Polarised Neutron Scattering at ANSTO

Report of a Workshop Held at the
Australian Nuclear Science and Technology Organisation

28-29 November 2007
Polarised Neutron Scattering at ANSTO

Report prepared by the participants of a workshop held at the Bragg Institute, 28-29 November 2007

Edited by Frank Klose

Executive Summary

1. Introduction: Polarised Neutrons at ANSTO

2. Polarised Neutron Scattering - An Introduction

3. Scientific Case for Polarised Neutron Scattering
   3.1 Crystallography - Diffraction
   3.2 Magnetic thin films - Reflectometry
   3.3 Large scale structures - SANS
   3.4 Excitations - Inelastic scattering (triple-axis and TOF spectroscopy)

4. Polarised Neutron Instrumentation
   4.1 Supermirror-based analyser systems
   4.2 Heusler crystals
   4.3 Polarised $^3$He - MEOP and SEOP spin filters

5. Recommendations for the Polarised Neutron Setup at Particular OPAL Instruments
   5.1 Wombat - High Intensity Diffractometer
   5.2 Platypus - Reflectometer
   5.3 Quokka - Small-Angle Neutron Scattering
   5.4 Sika - Cold Neutron Triple-Axis Spectrometer
   5.5 Taipan - Thermal Neutron Triple-Axis Spectrometer
   5.6 Pelican - TOF Spectrometer
   5.7 Overview: Polarising options and scientific case for OPAL instruments


Appendix A - Workshop Attendees
Appendix B - Workshop Photo
Appendix C - Workshop Program

07.01.08
Executive Summary

A workshop on "Polarised Neutron Scattering at ANSTO" was held at Lucas Heights, on 28-29 November 2007. Thirty-five participants attended, from eight Australian and two overseas universities, two ANSTO Institutes, and three leading overseas neutron scattering laboratories.

The purpose of the workshop was (1) to discuss the scientific case for further polarised-neutron capability, beyond that funded with the initial set of eight instruments at OPAL, and (2) to define which are the most appropriate polarisation technologies to do this science.

We concluded that there is a compelling case for polarised neutrons and polarisation analysis for inelastic neutron scattering (particularly on Pelican, but also on Taipan and Sika) and neutron diffraction (particularly on Wombat, but also on Taipan). We also support polarisation analysis of high-intensity specular and diffuse scattering for reflectometry as well as small-angle neutron scattering, though the scientific case for SANS may not be as strong.

1. The majority of our needs can be met with polarised $^3$He gas technology, as implemented at the ILL or NIST. The particular choice between metastable exchange and spin-exchange optical pumping will depend on an assessment of relative cost, scheduling times and risk, by ANSTO.

2. There is also support for a focussing Heusler-alloy monochromator on Taipan.

3. While commercial polarising supermirrors will continue to find a role at OPAL, particularly for well-collimated incident neutron beams, we do not recommend that ANSTO invest in its own supermirror production – it is only suitable for one of our instruments and is more expensive than $^3$He technology.

Estimates of capital and operating cost, lab-space requirements, and staffing levels are given in the body of the report. We recommend that ANSTO proceed with an effort to install $^3$He polarizers/analysers on five of our instruments with all haste, subject to providing staffing and making a technology choice between the metastable-exchange and spin-exchange optical pumping methods. In parallel we recommend that a Heusler-alloy polarising monochromator be procured for Taipan.
1. Introduction: Polarised Neutrons at ANSTO

Australia has a long history of polarised neutron scattering, dating back to 1974 with the LONGPOL instrument at the HFIR reactor as one of the first demonstrations of neutron polarisation analysis. LONGPOL has served the Australian magnetism community for over 30 years and has produced important scientific results, for example in the areas of spin glasses, short range order phenomena, flux relaxation in high $T_C$ superconductors, crystal field transitions, domains in amorphous magnets, etc. It is evident from the program of this workshop that the magnetism community is still very active, particularly in modern areas of magnetism such as multiferroics (Curtin, UWA, UNSW, Bragg), high-energy product magnets (CSIRO), colossal magnetoresistive materials (Sydney Uni), nanostructured bulk magnets (UNSW@ADFA), nanomagnetism & thin film spintronic materials (UWA, UNSW, UW, Bragg) and magnetisation dynamics (UWA).

The new OPAL research reactor and the initial suite of neutron scattering instruments will provide the Australian users with unprecedented experimental capabilities that, in many cases, will rival the current state-of-the-art neutron beam lines found at the Institute Laue Langevin, Grenoble. The Bragg Institute is now developing plans to ensure that not only the neutron scattering instruments are competitive on an international level, but that also state-of-the-art polarised neutron scattering facilities will be made available for the Australian users. This has to be seen on the background that the use of polarised neutrons is on the rise internationally, and all modern facilities have, or will soon have, major capabilities for polarised neutron scattering.

The purpose of this workshop was to demonstrate the scientific value of polarised neutron scattering to Australian industry, government and universities, to discuss the current and future polarised neutron science applications with the Australian user community, and to define specifications for state-of-the-art polarised neutron capabilities at the OPAL beam instruments.

2. Polarised Neutron Scattering - An Introduction

One of the most remarkable features of the neutron scattering technique is that magnetic interaction strengths are often of the same order of magnitude as nuclear interactions such that magnetic and structural properties of the sample can be probed simultaneously. Both the nuclear and magnetic potentials experienced by neutrons interacting with condensed matter depend strongly on the spin polarisation of the neutron. This polarisation-dependence can be exploited to extract quantitative information about spatial and temporal variations of atomic and magnetic densities in condensed matter that cannot be obtained with unpolarised neutrons. The use of spin-polarised neutrons in neutron-scattering experiments provides the capability to study scientific phenomena and/or achieve levels of instrument performance not otherwise accessible.

Magnetic neutron scattering experiments can be performed on a large variety of samples, including, for example, single crystals, powders, and even artificially grown thin film structures. Physical quantities that can be measured by magnetic neutron scattering include:
i) Magnetic structures across various length scales (e.g., ranging from ferro- and antiferromagnetic order at atomic length scales to mesoscopic structures like flux lattices of superconductors, magnetic spirals or magnetic depth profiles in thin films)

ii) Magnetization density (e.g., how the moment is distributed in the vicinity of magnetic atoms)

iii) Magnetic excitations (e.g. spin waves)

For the characterisation of magnetic materials the analysis of the polarisation of the scattered beam is an essential part of the scattering experiment (C.G. Shull, E.O. Wollan, W.C. Kohler, Phys. Rev. 84, (1951) 912). If the beam incident on the sample is polarised, performing this analysis allows one to separate nuclear and magnetic scattering.

The nuclear scattering potential $\hat{V}_{\text{nucl}}$ sums the individual $b$’s, which for nuclei with spin can be written as (S. W. Lovesey, Theory of Neutron Scattering from Condensed Matter Clarendon Press, Oxford, 1984):

$$\hat{b} = A + \frac{1}{2} B \hat{s} \cdot \hat{i}$$

where $A$ and $B$ are isotope-specific numbers, and $\hat{s}$ and $\hat{i}$ are the spin operators of neutron and nucleus, respectively. The spin-independent part of the potential gives rise to scattering without spin flip, because the neutron spin is not involved (usually referred to as coherent nuclear scattering). If the sample contains isotopes with different scattering lengths, local fluctuations around the mean value of $A$ give rise to isotope-incoherent scattering (also without spin flip). The separation of nuclear incoherent scattering from coherent nuclear scattering is particularly important in soft and complex matter, for example biological systems. Currently, such separation can only be achieved by using specially protonated and deuterated samples in which the chemistry and therefore also the material properties may be altered.

The $\hat{s} \cdot \hat{i}$ term tells that, if the nucleus has a spin, two different compound nuclear states with total spins $(i+1/2)$ and $(i-1/2)$ may be formed during scattering, with probabilities $(i+1)/(2i+1)$ and $i/(2i+1)$, and in general their scattering lengths will be different. As for different isotopes, this creates incoherent scattering, but this time a spin flip is involved.

Generally, scattering from a magnetic moment $\mu$ or a nuclear magnetic moment $i$ is without spin flip for the component of $\mu$ or $i$ parallel to $\hat{s}$, whereas the two components perpendicular to $\hat{s}$ will scatter with spin flip (R. M. Moon, T. Riste, and W. C. Koehler, Phys. Rev 181 (1969) 920). Usually nuclear spins are not ordered and this contribution to the scattering (hence called spin-incoherent scattering) is then 2/3 with spin flip and 1/3 without spin flip. At extremely low temperatures ordered nuclear moments may give rise to magnetic scattering effects.
Given an initial beam polarisation $P$, we may summarize the effect of the different types of scattering on the scattered beam polarization $P'$ as follows:

Nuclear scattering (coherent or isotope-incoherent):

\[ P' = P \]

Spin-incoherent scattering:

\[ P' = -\frac{1}{3} P \]

Magnetic scattering from macroscopically isotropic magnetic systems (usually from unpaired electrons; at extremely low temperature also from nuclear magnetic moments):

\[ P' = -\frac{q(q \cdot P)}{q^2} \]

The last formula was first obtained by Halpern and Johnson in their classic paper on magnetic neutron scattering (O. Halpern and M. H. Johnson, Phys. Rev. 55 (1939) 898). Its meaning is: The scattered beam is polarised in the direction of the scattering vector $q$, the spin is flipped, and the polarisation also depends on the relative orientation of $q$ and $P$. The formula is not universal, however. It holds only for macroscopically isotropic cases, for example paramagnets, collinear antiferromagnets, generally powder samples, and (non-magnetized) multidomain ferromagnets (as long as they do not depolarise the beam), but not for macroscopic single crystals with non-collinear magnetic order.

In the most general case, when the Halpern-Johnson formula can not be used, we have to write

\[ P' = \hat{S}P + P'' \]

where $\hat{S}$ is called the polarisation tensor and $P''$ is the polarisation created by the scattering process. $\hat{S}$ has (at most) six independent elements. These can be measured if the magnetic sample is kept in zero external magnetic field. The corresponding technique is called spherical polarisation analysis (P. J. Brown, J. B. Forsyth, E. Lelièvre-Berna, and F. Tasset, J. Phys.: Condens. Matter 14, (2002) 1957). The required formulae for the individual elements of $\hat{S}$ and $P''$ can be found in the literature in a handy form (P. J. Brown, Physica B 297 (2001) 198). Since the experimental setup is difficult (see Fig. 1), and the diagonal elements of $\hat{S}$ can be measured in an easier way (see below), the technique is only applied if $\hat{S}$ has off-diagonal elements. Such elements may appear in magnetic crystals with non-collinear magnetic order (for example, canted or helical structures), magneto-electric crystals (for reference and examples, see Brown 2001). If they do, spherical polarisation analysis is the only way today to access them experimentally.
Using a magnetic guide field at the sample position in order to keep the neutron beam polarisation is experimentally easier to realize (see Fig. 2) and allows one to measure the three diagonal terms of $\hat{S}$. This technique is called three-directional polarisation analysis (O. Schärpf and H. Capellmann, Phys. Stat. Sol. A 135 (1993) 359). Nuclear and spin-incoherent neutron scattering always appear in the diagonal elements of $\hat{S}$, because $P$ and $P'$ are parallel. The same holds for magnetic scattering, if the Halpern-Johnson formula can be applied.

Thus, in many cases the three diagonal terms of $\hat{S}$ contain all information about the sample one wants to obtain in a neutron scattering experiment. The separation of magnetic and nuclear cross sections, achievable through X, Y, Z polarisation analysis, is particularly important for studying magnetic fluctuations of correlated electron systems such as high-$T_C$ and CMR materials as well as for spin glass systems which often only show short-range magnetic order.

**Figure 1** Spherical polarisation analysis (schematic)

Note: Sample is placed in rotatable guide field $H$

**Figure 2** Three-directional (X, Y, Z) polarisation analysis (schematic)
In most experimental setups, for example at the Platypus reflectometer, only a single magnetic axis is available (usually provided by an electromagnet or by a superconducting cryo-magnet). This technique is called uni-directional polarisation analysis and was first demonstrated by Moon, Riste and Koehler in 1969 (R. Moon et al., Phys. Rev. 181 (1969) 920). In such experiments, four neutron intensity cross sections ($I^{++}$, $I^{+-}$, $I^{-+}$ and $I^{-}$) are measured.

Figure 3 Uni-directional polarisation analysis (schematic)

3. Scientific Case for Polarised Neutron Scattering

3.1 Crystallography - Diffraction

The high-intensity powder diffractometer Wombat deserves serious consideration as an instrument for neutron polarisation analysis studies. Its extremely high intensity is ideal for magnetic scattering (which is generally weak) while its resolution is more than adequate to discriminate magnetic Bragg peaks (which generally occur at low angles). Wombat therefore appears to possess all the features appropriate for uni directional neutron polarisation analysis as outlined in detail in the classic paper of Moon, Riste and Koehler (Phys. Rev 181, (1969) 920).

While magnetic information is always present in neutron scattering data, its intensity is often close to the background of the nuclear scattering. A polarised incoming neutron beam, neutron spin flippers, and an analyser allows spin-flip (magnetic) scattering events to be unambiguously distinguished from non-spin-flip (nuclear) scattering. Neutron polarisation analysis thereby offers the ability to separate unequivocally magnetic from nuclear scattering events, be they coherent or incoherent. This is particularly important where the magnetic and nuclear scattering coincide, as for ferromagnets and (sometimes) ferrimagnets, but is also important for complex magnetic structures such as spirals and other incommensurate spin states which occur in many magnetic materials of current interest (e.g. multiferroics).

The potential use of Wombat as a single crystal diffractometer adds a significant new dimension. With its large area detector, Wombat will rival D19 at the ILL as the world's fastest monochromatic single crystal neutron diffractometer for the collection of high-resolution Bragg and (in particular) diffuse scattering. A commissioning experiment has already demonstrated the viability and the potential of this use of Wombat. The addition
of polarisation analysis would elevate Wombat from a world-class single crystal diffractometer to a truly unique machine, especially for the collection of incommensurate and magnetic diffuse scattering where it would be unrivalled.

Australian science has a substantial history and record of achievement in studies of magnetism and magnetic materials. This is demonstrated clearly by the awarding of The International Conference in Magnetism to Australia (ICM1997), and the recent International Conference of Neutron Scattering (ICNS2005) to the Australian scientific community. Magnetic systems currently being pursued through structural studies by Australian researchers include the following:

- Rare-earth intermetallic compounds:
  
  Competing Magnetic Interaction in La$_{0.8}$Y$_{0.2}$Mn$_2$Si$_2$ – Coexistence of Canted Ferromagnetism and Antiferromagnetism, M. Hofmann, S.J. Campbell and S. J. Kennedy, Journal of Physics: Condensed Matter, 12, (2000) 3241-3254.


  Molecular Mean Field Study of Rare-Earth Intermetallic Compounds $R_3$Co$_{26}$Si$_4$B$_{10}$, Heng Zhang and S. J. Campbell, Journal of Applied Physics, 93 (2003) 9177-9181.


- Multiferroics


  Three-layer Aurivillius Phases Containing Magnetic Transition Metal Cations: Bi$_2$$x$Sr$_{2+x}$(Nb,Ta)$_{2+y}$M$_{1.4}$O$_{12}$, $M = Ru^{4+}$, Ir$^{4+}$, Mn$^{4+}$, $x \approx 0.5$


- Magnetic Nanostructures


  The Magnetic Behaviour of Nanostructured Zinc Ferrite, M. Hofmann, S. J.


- **CMR Manganites**


  *Interplay of Spin and Orbital Ordering in the Layered Colossal Magnetoresistance Manganite La$_{2-2x}$Sr$_{1-2x}$Mn$_2$O$_7$ ($0.5 \leq x \leq 1.0$)*, C.D. Ling, J.E. Millburn, J.F. Mitchell, D.N. Argyriou, J. Linton, and H.N. Bordallo, Physical Review B \textbf{62} (2000) 15096-15111.


- **Molecular Magnets**

3.2 Magnetic Thin Films - Reflectometry
Great advances in growth and fabrication technologies have led to an unprecedented ability to atomically engineer materials that do not occur naturally. It is possible in these structures to drastically modify electronic, optical, and magnetic properties by strategic design of interfaces between dissimilar materials. An example that has completely transformed magnetic thin film research was the discovery, and subsequent research into, the phenomena of giant magneto-resistance.

Studies of this and related properties rely heavily on an ability to resolve the orientation and distribution of magnetic moments at and near buried interfaces. A wide range of phenomena in nanometer thick films and multilayers are open to study using neutrons: chiral and helical orderings in structures with competing interactions, temperature driven phase, and reorientation transitions nucleated at interfaces, enhanced magnetic moments at ferromagnetic interfaces, proximity induced magnetic moments in nonmagnetic metals (such as Pd) and frustration induced at interfaces involving combinations of ferromagnets, ferrimagnets, and antiferromagnets. The range of materials extends across the transition and rare earth metals in a variety of alloys and multilayered geometries.

The forefront of magnetic materials research involves understanding static order and dynamics of ordering in thin film structures patterned into geometries with nanometer dimensions. This also includes nanocrystalline materials and techniques for nanostructuring produced using "self-organization". In addition to using neutrons for studies of static magnetic order and distributions of magnetization in buried ferromagnetic and antiferromagnetic components, new directions in technological applications require understanding the relationship between geometrical structure and low frequency spin wave dynamics. In particular, mode diffusion and damping mechanisms are of particular importance. Spin wave scattering and interactions involving scattering from conduction electrons in magnetic metals is of especial interest at present, especially in regards to current driven reversal schemes and high frequency magnetoresistance.

Novel Spintronics Materials - Some Examples
Presently, electronic technologies are largely dominated by semiconductor based devices in which the charge of the electron is used for processing, storing and retrieving of information. Processor and Random Access Memory chips in computers are examples for fast and cost effective devices. However, in order to keep up with the increasing requirements for further miniaturization, higher speed and lower power consumption of devices, novel scientific solutions for fast, reliable and energy efficient processing and storing of data must be developed.

Spintronics (or spin electronics) is believed to be a very promising approach. Spintronic devices specifically exploit the spin properties of the electrons (i.e. its magnetism) instead of or in addition to charge degrees of freedom. Spin transport in metals and semiconductors, for example, is of fundamental research interest not only in terms of basic solid state physics, but also for applications, some already realised, in electronic technology (S. Parkin et al., Proceedings of the IEEE 91(5) (2003) 661). The prototype device that is already in use in industry as a read head and a memory-storage cell is the giant-magnetoresistive (GMR) sandwich structure which consists of alternating ferromagnetic and nonmagnetic metal layers (the 2007 Nobel price was awarded to
Peter Grünberg and Albert Fert for this discovery). Depending on the relative orientation of the magnetisations in the magnetic layers, the device resistance changes from small (parallel magnetisations) to large (antiparallel magnetisations). This change in resistance (also called magnetoresistance) is used to sense changes in magnetic fields (for example the dipole field of a magnetic bit stored on a hard disk drive). Recent efforts in GMR technology have also involved magnetic tunnel junction devices where the tunnelling current depends on spin orientations of the electrodes.

*Multiferroics* are another class of materials which potentially could have applications in spintronic devices. Multiferroics are materials that simultaneously have ferroelectric and ferromagnetic properties. Ferroelectric and ferromagnetic materials are analogous materials in many ways, belonging to a broader family called as ferroics - both show features such as a spontaneous moment (dipole vs. electron spin), sensitivity to applied bias (electric vs. magnetic), complex domain structures and finally strain effects under an applied bias (electrostriction/piezoelectricity vs. magnetostriction). Both types of materials have been used for traditional functional applications such as storage memory media, sensors and actuators, and also emerging applications such as templates for biological systems and self assembled patterns. Naturally there has been tremendous interest in designing systems which are "multiferroic", i.e. possessing both ferroelectric and ferromagnetic properties. Multiferroics offer the unique possibility to control electron spin polarisation, ferroelectric lattice polarisation, and stress through cross-coupled interaction parameters. The key idea for device applications is the possibility to control magnetic properties (for example the direction of a magnetic bit) by applying electric fields across the material or, vice versa, to control the flow of current by externally controlling the magnetisation of the same material. Spintronic applications of multiferroic materials, due to the necessary miniaturisation and for cost reasons, will require multiferroic materials in thin film form. Since bulk multiferroic materials are extremely rare anyway, thin film hybrid structures (made by interfacing ferroelectric and ferromagnetic materials) are believed to have enormous potential for exciting research and applications.

Another potential approach for developing novel spintronic materials is to interface high Tc superconductor films with diluted magnetic semiconductors. The basic idea is that a magnetic field can be applied perpendicular to the surface of the superconductor layer which will penetrate it in form of flux tubes. These flux tubes concentrate the field inside each tube, so that they create spots of high-intensity magnetism on the semiconductor layer below, which, in turn, creates patches of closely aligned electron spins. The resulting spin patches, one for each flux tube, are then available for encoding information. The spins in these magnetic patches can then be manipulated, for example, by moving the flux tubes.


Applications for magneto-electronics involve devices that may incorporate a number of different magnetic materials and rely on several types of interface effects. An active frontier of exploration in this area is the use of nanostructured films. An example of nanostructuring effects on magnetic properties was demonstrated using 30 nm thick Pt$_{50}$Mn$_{50}$ films layered with Fe, and grown using molecular beam epitaxy. Magnetometry results showed the puzzling existence of a four-fold exchange anisotropy that could be strongly modified by cooling field direction. Polarised neutron
reflectometry proved the existence of a complex magnetic structure associated with a twinned nanostructure in the PtMn. This structure was shown to create high order exchange coupled anisotropies in the Fe in addition to a unidirectional anisotropy presumed to arise from pinned spins at grain boundaries. This study highlights the importance of having detailed knowledge of spin orientations for understanding material parameters of thin film nanostructures.

**Figure 4** Left: (a) Sketch of magnetic configuration in twinned grain structure of MnPt. (b) TEM images of twinned structure. Right: sketch of magnetic orientations determined from neutron scattering.

### 3.3 Large Scale Structures - SANS

The case for incident beam polarisation has been stated in detail in the 2001 workshop report (E.P. Gilbert, Dec 2001) and 2002 instrument acquisition proposal (E.P. Gilbert, NBIP-SS-404-1003, Feb 2003). Polariser and spin flipper design have concluded and installation is expected to be completed (spin flipper) in early 2008.

**Polarisation analysis**

Polarisation analysis enables evaluation of the spin flip channel and is of value when the material moments are perpendicular to the quantisation direction. Polarisation analysis has been tested on NG3 (NIST), V4 (HMI) and D22 (ILL), see the examples below. Depolarisation of the incident beam may be used to evaluate domain sizes of randomly directed magnetic structures (e.g. Pd-Ni-Fe-P ribbons, D.H. Yu et al., Physica B: Condensed Matter Volume 397 (2007) 30-32). Incident beam polarised SANS has been used to investigate the structure of ferrofluids, magnetic materials and spin chirality.

There is also the opportunity of evaluating the spin incoherent scattering that, in SANS, contributes to a background which limits the spatial resolution in the structure determination. The ability to reach higher q, in principle, enables models of the scattering that are similar in the low-mid q region but differ in the high q region to be
distinguished. This background often generates limitations as far as maximum count rate is concerned (i.e. selection of source-to-sample distance). Other interesting applications of polarized neutrons in regard to SANS include:

- Time-resolved polarisation: magnetorheological kinetics and dynamics (Langevin statistics) oscillatory field application
- Storage and loss moduli of magnetic nanoparticle interactions
- External field responses of particles under shear flow i.e. vary field direction with regard to flow field

**Examples:**

**More Literature:**
- Ferrofluids
- Magnetic nanocrystals
- Magnetic alloys
- Soft metallic glasses
- Spin chirality

### 3.4 Excitations - Inelastic Scattering

**Cold/Thermal Triple-Axis Spectroscopy**
A number of areas of condensed matter physics are incredibly well suited to being probed by polarised inelastic scattering. It is used to separate the nuclear and magnetic components of the scattering. Spin-lattice coupled systems are a perfect example and cover a vast range of systems including multiferroics, high-$T_c$ superconductors, quantum critical point systems, spin-Peierls materials and helimagnons in systems with novel magnetic order, to name a few. This technique is also very effective when studying dilute magnets and frustrated magnets and Haldane gap systems. A subcategory is in measurements of very small magnetic signals such as superlattice structures, when removing the nuclear signal improves the sensitivity of the measurement greatly.

A related direction where polarisation analysis proves useful is to separate the coherent and incoherent neutron cross-sections, such as in studies of liquids and diffusion. Here,
the incoherent signal can be studied with higher sensitivity if the coherent signal can be effectively removed. This method can be made much more effective than it has been in the past if the machine was setup such that the measurements and data analysis were made more convenient.

A possible zero-field spin-echo option requires polarised neutrons but does not affect the choice of Heusler versus $^3$He and opens up a variety of further studies on many of the same systems mentioned above, only with considerably higher resolution.

**Time-of-Flight Spectroscopy**

For non-magnetic materials the separation of spin-incoherent scattering from the coherent scattering, based on Q-dependent of the Debye-Waller factor is of great importance. Apart from hydrogenous materials, a large group of other materials, eg. Cu, has strong spin incoherent scattering. This separation is important to get a good structure factor. The presence of Bragg peaks can severely limit the available incoherent Q-range, of interest in the study of lattice dynamics and diffusion. Uni-axial PA will eliminate this and will make *Pelican* unique in this respect.

In terms of inelastic or quasielastic scattering, it is important to separate co-operative excitations from the diffusion mode. The spin-incoherent scattering contains diffusive excitations, while the coherent scattering contains both diffusive and co-operative excitation. These effects can be separated, e.g. L-Na and has never been fully utilised despite having applications across applications in chemistry, materials science, physics and even simple biological materials.

Polarised neutrons with polarisation analysis can distinguish magnetic from non-magnetic scattering. This works for a large range of magnetic materials like ferro- and antiferromagnets, spin glasses, spin ices and molecular magnets which are all of fundamental importance. It also enables to identify magnetic moment directions, like, chiral magnetic structures.

The importance of separating dynamic from the static magnetic contributions is of primary importance in low-dimensional and frustrated magnetic materials. Possible Spin wave excitations confined in low dimensional systems can be done as *Pelican* got the often required large (Q,ω) space.

### 4. Polarized Neutron Instrumentation

This section summarises the present status of polarised neutrons technologies that are relevant for the current suite of OPAL instruments. An accepted figure-of-merit is $P^2 \times T$ where $P$ is the polarisation and $T$ the transmission of an initially unpolarised beam after passing through a polarising device.

#### 4.1 Supermirrors Based Polarizer and Analyzer Systems

Supermirror based polarisers are the method of choice for well collimated neutron beams in the cold and cold/thermal wavelength range. Typical applications include SANS and reflectometry. High-quality supermirror transmission polarisers such as the one planned for *Platyus* achieve $P^2T$ quality factors of about 0.4 for an extended wavelength interval ranging from 3 Å to above 10 Å (Fig. 5). In current instruments, $m$
= 2-3 coatings are used but prototype coatings of \( m = 4-5 \) coatings have already been produced at the ILL and in Japan. These coatings will extend the applicability of supermirrors towards shorter wavelengths.

Supermirrors show also an excellent performance as polarisation analyser system for wide angle diffraction experiments (\( P^2 T \) quality factors of typically 0.3 are achievable). However, due to the small angular coverage of an individual supermirror, curved arrays of thousands of mirrors have to be assembled in order to cover a significant angular range of scattering angles. The most ambitious supermirror analyser project was the recently completed upgrade of ILL's D7 where 270 m\(^2\) of \( m = 2.8 \) supermirror coatings were used. Due to the high cost of producing such supermirrors (>10 k€/m\(^2\)) in many cases the use of supermirror based wide-angle analysers is unrealistic.

4.2 Heusler crystals

The (111) reflection from the ferromagnetic Heusler alloy \( \text{Cu}_2\text{MnAl} \) can be used to polarise cold and thermal neutrons. This is convenient for instruments that use a monochromatic beam (for example, diffractometers and triple-axis spectrometers at reactor installations) because polarisation and monochromatisation is done simultaneously. As for all monochromators, the peak reflectivity depends on the neutron wavelength and on the mosaicity of the crystals (see Fig. 6). Heusler crystals with 0.45° mosaicity have 25% reflectivity at 1.8 Å wavelength. For this case, the reflected beam has a polarisation of 95% (a typical value for Heusler crystals) and a \( P^2 T \) of 20%. Heusler crystals have the best reflectivity for cold neutron beams but are often also employed for thermal spectrometers. Focusing monochromator assemblies allow vertical and horizontal focusing but the overall size is restricted to about 15 cm by the magnetic field gap (see Fig. 7).

For cold neutron instruments it can be advantageous to polarize with a supermirror and monochromatize independently using pyrolytic graphite crystals. This works best when there is no horizontal focusing at the monochromator. Significant horizontal focusing
increases the divergence, which reduces the transmission of the supermirror polariser. Compared to a Heusler monochromator, this approach has the advantage that, due to the low neutron absorption of graphite, the spectrum transmitted by the monochromator can be used to feed neutrons to other instruments further down the neutron guide. Furthermore, the decoupling of monochromatization and polarization can be an advantage for triple-axis spectrometers since it allows for a more flexible resolution setting.

Heusler crystal polarisers are a well developed technology and further major improvements are not expected. Heusler monochromators have similar advantages as typical supermirror polarisers, in the sense that they do not require further maintenance after installation, and once they are set up and aligned, an instrument can change from unpolarised to polarised mode by a computer controlled exchange of the non-polarising monochromator for a Heusler.

Figure 6  Peak reflectivity of Heusler crystals as function of the mosaicity (top) and comparison of Heusler and graphite crystal properties (bottom) (from Ken Andersen)
4.3 Polarised $^3$He - MEOP and SEOP spin filters

Polarising filters based on preferential scattering or absorption of one of the neutron spin states have been known for decades. Various techniques have been developed but, for various reasons, none of them has become widely accepted (insufficient polarising efficiency, unfavourable neutron energy-dependence, low transmittance, too complicated setup, high cost, etc.). A more recent and very promising development, however, is the helium spin filter. Although it has been recognized since the 1960s that polarized $^3$He gas might be an extremely useful spin filter for thermal and epithermal neutron beams, the feasibility could be demonstrated only recently. The device is based on the spin dependence of the neutron absorption by the $^3$He isotope. At neutron energies typically used in neutron scattering, absorption is largely dominated by the reaction $^3$He- + n $\rightarrow$ $^4$He* $\rightarrow$ $^1$H + $^3$H, which goes entirely through the singlet state of the compound nucleus with zero spin, that is, only the neutron spin state with spin antiparallel to the $^3$He spin contributes to the absorption cross section for capture of neutrons. At a neutron energy of 25 meV, the cross section is 10666 barns for neutrons with spin antiparallel to the $^3$He nuclear spin, while the total cross section for absorption or scattering of neutrons with parallel spin is only a few barns. This makes it possible to construct a spin filter device provided the $^3$He can be polarised. For a sufficient column density (atomic density x length of the cell) of 100% polarised $^3$He, the transmission of neutrons with parallel spin would approach 100%. This transmitted neutron beam would be 100% polarized since virtually no neutrons with antiparallel spin could pass through the cell.

Highly polarised $^3$He can be obtained by two methods that use optical pumping techniques: spin exchange with optically pumped Rb (SEOP), and metastability.
exchange optical pumping in $^3$He (MEOP). In recent years, both approaches have been used successfully in polarisation and analysis experiments of neutron beams.

$^3$He spin filters show many favourable characteristics:

i) They are appropriate for polarising/analysing neutrons of a very broad energy range from cold to epithermal.
ii) They are suitable for broad wavelength band experiments.
iii) Their beam polarisation is highly homogeneous.
iv) They have a predictable transmission function.
v) A large solid angle of detection is possible.
vi) Their additional contribution to the beam divergence is minimal.

Due to these features, $^3$He spin-filters are particularly well-suited for polarisation analysis in experiments that require large angular coverage, e.g. high-angle diffraction, diffuse scattering, small-angle scattering, off-specular neutron reflectometry, etc. For these applications, the use of $^3$He is a good alternative compared to a complicated and expensive arrangement of supermirrors to cover large solid angles (although, once installed, the latter do not require further maintenance). In contrast, supermirrors are usually superior in experiments that require only small angular coverage at lower neutron energies, e.g. specular reflectometry.

Although $^3$He spin filters are already today often competitive with or sometimes even superior to supermirror/Heusler crystal based polarization methods, they are, however, not yet fully mature devices. The technology still has potential for major improvement and, because it has only recently been developed and that only at a small number of neutron labs, is has not yet been implemented on many neutron instruments. Issues that require further technical development include:

i) Improving the $^3$He polarisation reliably beyond the current experimental limit (in state-of-the-art cells, polarisation values up to 80% have been achieved directly after polarising the cells but after gas transfer and/or cell installation at an instrument, typical gas polarisations are currently in the 70% to 75% range)
ii) Achieving reproducible and very long relaxation times (in state-of-the-art cells, relaxation times of several 100 hours have been achieved)
iii) Fabricating large solid angle cells for SEOP
iv) Shielding the cell from magnetic field gradients resulting from high sample fields (ILL has recently designed a Meissner-screened cell cavity for a 10 Tesla superconducting magnet at the D3 instrument; at the location of the $^3$He cell the stray field can be up to 500 Gauss)

The first point is of particular importance. Due to the non-perfect $^3$He polarisation, the "wrong" neutron polarisation state (antiparallel) is partially transmitted, whereas the desired parallel neutron spin state is partially absorbed. Therefore, in order to achieve high neutron beam polarisation, a relatively large column density of $^3$He gas is required, which implies low transmission (see Fig. 8, left side). A state-of-the-art $^3$He cell designed for achieving a neutron beam polarisation of 95%, a typical value for a polarising supermirror, will provide approximately two times less neutron flux than a supermirror polariser (in this comparison we assume a well collimated neutron beam which can be covered by a simple transmission supermirror polariser).
Another problem related to the non-perfect polarisation of the $^3$He gas is that neutron polarisation power and transmission are coupled and neutron wavelength dependent. For experiments that require using broad neutron bandwidth, optimum conditions (in terms of achieving a particular set of values for neutron polarisation and transmission) can be achieved only for a limited range of wavelengths. However, the location of the optimal $P^2T$ product can be conveniently set to a particular value of neutron wavelength by varying the $^3$He cell pressure or the length of the cell (see Fig. 8, right side).

Figure 8 Left: Polarisation, transmission, and figure-of-merit of $^3$He polarisers as function of the cell opacity (product of $^3$He pressure inside the cell, length of the $^3$He gas along the beam path and neutron wavelength). Right: $P, T$ and $P^2T$ as function of neutron wavelength for a particular set of $^3$He gas pressure and cell length. In both figures, the assumed $^3$He polarisation is 75%. (from Ken Andersen)

MEOP based $^3$He polarising systems as the one developed by the ILL require a relatively large (laboratory room size) setup of equipment. In this method, the
polarisation of the gas is carried out at relatively low gas pressures and a compressor system is employed to achieve gas pressures that are needed for the actual use of the cell at a particular neutron scattering instrument (typical $^3\text{He}$ gas pressures inside a cell are in the range of 1 to 3 bar). Therefore, MEOP systems are not intended for on-line gas polarisation, i.e. *in-situ* at the actual point of use at an instrument. Usually, cells are filled with freshly polarised $^3\text{He}$ gas at a filling station attached to the compressor and are subsequently transported in a magnetic holding field to the instrument. A major advantage of the MEOP method is that the gas polarisation rate is about ten times faster compared to SEOP.

The ILL has recently implemented a new technique for re-filling cells directly at the instrument (see Fig. 9). In this approach, a buffer cell is filled at the filling station and subsequently transported to the instrument location. The buffer cell is then connected to the (evacuated) instrument cell using a capillary. The volume and gas pressure of the buffer cell is chosen such that the desired $^3\text{He}$ pressure is achieved in the instrument cell after the pressures in both cells are in equilibrium. The advantage of this re-filling method is that the instrument cell does not need to be accessed or removed which can sometimes be quite difficult, for example if the cell is located inside a scattering tank (see Fig. 9).

![Figure 9](image)

**Figure 9** Re-filling of instrument cells through buffer cells (example: the D17 reflectometer at the ILL)

Using the SEOP method, the $^3\text{He}$ gas can be polarised directly at its desired final pressure. The polarisation is a two-step process in which a laser polarises Rb atoms which subsequently transfer their polarisation to the $^3\text{He}$ atoms. For this reason, the cell must contain some amount of Rb metal. In order to achieve the required Rb gas partial pressure inside the cell, the Rb metal is evaporated by heating the cell to about 200°C. The heating is usually done by streaming hot air along the outside of the cell. Once the cell is polarised and cooled down to room-temperature, there is, compared to the MEOP
method, no difference in the subsequent handling of the polarised gas. However, since the SEOP method is a relatively compact set-up (table top size) it offers the possibility to continuously re-polarise the gas in-situ at the location of the cell in the neutron beam thereby avoiding the exponential decay of the polarisation (see Fig. 10). Small changes of the \(^3\)He polarisation, however, are still possible (for example due to the temperature stability of the cell heating system) but the degree of polarisation can be monitored in-situ using an NMR method. Even though the \(^3\)He polarisation decay theoretically follows a predictable exponential law, in-situ monitoring of the polarization is highly desirable also for non-continuously polarised cells since external magnetic field fluctuations may result in non-stable decay times (for example changes of the sample magnetic field with enough leakage to the cell area). Again, this is independent of what method (MEOP or SEOP) was initially used for polarising the gas.

**Figure 10** In-situ SEOP \(^3\)He polarisation analyser set-up at the SNS Magnetism Reflectometer (courtesy Wai-Tung Lee, SNS). The polarising laser and the necessary optics are contained in the black box. The optics expands the laser beam to about 2 inch diameter. A large Silicon wafer located directly under the optics box deflects the laser beam towards the cell into a direction parallel to the neutron beam. The complete \(^3\)He analyser system can be moved in and out of the neutron beam (vertical translation table) allowing a convenient change between polarised and unpolarised scattering experiments. The design of this SEOP system is based on technology developed by Thomas Gentile and co-workers, NIST.
5. Recommendations for the Polarised Neutron Setup at Particular OPAL Instruments

5.1 Wombat - High-Intensity Diffractometer
Given the large area detector on Wombat, polarisation analysis of the scattered beam using $^3$He is the only real option. Concerning the polarisation of the incoming beam, the take-off angle of the instrument is coupled to the sample position such that it would be strongly preferable to use an "in-line" system. This rules out supermirrors, which deflect the beam. Since the beam transmitted through the Wombat monochromator is used for Echidna, a Heusler monochromator is likely not an option for WOMBAT. Inserting a Heusler monochromator would not allow use of the transmitted beam, due to the absorption of the crystals themselves and the steel yoke required for the magnetisation of the crystals. This leaves $^3$He as the only option.

High-angle magnetic neutron diffraction (available at the Wombat diffractometer) is an extremely powerful technique for investigating atomic-scale antiferromagnetism in thin films. The latter is very important in regard to the exchange bias effect created at interfaces between ferromagnetic and antiferromagnetic layers. Also this effect is used, often in conjunction with the GMR effect, in contemporary magnetic storage technology. Diffraction measurements on thin films are usually carried out using a high-intensity/low-resolution beam (the incident beam divergence may be as large as 1°).

5.2 Platypus - Reflectometer
Platypus, OPAL's new polarised neutron reflectometer is an ideal tool for investigating vector magnetisation/superconductivity profiles in thin film systems with a vertical depth-resolution of a few monolayers. Generally, one would like to distinguish and quantify, the orientation of magnetic moments oriented parallel or perpendicular to an applied magnetic field. Polarised neutron reflectometry (PNR) can determine these components if the scattered beam is analysed (see Fig. 11). Spin flip scattering results from the moments that are perpendicular to the applied field and non-spin flip scattering results from moments that are parallel to H. The two major advantages of the reflectometry technique relative to SQUID magnetometry or SMOKE is that

i) PNR allows the determination of chemical and magnetic depth profiles (layer resolved magnetism) and
ii) PNR allows the determination of the magnitude of magnetization and its direction in space.
For standard specular polarised neutron reflectometry experiments supermirror based transmission polarisers and analysers are the best choice due to their high polarisation capability (usually 96% - 97%) and low beam absorption/scattering (only a few percent beam loss for cold neutrons) which results in a $P^2T$ factor of about 0.40. However, *Platypus* offers a high-intensity/low-resolution mode of operation in which large divergent beams are used. In this case, the angular and spatial coverage of a supermirror transmission analyser may be insufficient and a $^3$He based analyser is the best choice.

Recently developed polarised off-specular/diffuse scattering methods also allow investigations of lateral (in-plane) magnetic correlations on length-scales between 1 nm and 100 $\mu$m, for example lithographically produced patterns, self-assembled magnetic structures, or the aforementioned flux tubes. For such measurements, since the scattered beam is distributed over a few degrees of exit angles, a $^3$He based wide-angle polarisation analyser is indispensable.

### 5.3 Quokka - Small-Angle Neutron Scattering

*Quokka* has been specifically designed with polarisation analysis in mind (viz. minimal magnetic materials in construction, large sample area - 1.2 m between gate valves, in principle, can be increased to 3.2 m.). The sample area allows large space for magnetic shielding to minimise field gradient effects from sample environment influencing analyser efficiency. The *Quokka* detector has the advantage of having a very high angular acceptance (up to 45° - required for spin incoherent background reduction). The polarisation analyser for *Quokka* should have a wide wavelength bandwidth, a high polarisation efficiency, and minimal (ideally none) small-angle scattering. This makes a $^3$He analyser system by far the best choice. A 5T cryomagnet was specifically manufactured with large angular exit. Therefore, it does not limit the access to high Q. The same requirement is valid for the polarisation analysis system. The access to higher Q values may open up a unique niche market for polarisation analysis experiments (no instrument in the world has this capability). Other requirements for the polarisation analyser system include simple and reasonably smooth corrections for its efficiency (*seamlessly incorporated into instrument software*). Typical SANS experiment times (2 - 6 h max) mean that typical $^3$He relaxation times of 100 h - 200 h are not too problematic.
### 5.4 SIKA / TAIPAN - Cold / Thermal Neutron Triple-Axis Spectrometry

Pros and cons for polarising options:

<table>
<thead>
<tr>
<th></th>
<th>$^3$He</th>
<th>Heusler</th>
<th>Supermirror</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Divergence</strong></td>
<td>Can accept high divergence; the only option for area detectors</td>
<td>Current state-of-the-art accepts high divergence</td>
<td>NOT a reasonable option especially for thermal beam, too well collimated and precludes horizontal focusing</td>
</tr>
<tr>
<td><strong>Focusing</strong></td>
<td>Works</td>
<td>Works in one direction (can be fixed focus in the other direction)</td>
<td>Works in one direction</td>
</tr>
<tr>
<td><strong>Performance</strong></td>
<td>High (comparable Figure of Merit with Heusler); high flipping ratio possible by choosing appropriate gas pressure/thickness</td>
<td>High (comparable Figure of Merit with $^3$He); high flipping ratio</td>
<td>Low intensity for $E &gt; 10$ meV, high flipping ratio - but much lower Figure of Merit compared to Heusler or $^3$He for thermal neutrons</td>
</tr>
<tr>
<td><strong>Ease of Use</strong></td>
<td>Maintenance (on or off line) downtime of up to 1 hour every 24 h to change out cell, check polarisations, and do calibration scans for offline system - hence STRONGLY prefer online polarisation system</td>
<td>Zero maintenance - can changed to polarised in automated way No time-dependent polarisation correction</td>
<td>Zero maintenance - can changed to polarised in automated way No time-dependent polarisation correction</td>
</tr>
<tr>
<td><strong>Stability</strong></td>
<td>Polarisation correction would have to be incorporated in data reduction software. Polarisation corrections would need to be appended to data files after calibrations</td>
<td>Setup once, calibrate occasionally</td>
<td>Setup once, realign occasionally</td>
</tr>
<tr>
<td><strong>Flexibility</strong></td>
<td>Allows for arbitrary monochromators such Si(111) or Cu(200) etc.</td>
<td>Fixed to 5 - 105 meV incident energy; energy range and resolution equivalent to PG 002.</td>
<td>Realistically, not much above 15 meV</td>
</tr>
<tr>
<td><strong>Sensitivity</strong></td>
<td>To magnetic field gradients, which would affect 50% of all polarised experiments - need s/c shield. Increasing length of instrument strongly reduces flux on sample</td>
<td>INSENSITIVE</td>
<td>INSENSITIVE</td>
</tr>
</tbody>
</table>

Notes: Heusler/Heusler for TAIPAN would allow for automated changing to polarized mode available on a routine basis. This was considered really useful and would considerably increase the use of polarized mode use.

Consensus: Heusler/Heusler for TAIPAN and $^3$He/$^3$He for SIKA
5.5 Pelican – Time-of-Flight Spectrometer
In principle, both $^3$He and SM based polarisers and analysers can be used for Pelican. For the polariser, $^3$He will be a better option to accommodate the large divergence of the incident neutron beam, however, the PELICAN team has determined that the required space of approximately 400 mm is not available.

Due to wide angle ($125^\circ$ horizontal and $23^\circ$ vertical) coverage of the detector, $^3$He is the only practical option for the Pelican analyser (see the cost comparison in section 6). In terms of $^3$He technology, either a continuously pumped SEOP system or filling mechanism is required (*in-situ* filling would be advantageous). Normalisation of the cell polarisation when placed into the instrument would need to be carefully addressed. A compact cell geometry must be used to enable a compact cell size without significant loss of solid angle coverage.

5.6 Overview: Polarising options and scientific case for OPAL instruments
(polarizer/analyzer)

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Current</th>
<th>Best</th>
<th>Realistic</th>
<th>Science Case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wombat</td>
<td>None</td>
<td>$^3$He / $^3$He</td>
<td>$^3$He / $^3$He</td>
<td>strong</td>
</tr>
<tr>
<td>Taipan</td>
<td>SM / SM</td>
<td>Heusler / Heusler</td>
<td>Heusler / Heusler</td>
<td>strong</td>
</tr>
<tr>
<td>Sika</td>
<td>None / None</td>
<td>$^3$He / $^3$He</td>
<td>$^3$He / $^3$He</td>
<td>strong</td>
</tr>
<tr>
<td>Pelican</td>
<td>SM / None</td>
<td>$^3$He / $^3$He</td>
<td>SM / $^3$He</td>
<td>strong</td>
</tr>
<tr>
<td>Quokka</td>
<td>SM / None</td>
<td>SM / $^3$He</td>
<td>SM / $^3$He</td>
<td>weak</td>
</tr>
<tr>
<td>Platypus</td>
<td>SM / SM</td>
<td>SM / $^3$He</td>
<td>SM / $^3$He</td>
<td>strong</td>
</tr>
</tbody>
</table>

This table is compiled based on information provided by Ken Andersen, ILL and Thomas Gentile, NIST.

<table>
<thead>
<tr>
<th></th>
<th>SEOP 2 polarizing systems</th>
<th>SEOP 4 polarizing systems</th>
<th>MEOP</th>
<th>Supermirrors</th>
<th>Heusler</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Capital Cost (A$)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Equipment</td>
<td>114,000 x 2 stations</td>
<td>114,000 x 4 stations</td>
<td>1,200,000</td>
<td>1,690,000</td>
<td>300,000</td>
</tr>
<tr>
<td></td>
<td>80,000</td>
<td>80,000</td>
<td>86,000 x 3 instruments</td>
<td>80,000 x 3 instruments</td>
<td></td>
</tr>
<tr>
<td>3He Cell Preparation Lab</td>
<td>80,000</td>
<td>80,000</td>
<td>86,000 x 3 instruments</td>
<td>80,000 x 3 instruments</td>
<td></td>
</tr>
<tr>
<td>3He Holding Fields (3 instruments)</td>
<td>86,000 x 3 instruments</td>
<td>86,000 x 3 instruments</td>
<td>86,000 x 3 instruments</td>
<td>86,000 x 3 instruments</td>
<td></td>
</tr>
<tr>
<td>SM Production Cost</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SM Equipment (mechanics etc)</td>
<td>845,000 (Pelican only)</td>
<td>40,000 (Pelican only)</td>
<td>57,000 x 7 years</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sputter equipment operation cost</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Total Capital (A$)</strong></td>
<td>566,000</td>
<td>794,000</td>
<td>1,538,000</td>
<td>2,974,000 (Pelican only)</td>
<td></td>
</tr>
</tbody>
</table>

**Ongoing Operation Costs (A$)**
(from year one)

<table>
<thead>
<tr>
<th></th>
<th>SEOP 2 polarizing systems</th>
<th>SEOP 4 polarizing systems</th>
<th>MEOP</th>
<th>Supermirrors</th>
<th>Heusler</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equipment Operating cost (per yr)</td>
<td>70,000</td>
<td>100,000</td>
<td>135,000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cell Replacements (per yr)</td>
<td>6,000 x 3 instruments</td>
<td>6,000 x 3 instruments</td>
<td>6,000 x 3 instruments</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Total Operation Cots (per yr)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lab Space (m^2)</td>
<td>60</td>
<td>80</td>
<td>80</td>
<td>50</td>
<td></td>
</tr>
<tr>
<td>Timescale (Yr)</td>
<td>2.5</td>
<td>2.5</td>
<td>2.5</td>
<td>7 (3 years for set up &amp; 4 years for production)</td>
<td></td>
</tr>
<tr>
<td>Labour (FTE, from year one)</td>
<td>15% glassblower</td>
<td>15% glassblower</td>
<td>15% glassblower</td>
<td>1 scientist</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1 scientist</td>
<td>1 scientist</td>
<td>1 scientist</td>
<td>1 scientist</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1 technician</td>
<td>1 technician</td>
<td>1 technician</td>
<td>1 technician</td>
<td></td>
</tr>
<tr>
<td>Surname</td>
<td>First Name</td>
<td>Email</td>
<td>Affiliation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
<td>-------</td>
<td>-------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Andersen</td>
<td>Ken</td>
<td><a href="mailto:andersen@ill.fr">andersen@ill.fr</a></td>
<td>Institute Laue Langevin, France</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Best</td>
<td>Stephen</td>
<td><a href="mailto:spbest@unimelb.edu.au">spbest@unimelb.edu.au</a></td>
<td>University of Melbourne</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Campbell</td>
<td>Stewart</td>
<td><a href="mailto:Stewart.Campbell@adfa.edu.au">Stewart.Campbell@adfa.edu.au</a></td>
<td>UNSW @ADFA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Danilkin</td>
<td>Sergey</td>
<td><a href="mailto:Sergey.Danilkin@ansto.gov.au">Sergey.Danilkin@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Divakar</td>
<td>Ujual</td>
<td><a href="mailto:divakar@physics.uq.edu.au">divakar@physics.uq.edu.au</a></td>
<td>University of Queensland</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Finlayson</td>
<td>Trevor</td>
<td><a href="mailto:trevor@unimelb.edu.au">trevor@unimelb.edu.au</a></td>
<td>University of Melbourne</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Garvey</td>
<td>Chris</td>
<td><a href="mailto:Chris.Garvey@ansto.gov.au">Chris.Garvey@ansto.gov.au</a></td>
<td>ANSTO - IER</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gentle</td>
<td>Thomas</td>
<td><a href="mailto:thomas.gentile@nist.gov">thomas.gentile@nist.gov</a></td>
<td>NIST, USA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gilbert</td>
<td>Elliot</td>
<td><a href="mailto:elliot.gilbert@ansto.gov.au">elliot.gilbert@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Goosens</td>
<td>Darren</td>
<td><a href="mailto:goossens@rsc.anu.edu.au">goossens@rsc.anu.edu.au</a></td>
<td>ANU</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hambe</td>
<td>Michael</td>
<td><a href="mailto:michael.hambe@gmail.com">michael.hambe@gmail.com</a></td>
<td>University of New South Wales</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hamilton</td>
<td>William</td>
<td><a href="mailto:bill.hamilton@ansto.gov.au">bill.hamilton@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hicks</td>
<td>Trevor</td>
<td><a href="mailto:Trevor.Hicks@sci.monash.edu.au">Trevor.Hicks@sci.monash.edu.au</a></td>
<td>Monash University</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kearley</td>
<td>Gordon</td>
<td><a href="mailto:gordon.kearley@ansto.gov.au">gordon.kearley@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Keller</td>
<td>Thomas</td>
<td><a href="mailto:thomas.keller@fm2.tum.de">thomas.keller@fm2.tum.de</a></td>
<td>Max-Planck Institute Stuttgart, Germany</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kennedy</td>
<td>Shane</td>
<td><a href="mailto:shane.kennedy@ansto.gov.au">shane.kennedy@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Klose</td>
<td>Frank</td>
<td><a href="mailto:Frank.Klose@ansto.gov.au">Frank.Klose@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lee</td>
<td>Chih-Hao</td>
<td><a href="mailto:chlee@mx.nthu.edu.tw">chlee@mx.nthu.edu.tw</a></td>
<td>National Tsing Hua University, Taiwan</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Li</td>
<td>Sean</td>
<td><a href="mailto:sean.li@unsw.edu.au">sean.li@unsw.edu.au</a></td>
<td>University of New South Wales</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Li</td>
<td>Wen-Hsien</td>
<td></td>
<td>National Central University, Taiwan</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ling</td>
<td>Chris</td>
<td><a href="mailto:c.ling@chem.usyd.edu.au">c.ling@chem.usyd.edu.au</a></td>
<td>The University of Sydney</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liu</td>
<td>Yun</td>
<td><a href="mailto:yliu@rsc.anu.edu.au">yliu@rsc.anu.edu.au</a></td>
<td>The Australian National University</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mulders</td>
<td>Annemieke</td>
<td><a href="mailto:A.Mulders@curtin.edu.au">A.Mulders@curtin.edu.au</a></td>
<td>Curtin University of Technology</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nigam</td>
<td>Rashmi</td>
<td><a href="mailto:m393@uow.edu.au">m393@uow.edu.au</a></td>
<td>University of Wollongong</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P. Sushkov</td>
<td>Oleg</td>
<td><a href="mailto:sushkov@phys.unsw.edu.au">sushkov@phys.unsw.edu.au</a></td>
<td>University of New South Wales</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Photongkam</td>
<td>Pat</td>
<td><a href="mailto:p.photongkam@unsw.edu.au">p.photongkam@unsw.edu.au</a></td>
<td>University of New South Wales</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rehm</td>
<td>Christine</td>
<td><a href="mailto:Christine.Rehm@ansto.gov.au">Christine.Rehm@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Robinson</td>
<td>Robert</td>
<td><a href="mailto:robert.robinson@ansto.gov.au">robert.robinson@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stampfl</td>
<td>Anton</td>
<td><a href="mailto:Anton.Stampfl@ansto.gov.au">Anton.Stampfl@ansto.gov.au</a></td>
<td>ANSTO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stamps</td>
<td>Robert</td>
<td><a href="mailto:stamps@pd.uwa.edu.au">stamps@pd.uwa.edu.au</a></td>
<td>University of Western Australia</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Studer</td>
<td>Andrew</td>
<td><a href="mailto:andrew.studer@ansto.gov.au">andrew.studer@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Valanoor</td>
<td>Nagarajan</td>
<td><a href="mailto:nagarajan@unsw.edu.au">nagarajan@unsw.edu.au</a></td>
<td>University of New South Wales</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vorderwisch</td>
<td>Peter</td>
<td><a href="mailto:peter.vorderwisch@ansto.gov.au">peter.vorderwisch@ansto.gov.au</a></td>
<td>National Central University, Taiwan</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Yethiraj</td>
<td>Mohana</td>
<td><a href="mailto:mohana.yethiraj@ansto.gov.au">mohana.yethiraj@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Yu</td>
<td>Dehong</td>
<td><a href="mailto:dyu@ansto.gov.au">dyu@ansto.gov.au</a></td>
<td>ANSTO – Bragg Institute</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix B - Workshop Photo
Appendix C - Workshop Program

"Polarised Neutron Scattering at ANSTO"

OPAL Conference Room, Building 83, ANSTO, New Illawarra Road, Menai, NSW 2234
28-29 November 2007

WEDNESDAY, 28 November 2007

<table>
<thead>
<tr>
<th>Time</th>
<th>Presentation</th>
<th>Presenter</th>
<th>Chair</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>Arrival at ANSTO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9:00</td>
<td>Opening and Welcome</td>
<td>Rob Robinson, ANSTO</td>
<td>Michael James, ANSTO</td>
</tr>
<tr>
<td>9:05</td>
<td>Neutron Scattering at OPAL</td>
<td>Shane Kennedy, ANSTO</td>
<td></td>
</tr>
<tr>
<td>9:30</td>
<td>Charge to the Workshop</td>
<td>Rob Robinson, ANSTO</td>
<td></td>
</tr>
<tr>
<td>9:35</td>
<td>Introduction to Polarised Neutron Scattering</td>
<td>Frank Klose, ANSTO</td>
<td></td>
</tr>
<tr>
<td>10:00</td>
<td>Coffee</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:15</td>
<td>Science Applications of Polarised (^3)He Spin Filters in the USA</td>
<td>Thomas Gentile, NIST</td>
<td>Trevor Hicks,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Monash University</td>
</tr>
<tr>
<td>11:00</td>
<td>First Science Results From TRISP, the New Triple Axis Spin-Echo Spectrometer at FRM2</td>
<td>Thomas Keller, MPI Stuttgart/FRM2</td>
<td></td>
</tr>
<tr>
<td>11:45</td>
<td>Instrumentation Choices for Science With Polarised Neutrons at ILL</td>
<td>Ken Andersen, ILL</td>
<td></td>
</tr>
<tr>
<td>12:30</td>
<td>Lunch</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13:15</td>
<td>Scientific and Technical Visions: (Introduction of workshop participants)</td>
<td>Frank Klose, ANSTO</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Neutron Scattering From Lightly Doped (\text{La}_2\text{Sr}_x\text{CuO}_4): The Incommensurate Spin Structure is a Fingerprint of the Underlining Physics of Cuprate Superconductors</td>
<td>Oleg P. Sushkov, UNSW, Sydney</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NSE Studies of Diffusive Dynamics in Concentrated Biopolymer Solutions</td>
<td>Chris Garvey, ANSTO, Environmental Research</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mesoscopic Phase Separation in CMR Manganites</td>
<td>Chris Ling, Sydney University</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Magnetic Spirals and Ferroelectricity</td>
<td>Annemieke Mulders, Curtin University</td>
<td></td>
</tr>
</tbody>
</table>
Separation of Magnetic Scattering - From Intermetallic Magnetism to Nanocrystalline Spinels
Stewart Campbell, UNSW @ ADFA

The Role of Polarisation Analysis in Diffuse and Diffusive Scattering
Trevor Hicks, Monash University

Magnetic Configurations and Dynamics
Bob Stamps, University of Western Australia

Linking Surface Science to Neutron Scattering
Anton Stampfl, ANSTO

14:45 Polarised $^3$He Spin Filters at ILL
Ken Andersen, ILL John Stride, UNSW, Sydney

15:15 Technical Aspects of Resonance Spin-Echo Spectroscopy
Thomas Keller, MPI Stuttgart/FRM2

15:45 Workshop Photo

16:00 Afternoon Tea

16:15 Development of Polarised $^3$He Spin Filters in the USA
Thomas Gentile, NIST

16:45 Discussion of "Scientific Opportunities for Polarised Neutron Scattering at ANSTO"
Shane Kennedy / Mohana Yethiraj / Frank Klose

Goals:
- Identify a list of "hot" polarised neutron science applications that could be addressed by OPAL instruments provided that state-of-the-art polarised neutron instrumentation would be available.
- What are the polarised neutron science areas that we should focus on in the immediate/intermediate future?
- What polarised neutron science does OPAL's user base currently pursue? What are likely future directions?
- What polarised neutron science is currently carried out at the Bragg Institute? What are likely future directions? (This session should not focus on instrumentation!)

18:00 Move to dinner

18:30 Workshop dinner

Wednesday Evening

Thai Peninsular Restaurant at Woronora
2 Prices Circuit
Woronora, NSW 2232
Ph: 9545 4357

Exit bridge to left.
Follow road underneath.
Cross river again.
Turn left into Prices Circuit.
Thursday, 29 November 2007

<table>
<thead>
<tr>
<th>Time</th>
<th>Presentation</th>
<th>Presenter</th>
<th>Chair</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:55</td>
<td>Welcome Back</td>
<td>Frank Klose, ANSTO</td>
<td></td>
</tr>
</tbody>
</table>

Goals for the instrument session:
- To identify what equipment we need for the individual instruments (wavelength/energy range, scattering angle, etc.).
- Pros and cons of different solutions for polarised neutron equipment should be discussed for each of the OPAL instruments (incident beam polarisation, spin flippers, spin analyser, supermirror based devices / $^3$He / Heusler crystals/other solutions?)

9:00 Plans for Polarised Neutrons at Pelican (10-15 min presentation & discussion)  
Dehong Yu  
Trevor Finlayson, U. of Melbourne

9:30 Plans for Polarised Neutrons at Sika (10-15 min presentation & discussion)  
Peter Vorderwisch

10:00 Coffee

10:15 Plans for Polarised Neutrons at Taipan (10-15 min presentation & discussion)  
Mohana Yethiraj  
Shane Kennedy, ANSTO

10:45 Plans for Polarised Neutrons at Quokka (10-15 min presentation & discussion)  
Elliot Gilbert

11:15 Plans for Polarised Neutrons at Platypus (10-15 min presentation & discussion)  
Frank Klose

11:45 Plans for Polarised Neutrons at Wombat (10-15 min presentation & discussion)  
Andrew Studer

12:15 Lunch

13:15 Charge for writing workshop report  
Rob Robinson, ANSTO

13:20 Split into groups for report writing  
(Workshop report sections should have science and instrumentation parts!)

Working groups:  
- TOF inelastic (Pelican)  
  - Dehong Yu
- Cold and thermal triple axis (Sika & Taipan)  
  - Mona Yethiraj / Sergey Danilkin / Peter Vorderwisch
- SANS (Quokka) & Reflectometer (Platypus)  
  - Elliot Gilbert / Bill Hamilton / Michael James
- Diffraction (Wombat)  
  - Andrew Studer / Chris Ling
- Polarised Neutron Technology  
  - Tom Gentile / Ken Andersen

16:00 Reports from working groups (5 min each)  
Frank Klose, ANSTO

16:30 Discussion: Requirements for the Polarised Neutron Infrastructure at OPAL  
Don Kearley, ANSTO

Goals:
- What resources are needed for providing polarised neutron capabilities to the initial 6 OPAL instruments (investments, operation cost, manpower)?
- What infrastructure and resources are needed for a polarized $^3$He (MEOP versus SEOP, investments, manpower, lab space)?
- What approach do other facilities have for their polarised neutron infrastructure?

17:00 Closing  
Frank Klose