Report on Small-Angle Neutron Scattering for the Australian Replacement Research Reactor

Small-Angle Neutron Scattering Workshop
Australian Nuclear Science and Technology Organisation.

13th – 14th December 2001

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Report on Small-Angle Neutron Scattering for the
Australian Research Reactor

Prepared by participants at the Small-Angle Neutron Scattering Workshop,
held at ANSTO on the 13th – 14th December 2001.

Edited: Elliot Gilbert

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Executive Summary

There is a clear need and strong desire for at least one state-of-the-art pinhole small-angle neutron scattering (SANS) instrument at the Australian Replacement Research Reactor when it commences operation in 2005.

The participants at the SANS Workshop have identified that the SANS instrument to be built at the Australian Replacement Research Reactor should:

• be in the spirit to the 40 metre D22 instrument at ILL, France and the 30 metre instruments on NG3 and NG7 at NCNR, NIST in the United States.

and must:

• be sufficiently flexible to enable user-defined and –constructed sample environments to be used
• be capable of time-resolved, dynamic measurements
• have incident beam polarisation
• have easy to use software

Other important issues identified were:

• benefits of polarisation analysis and quantifying spin incoherent background
• provision for TISANE-type measurements and inelastic studies
• provision for higher resolution studies (down to 5%)
• the ability to access the ultra-low q domain to study larger scale structures
• the need for education / outreach on the opportunities with SANS
• the development of interactions with New Zealand
• in-house SAXS facilities
• facilities for deuteration of chemicals

This report contains a scientific case for a small-angle neutron scattering (SANS) instrument to be built at the Australian Replacement Research Reactor that is based on the areas of scientific research expressed by the workshop participants. In addition, trends in SANS research conducted at major overseas neutron facilities are noted.

Basic aspects of SANS design are discussed which meet the above-stated scientific criteria and include a preliminary list of instrument specifications, capabilities and ancillary equipment requested by the workshop participants. The report lists a number of questions that require calculation to optimise the instrument design.
1. Introduction

On the 13th and 14th December 2001, a workshop to define the Small-Angle Neutron Scattering (SANS) requirements for Australia’s Research Reactor was held at ANSTO, Lucas Heights. At present it is anticipated that there will be one dedicated SANS instrument at the reactor when it commences operation in late 2005.

The workshop attracted 55 participants from Australia, New Zealand, Argentina, France, and the United States from university, industry, international neutron and research facilities. The participants’ interests were equally diverse from scientific fields such as chemistry and industrial chemistry; physics; biochemistry; biology; polymer and colloid sciences; mechanical, chemical, polymer and materials engineering; environmental sciences; steel processing; geology and geosciences; and neutron optics. 26 other researchers from Australia, New Zealand, Germany, Switzerland, Israel, Hungary, Russia, Argentina and the United States expressed an interest in attending the workshop, but were unable to attend due to other commitments.

The purpose of the workshop was to:

• promote the techniques of SANS to the Australian Scientific community
• identify the future needs and opportunities in this area, and
• specify instrument requirements based on the future needs.

This document represents the accumulated views of the participants at the workshop.

Figure 1.1 – Attendees of ANSTO SANS workshop gather for group photograph during short break in busy schedule.

A detailed list of workshop attendees and affiliations is in Appendix A.
2. Small-Angle Neutron Scattering – An Introduction

a) Basics of the Technique
Small angle neutron scattering (SANS) is a key tool in the study of a variety of phenomena at the nanoscale (Figure 2.1), probing the structure of materials on a length scale from ten to several thousand Angstroms (1 Angstrom = 0.1 nanometres). The size range spans a vast range of science, from proteins and viruses (biology and medical sciences) to emulsions and microemulsions (polymer and materials science) to phase separation and fractal growth (physics, geology and metallurgy). Evidence of the wide application is borne out by attendees of the workshop from across these research interests.

For scattering to occur from an object, a contrast difference is required between the atoms or molecules in the object and its surroundings, and depends on the type of radiation used. Differences in scattering are thus caused by chemical or physical
inhomogeneities and thus one speaks of ‘scattering particles’. A SANS experiment measures the scattered intensity versus the scattering vector, $q^1$. $q$ is defined as:

$$q = \frac{4\pi}{\lambda} \sin \theta$$

where $\theta$ is half the angle through which the neutrons are scattered and $\lambda$ is the wavelength of the incident radiation. The assumption is made that the scattering is predominantly elastic (the energy of the incident and scattered neutrons is unaltered as a result of the scattering) and inelastic effects may be neglected. The influence of inelastic effects in SANS is currently the subject of investigation by several researchers and is likely to contain interesting science (2); opportunities for study will be discussed briefly below.

Several parameters can be evaluated directly from the scattering data. These include the molecular weight, the radius of gyration ($R_g$) from application of the Guinier approximation, and the particle surface area (Porod’s law). Further quantitative information, such as number of microemulsion droplets in a solution, may be obtained if the data are on an absolute scale. Information on the shape of scattering particle may also be obtained from the slope of a log-log plot of the intensity versus $q$ provides; this is illustrated in Figure 2.2 for disk-like particles.

![Figure 2.2 – SANS pattern from a dilute solution of randomly oriented monodisperse disks of thickness 40 Å and diameter 1600 Å. Characteristic power-law behaviour is observed whose limits are related to the dimensions of the particle.](image)

For systems containing particles that are more complex than simple spheres, disks or rods, they are typically best analysed using scattering models; these are inverted,

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1 The reader may find $q$ written as $Q$ and referred to either as the wavevector transfer or momentum transfer vector. For isotropic scatterers, data are typically radially averaged to give the scalar quantity $q$ (or $Q$).
compared with the experimental data and refined iteratively. At higher particle concentrations (non-dilute regime), SANS provides information concerning interparticle correlation and potential. A Fourier transform of the data provides real space information such as the distance distribution function, \( P(r) \); this method can be applied to dilute systems studied over a sufficiently wide \( q \) range.

b) Scattering and microscopy techniques
Where possible, complementary imaging techniques such as transmission and scanning electron microscopy (TEM and SEM) should be used in conjunction with SANS to obtain the best results. However in many cases SANS is either the best or the only experimental technique available that is capable of providing structural and kinetic information concerning nano-sized inhomogeneities in the medium of interest, whether that be a matrix, a solution or one or more components in a mixture. For example, SANS does not require the production of very thin specimens as is the case for TEM; this process can destroy the very region of the material that is of interest. Microscopy is also less attractive for aqueous samples. Further, a microscopy image may include artefacts and may not be truly representative of the sample. While SANS does not provide real-space structure directly, the technique does probe the sample in its entirety.

The major strength of the SANS technique is that it can be used as a probe on a host of materials, which cover a wide range of research disciplines. Materials that are routinely characterised using the SANS technique include, alloys and ceramics, biological materials, colloidal materials, complex fluids, polymers, surfaces and interfaces and flux lattices in superconductors. Each of these areas have existing or potential industrial interest. The presence of a world-class SANS instrument in Australia will also allow for curiosity-driven, higher-risk, greater-return experiments to be performed locally.

c) Why use neutrons as opposed to X-rays?
Neutrons provide a unique probe for the study of structure for the following:

Neutrons are uncharged and are therefore highly penetrating.

(i) This means that bulk structure can be studied as opposed to micron-depth with X-rays.
(ii) Neutrons can penetrate a number of materials such as silicon, quartz, and sapphire with little attenuation. These materials can act as both substrates for samples and windows for cells.
(iii) Similarly neutrons can penetrate materials such as aluminium that are used in the construction of closed-cycle refrigerators, cryostats and furnaces.

The scattering length of neutrons varies in a non-uniform fashion between elements as well as between different isotopes of the same element, while for X-rays it varies monotonically with increasing atomic number.

(i) As a result, neutrons scatter differently from hydrogen and deuterium. This offers the experimenter a wealth of possibilities. For example, the structure of a complex multiphase system may be solved by either contrast matching (matching the scattering length density of two phases or by selectively
labelling a component (replacing hydrogen for deuterium) (Figure 2.3). This approach is particularly beneficial in aqueous and soft matter systems. There is considerable scope for conducting parallel contrast variation experiments and simultaneous refinement scattering models (3);

(ii) Neutrons can scatter from adjacent elements such as iron and manganese with high contrast; whereas X-rays show very little contrast (e.g. bicopper tetracarboxylate and metalloporphyrins, (4));

(iii) Light elements (such as hydrogen, carbon, nitrogen and oxygen) may be readily observed in the presence of heavy elements (such as barium, lanthanides and actinides).

In addition, neutrons have a magnetic moment enabling them to interact with unpaired electrons in materials that gives rise to magnetism. Neutrons thus provide a unique tool for the structural study of magnetic and superconducting systems.

**CONTRAST VARIATION**

\[
\rho(\text{shell}) \approx \rho(\text{core}) \ll \rho(\text{solvent})
\]

Figure 2.3 – Schematic illustrating the power of the contrast variation technique.

However, neutrons are more expensive to produce and have a lower intensity than X-rays (the latter is sometimes advantageous !). Major benefits may be gained by taking advantage of these differences and employing the complementarity of SANS and SAXS (small-angle X-ray scattering) (4,5).

References:

3. Scientific Case for Small-Angle Scattering Instrumentation at the RRR.

In discussing the widespread application of SANS to areas of interest to the workshop participants, the following categories were selected. However, the majority of researchers are interdisciplinary in their approach and thus substantial overlap exists between categories. All areas have direct industrial application.

a) Life and Biomedical Sciences

Proteins: Proteomics is a rapidly growing field in the post-genomic era. Proteins are molecules with sizes ranging from approximately 10 to 150 Å and hence are amenable to study by SANS. One third of all proteins reside in cell membranes and are difficult to crystallise therefore SANS is useful. Important questions to be addressed include protein-protein interactions, protein nucleic acid interactions, and protein-lipid interactions (1).

Medicine: Iron overload diseases affect approx 0.5% of the Australian population. Iron builds up, in the form of inorganic nanoparticles of iron oxyhydroxide, in tissues of the body. These particles act as catalysts for cell-damaging reactions that ultimately result in cell death and associated organ failure. The physical structure and properties of these particles can be probed using SANS. Whole tissue specimens from both animal models and human tissue can be used to unravel the relationship between iron toxicity and the physical structure of the particles e.g. surface-to-volume ratios.

Gall stones and kidney stones are formed as a result of proteins intercalated in calcium oxalate. Proteins are also relevant as both templating agents for inorganic mineralisation (biomineralisation) and as a model for the production of new materials that mimic those naturally produced (biomimetic materials) such as in the formation of artificial skin.

Structural biology and biotechnology: Biologists have a direct interest in the study of molecular and molecular assemblies at low resolution e.g. proteins in solution, viruses, liposomes, and also protein complexes with, for example, polyelectrolytes such as DNA (2), (Figure 3.1). Contemporary research areas in biology and the life sciences include membrane biophysyics, drug-delivery systems and pharmacology, dental and medical composites, biomaterials, fillings and implants. In enzyme-catalysed processes, protein folding and denaturation due to pH, temperature (e.g. heat shock) can be studied using SANS enabling further understanding of structure-function relationships; the kinetics of these processes may be studied with time resolved SANS.

Further relevant areas are:

- Complexes that are not possible to be crystallised can be studied in solution systematically with different contrasts;
- Organisation of sub-units – nucleosomes, ribosomes, chaparonins;
- Conformational changes in regulatory proteins; DNA binding proteins, cell framework proteins etc.;
- Phase transitions and supramolecular assemblies of peptides in membranes;
- Membrane systems;
- Structure of integral membrane proteins;
- Alignment of membrane proteins in magnetic field.

Figure 3.1 – Application of SANS to structure-determination of calmodulin (2). Left shows the crystal structure of calmodulin (top) and nmr structure of calmodulin-myosin light chain kinase (MLCK-1) (bottom). SANS (right) provided the first evidence that the interconnecting matrix in calmodulin is flexible, enabling the dramatic conformational collapse upon binding to the target sequence in MLCK-1.

b) Physical Sciences

Nanomagnetic materials: The physical properties and magnetic behaviour of magnetic materials change dramatically when they are reduced to small particle sizes. Recent studies of nanomagnetic particles have shown tantalising evidence of macroscopic quantum tunnelling of magnetisation. The study of this phenomenon will shed light on the limits of scale under which quantum mechanical phenomena can be observed. The combination of the magnetic moment of neutrons, with the ability of scattering techniques to probe nanoscale phenomena, make SANS an ideal tool for these studies. Nanomagnetic materials are of great interest in the magnetic recording industry since the physics of these systems will ultimately limit the information density of new magnetic recording media and the speed with which information can be written to such media. Application of nanomagnets in the biomedical/biotechnological field include magnetically targeted drug delivery, magnetic hyperthermia treatment, and novel biosensors.
Fuel cells and hydrogen storage: Hydrogen as a potential future clean fuel needs to be stored at high density. Since high pressure is unsafe and expensive, alternative methods of storing hydrogen in the solid state are being investigated by combination with such materials as metals as hydrides and carbon as nanotubes and intercalated carbons. As hydrogen is introduced into the material, SANS will be able to map the phase changes that manifest themselves on the nanometer scale in-situ.

c) Polymer Science and Engineering

Polymers are long chain molecules that play an important role in biology, medical applications, new materials, biotechnology, and nanocomposites. The final properties of the polymeric materials are determined by their nanostructure. SANS will be used to study crystallisation kinetics, blend structure (interpenetrating networks), and polymers under shear. In the next few years the new RAFT (reversible-addition-fragmentation transfer polymerisation) processes developed in Australia will revolutionise polymer science because of the highly increased control over the final product. Low perturbations are important in studying polymers thus SANS offers a non-invasive alternative to staining and sectioning.

Other applications of SANS to Polymer Science and Engineering include:
- Chain Conformation and Interactions Affecting Miscibility in Polymer Blends (4);
- Mechanisms and Effectiveness of Blend Compatibilizers (diblock copolymers, graft copolymers, hydrogen-bonding side groups, etc.);
• Real-Time Studies of Microphase Separation of Block Copolymers / Blends (5);
• Effects of Pressure and Shear on Polymer Phase Behaviour (6);
• Effects of Confinement (e.g. in thin films or porous media) on Chain Conformation and Phase Behavior (7,8);
• Critical fluctuations and determination of $\chi$ parameter;
• Conformations of polymer chains;
• Miscibility, Interactions and Blends;
• Real-time studies of micro-phase separation of block copolymers;
• The effect of pressure, shear and history on polymer phase behaviour in polymer processing and injection moulding;
• Morphology and Phase Behaviour of Block Copolymers in Selective Solvents: mesoemulsions, viscosity modifiers, solubilizers, etc. (9,10); (Figure 3.3);
• Novel Macromolecular Architectures and Resulting Phase Behavior e.g. dendrimers, hyperbranched polymers, star polymers and liquid crystalline polymers;
• Electrochemical processes and conducting polymer kinetics;
• PET - poly(ethylene terephthalate) - manufacturing with improved properties;
• Effect of humidity on cellulose fibres

Figure 3.3 – SANS from 450K Da poly(styrenesulphonate) polyelectrolyte, in zero average contrast condition, in bulk and confined geometry (Vycor glass) (7). Bulk data have been fitted to a Sharp and Bloomfield model for wormlike chains for $q l_p < 2$ where $l_p$ is the chain persistence length. $q^{-2}$ and $q^{-1}$ power-law regions crossover at $q^*$. 

d) Chemistry, Chemical Engineering and Materials Science

Mixing, separation, and precipitation are of significant importance to the application of materials. Manipulation of the phase behaviour of pure materials such as partially
stabilized zirconia can be followed by SANS through the difference between the
scattering length density of the constituent phases. SANS is widely used to study
organic-inorganic composites and templating processes, for example, in zeolites and
mesoporous materials typically associated with self-assembly of precursor molecules.

Other relevant areas for study are:
- Engineered Nanostructures and Mesostructural materials;
- Intercalated carbon;
- Helium bubble growth in martensitic steel for fusion reactors;
- Radiation-Induced Microstructural Changes in Reactor Pressure Vessels (making
  use of the magnetic contrast between phases using unpolarised neutrons);
- surface properties of catalysts;
- metal physics;
- phase stability of alloys, precipitates, interfaces, grain boundaries
- structural tailoring and testing, stability under load;
- nanocrystalline materials and influence of grain size, interface, porosity;
- Colloid structure, interactions and stabilisation;
- Surfactant and Micro-emulsions microstructures and phase transitions;
- Measurement of rheological properties (simultaneously with SANS) e.g. shear
  thinning / thickening / shear induced mixing / demixing; viscoelasticity and
  thixotropy;
- Kinetics of micro-emulsion polymerisation;
- Molecular templates for controlled synthesis of nano-phase materials;
- Stages of growth in inorganic templated materials;
- Metals and Ceramics;
- Nucleation and Growth of Precipitates in Alloys;
- Characterization of Distributed Damage in Metals and Ceramics Subjected to
  Creep, Fatigue, etc.;
- In-Situ Densification of Ceramics; Grain Size and Defect Structure in
  Nanocrystalline Materials
- Environmentally benign solvents (e.g. supercritical CO₂) and modification of
  polymer processing techniques

e) Industrial Research

Colloids/emulsion/Micellar Systems: Amphiphiles (surfactants detergents and
soaps) self-assemble in solution to form aggregates on the nanometer length scale.
These structures lead to fluids of widely varying rheological properties used in the
food (e.g. ice cream, mayonnaise, milk), cosmetic/personal care products,
pharmaceuticals and drug-delivery, and the mining industry. SANS in parallel with
isotopic substitution enables the detailed study of these systems and, drawing ideas
from membrane biophysics, a greater understanding of the stabilising mechanisms.
Emulsions can also be used as templates for the synthesis of new materials such as
extremely low-density silicas. For the polymer industry, benefits include an improved
understanding of the miscibility of polymers and solvents, an increased product range,
improved moulding and improved recycling, plastic degradation and responsive
materials.
**Agriculture and Natural products:** Production of structural materials such as fibreboard from pine chips is a current technology. Production of these materials from eucalypt or bagasse or other biowaste often produces unsatisfactory product because of poor adhesion of the resin to the fibre. Current treatments are expensive and the mechanism of adhesion at the nanoscale is not known.

Other applications of SANS are:
- Bioremediation;
- Paper and pulp manufacture;
- Timber industry and associated fibre technology including timber industry (diffraction from timber is a useful technique in the classification of timber quality);
- Wool and cotton;
- Cereals, grain products, maize. (Starch structures have a characteristic SANS signatures that can be used to elucidate differences between varieties and treatments).

**Cement/concrete:** The mechanism of concrete hardening by hydration is still not understood after 2000 years. It is highly likely that an understanding these processes are intimately involved with the changes in nanostructure during the hardening process can be revealed by isotopic substitution in conjunction with SANS.

**Wine science:** Protein clouding of wines is a poorly understood problem for the Australian wine industry as are the changes in grape skins on fermentation. In both cases the underlying causes are related to biological structures in the nanometer length scale range.

**Porosity:** Relevant to zeolites, catalysts and MCM-type materials discussed above, SANS has the capability of studying porosity as well as particle size but differs from conventional techniques in measuring both closed and open pores. The smaller pore systems are synthesized in tens-of-thousands of tons, as supports for catalysts, with unique properties. Aluminium/silicon based inorganic polymers are being investigated as a replacement for structural materials such as cement. As with cement, the nanostructure of these inorganic polymers are not well understood. The influence of aggregates in the inorganic polymer nanostructure needs to be investigated.

**Petroleum and Mining Industry:** Problems to be investigated using SANS include the interaction of drilling muds with porous oil bearing rocks in the oil and gas industry. The benefits to the mining industry include improved product quality and environmental care; and for the Petroleum industry, benefits include enhanced oil recovery. Froth flotation used in mineral processing is a black art. The interaction of the collector molecules with the mineral and the gangue are not well understood at present. If understood, suitable collector systems could be designed which are cheaper than the current expensive chemicals.

Other areas of research include:
- Organic/inorganic systems including talc contaminants in Nickel;
- Sodium oxalate & the Bayer process
- novel nanocomposites.
**Pyrolysis experiments:** The *in-situ* capability of SANS and ability to use conventional furnaces allows us to monitor structural changes as materials such as coal and oil shale are heated. It is difficult to monitor these changes using other techniques. The ability of neutron beams to penetrate large quantities of bulk specimens makes it ideal for such *in-situ* studies.

**Barriers and the microstructure of radioactive waste materials:** Synroc is a patented material developed by the CSIRO that is a potential medium for high level radioactive waste storage. Synroc is composed of many different inorganic phases and the leaching of undesirable radioactive material from Synroc depends on the crystallite quality and dimension and possibly surface effects.

Other areas in which SANS can be utilised:
- Study of porosity in concrete;
- Clays and barrier materials to water.

**Degradation of polymers:** New materials derived from crops will revolutionise the plastics industry by removing the waste problem. The rates of degradation of these new polymer materials are of crucial importance and may be studied with SANS.

**References:**

4. Recent Developments in Small-Angle Neutron Scattering

i) Time-Resolved SANS and ‘Time-Involved’ SANS (‘TISANE’)

There is extensive interest in minimising the collection time of SANS data to enable more rapid kinetic measurements. In conventional time-slicing, data is collected for some time interval, $\Delta t$, in a block of histogramming memory, and then collected in another block of memory for the next $\Delta t$ and so forth. A series of such measurements, i.e. time slices, must be repeated many times, of course, to build up reasonable statistics in every time interval. With this approach, time resolution down to 50-100 millisecond is straightforward.

![Figure 4.1 – Time-resolved studies of Photoactive Yellow Protein response to cyclic flash-light illumination (1).](image)

It may be that a single sample could be studied many times if it responds in the same way to an external effect. For example, if a single 100-second snapshot could be collected that has appropriate statistics for data analysis then 1000 repetitions could provide, in principle, 100 millisecond time-resolution. Such is the case for studies of Photo-active Yellow Protein (PYP) whose response was studied to a cyclic flash-light illumination (1) (Figure 4.1).

Beyond this, however, the spread in arrival times at the detector, due to the wavelength spread in the incident beam, limits what can be achieved this way (Figure 4.2). For a spread of 10%-20%, the variation in arrival time is between $\approx 5$ and $50$ ms. Consequently, for better time resolution, an alternative approach is required.

In ‘TISANE’, a simple chopper is located prior to the sample (2) and the wavelength resolution of the experiment may be relaxed further. The beam is then pulsed such that the pulsing may be correlated with the cycling of the external stimulus, e.g. chopper synchronised with shear flow. The aim is to have a one-to-one correlation between the scattered neutron arrival time and the stimulus from different pulses. Thus neutrons arrive at the same point of the periodic stimulus cycle and then are added together. For a system that can be repeatedly stimulated so that sufficient statistics may be obtained, with available technology, 50-100 microsecond time-resolution is achievable (Figure 4.3).
Time resolution of 'conventional' time-slicing experiments is limited by the wavelength spread \( \Delta \lambda / \lambda \) (typically 10% - 20%, fwhm)

\[ \Delta t = \frac{2L \lambda}{c} \left( \frac{\Delta \lambda}{\lambda} \right) \]

\( c \approx 4 \text{m-A/\text{ms}} \)

\( \Delta t \approx 5 - 50 \text{ ms} \)

Figure 4.2 – Time-resolution limit in conventional time-slicing experiments.

Figure 4.3 – TISANE's ability to obtain sub-millisecond time resolution relies on the one-to-one correlation between the scattered neutron arrival time and the stimulus from different pulses (2).
A stopped flow apparatus has been incorporated into D22 to enable SANS data to be collected from samples immediately after mixing that uses stepper motor controlled syringes (Figure 4.4). The current limitation on time-resolved measurements is also the finite time required for mixing precursors and flowing to the sample position. At present, the minimum collection time is down to $\approx 100$ ms but, in principle, could be reduced to 10 ms. This approach has been used to study, for example, the phase diagram of AOT [bis(2-ethylhexyl)sulphosuccinate sodium salt] in brine (3) and the formation of cationic vesicle/DNA complexes (4). For irreversible responses to a stimulus, the limit remains the precision of cutting frames and the wavelength spread of the beam.

Figure 4.4 - Stepper motor controlled syringe apparatus used in conjunction with stopped flow on D22 (courtesy of Isabelle Grillo).

### ii) Inelastic SANS

Generally SANS data are reduced assuming that the scattering process is purely elastic. By incorporating a chopper in the pre-sample flight path, it is possible to ascertain whether inelastic effects are taking place however. The SANS from SiO$_2$ precipitates in a single crystal of silicon which has been heat treated for 500 hours at 600 °C is shown in Figure 4.5 (4) with the neutron beam incident along a $<100>$ direction. The central cross arises from the cushion shaped SiO$_2$ precipitates lying on (100) planes with their edges along $<110>$ directions. The use of a chopper indicated that the outer features were in fact inelastic in origin and associated with Umklapp processes.

### iii) Refractive Lenses and Improvements in $q_{\text{min}}$

Since the scattering signal is proportional to sample size, a lens system can be used to improve resolution more efficiently, by reducing the size of the source aperture, than is possible with pinhole collimation where both the source aperture and sample size must be reduced proportionally to improve angular resolution. Figure 4.6 shows a 6-lens array for $\lambda = 18.1$ Å and a 28-lens array for $\lambda = 8.44$ Å that are available on the

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2 The volume of sample required for this type of experiment can be estimated as follows assuming 1. a 10-second exposure contains sufficient statistics for data analysis and 2. required 10 ms time-resolution: Typical sample volume = 200 µL. Number of experimental repetitions required = 10 s / 10 ms = 1000. Total volume required = 200 mL. This quantity of material may be prohibitively expensive for certain samples.
NIST 30 m instruments (5). These lenses are composed of MgF$_2$ and are installed just in front of the sample position. It has been shown that for $q < 0.0038$ Å$^{-1}$, the lenses outperform pinhole collimation (Figure 4.6).

Figure 4.5 – Inelastic effects in SANS region from heat-treated single crystal of silicon (4).

Figure 4.6 - MgF$_2$ lens arrays installed on NG3/NG7. Top) 6-lens array for $\lambda = 18.1$ Å; 28 lens-array for $\lambda = 8.44$ Å (Transmission $\approx$ 70%). Bottom) Use of lenses is more effective than pinhole collimation for $q < 0.0038$ Å$^{-1}$ and enhances resolution (5).
iv) Polarised proton clusters

Figure 4.7 shows the Chromium (V) complex, CrO$_7$C$_4$(C$_2$H$_5$)$_4$: essentially a Chromium core surrounded by an organic shell. Using microwave pumping (i.e. electron spin resonance or paramagnetic resonance) and nmr, with a 3.5 T cryo-magnetic system and a $^3$He insert operated at 1 K, the unpaired aligned electrons are able to transfer their spin ordering to nearby protons. Since neutrons are sensitive to proton polarisation, the decay of the polarisation may be studied by SANS. To achieve the necessary sub-second statistics, scattering data were taken in a stroboscopic manner using short time frames. Two time constants are obtained, one for the “close proton” polarisation within the Cr complex and the slower one being the bulk time constant. The proton depolarisation may be directly compared with ‘bulk’ nmr measurements (6).

![Figure 4.7 – Proton depolarisation measurements with SANS has been compared with nmr from a Cr(V) complex (6); submitted for publication to E. P. Lett.](image)

References:

1. Roland May and collaboration with W. Crielaard et al., University of Amsterdam
6. B. van der Brandt et al., submitted for publication to E. P. Lett.
5. Requested Performance

Introduction

The participants stressed the need for a world-class instrument. The design will therefore be strongly influenced by the 40 m D22 instrument at ILL (1) and the two 30 m SANS instruments at NIST (2); these instruments are widely considered to currently be the best in the world (Figure 5.1); Table 5.1, Table 5.2.

![Diagram of CHANS 30 METER SANS INSTRUMENT](image)

Figure 5.1 – Top: 40 m D22 instrument at ILL; Bottom: 30 m NG3 SANS instrument at NIST.

Time-Resolved Data Collection

Time-resolved measurements were identified as important but it is unclear what time resolution is required. The TISANE approach is attractive but is still under development. Consideration should be given to designing the instrument such that this could be implemented at a later stage if proven and developments in this area should be monitored.

Instrument Length

Since $q_{\text{min}}$ is primarily determined by instrument length, the participants requested the maximum length achievable; a 40 m instrument is envisioned.
**Instrument Resolution**

An instrument resolution of as low as 5% would be beneficial for certain studies (3).

Table 5.1 – Instrument Parameters for Proposed Pinhole SANS Instrument at the RRR

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Without Lenses</th>
<th>With Lenses</th>
</tr>
</thead>
<tbody>
<tr>
<td>q range (Å⁻¹)</td>
<td>0.0015 – 0.7</td>
<td>0.0008 – 0.7</td>
</tr>
<tr>
<td>Wavelength Range (Å)</td>
<td>4 – 20</td>
<td></td>
</tr>
<tr>
<td>Wavelength Resolution (Δλ/λ)</td>
<td>5% – 20%</td>
<td></td>
</tr>
<tr>
<td>Δq/q</td>
<td>5% – 20%</td>
<td></td>
</tr>
<tr>
<td>Incident Polarisation</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Polarisation Analysis</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Chopper for TOF/inelastic</td>
<td>Not initially,</td>
<td></td>
</tr>
<tr>
<td></td>
<td>but include provision</td>
<td></td>
</tr>
<tr>
<td>Pre-sample chopper (TISANE)</td>
<td>Include provision</td>
<td></td>
</tr>
<tr>
<td>White Flux at sample</td>
<td>To be determined</td>
<td></td>
</tr>
<tr>
<td>Sample size</td>
<td>Up to collimator dimensions</td>
<td></td>
</tr>
<tr>
<td>Beam size</td>
<td>Up to collimator dimensions</td>
<td></td>
</tr>
<tr>
<td>Source-Sample Distance (m)</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>Sample-Detector Distance (m)</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>Detector Type</td>
<td>³He wire</td>
<td></td>
</tr>
<tr>
<td>Detector Area (cm²)</td>
<td>4096 minimum; 10000 to be determined</td>
<td></td>
</tr>
<tr>
<td>Detector Resolution</td>
<td>5 mm</td>
<td></td>
</tr>
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</table>

Table 5.2 - Instrument Parameters for NG3/NG7 (NIST) and D22 (ILL)

<table>
<thead>
<tr>
<th></th>
<th>NG3/NG7(NIST)</th>
<th>D22 (ILL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Detector Dimensions (cm)</td>
<td>64 x 64</td>
<td>100 x 100</td>
</tr>
<tr>
<td>Detector Resolution (cm)</td>
<td>0.5</td>
<td>0.75</td>
</tr>
<tr>
<td>Detector Supplier</td>
<td>ORDELA</td>
<td>In-house / CERCA Changing to array of linear PSDs</td>
</tr>
<tr>
<td>Counselate (kHz)</td>
<td>100 – (linear PSD array ≈ 13000)</td>
<td></td>
</tr>
<tr>
<td>Deadtime Losses</td>
<td>10%</td>
<td></td>
</tr>
<tr>
<td>Velocity Selector</td>
<td>MIRROTRON</td>
<td>DORNIER</td>
</tr>
<tr>
<td>Maximum velocity selector transmission</td>
<td>75%</td>
<td>94%</td>
</tr>
<tr>
<td>Wavelength Range (Å)</td>
<td>5 – 20</td>
<td>5 - 42</td>
</tr>
<tr>
<td>Wavelength Resolution</td>
<td>10 – 30%</td>
<td>8 – 20%</td>
</tr>
<tr>
<td>q range (Å⁻¹) (with lenses)</td>
<td>0.0015 – 0.7 (0.0008)</td>
<td>0.0007 – 1.0</td>
</tr>
<tr>
<td>Total Instrument Length (m)</td>
<td>30</td>
<td>40</td>
</tr>
<tr>
<td>Min. Sample-Det. Dist. (m)</td>
<td>1.3 (NG3); 1.0 (NG7)</td>
<td>1.35</td>
</tr>
<tr>
<td>Max. Sample-Det. Dist. (m)</td>
<td>13.2 (NG3); 15.3 (NG7)</td>
<td>18</td>
</tr>
<tr>
<td>Max. Detector Offset (cm)</td>
<td>25</td>
<td>50</td>
</tr>
<tr>
<td>Sample Diameter (mm)</td>
<td>5 – 25</td>
<td>1.8 – 10</td>
</tr>
</tbody>
</table>
**Inelastic Measurements**

Inelastic studies require a chopper and a time-of-flight approach to data analysis. While a chopper is not envisioned in the instrument immediately, the design should make provision for one at a later stage if appropriate.

**Sample Position**

There is significant scope for improvement. The largest dimension envisioned for ancillary equipment is 1 m but it was considered that 0.5 m would be sufficient (although less if a polarised option were available). This space is also considered suitable for the possible addition of optical probes for simultaneous measurements, e.g. UV absorption / fluorescence. The requirement must be balanced with the need to minimise air scatter between the sample and the detector.

Other related issues:
- The sample position should have standard connectors for user-defined and -produced unique environments.
- A removable sample chamber would be required.
- The sample position should be easily accessed and the multi-position sample holders should have the ability to be easily translated for insertion of sample cells, i.e. without the need to unscrew and lift out.
- There should be sufficient space around the instrument to position large pieces of equipment e.g. polymer extruder.
- There should be a 30-minute maximum changeover time without crane for changing samples.
- Maximum height between support and beam of ≈ 0.5 m.

**Sample Environment**

Many of the following need to be designed specifically for the SANS sample position. Requested specifications are:
- Samples should have complete \( x, y, z \) and \( \theta, \phi, \psi \) motion, enabling, e.g. study of single crystal, oriented silica films; this motion would be valuable for cryostat-enclosed samples also.
- A 25-position automatic sample holder (≈ 80 cm wide) or possibility of 2-stack of samples in a row arrangement
- Electric Field
- Pressure
- Temperature-ramping / thermal shock (±200° min\(^{-1}\)) to \( T_{\text{max}} \) of ≈ 1000°C
- Furnace up to 2000°C
- Cryostat down to 2K (wide window is required at short sample-detector distances)
- Laser beam for sample alignment
- Circulating bath (-10 to 80°C)
- Thermostatted sample holders (0.1° precision)
- Sample changer robot for dangerous (e.g. active) samples and for precise sample handling
- Magnetic field > 10 T
• magnetic field shielding (0 T)
• vacuum chamber for weakly scattering samples
• humidity / atmospheric control
• 200 microSv/h radiation shielding (transport of nuclear waste)
• micro-flow cell (auto-mixing and injection)
• shear cells
• sample table
• flexible cells e.g. for electrochemical inserts
• stopped flow apparatus
• rheometer for shear flow measurements concurrent with SANS measurement

Figure 5.2 – *In-situ* rheometry on D11 (courtesy of Peter Lindner, ILL).

**Sample size**

Users should be discouraged from bringing small samples since beam time is (generally) more expensive than larger sample production although it is understood that this is not always possible.

**Data acquisition, reduction and analysis software**

Data acquisition, reduction and analysis software must be easy to use. Software should provide inexperienced users with necessary prompting and presented only with available options for instrument configuration with parameter files. An operating manual should be made available that can be accessed remotely, prior to experiments, enabling users to familiarise themselves with instrument control.

**The case for Polarised Neutrons**

The use of polarised neutrons enables the contribution of magnetic and structural information to be separated thus opening the way for detailed studies of the relationship between the structure and magnetic behaviour of materials, e.g. ferrofluids (4). The use of polarised neutrons in SANS is in its infancy but it is believed that this area will expand greatly in the future. A polarised instrument is also likely to be a significant drawcard for researchers.
The case for Polarisation Analysis

Spin incoherent background is a prominent source of background scattering and thus signal-to-noise in typical SANS measurements. Spin incoherent scattering spin-flips two-thirds of the proton nuclear spins whereas the coherent signal – containing structural information - does not spin-flip. This ratio can be quantitatively used to determine the extent of spin incoherence and to separate it from the coherent signal. Test neutron reflectivity experiments on the ISIS reflectometer, CRISP, have shown that at least an order of magnitude increase in signal to noise can be obtained by this method (5). One of the important consequences of this is extension of useful SANS data to higher q and thus higher spatial resolution revealing details on a much finer scale. Other benefits to having polarisation analysis are the enhanced sensitivity to magnetic scattering.

Non-instrument-specific Requests

• Deuteration of chemical facilities for sample preparation

The participants emphasised the need for a facility in which deuterated materials may be manufactured; this view is in common with that expressed at the ‘Neutrons in Biology Workshop’. The required infrastructure development is outside the reactor instruments’ budget and scope but should be investigated outside this.

• Small-Angle X-Ray Scattering Facilities

There is clear support for the availability of in-house SAXS facilities. There is interest in conducting parallel SANS and SAXS measurements although it is unclear what design such an experimental set-up would take.

• Educational outreach

The participants expressed a desire for greater exposure of small-angle techniques to Australian researchers particularly given the wide range of application across many research fields.

• Simultaneous or Complementary Techniques

There is insufficient demand to have a dedicated instrument for grazing-incidence SANS measurements; the user should be prepared to adopt their own set-ups on SANS / reflectometers designed as part of the Replacement Research Reactor project.

• Design of Laboratories

Consultation should be made with community regarding fitting out of laboratories. They need to have several locations so that harmless laboratory work can be separated from Biohazard cabinet. It would be useful to have the ability to seal samples into quartz cells in an automated way.
References:

(1) http://www.ill.fr/YellowBook/D22/
(5) P. Reynolds (private communication).
6. Instrument Design

The 40 m D22 instrument at ILL and the two 30 m instruments at NCNR at NIST are widely regarded as the best SANS instruments in the world. Two new SANS instruments of 35 m and 40 m length are currently being designed for installation at HFIR at Oak Ridge National Laboratory with similar design. The general philosophy is to construct a similar instrument at the Australian Replacement Research Reactor.

The following questions require particular emphasis during the design-study to optimise aspects of the instrument design.

- The active area and spatial resolution of the detector
- The optimal guide coating

Velocity Selector

DORNIER and MIRROTRON are the main suppliers of velocity selectors. Whichever model is chosen, a spare is required to enable regular maintenance work to be conducted; it may be appropriate to purchase a spare with different resolution. A 5% selector is available from MIRROTRON that may be suitable for high-resolution studies. Selectors may be calibrated using time-of-flight with a simple chopper at the sample position.

One might wish to choose between a low resolution and a high resolution selector, choosing one for a particular run cycle and then replace. This approach is suitable in principle, as long as the selector position can be maintained otherwise calibration is required that may take as much as two days using calibration equipment and skilled technical staff. There are disadvantages in using $\lambda_{\text{min}} \leq 4$ Å due to velocity selector effects on tilting. $\lambda_{\text{max}}$ should be $\approx 20$ Å since longer wavelengths result in greater multiple scattering, flux decrease due to absorption and smearing effects due to gravity.

Instrument Resolution

To obtain a high-resolution mode of operation (5% requested), a monochromator option should be investigated. A double monochromator option (ex-D11, ILL) should not be considered as a full-time option. Band-pass filters from XENOCS (ex-ILL) could be investigated. The instrumental resolution is of course also determined by geometrical smearing due to the finite beam size. To obtain the required resolution, smaller beams would be necessary with a corresponding decrease in flux.

Inelastic Measurements

The necessary time-binning capability is a feature of the current ORDELA area detectors. ILL already has a chopper for inelastic studies and NIST will be installing in a custom-made first guide section.

A 4-position, automated and removable guide system is needed. ORNL have made mechanical improvements by employing more precise motors. A carousel design offers no advantage over a translational table design.
Choice of coating for guide material after the velocity selector needs to be investigated. Both D22 and NG3/NG7 use natural Nickel guides; D11 uses glass guides. While improvements in guide reflectivity results in an increased flux, the enhancement occurs at shorter wavelength. Imperfections in the coating quality result in a loss of long wavelength neutrons (through off-specular scattering) and an increase in instrument background. There may be gains in using supermirror guide coating for $q_{\text{max}}$ (shortest sample detector distance, short wavelength neutrons). Simulations should enable consideration of benefits at $q_{\text{max}}$ (gain in short wavelength neutrons) against potential limitations for $q_{\text{min}}$ (increased background, reduced flux) for smooth, uncoated borated glass, natural nickel, $^{58}\text{Ni}$ (m=1) and supermirror guide (m=2). The use of m=2 supermirror guide prior to the velocity selector, as per contract with INVAP (1) and Mirrotron, is suitable (2).

Polarisation of incident beam should be included whether or not polarisation analysis is included in initial design. This will be a drawcard for researchers. Instrument should be made of non-magnetic material such as aluminium and some grades of stainless steel but excludes mild steel. Polariser cost is inexpensive. The challenges are in producing efficient polarisers and analysers with wide angular and wavelength acceptance and to produce analysers free from small-angle scattering. Thus while the polariser is located upstream from the collimation, the same approach is inappropriate for analysis. $^3\text{He}$ is being actively studied as a polariser. The efficiency in polarisation has to be balanced with the lower associated transmission. At present, best results are for 50% transmission and $\approx 60-70\%$ polarisation. This approach is far from optimised and is still at the development stage.

Automatic attenuation of the beam is required.

Length of instrument and minimum q. A 20MW reactor and good cold source would justify 40 m. Considerations are that for wavelengths greater than the maximum in the incident cold source spectrum, the number of neutrons decreases approximately to $\lambda^{-4}$. Also, for a fixed instrument length, slower neutrons are more greatly affected by gravity, giving rise to smearing effects. In addition, the diminishing number of long-wavelength neutrons are more strongly absorbed and have a higher multiple scattering probability. To access lower values of $q_{\text{min}}$, there is thus a desire to build the longest instrument that can be fitted within the guide hall. The capacity for studying even greater distances than available by SANS will be discussed below as part of ‘The Case for a USANS instrument at the RRR’.

The use of multiple refractive lenses should definitely be considered. They offer a cheap and simple method of improving the resolution of the instrument and accessing a lower minimum q without the significant intensity losses associated with reducing both source and sample size. Lenses employed at NIST are 2.5 cm in diameter, on a cradle and can be moved in and out of position. The 18.1 Å lens array must be used in conjunction with MgF$_2$ prisms to minimise gravity effects. The effect of background scattering and transmission from prisms must be considered (3).

The application of adaptive optics’ methodology may be suitable for correcting for chromatic aberration from the lenses for finite wavelength resolution (4).
**Toroidal Mirrors.** Toroidal mirrors may also be used to reduce $q_{\text{min}}$ and are being investigated at Jülich (5). Surface roughness from grazing incidence on mirrors is problematic however, as a mean square roughness of $< 2 \, \text{Å}$ is required over their typically large area. Advantages are that the resolution does not depend on the size of the sample nor sample-detector distance but very large samples are needed to use the entire beam widths at the shorter sample-detector distances.

The sample chamber requires creative engineering. Conflicting requirements are the minimisation of the air path and collimation as close as possible to reduce signal to noise but with the availability to access a large sample space and flexibility.

NIST has a two-position option. There is either a permanent and evacuable sample chamber or alternatively a sample table further upstream. When the table is not used, a tube bridges the sample table to extend the pre-sample flight path to the chamber. When the table is used, the chamber is evacuated to form part of the post-sample flight path thereby increasing the minimum sample-to-detector distance. There may be scope in consideration of a sliding chamber or a more versatile, section-separated approach.

Sophisticated control / interlock system is required with gate valves for vacuum. Motivation against a single permanent chamber is time required to evacuate. An ultra high vacuum is not necessary; a vacuum no better than $\approx 50 \, \text{microns}$ is needed to remove background due to air scattering.

Sample alignment method is required. Options include semi-transparent silicon wafer with laser and light alignment.

A simple method to change aperture system is required. Sample-defining aperture should be as close to sample as possible. A variable iris would be ideal but has not yet been made. This may be considered by a lens or camera manufacturer.

Aperture Shape and Beam Stop. The relative benefits of a rectangular over circular need to be considered.

ORDELA 2660N detector ($64 \times 64 \, \text{cm}^2$) has proven to have a reliable track record for 2 years at NIST. The new instruments at ORNL will use the ORDELA 21000N with an active area of $100 \times 100 \, \text{cm}^2$ enabling a larger dynamic $q$ range as per D22 at ILL $^3$. The detector carriage should have ability to be offset at ANY sample-detector distance beyond the minimum SDD and up to half the detector diameter while maintaining full illumination (Table 6.1). There are potential countrate gains to be made by detectors being developed at ILL using multi-one dimensional detectors. While the linear detectors are available from Reuter-Stokes, the multi-1D detector is not yet commercially available. They will have, initially, a minimum resolution of 8 mm. CERCA detectors should also be considered.

Image plates should not being actively considered due to inherent low time resolution as a result of processing time. An alternative approach is to use of an Anger camera, as is the case at Julich (6).

$^3$ Associated parallax issues need to be carefully considered.
A spare detector is required but it need not be available initially and not necessarily of the same size and resolution. There may be benefits to having a spare detector with smaller area but better resolution. However, one should generally avoid exchanging detectors for this benefit due to risks associated with detector movement.

Table 6.1 Comparison of specifications for two ORDELA PSPC (7).

<table>
<thead>
<tr>
<th></th>
<th>Ordela 2660N</th>
<th>Ordela 21000N</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Active area</strong></td>
<td>64.5cm × 64.5cm</td>
<td>98cm × 98cm</td>
</tr>
<tr>
<td><strong>Active depth</strong></td>
<td>2.54cm</td>
<td>6.4cm</td>
</tr>
<tr>
<td><strong>Spatial resolution</strong></td>
<td>128 × 128 pixels</td>
<td>192 × 192 pixels</td>
</tr>
<tr>
<td><strong>Pixel size</strong></td>
<td>0.5cm × 0.5cm</td>
<td>0.51cm × 0.51cm</td>
</tr>
<tr>
<td><strong>Spatial uncertainty</strong></td>
<td>0.5cm</td>
<td>0.5cm</td>
</tr>
<tr>
<td><strong>Countrate capability</strong></td>
<td>10^4 n/s/anode (10^6 n/s total)</td>
<td>10^5 n/s/anode (10^7 n/s total)</td>
</tr>
<tr>
<td><strong>Spatial uniformity</strong></td>
<td>±2% integral, ±10% differential</td>
<td>±2% integral, ±10% differential</td>
</tr>
<tr>
<td><strong>Counting gas</strong></td>
<td>77%^3He+23%CF_4 260kPa</td>
<td>60%^3He+40%CF_4 125kPa</td>
</tr>
<tr>
<td><strong>Detection efficiency</strong></td>
<td>80%(5), 65%(3), 50%(2)</td>
<td>80%(5), 65%(3), 50%(2)</td>
</tr>
<tr>
<td><strong>Overall dimensions</strong></td>
<td>122cm diameter × 50cm depth</td>
<td>122cm × 122cm × 38cm</td>
</tr>
<tr>
<td><strong>Weight</strong></td>
<td>~800kg</td>
<td>~1250kg</td>
</tr>
</tbody>
</table>

The spare detector should not be installed simultaneously with the main detector to provide a wide-angle bank since sample geometry cannot be optimised for both detectors simultaneously. Other factors relate to expense and low use (8). Spare electronics, which represent a significant fraction of the detector cost, may not be required depending on the choice of spare detector.

A countrate of 100kHz with 10% loss is sufficient for a 64 cm × 64 cm detector but a larger detector would benefit greatly from a faster collection rate. The emphasis of higher count rates, at slightly relaxed resolution, is being actively pursued through the Millennium Project at ILL.

SANS instruments located on lower intensity sources are more competitive at shorter sample-detector distances than their more intense counterparts, since the latter need to
either attenuate incident beam intensity or move the detector further away due to current limitations on detector performance.

**Data acquisition, reduction and analysis software.** Software requirements depend on the detector chosen and need to be instrument specific. All components should be under computer control, ideally including the sample aperture. It is considered advisable to design software that is based upon a commercial package (e.g. MATLAB, IDL, IGOR by WaveMetrics) operating on and with well-known (multi-)platform / operating system. Alternatives would be to base on an existing facility-based structure (e.g. MAD at ILL) or to design from scratch. JAVA should be considered for web-based access. ILL has a program GRASP that is MATLAB-based. It is a multi-platform GUI enabling data to be observed as it is being collected and also auto-analysis. The International Commission on SAS in IUCr is trying to establish data standards but no decision has yet been made. Universal standard for data formats could however be considered (PSI - NEXUS; clickable options for different data formats, ASCII as default).

**Signal to noise.** Parasitic Scattering and Detector Shielding need to be carefully considered, particularly beam apertures and adjacent instruments to enable traditionally background-limiting experiments to be studied. The ability to conduct experiments on aerosols for example is reliant on minimisation of instrument background.

**References:**

(1) http://www.invap.com.ar
(2) http://ns.kfkipark.hu/~mirrot
(5) D. Schwann (personal communication).
(6) D. Schwann (personal communication).
(7) http://www.ordela.com/.
(8) C. Glinka (personal communication).
7. Summary

The workshop participants came to the following conclusions:

- that the SANS instrument at the Australian RRR be in the spirit to the 40 metre D22 instrument at ILL, France and the 30 metre instruments on NG3 and NG7 at NCNR, NIST in the United States.

and must:

- be sufficiently flexible to enable user-defined and –constructed sample environments to be used
- be capable of time-resolved, dynamic measurements
- have incident beam polarisation; this requires construction with non-magnetic materials
- have easy to use data acquisition, reduction and analysis software

Other important issues identified were:

- benefits of polarisation analysis and quantifying spin incoherent background
- provision for TISANE-type measurements and inelastic studies
- provision for higher resolution studies (down to 5%)
- the ability to access the ultra-low q domain to study larger scale structures either using the traditional USANS approach or via the use of specialised optics and / or modification to the classical pinhole SANS method
- the need for education / outreach on the opportunities with SANS
- the development of interactions with New Zealand
- in-house SAXS facilities
- facilities for deuteration of chemicals
## Appendix A - Workshop Attendees and Interested Persons

### 1. Workshop Attendees

<table>
<thead>
<tr>
<th>Name</th>
<th>Last Name</th>
<th>Affiliation</th>
<th>Email</th>
</tr>
</thead>
<tbody>
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</tr>
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</tr>
<tr>
<td>Tanya</td>
<td>Elliott</td>
<td>Curtin U.</td>
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</tr>
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<tr>
<td>Kim</td>
<td>Finnie</td>
<td>ANSTO - Materials</td>
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<tr>
<td>Gerry</td>
<td>Gadd</td>
<td>ANSTO - Physics</td>
<td><a href="mailto:geg@ansto.gov.au">geg@ansto.gov.au</a></td>
</tr>
<tr>
<td>Patricia</td>
<td>Gadd</td>
<td>ANSTO - Environment</td>
<td><a href="mailto:psp@ansto.gov.au">psp@ansto.gov.au</a></td>
</tr>
<tr>
<td>Chris</td>
<td>Garvey</td>
<td>U. Sydney</td>
<td><a href="mailto:c.garvey@chem.usyd.edu.au">c.garvey@chem.usyd.edu.au</a></td>
</tr>
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### 2. Interested Persons Unable to Attend Workshop

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<th>Affiliation</th>
<th>Email</th>
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Appendix B – Workshop Programme

Thursday, 13th December 2001

**Purpose:**

Morning: to disseminate information on scientific opportunities, techniques and state-of-the-art instrumentation at overseas facilities.

Afternoon: to discuss scientific issues associated with instrument design specifications.

<table>
<thead>
<tr>
<th>Time</th>
<th>Presentation</th>
<th>Presenter</th>
<th>Chair</th>
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<tbody>
<tr>
<td>8:30</td>
<td>Arrival at ANSTO</td>
<td></td>
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</tr>
<tr>
<td>9:00</td>
<td>Opening and Welcome</td>
<td>Helen Garnett, ANSTO</td>
<td>John White, ANU</td>
</tr>
<tr>
<td>9:05</td>
<td>An Overview of Instrument Opportunities at the Australian Replacement Research Reactor</td>
<td>Rob Robinson, ANSTO</td>
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<tr>
<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>An Introduction to Small-Angle Neutron Scattering</td>
<td>Elliot Gilbert, ANSTO</td>
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<tr>
<td>10:15</td>
<td>Coffee</td>
<td></td>
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<tr>
<td>10:30</td>
<td>Scientific Opportunities and Technical Challenges for SANS - Europe</td>
<td>Roland May, ILL (France)</td>
<td>Rob Burford, UNSW</td>
</tr>
<tr>
<td>11:30</td>
<td>Scientific and Technical Visions</td>
<td>5 minutes for each interested attendee</td>
<td>Robert Robinson, ANSTO</td>
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<tr>
<td>12:45</td>
<td>Lunch</td>
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<tr>
<td>13:45</td>
<td>Scientific Opportunities and Technical Challenges for SANS – North America</td>
<td>Charlie Glinka, NIST (USA)</td>
<td>Ian Dagley, CRC for Polymers</td>
</tr>
<tr>
<td>14:45</td>
<td>Summary of “Neutrons in Biology Workshop” Implications for SANS at the RRR</td>
<td>Robert Knott, ANSTO</td>
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<tr>
<td>15:00</td>
<td>Case for a USANS Instrument at the RRR</td>
<td>Terry Sabine, UTS</td>
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<td>Workshop Photo</td>
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<tr>
<td>15:30</td>
<td>Afternoon Tea</td>
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<tr>
<td>15:45</td>
<td>Interesting Emulsions Studied by SANS</td>
<td>John White, ANU</td>
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<tr>
<td>16:00</td>
<td>Industrial Opportunities for Research and Development using SANS</td>
<td>Robert Knott, ANSTO</td>
<td></td>
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<tr>
<td>16:15</td>
<td>Discussion of Scientific Opportunities</td>
<td>Forum for Discussion</td>
<td>Ian Gentle, U. Queensland</td>
</tr>
<tr>
<td>18:00</td>
<td>Move to Dinner</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18:30</td>
<td>Dinner – at Dijon’s Restaurant</td>
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</table>
Friday, 14\textsuperscript{th} December 2001

**Purpose:** to draft *Report on the Science and Technical Requirements for Small-Angle Neutron Scattering at Australia’s Replacement Research Reactor.*

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<tr>
<td>9:00</td>
<td><strong>Welcome Back</strong></td>
<td>Elliot Gilbert, ANSTO</td>
<td>Craig Buckley, Curtin U.</td>
</tr>
<tr>
<td>9:05</td>
<td>Design Issues: i. Time-Resolved Measurements and ii. Polarisation Analysis</td>
<td>Charlie Glinka, NIST (USA)</td>
<td></td>
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<tr>
<td>10:05</td>
<td>Measuring the Phase of a Neutron Wave</td>
<td>Keith Nugent, U. Melbourne</td>
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<td>10:20</td>
<td>Characteristics of the Cold Neutron Source and Neutron Guides at the Australian RRR</td>
<td>S. J. Kennedy, ANSTO</td>
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<tr>
<td>10:40</td>
<td><strong>Coffee</strong></td>
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<tr>
<td>10:55</td>
<td>Discussion of SANS Instrument Design</td>
<td>Forum for Discussion</td>
<td>Shane Kennedy, Elliot Gilbert, ANSTO</td>
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<tr>
<td>12:00</td>
<td>Charge for Writing Workshop Report</td>
<td></td>
<td></td>
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<tr>
<td><strong>13:00</strong></td>
<td><strong>Lunch</strong></td>
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<tr>
<td>13:30</td>
<td>Report Writing</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16:30</td>
<td>Workshop Summary and Close</td>
<td>Elliot Gilbert, ANSTO</td>
<td></td>
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</table>
Appendix C - Research Trends at Overseas Facilities

ILL (April 2001-April 2002):

D22 college system for beam time:
≈ 50% for colloids and polymers
20-25% for biology
20-25% for flux lines in type II superconductors
≈ 10% for other

NIST:

Figure C.1 – Statistics for NIST SANS research and beamtime usage.
About 12 years ago collaboration between Czech and East German scientists led to the development of Ultra Sans, an instrument that extended the range of the conventional SANS instruments. Two types of USANS instruments have been developed. A bent perfect crystal analyser and monochromator at HMI and Prague, and a triple bounce analyser and monochromator at ORNL, ILL, NIST and GKSS.

The advantages of the triple-bounce machine (e.g. the NIST instrument on the thermal guide BT5, Figure D.1) are the high peak to background ratio, better resolution and superior q range. In addition the calibration of q is straightforward. The disadvantage is the time that is required for the experiment (typically 24 hours to measure single spectrum). The bent-crystal instrument (e.g. V12 at HMI as shown in Figure D.2) has the advantage that a typical USANS pattern can be determined in ten minutes. The disadvantage is the high background and the lower resolution and q range. Australian scientists have extensively used both types of machines.

![USANS Beam Optics Schematic](image)

Figure D.1 – Triple-bounce optics as used on NIST’s recently commissioned for USANS instrument (1).

This equipment is complementary to the conventional SANS and when combined with SANS allows the characterisation of microstructure over 11 orders of magnitude (Figure D.3). In common with SANS, the technique provides information on bulk properties with minimum sample preparation and can be used to analyse material in a non-destructive manner. Further, the extension of q will extend the range and capacity of the scattering at the RRR and should provide the basis for a regional and international centre for microstructural characterisation of industrially useful and economically important materials in the plastic, polymer, minerals and manufactured materials arena.

Australian scientists were early users and developers of this technique. They have carried out a number of experiments overseas using all of the available instruments for studies on determination of petroleum geology (by studying the porosity of source and reservoir rocks, (3), Figure D.3), coal characterisation, mineral and Synroc characterisation, hydrogen in metals (4) and cement hydration. Examples of the
Australian organisations that have used this instrument in the last year are UTS, ANSTO, AGSO and Curtin University.

Figure D.2 – Bent-Crystal USANS instrument, V12, at HMI, Germany (2).

Figure D.3 - SANS and USANS data from sedimentary rock showing that the pore-rock interface is a surface fractal (Ds = 2.82) over three orders of magnitude in length scale and ten orders of magnitude in cross section (intensity).

In particular USANS would be used for:
1. The measurement of the shape and size of particles in the range 30-0.3 µm with the bent-crystal and 30-0.01 µm with the triple-bounce machine;
2. The characterisation of the interactions of these particles with liquids;
3. The characterisation of porous materials.

**It is recommended**

1. That the users form a consortium and approach the ARC for funding to construct and operate a USANS instrument.
2. That a dual-purpose machine be constructed for bent-crystal and triple-bounce using thermal neutrons (wavelength 2.1 Å).

**References:**

(1) [http://www.ncnr.nist.gov/instruments/usans/](http://www.ncnr.nist.gov/instruments/usans/)
(2) [http://www.hmi.de/bensc/instrumentation/instrumente/v12/v12.html](http://www.hmi.de/bensc/instrumentation/instrumente/v12/v12.html)
Appendix E: Scope for Co-operation between Australian RRR and New Zealand researchers

(Submitted by Dr. Murray Bartle)

I strongly support the reactor as a high-tech facility to help stimulate the work of our future students. Without top class facilities to work at, students will look for other opportunities. The presence of so many students at the workshop shows the level of interest of students in new facilities. In nuclear science it has been traditionally the task of each generation of students to invent the next stage of instrumentation to carry the technology forward. The central facility such as the new reactor will form the focus for these developments.

In the case of New Zealand the government is stating the need to encourage more students to work in the sciences and engineering. They are also telling us about its need to limit expenditure. Thus it is obvious there should be strong support and collaboration over research activities on the proposed reactor. It's a win-win situation all round. The best means must be found to promote these ideas to the government. The top management or boards of the Crown research Institutes meet directly with the Minister from time to time.

Part of the plan should include presenting information on what the new reactor will be able to do to as wide an audience as possible. In New Zealand this could include presentations on the Gracefield campus at Lower Hutt. This campus includes a number of Crown Research Institutes.
Appendix F – Detailed list of participants scientific interests

**Polymers**
Intelligent Polymers
electrically insulating components, electrochemistry and conducting polymers
kinetics and time-studies of polymers
polymer blends
polymer kinetics
interpenetrating polymer networks
polymer-polymer interfaces and coatings
polymer films
Polymer blends and phase separation

**Porous materials and porosity**
porous polymers
rock structure - pore correlation
porosity in barrier materials

**Biology and Medicine**
membranes
biological systems
protein crystallisation
protein-folding
magnetic fluids in medicine and biology
biophysics and biopolymers
enzyme-catalysed reactions
haemoglobin, clustering and concentrated solutions in cells
drug delivery
biomimetic materials
poisons
artificial blood
proteins and lipids in lung surfactants
iron-loading diseases
protein cages encapsulating anti-ferromagnetic particles; ferritin

**Materials Science**
sol gels
composites under shear
nanoparticle formation in reverse micelles
nanostructure of amorphous materials
inorganic polymers (e.g. zirconias and aluminas) and influence of aggregates
metal-inorganic polymer hydrates
organic/inorganic hybrids
foams
nanotubes
encapsulated materials
metal complexes in colloids
magnetic nanoparticles and nanoclusters suspended in polymers
geology, geosciences and rock structure
self-assembly
metallurgy
time-resolved studies of growth in multiple metals
phase separation in metals
cement including hydration thereof and concrete
functionalised carbons
inorganic complexes and supramolecular complexes
spray-dried powders, aerosols and droplet formation
mesoporous materials
functional materials
organic/inorganic domains in matrices

**Colloids**
emulsions
microemulsions
foams
surfactant self-assembly
lyotropic liquid systems
aggregation of colloids in polymers
surfactant-based systems
phase behaviour
magnetic nanoparticles

**Physics**
Nanomagnetism
Ferrofluids
Magnetic relaxation