 1.5 metres wide!


Initially, the Coat of Arms consisted of a shield in the centre, the seven pointed star on a wreath as the crest above it, and a Kangaroo and an Emu supporting the shield, all on a bed of green grass with a scroll containing the motto "Advance Australia". The selection of the kangaroo, the Emu and the words, "Advance Australia" was tied together symbolically.