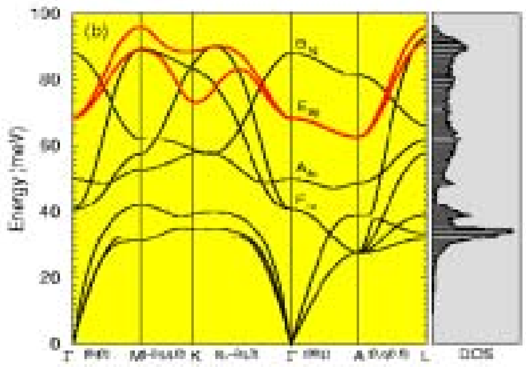
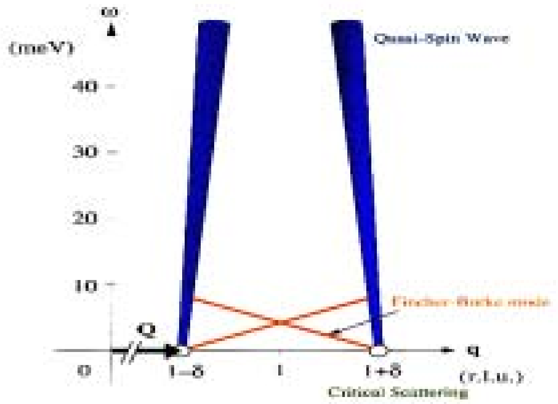
Dynamics, Excitations and Magnetism - Neutron Inelastic Scattering





The measured phonon density of states and modelled dispersion relations for the high temperature superconductor $Mg^{11}B_2$ at 39K. (Courtesy of J. W. Lynn, NIST [1])

Dispersion relations for Chromium. (Courtesy of Y. Endoh, Tohoku University)

[1] Giant anharmonicity and non-linear electron-phonon coupling in MgB_2: Combined First-principles calculations and inelastic neutron scattering study, T. Yildirim, O. Gülseren, J. W. Lynn, C. M. Brown, T. J. Udovic, Q. Huang, N. Rogado, K.A. Regan, M.A. Hayward, J.S. Slusky, T. He, M.K. Haas, P. Khalifah, K. Inumaru, and R.J. Cava, Phys. Rev. Lett. **87**, 037001 (2001).

Neutron Inelastic Scattering at the Australian Replacement Research Reactor

Edited by Leo Cussen from the work and comments of participants at the Workshop on Dynamics, Excitations and Magnetism held at ANSTO on 27-28th of August 2001.

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Executive Summary

The Replacement Reactor Project includes a sub project – the Neutron Beam Instrument project – to construct a suite of eight leading edge neutron scattering instruments to be ready at reactor start up in 2005. Amongst these will be an inelastic scattering instrument and a workshop was run on the 27th and 28th of August 2001 to explore the options that would best serve the future needs of the Australian neutron scattering community.

Three viable options became apparent during the two day meeting.

1. a state-of-the-art thermal neutron three-axis spectrometer, ideally with two analyser options; a crystal analyser to accommodate the needs of the condensed matter physics community and a filter-analyser for the investigation of molecular vibrations and phonon density of states.
2. a cold neutron three-axis spectrometer, to address primarily the needs of the low-temperature condensed matter physics community.
3. a cold neutron time-of-flight spectrometer to address primarily the needs of the physical chemistry community.

Considering the dynamic range of each of these instruments and the ability to address the needs of the widest group of problems, it is our opinion that a thermal neutron three-axis spectrometer offers the project the best opportunity and flexibility in terms of the available wave-vector and energy range. We also recommend that priority consideration be given to developing cold neutron three-axis and time-of-flight spectrometers, perhaps in collaboration with outside organisations, after completion of the initial project.

To help bolster the on-site expertise and provide additional expert capability, we recommend that management institute a long-term visitor program, to take advantage of specialised skills in developing the new instrumental suite. This program would offer international experts an opportunity to spend between four and six months at ANSTO to pursue their own work. This would give the dual benefits of producing high quality scientific research and providing an opportunity for local researchers to meet, collaborate with and learn from these experts.

Key design issues for this instrument are the in-pile collimation and monochromator design to produce an extremely intense beam at the sample position with control over wave-vector and angular spread. The choice of a thermal neutron beam essentially dictates a reactor face position for this instrument. The user community requested ancillary equipment enabling samples to be measured at low and high temperatures (0.5 – 1900 Kelvin) and in large magnetic fields (up to 12 Tesla).

We anticipate that participants from the workshop will also participate in an ongoing Instrument Advisory Team that will contribute to specifying, designing and commissioning the instrument over the five year life of the construction project.

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Row 4: Stephen Collocott, Shane Kennedy, Jeffrey Sellar, Ross M[c]Kenzie, Roger Lewis, Catherine Pappas, Yasuo Endoh

Row 3: Glen Stewart, Wim Klooster, Des McMorrow, Julia Chadwick, Mike Fitzsimmons, David Robinson, Steve Burke, Trevor Hicks

Row 2: Jeff Lynn, Sungjoong Kim, Eddy Bakshi, Anthony Bartels, Simon Redfern, Andrew Studer

Front row: Rob Robinson, Trevor Finlayson, Mukunda Das, Margaret Elcombe, Darren Goossens, Ross Piltz, Tim St. Pierre, Leo Cussen

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Introduction

On the 27th and 28th of August 2001 a group of 40 participants from Australia, Denmark, Germany, Japan and the USA assembled at ANSTO to discuss the optimum choice of instruments for neutron inelastic scattering and polarised neutron scattering at Australia's Replacement Research Reactor. We plan to have one instrument of each type when the reactor starts operation in late 2005. A full list of participants is included as appendix A.

This report deals only with the inelastic scattering instrument.

Neutron Inelastic Scattering is a widely used technique in condensed-matter physics. It is a key technique for the measurement of excitations in materials - collective excitations such as phonons and magnons, diffusive excitations like spin fluctuations and localised excitations arising from the hopping of charge in materials, crystal-field levels and some intramolecular modes. It is likely that it will become important in soft matter studies in the future. In recognition of the importance of this technique, Bertram Brockhouse was awarded the 1994 Nobel Prize in Physics.

While measurements of the structure of materials yield interatomic separations, measurements of the structural excitations in materials yield interatomic forces and measurements of magnetic excitations yield the force between magnetic spins. Neutron inelastic scattering is a key technique for extracting fundamental information about materials and this knowledge has been of great importance in understanding phenomena such as superconductivity and in the development of advanced materials.

Neutron inelastic scattering instruments must measure the neutron energy change on scattering, ΔE, and are conducted on a wide variety of instruments classified by the means used to measure ΔE. These instrument types include

- Time-of-flight (TOF) instruments where ΔE is measured by timing the travel of neutrons between fixed points. On reactor sources, the incident beam is chopped with a duty cycle of about 1%. This greatly reduces the time averaged intensity at the sample but all scattered neutrons can be counted with full knowledge of their change in energy.
- Three-axis spectrometers (TAS) which use Bragg diffraction of neutrons before and after the sample to determine ΔE. Here the intensity at the sample is high but only a small fraction of the scattered neutrons are counted.
- Spin-echo spectrometers which measure ΔE by the neutron speed dependent precession of neutron spins in a magnetic field. The energy resolution of such spectrometers is very high but the energy range is restricted unless the spin echo is installed on a TAS. Such machines are quite complex.
- Backscattering spectrometers which are highly specialised spectrometers that use Bragg back reflection before and after the sample to determine ΔE to extremely high precision but within quite restricted energy ranges determined by the choice of crystals. Typically they use an enormous static array of analyser crystals.

Neutron inelastic scattering measurements are hampered by the weak scattering observed – typically between three and six orders of magnitude weaker than that observed for elastic scattering. Driven by the difficulty of the measurements, scientists involved in neutron inelastic scattering have developed instruments of great power. This power is manifested in extremely high beam intensities at the sample position and great versatility in resolution characteristics. As an example, IN8C at the Institut Laue-Langevin (ILL), the most powerful three-axis spectrometer in the world, will have a peak monochromatic intensity at the sample position of 10^9 n.cm^{-2}s^{-1} [1]. This compares with the intensities of $8x10^4$ n.cm^{-2}s^{-1} and 10^6 n.cm^{-2}s^{-1} on the powder diffractometers HRPD and MRPD at HIFAR.

As for all neutron scattering instruments, intensity can be traded for resolution. Inelastic scattering instruments are often designed to be useful in particular ranges of energy transfer. To cover the myriad requirements, most institutes have several inelastic scattering spectrometers.

For instance, at the Institut Laue-Langevin 15 of the 36 instruments are designed purely for inelastic scattering and another 5 have some capability for energy analysis.

The most versatile neutron scattering instruments are three-axis spectrometers which are designed to provide great flexibility in the choice of resolution. Because of their powerful beams and flexibility in resolution, TAS have also proved to be very useful in solving difficult problems in elastic scattering.

Key questions for the workshop were identified beforehand. These were

- What are the scientific interests of the community?
- Should we build a time-of-flight or a three-axis spectrometer or something else?
- Should the instrument use cold or thermal neutrons?
- Should the instrument be at the reactor face or on a guide tube?
- Do we need a polarisation analysis option and if so how should it be implemented?
- What types of ancillary equipment (sample environment) are needed and what space do they need?

Scientific Case

The scientific case for a neutron inelastic scattering facility at Australia's replacement research reactor can be summarised as follows. Reference can also be made to documents such as the AUTRANS [2] assessment of the future of neutron scattering in Europe.

1. International practice shows that existing sources generally include a significant emphasis on inelastic neutron scattering. Publication rates are typically high for instruments which collect data fast and low for instruments which collect data slowly. When this is considered, publication rates are comparable for inelastic and elastic scattering machines. Citation rates show that a very significant fraction of significant neutron science publications involve inelastic scattering. International projections and planning documents for neutron scattering place a strong emphasis on inelastic scattering.
2. The requirements of the local community, both now and in five years time, are the primary criteria for the choice of instrument. The views presented by the participants in two sessions on Monday and Tuesday afternoon are summarised below. Full details are included as appendix C. Any instrument constructed should be capable of addressing as many of these areas of interest as possible.
   - There was much interest in the physics of high temperature superconductivity where the mechanism of the superconductivity is still not understood and neutron inelastic scattering is likely to make a key contribution. The structural and magnetic excitations in these materials are key areas of research.
   - The study of excitations and quantum effects in low-dimensional magnets is a key test of theoretical models of magnetism. Neutrons are a particularly powerful microscopic probe of magnetic properties and much of the interest in inelastic scattering is in the magnetic properties of materials. Inelastic magnetic scattering yields the exchange constants between neighbouring magnetic spins in materials. An excellent resource in looking to future studies is a special volume of the Journal of Magnetism and Magnetic Materials entitled "Magnetism beyond 2000" [3].
   - The study of excitations near quantum phase transitions enables tests of models. One example among many is the magnetic field induced superconductivity in the layered organic crystal λ-$(BETS)_2FeCl_4$ [4] described by Dr. Ross M^{c}Kenzie at the workshop.
   - Colossal magneto-resistance materials are of great current interest and polarised neutron inelastic scattering is ideal for examining magneto-elastic coupling.
   - The magnetic excitations in chromium are still unexplained despite intensive study over many decades and continue to excite interest.

- Excitations and magnetic structures in thin films and small particles are a key growth area for these technically vital materials.
- Crystal field excitations remain interesting to some participants.
- The modelling of lattice excitations (phonon physics) has advanced to the point where measurements are now needed mainly to confirm the models rather than to form them. However, key areas of study overseas are phonon lifetimes and the excitations in low symmetry solids. There was a surprisingly large degree of interest in phonons among those present at the workshop. Specific interests discussed include
  - ♦ work at high temperatures and high pressures
  - ♦ soft phonon modes
  - ♦ phonon line-width broadening
  - ♦ phase transformations
  - ♦ semiconductors
  - ♦ minerals – excitations to improve our understanding of earth science
  - ♦ low symmetry materials
- Some interest was expressed in low energy scattering as seen in
  - ♦ quasi-elastic scattering in silicates and cement
  - ♦ dynamics in disordered and amorphous materials
  - ♦ vortex matter.
  - There was much interest in distinguishing between surface and bulk effects requiring complementary neutron and X-ray studies.

3. There is great potential for growth in the local community's interests. It was surprising that there was little interest in neutron inelastic scattering from Australian chemists. This would explain the lack of support for a TOF spectrometer. Neutron inelastic scattering is not very widely used in Australian chemistry by comparison with probes such as infrared spectroscopy. This situation is in marked contrast to that in Europe where many chemists are active neutron scatterers and have produced many interesting results. Once the new neutron source is operational we should try to engage Australian chemists in this field.

Design Considerations

This section is structured to address the questions posed for the workshop in order.

On Tuesday afternoon, the group separated by interest area and those remaining to discuss inelastic scattering were:

Eddy Bakshi, Anthony Bartels, Olivier Cepas, Leo Cussen, Margaret Elcombe, Yasuo Endoh, Trevor Finlayson, Miklos Gulacsi, Jeff Lynn, Ross McKenzie, Des McMorrow, Simon Redfern and Glen Stewart.

It was made clear that the workshop would make a recommendation on the choice of instrument but that the final decision on the choice rests with ANSTO management, in particular with the Neutron Beam Instrument and Project Coordination Group, with advice from the Beam Instruments Advisory Group.

1) **Should we build a Time-of-Flight, a Three-Axis Spectrometer or something else?**

Many people felt strongly that any instrument should only be built if it is the "best in its class" internationally. The point was made that it is the science which must be best in class and the instrument must be capable of doing the science. It was suggested that the two instruments under consideration at this workshop – polarisation analysis and inelastic scattering – could be considered to be a condensed matter suite and chosen to be complementary. It was then emphasised that we are building only one inelastic scattering instrument and should be wary about excluding the science of any member of the community. It was stated that the person constructing the instrument must have a large say in the choice as their motivation significantly impacts the final instrument quality.

There was general agreement that backscattering, neutron spin echo or resonant spin echo spectrometers are (immensely) complex systems and probably beyond our immediate capability. Such instruments would be too specialised to be chosen as the first inelastic scattering spectrometer at the replacement reactor.

There was little support for a time-of-flight spectrometer. Given the absence of any significant representation of the Australian chemistry community at the workshop, despite widespread advertising through the RACI, this is not surprising. It was also noted that TOF instruments compete directly with rapidly improving spallation sources and may be uncompetitive at reactor sources in the near future. It was pointed out that IN5 and IN6, the cold neutron TOF machines at ILL, are the most productive inelastic neutron scattering instruments there. It was also noted that we could build an equivalent machine here that would exceed the current performance of those instruments. Inelastic scattering from soft matter is probably a growth area and would benefit most from a cold neutron TOF. It was stated that a TAS cannot measure crystal fields competitively.

There was a widespread view that the instrument must serve the potential community.

The choice remaining is thus a three-axis spectrometer. There was a lengthy discussion of the challenge of providing the large single crystal samples needed for such a machine from the Australian community. The community requires resourcing – suitable mirror furnaces to grow crystals cost US$100,000 – and we face the challenge of convincing the funding authorities that the best science requires the best possible samples to test the latest ideas produced by theory.

It was accepted that it is relatively cheap to build several secondary spectrometers for a TAS such as a conventional analyser, a multi-crystal multi-detector arrangement (SPINS/RITA [5]) or a filter analyser system (FANS [6]). It was also stated that trying to develop too many options compromises competitiveness and that we should not try to do everything. We may get the chance to build other instruments later if the first is successful.

Experience overseas is that TAS are almost always heavily over-booked even when they represent a large fraction of the instruments at a source. It was stated that if a good thermal neutron TAS was built, Japanese scientists would be happy to come to Australia bringing their single crystal samples.

2) Should the instrument use cold or thermal neutrons?

Despite the fact that most recent international development has been of cold neutron TAS, the relatively large interest in phonon physics in Australia requires a thermal neutron TAS. Such a machine also gives the greatest versatility in science tackled but it was emphasised that thermal neutron TAS are not competitive with cold neutron machines for low energy work. The cross over in flux between the thermal and cold sources at the RRR reactor face is at 2.4 Å (15 meV). Figure 1 shows the relevant predicted flux curves.

Leo Cussen suggested that thermal neutron instruments do cold neutron work better than cold neutron instruments do thermal neutron work but Des M^{c}Morrow pointed out that

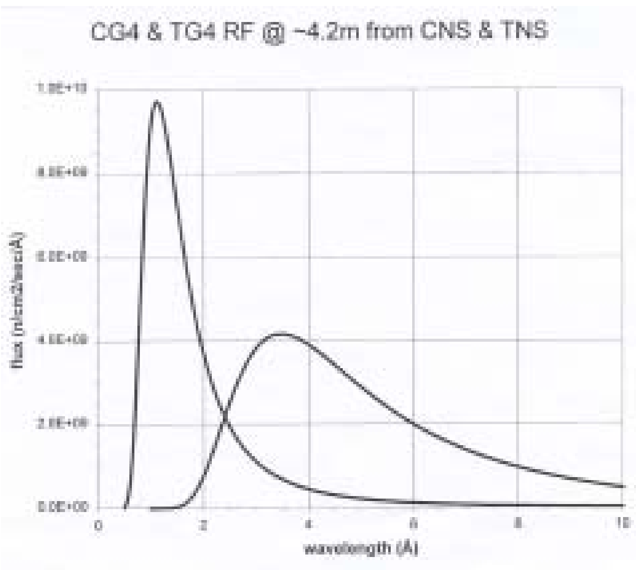

Figure 1: Predicted intensity as a function of

wavelength for thermal and cold beams at RRR.
thermal neutron instruments remain uncompetitive for cold neutron work.

If the focus is on building a best in class instrument, we should be able to build an instrument superior to the IN14 cold neutron TAS at ILL as the scientists at the Paul Scherrer Institute (PSI) can do this already. It was stated that it is unlikely that we could beat IN8C with a thermal beam.

The consensus in the room was for a thermal neutron TAS with Des M[c]Morrow's the strongest dissenting voice. It is noted that growth seems to be in cold neutron TAS and that synchrotrons may be competitive with thermal TAS for phonon measurements.

3) Should the instrument be at the reactor face or on a guide tube?

The instrument chosen is thus a thermal neutron TAS. When considering thermal beam TAS with polarisation analysis (as decided – see section 4) the bench mark instruments at present are IN22 and IN20 at ILL. IN22 is on a guide tube position while IN20 is at the reactor face.

A face position gives more intensity and access to more divergent beams suitable for double focussing monochromators. Indeed if the instrument is at the face it should have double focussing monochromators. A guide position can deliver better signal to noise ratios due to the far lower fast neutron flux in a guide than at the reactor face. It was stated that if the instrument is primarily designed for using collimators it should be on a guide. Our thermal guides will give only 0.5^{o} horizontal divergence and 0.7^{o} vertical divergence – much less than can be used even by a conventional collimator instrument.

The conclusion is that the best thermal beam is at the reactor face.

4) Do we need a polarisation analysis option and if so how should it be implemented?

Our overseas visitors were unanimous in saying that the instrument must be built with polarisation analysis (PA) in mind (i.e. the instrument components must all be non magnetic) even if PA is not implemented initially. The recommendation was strong that polarisation analysis be included. The polarising method used for a thermal TAS should be a Heusler alloy monochromator and analyser unless ^{3}He spin filters progress greatly in the near future.

5) What type of ancillaries (sample environment) are needed and what space do they need?

Magnetic studies require low temperatures and high magnetic fields. It was assumed that closed cycle refrigerators would be available for the temperature range from 5 Kelvin to 300 Kelvin. A cryofurnace for temperatures between 4K and 750 K was requested.

We also need temperatures below 1 Kelvin. From a technical view, this requires a dilution refrigerator and support staff for it (one full time expert). There are now closed cycle devices which can reach 50 mK with much less support. We need a 7 Tesla cryomagnet and should aim for a 15 Tesla cryomagnet. There was no expressed view about whether the field should be horizontal or vertical. Again such devices need technical support.

There was lots of interest in high pressure and high temperature for studies of Earth science and phase transitions. A furnace which can reach 1500°C should be available. Gas control should be available within the furnace. The high pressure capability requested was 10 GPa. The requirements are summarised in the following table.

Closed-cycle refrigerator	Temperature	3 – 300K
Cryofurnace	Temperature	10 – 750K
Dilution Refrigerator (possibly closed-cycle)	Temperature	50 mK – 4K
Cryomagnet	Magnetic Field	Up to 15T
Simultaneous high temperature and pressure with gas control	Pressure Temperature	Up to 10 GPa Up to 1500°C

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6) User Interface

We were advised that the PSI and Oak Ridge National Laboratory (ORNL) software is much better than that at ILL which should be avoided. The instrument control software should have low level modules for motor control and counting and a macro type language such as IDL above for more sophisticated instrument control functions. NIST and ILL are switching to LINUX/UNIX operating systems.

The data files should include the values of all instrument variables. The technology exists to make this automatic and also to include photographs of parts of the instrument at regular intervals during experiments.

7) Other issues

High flux and low background are vital on a TAS.

Intensity

Horizontal focussing increases count rates in the detector by about a factor of 10 but at a significant cost in resolution for dispersive modes. The monochromator assembly cost is the major expense in a TAS and thus multiple analyser modules make sense but multiple monochromator assemblies do not. The instrument needs at least three double focussing monochromators (Pyrolytic Graphite, Cu_2MnAl Heusler and the best of Cu200/Si311/Ge311). A better option than a carousel for changing the monochromator is a lifting frame with the Heusler and its magnets in one position and a double sided monochromator above or below. However, this method requires a higher monochromator shielding drum which can lead to problems with floor loading limits.

The new double focussing NIST monochromators [7] use carefully shaped (bow like) solid vertical 6061 aluminium blades which bend cylindrically under compression. The mechanism is illustrated in reference 7. The monochromator crystals are drilled and screwed to the blades. Focussing is by a screw mechanism to compress the blades. The cost is about US$400,000 for the mechanism plus US$50,000 for the graphite plus US$200,000 for the Heusler crystals.

NIST use a different form of horizontal focussing to that used at ILL. Individual vertical arrays are misaligned in angle but aligned along the line of sight to the sample. This gives small angular spread but large wave-vector spread. Each of the 13 vertical blades thus has a motor and angle encoder on it. Johns Hopkins University built the mechanism.

Note that with proper beam tube design for horizontal focussing monochromators the low angle range in monochromator take-off angle (below 40 degrees!) is compromised because of the horizontal divergence of the beam incident on the monochromator. This may impose severe limits on instrument performance.

Background

Reducing background is largely about choosing the shielding.

NIST use 7 ft diameter monochromator shielding drums lined with 2mm thick plates of ^6LiF. The drum is filled with paraffin with 4" of lead on the outside. It should be possible to use steel shot in the paraffin. NIST also include 4" of tungsten in the beam stop. Cadmium should not be used in the main beam.

Non magnetic heavy concrete is now available with a density of 6.4 g cm^{-3}

If the instrument is on air pads it is relatively easy to increase the shielding on the secondary spectrometer – cantilevered designs are restricted this way.

- Sapphire (Al_2O_3) and beryllium filters should be available before the monochromator.
- A pyrolytic graphite filter is needed for the analyser.
- "Sloppy choppers" to reduce λ/n beam contamination are relatively ineffective on thermal TAS as the choppers usually cannot spin fast enough. The new instrument at FRM-II in Munich, PUMA, is designed to operate with such a filter but as at September 2001 the device had not been constructed and the technical challenges in its development appear formidable.

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Movement

Backlash and flexibility in control arms cause problems with the heavy instrument modules used on a TAS. NIST dance floors are anodised aluminium plates press fitted into a frame. The drives on BT7 at NIST are HUBER tables with stepper motors and no angle encoders for the drives. Care is taken to remove the backlash. Encoders may be more trouble than they are worth. The NIST airpads are of a bladder type which give a very low compressed air consumption. Thus the compressed air is not switched on and off but is always left on.

Multiple Analysers

Not all analysers are needed at startup and development of analyser modules is relatively cheap by comparison with the monochromator assembly. The following options will be considered:

- Single analyser and detector (Pyrolytic Graphite and Heusler alloy)
- RITA [5] style which increases flexibility by giving a mapping or focussing option. Use a 1D microstrip type detector 48 wires at 5mm spacing => higher peak count rate.
- FANS [6]– a large cooled beryllium filter with a large angular acceptance position sensitive detector (multiwire).
- Polarised reflectometer option

Several people requested out of plane detector movement. We could equivalently and more simply have a 4-circle attachment at the sample position with its own specialised displex and furnace.

We should consciously choose to buy everything we possibly can and not try to build instrument components ourselves.

Upgrading the existing TAS at HIFAR at a minimal cost may help to develop the user community before the new instrument becomes available. The upgrade needed is to replace the existing motors, coders, computer and software.

Professor Endoh has recommended that spectrometers must be designed with a concrete mission in mind. An example would be a mission to measure magnetic excitations. This is a view which was also expressed by Des McMorrow.

The consensus on design reached at the workshop is thus a thermal neutron three axis spectrometer at the reactor face with double focussing monochromator and analyser and a polarisation analysis option.

Recommended actions during the design and construction phase

- Conduct a market review of leading neutron scattering facilities, to include: NIST, ORNL, JAERI, ILL and FRM-II. This should result in a report to form the basis of the final conceptual design.
- Where possible, extensive in-house engineering development should be avoided where solutions exist and can be purchased.
- Key questions that should be answered in this phase:
    - Choice of monochromator
    - Possibility to mount several monochromators in shielding
    - Polarized beam capability, built in guide fields
    - Future options for sample environment should be part of design
    - Analyser options – conventional TAS or RITA style or FANS style
    - Make decision on multi-analyser/PSD options (RITA/SPINS type)

Establish a small international consultation and working group.

Recommended actions for optimum use of the instrument

- Establish a visiting scientist programme to encourage overseas scientists to work at ANSTO. An example would be a sabbatical programme for stays of 6 months to 1 year.
- Explore possibilities for a formal collaboration on neutron scattering between Australia and Japan and other southern Asian countries (Hong Kong, Singapore, India, China).

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- ANSTO management should make it a top priority to establish joint positions in neutron scattering with Australian universities.
- The facility must be very user friendly – as a starting point, establishing e-mail and internet access for visitors must be much simpler than it is now.
- Work to establish crystal growing labs in Australia. It is hard to get the message to the funding authorities, but leading-edge science requires the best possible samples. If we build a superb facility people will be happy to work here - once they see that it is superb.

Proposed plan of action

The following issues need resolving in the next six months.

- Develop in-house understanding of focussing monochromator systems (an analytical understanding is needed to use Monte Carlo simulation programs effectively).
- Investigate the Flux depression effects of large beam tube thimbles - MCNP studies by the Nuclear Technology group at ANSTO.
- Optimum design of beam tube to exploit focussing monochromator
  (Analytic model followed by a McSTAS Monte Carlo check and optimisation)
- Modelling of beam characteristics at the sample position.
- Calculations of monochromator shielding required.
- Ideally we would also simulate the performance characteristics offered by the new reflecting Soller slit collimators. Time restrictions will probably prevent this.
- Produce an estimate of instrument background.
- NBI management team agreement on broad conceptual design.
- Detailed conceptual design including projections of cost, schedule and performance

The work needed to complete this has been developed as a work breakdown structure for project management and is attached as appendix E.

Summary

In summary, the Australian user community was invited to participate in a workshop with ANSTO regarding the choice of a neutron inelastic scattering facility for the replacement research reactor. A significant number of local and international experts gathered at Lucas Heights on the 27th and 28th of August 2001 to discuss the choice. The workshop endorsed the recommendation of the Beam Facilities Consultative Group to build a thermal neutron three axis spectrometer. The workshop recommended that such an instrument should be built at the reactor face on a thermal beam, using a double-focussing monochromator and analyser. Polarisation analysis should be available as an option. It is important that the instrument perform at or close to world's best level. Recommendations were received on sample environment requirements and low temperature, high temperature and strong magnetic fields are seen as necessary.

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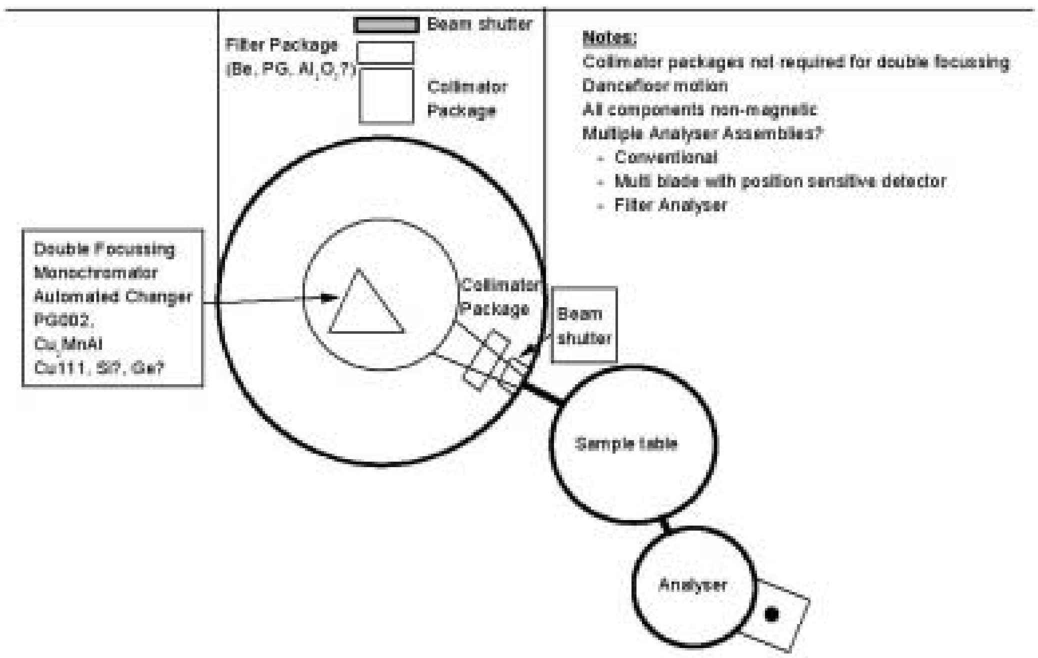

Preliminary Conceptual Schematic of RRR TAS
This diagram produced by L.Cussen based on
input at workshop.

Appendix A: List of participants and their affiliation.

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Other People who expressed interest but were unable to attend the workshop

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Appendix B Summary of Presentations by Invited Speakers

Jeff Lynn (NIST) "An Introduction to Neutron Inelastic Scattering"

"There is always a trade-off between intensity and resolution"

Dr. Lynn mentioned spin echo spectrometers, thermal TAS and a Fermi chopper spectrometer and described the inelastic scattering instruments at NIST.

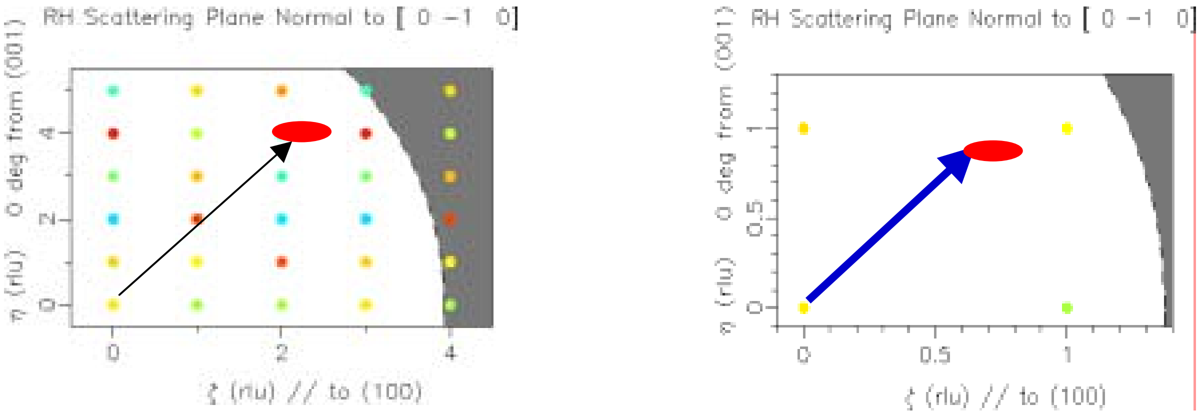
SPINS – a cold neutron TAS
FANS – a filter analyser spectrometer
HFBS – a backscattering spectrometer
DCS - A disc chopper time-of-flight spectrometer

His introduction described the key areas of neutron scattering science: crystallography, magnetism, SANS and reflectometry,

Inelastic scattering is used to measure lattice dynamics (phonon dispersion curves and density of states, interatomic forces, diffusion) and spin dynamics (magnetic exchange, anisotropy, fluctuations, crystal fields and coupling between the magnetic and structural properties).

He showed that participation in neutron scattering at NIST quadrupled between 1988 and 1999 and attributed this to advances in instrumentation.

He described the operation of a TAS and distinguished between cold and thermal neutron instruments by the larger range of reciprocal space accessible to a thermal instrument but the better resolution of the cold neutron instrument.



Thermal Beam   Cold neutron beam

Figure B1: This figure illustrates the range of scattering vector available for thermal and cold neutron spectrometers and displays an indicative effective resolution achievable with each type of beam

He then showed that many modern instrumentation developments have been to increase intensity by reducing the (too good) resolution of cold neutron TAS. A thermal TAS gives energy resolution of about 1000 μeV, a cold TAS 100 μeV and backscattering instruments give essentially perfect resolution – 1μeV.

He emphasised the usefulness of measurements of the phonon density of states given the advanced state of modelling theory for phonons. Among his scientific examples were studies of the newly discovered superconductor MgB_2. A measurement of the phonon density of states on FANS coupled with modelling showed that the superconductivity is phonon moderated and identified one optic phonon branch as the key mode without the need to measure the full dispersion relations.

He then spoke of the colossal magnetoresistive material $(La_{0.7}Sr_{0.3})MnO_3$. Such materials will be of key importance in the technology of magnetic recording. He showed that TAS measurements of spin waves and polarons have been vital in understanding the behaviour of these materials.

He emphasised that while TAS are powerful and versatile, because they measure only one point at a time and the scattering is usually weak the data collection rates are low. The use of multiple analysers and position sensitive detection can greatly speed data collection.

He expressed the view that since the secondary spectrometer represents only about 25% of the cost of a TAS it is cost effective to have several secondary spectrometers for one monochromator. His suggestion is to have two modules for use as a filter analyser and a multi analyser coupled to a position sensitive detector.

In conclusion he emphasised the ongoing instrument development at NIST. Of particular interest in choosing an instrument is this viewgraph from his talk.

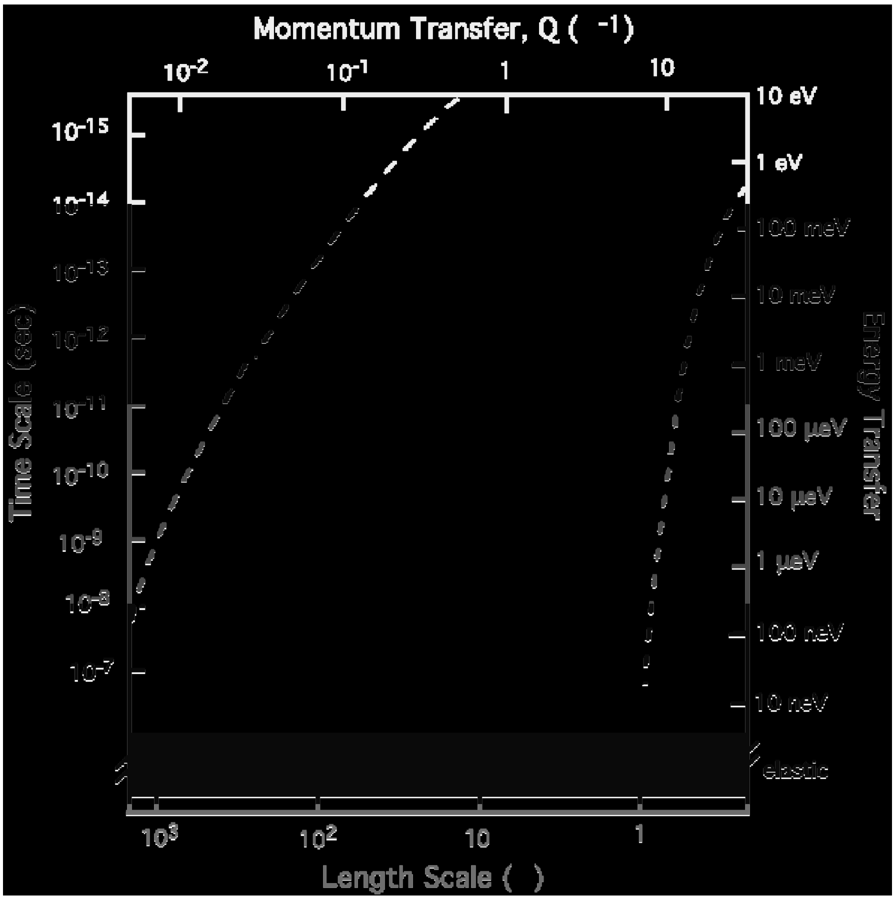


Figure B2: Diagram illustrating the range in length and energy of different types of neutron inelastic scattering spectrometers.

Des M^{c}Morrow (Risø) "Scientific Opportunities for Neutron Inelastic Scattering"

The key point of this talk was that the sensitivity of the instrument determines the science which can be done. Thus a good instrument needs high flux and low background and the ability to relax resolution in a controllable way. When measuring inelastic scattering, the cross sections are typically 10,000 times smaller than elastic cross sections. Most interesting science in this field involves studying matter under extreme conditions of magnetic field, pressure and temperature. This requires complex sample environments and requires that the instrument be designed to accommodate the sample environment. He spoke of key instruments. Those identified were RITA, RITA 2 (RISØ & PSI), SPINS (NIST) and PUMA (FRM II) at reactor sources and MAPS and MERLIN (ISIS) at spallation sources.

A description of RITA followed. RITA is a cold neutron three axis spectrometer which introduced the multiple analyser technique now being mimicked elsewhere. Des emphasised the flexibility and power of this system and also emphasised the extreme importance of reducing background. On RITA key features are filtering the beam before the monochromator using a "sloppy chopper", a velocity selector with broad acceptance, and a sapphire (Al_2O_3) fast neutron filter. New materials (polyethylene impregnated with lead shot cast into paraffin and soaked in boric acid (natural boron at 4.6g cm^{-1}) were developed for the main beam stop and this is critical in background reduction. The secondary spectrometer is housed in a large shielded vacuum tank. The multi analyser system permits operation in mapping and focussing modes.

Des showed data from MAPS, the relatively new inelastic spectrometer at ISIS which is extremely powerful and fast and ideally suited to a survey of the inelastic scattering which can be followed by examination of interesting features using TAS. This measurement was of the $LaSrCuO_4$ superconductor and was extremely impressive.

Des spoke of some of RITA's successes in

- Magnetic excitations in $LaSrCuO_4$
- Low dimensional quantum magnets
- Heavy Fermion physics
- Geometrically frustrated magnets

In examining future directions Des identified examinations of matter under extreme conditions as key.

In particular, opportunities exist in

- Superconductivity and magnetism
- Competing interactions
- Quantum transitions driven by temperature, pressure or magnetic field
- Magnetic frustration

Frontier areas include

- The dynamics of superlattices, thin films, wires and dots
- Quantum Phase Transitions
- Molecular Magnetism
- Organic Materials
- Exotic Interactions
- Coupled Excitations
- Spin Glass Dynamics

He advised that if we construct a TOF spectrometer for measuring crystal field levels and molecular rotations we should use pixellated position sensitive detectors at least for the small angle banks.

He also stated that the development of powerful machines producing data requiring lengthy analysis requires large user communities and good analysis software.

Yasuo Endoh (Tohoku University and JAERI)
"Inelastic Neutron Scattering in Japan – Present and Future Directions"

Professor Endoh spoke of his instrument TOPAN (Tohoku University Polarisation Analysis Neutron Spectrometer) [1] at JAERI, the Japanese 20MW reactor neutron source. He described the instrument as covering the same experimental conditions as IN20 at ILL which he used as a benchmark for performance. TOPAN is approximately half as fast as IN20 which corresponds to the difference in reactor power between the two sources. It was recommended that appropriate design of the in-pile collimation would further enhance performance.

At JAERI, 7 of the 21 neutron scattering instruments are three axis spectrometers which indicates the importance that the very productive Japanese neutron scattering community places on such instruments.

Professor Endoh emphasised that TAS are very important and indispensable tools to solid state physicists. Building a successful instrument requires that the flux must be maximised requiring optimised beam transport and neutron optics (double focussing monochromators). Polarisation analysis is necessary nowadays. It is vital that instrument background be minimised by the use of filters and beam choppers.

A range of high quality sample environments is also essential. In particular, a superconducting magnet is necessary to produce high magnet fields at the sample. This requires that the TAS must be constructed to be non magnetic and able to support the weight of the magnet.

He illustrated the value of powerful instrumentation via an extensive set of experimental results on the fascinating excitations in Cr (see front page) which after decades of intensive study are still not fully understood. He emphasised that neutron scattering is the only technique for studying this problem and that only experimentalists can solve this problem.

[1] http://www.issp.u-tokyo.ac.jp/labs/neutron/inst/6G/

Miklos Gulacsi Spoke about the explanation of High T_C superconductivity. The challenge here is that different communities believe different models. It is a very complex system.

Shane Kennedy
Emphasised our need for some cold neutron inelastic scattering capability.
Emphasised that most TOF is best done at spallation sources
Pointed out that we should build complementarity with Japanese facilities.

M.Fitzsimmons
While Dr. Fitzsimmons spoke mainly on polarisation analysis, some of his points were very relevant to this project. He discussed nanostructured materials and pointed out that magnetic studies produce 40% of ILL publications and 25% of NIST publications. He discussed the idea of length scales in magnetic and other problems.
For instrumentation:

Nobody knows what will be important in the future so we need instrument flexibility.
Devote equal attention to the instrument and to the sample environment
(Low and high Temperature, high pressure, high magnetic fields)
Removable filters.
Polarised and unpolarised beams.

C.Pappas
Dr. Pappas spoke mainly to the polarisation analysis side of the workshop with particular emphasis on spin echo measurements.

Appendix C Scientific Interests expressed by participants

Visitors expressed their scientific interests in two sessions on Monday and Tuesday afternoon. This list of interests is compiled from their written comments where available and notes from M. Elcombe, M.James and L.Cussen where not.

Laurie Aldridge
- Determination of bound and free water in cement paste extracted from concrete.
- A representative of the Australian Building Research Institute believes that up to ten such determinations per year are needed for their work.
- What is needed is polarised cold neutron measurement of quasielastic scattering and excitations in the range from –2 meV to 2 meV with a resolution of 0.1-0.2 meV.

Eddy Bakshi (Swinburne University)
Interested in state of the art neutron scattering techniques – Time-Correlated-Diffraction

Anthony Bartels (Swinburne University)
Interested in state of the art neutron scattering techniques – Time-Correlated-Diffraction

Steve Burke (DSTO & formerly on BFCG – previously ILL)
- Excitations in chromium
- Advises that the instrument should be a Three Axis Spectrometer.

Olivier Cepas (University of Queensland)
- Interested in low dimensional magnetism.
- $SrCu_2(BO_3)_2$
- Quasi 2-D spin gapped system $Na_2V_2O_5$
- Interested in polarisation effects
- Techniques such as neutron polarimetry

Stephen Collocott (CSIRO)
- Rare Earth magnetism and intermetallics
- Phonon physics

Leo Cussen (ANSTO)
- Magnetism
- Phase Transitions
- Neutron Scattering Instrumentation

Mukunda Das (ANU):
- Condensed matter theory.
- Flux lattices.
- Vortex matter.
- Phonon dispersion in high T_C superconductors must be re-examined.

Margaret Elcombe (ANSTO)
- Complexity of phonon studies – understanding isotope effects; Eigenvectors by isotopic substitution.
- The phase problem in inelastic scattering.
- Fundamental TAS work – small samples and out of plane phonons.
- Phonons in low symmetry structures.

- High Tc superconductor (123) phonons in non integral material
- Understanding transitions – interrelation with other properties
- Mineralogy

Yang Fei

- Colossal Magneto resistance
- Superconductivity
- Samples at less than 15K in a magnetic field greater than 15 Tesla
- Excitations at less than 1 meV

Trevor Finlayson (Monash University)

Current interests include:

- soft-phonon, martensitic systems, temperature dependence (20 K – 400K), and possibly pressure and/or stress dependence for certain modes.
- particular martensitic systems which also include magnetostrictive effects leading to the magnetic field dependence of certain soft modes.
- superconductors and soft-mode ferroelectrics.
- diffuse scattering development in the parent phase of soft-mode systems (e.g., Ni_2MnGa, NiAl, NiTi), where soft mode is not a zone-centred phonon, temperature range typically 150K ≤ T ≤ 350 K, including the resolution of this diffuse scattering into its inelastic and/or elastic components; (This could involve searching for diffuse scattering "out of the plane");
- similar studies in zone-centre systems (FePd, FePt);
- search for the onset of non-degeneracy for certain phonons in soft-mode systems, associated with the "tweed" microstructure in some of the above materials.
- Glancing incidence X-Ray scattering – surface versus bulk effects.

Miklos Gulacsi (Theoretical Physics/RSPhysSE/ANU)

Interested in fundamental problems related to heavy fermion alloys, high Tc ceramics and CRM materials. Magnetism is one of the most important areas to study from a theoretical point of view. INS data can explain the basic interactions, pairing mechanism in these materials. For heavy fermion system under pressure measurements at low temperatures is very important to understand their ground state properties, and the strongly correlated effects. For high Tc superconductors it would also be very useful to do high pressure measurements, as the theory predicts that Tc should increase with pressure, hence this will give us an opportunity to establish the pairing mechanism. I should mention that in this area it would not be a problem to obtain single crystals from my international collaborators. It should be also emphasised that connecting theoretical research with experiments will be beneficiary for attracting PhD students, and ARC grants.

Jan Hermann (CSIRO)

- Nanoparticles
- Superconductivity

Roger Lewis (University of Wollongong)

- Semiconductors (Si, Ge III-V& II-VI compounds)
- Perovskite compounds
- Phonon modes of $A(Co_{1/2}Mn_{1/2})O_3$
- Studies of MgO doped MgB_2
- Complementary optical and neutron measurements of phonons
- High temperature work (900^{o}C)
- Metamagnetism

Ross McKenzie (University of Queensland)
Low Dimensionality + Strong Interactions => Interesting Physics
- Competition between magnetism and superconductivity
- High temperature superconductivity
- Unconventional metals
- Fractional charge
- Separation of spin and charge
- Theorist with an interest in low dimensional magnetism

Jaan Oitmaa (UNSW)
- Low Dimensional antiferromagnets Chains & Ladders
- Competition between antiferromagnetic order and singlet formation
- Quantum phase transitions
- Interesting low energy excitations

Future directions:
- Multilayers, nanoparticles and molecular magnetism
- An excellent resource is a special volume of the Journal of Magnetism and Magnetic Materials entitled "Magnetism beyond 2000", JMMM **200** (1999)

Simon Redfern (Cambridge University and Australian National University)
Measurement of phonon softening associated with displacive (ferroelastic) and order-disorder phase transitions in silicates, carbonates and refractory oxides. In particular, the temperature-dependence of such phenomena elucidate the controlling processes responsible for phase stability and critical behaviour in Earth materials. General phenomena from model systems (in particular certain model systems provide insights readily transferable to important classes of ceramics and structural materials: SiO_2 polymorphs and $CaCO_3$ polymorphs have, for example, provided useful proving grounds for developing our understanding of structural stabilities and their relationship to lattice dynamics). The transition from long-range crystalline order to amorphous phases via metamictisation (radiation damaged "glass") and pressure-amorphisation may also be explored in terms of their dynamical effects, including the behaviour on "healing" on high-T annealing. Finally, pre-melting effects just below T_c should be explored, possibly in potential model analogues of refractory phases and ceramics.
Quasi-elastic scattering of NH_4 and H_2O in complex silicate structures (layer silicates and frameworks, including zeolites) will be important in understanding the dynamics of the molecular motions of these components in environmental scenarios within the Earth.

Tim St.Pierre (University of Western Australia)
- Nanoscale Magnetic particles
- PtCo
- Fe and Ni oxides
- Magnetic particles in biological systems
- Thin films
- Magnetic structure of nanoscale particles
- Biogenic Fe(III) oxyhydroxide particles
- Bulk/Surface effects

Jeffrey Sellar (Monash University)
- Phase transformations and associated anharmonic phonons.
- Must do in situ measurements under extreme conditions and not rely on quenching to retain phases.
- High temperature studies of oxides and hydrides.

- TAS not TOF
- Diffuse scattering studies in certain ceramics (e.g., YTZ), RT - 1500°C.
- Requires an ability to measure scattering "out of the plane" which may necessitate a special detector design.

Glen Stewart (ADFA)

Current research interests include

- Crystal field (CF) levels at the rare earth sites in intermetallics using Mössbauer spectroscopy
- CF interactions are important, for example, in their influence on the bulk properties of magnetic materials. It is useful to complement such investigations with more direct approaches such as INS or optical spectroscopy. Experience has indicated that CF characterisation for low symmetry sites requires the simultaneous description of as many different types of data as possible. CF splitting of rare earth ground states can range from the order of a hundred to over a thousand Kelvin.
- A thermal source with minimum wavelength of approx 0.8 angstrom would correspond to a maximum CF transition of order 500 K. This would provide a useful probe of the key lower energy CF levels in most circumstances.
- Such measurements could be conducted on a thermal TAS. The specimen must be close to liquid helium temperature,
- Spectra must be taken at several temperatures (different Boltzmann populations of the lower CF levels).

Bob Street (University of Western Australia)

- Nanoparticles
- Thin film structures
- Polarisation analysis thin films and nanoparticles
- PtCoCr – ferromagnetic-antiferromagnetic and non magnetic domain walls
- Small particle magnetism – mechanochemical processing
- Geopolymers to reduce CO_2 emissions – 10% of CO_2 comes from concrete!

Appendix D: A selected list of Three Axis Spectrometers Worldwide

Details obtained via the NSSA website http://www.neutronscattering.org/

Institute	Name	Type	Peak Intensity at sample n.cm^{-2}s^{-1}
ILL (International – France)	IN1	Hot	2x10^{7}
http://www.ill.fr	IN3	Thermal	2x10^{7}
Under construction	IN8C	Thermal	1x10^{9}
	IN12	Cold Guide	
	IN14	Cold Guide	3x10^{7}
Commissioning	IN20	Thermal Polarised	8x10^{7}
	IN22	Thermal Polarised	
LLB (France)	1T	Thermal	
Http://www-llb.cea.fr	2T	Thermal	
	4F1	Cold double monochromator	1.4x10^{7}
	4F2	Cold double monochromator	1.4x10^{7}
	G4-3	Cold guide	5x10^{5}
PSI (Switzerland)	RITA	Cold	
http://www.psi.ch/	TASP	Cold Polarised	5x10^{7}
	RITAII	Cold	
HMI (Germany)	FLEX	Cold	
http://www.hmi.de/	E1	Thermal Polarised	4x10^{6}
JULICH (Germany)	UNIDAS	Thermal	5x10^{6}
http://www.kfa-juelich.de			
FRM-II (Germany) http://www.frm2.tu-muenchen.de	PUMA PANDA	Thermal Cold	**Under construction**
ORNL (USA)	HB1	Thermal Polarised	3.5x10^{6}
http://neutrons.ornl.gov	HB1A	Thermal Fixed wavelength	3x10^{7}
	HB2	Thermal	3x10^{7}
	HB3	Thermal	1x10^{7}
Under Construction	STAR	Cold	
NIST (USA)	NG5 – SPINS	Cold Polarised	3.9x10^{6}
http://rrdjazz.nist.gov	BT2	Thermal Polarised	5x10^{7}
	BT7	Fixed wavelength	
	BT9	Thermal	
Under Construction	MACS	Cold	10^{8}
Chalk River (Canada)	C5	Thermal Polarised	
http://neutron.nrc.ca/	N5	Thermal	
JAERI (Japan)	TAS1	Thermal	
http://www.jaeri.go.jp	GPTAS	Thermal	
	PONTA	Thermal Polarised	
	TOPAN	Thermal Polarised	
	HQR	Thermal Guide	
	TAS-2	Thermal Guide	
HANARO (Korea)	ST3	Thermal	
http://hpngp01.kaeri.re.kr/hanaro	ST4	Thermal	

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APPENDIX E: Work Breakdown Structure

WBS	Name	Duration	Start Date	Finish Date	Notes
1	Design and Construct Thermal TAS - Focussing	248.18 wks	06/13/01	03/15/06	Plan is to hit three milestones 1) Instrument design approval by BIAG April 2002 2) Instrument delivered by guide hall completion date August 2005 3) Instrument commissioned by RRR startup Jan 2006 (With user base and crystals to measure!) This plan is a list of everything that needs to be done, bought, built and considered to put a TAS/TOF on the floor in working state in January 2006 Standardisation project.
1.1	Recurring/ongoing tasks	248.18 wks	06/13/01	03/15/06	Meetings with manager NBI & NS IAT meetings BIAG meetings Keep community informed (Web page, Newsletter, bulletins)
1.2	Phase 1 - Conceptual Design	53 wks	06/22/01	06/27/02	Duration is April 2001 - April 2002 Deliverable is a proposal to BIAG for the instrument Would like 3 instruments proposed of various costings
1.2.1	Preliminary Project Management Plan & WBS	1 wk	06/22/01	06/28/01	Need a detailed paper trail of reasons for conclusions All costings and all resources to be recognised in the plan Scope definition Schedule
1.2.2	Consult User Group	2 wks	10/08/01	10/19/01	Primary task here is organising the workshop. Output is the workshop report Identify stakeholders – ongoing Deliverable is a mailing list Uni departments Chemistry & Physics x 37 AIP, RACI, CSIRO, DSTO, Old AINSE grants, AMFRP grants, ANBUG
1.2.2.1	Write report on workshop	1 wk	10/08/01	10/12/01	
1.2.2.2	Set up IAT	1 wk	10/15/01	10/19/01	
1.2.3	Preliminary design	38.2 wks	10/04/01	06/27/02	
1.2.3.1	Web & literature search	12 wks	10/04/01	12/26/01	Design details other TAS Look at websites Exhaustive search of all recent 3 axis design stuff. In particular, monochromators, shielding
1.2.3.2	Make a choice of direction on instrument	27.4 wks	10/05/01	04/15/02	
1.2.3.2.1	Preliminary analytic Optimisation calculations	5 wks	10/05/01	11/08/01	Must know how to drive the machine best for realistic design simulations. If the optimisation is wrong you cannot even tell which configuration (W, plough, longchair or C) to use let alone which components and how to design them. Furthermore you cannot do effective MC simulation unless you know the effect of each element Outcomes: Journal papers, TASMASTER spreadsheet Focussing documents
1.2.3.2.2	Internal workshops	2 wks	11/01/01	11/14/01	Internal Resolution workshop Focussing Workshop Shielding workshop Detector workshop Modelling workshop
1.2.3.2.3	Analytic beam tube and monochromator design	2 wks	11/09/01	11/22/01	Analytic Design of 3 alternate beam tubes 1) Best monochromator for existing beam tube and analytically simulate 2) Best monochromator for beam tube with end 10 cm high x 15 wide 3) Best monochromator for beam tube with end 10 cm high x 5 wide Output is a set of numbers at the sample position I(k,gamma,delta,x,y)

					MCNP simulation of flux depression - 3 cases Guesstimate on background for 3 scenarios form opinion and document it Calculations of shielding needed for these 3 monochromators Key simulations are heavy concrete & layered materials, Beamstop area, Activation of drum
1.2.3.2.4	Numerical modelling of focussing monochromator/beam tubes	16.4 wks	11/23/01	03/18/02	Mosaic required in focussed and flat modes Crystal choices Precision of mounting required
1.2.3.2.4.1	MCNP simulation of flux depression - 3 cases	4 wks	11/23/01	12/20/01	
1.2.3.2.4.2	Calculations of shielding needed for these 3 monochromators	16 wks	11/23/01	03/14/02	
1.2.3.2.4.3	Assess MCNP/CEA code comments	2 days	12/21/01	12/24/01	
1.2.3.2.4.4	Length minimisation	2 days	03/15/02	03/18/02	A central feature of a high performance instrument may be the minimisation of its length
1.2.3.2.4.5	Install McSTAS & RESTRAX	1 wk	11/23/01	11/29/01	
1.2.3.2.4.6	Verify virtual source calculations	2 wks	11/30/01	12/13/01	Calculate through to sample for 3 scenarios Detailed pictures of I(k,gamma,delta,x,y) PLUS Integrated flux and spot size
1.2.3.2.4.7	Assess CEA transport methods - Critical	2 days	12/14/01	12/17/01	
1.2.3.2.4.8	Simulate Effect of monochromator mosaic	2 days	12/18/01	12/19/01	
1.2.3.2.4.9	Simulate effect of mis-set on monochromator elements	4 wks	12/14/01	01/10/02	
1.2.3.2.5	Cost monochromator assembly	4 wks	03/19/02	04/15/02	Costing of monochromator mechanism & crystals
1.2.3.3	Secondary spectrometer conceptual design	1 wk	01/11/02	01/17/02	
1.2.3.4	Secondary spectrometer preliminary design	24 wks	01/11/02	06/27/02	
1.2.3.4.1	Dance Floor considerations	2 wks	01/11/02	01/24/02	Granite If time constrained must choose this; Stainless Steel NON MAGNETIC; Marble; Aluminium; Glass
1.2.3.4.2	Sample tables & goniometer	2 wks	01/25/02	02/07/02	Sample tables = very complex assembly; May need two if the simulations show go short. Goniometer Choice
1.2.3.4.3	Analyser & its drum	2 wks	02/08/02	02/21/02	Start with PG002 issue is physical size and focussing required RITA?
1.2.3.4.4	Detector, shielding and electronics	2 wks	02/22/02	03/07/02	
1.2.3.4.5	Airpads	2 wks	03/08/02	03/21/02	
1.2.3.4.6	Connecting arms	2 wks	03/22/02	04/04/02	
1.2.3.4.7	Drive mechanisms	2 wks	04/05/02	04/18/02	
1.2.3.4.8	Motor drives, coders and drive cards	2 wks	04/19/02	05/02/02	
1.2.3.4.9	Guide fields and flippers	1 wk	05/03/02	05/09/02	
1.2.3.4.10	PG and Be filters	1 wk	05/10/02	05/16/02	
1.2.3.4.11	Sample environment	1 wk	05/17/02	05/23/02	Displex; Cryomagnet; Cryofurnace; Furnace; Pressure cell
1.2.3.4.12	Computers	1 wk	05/24/02	05/30/02	
1.2.3.4.13	Shielding wall around instrument space	1 wk	05/31/02	06/06/02	
1.2.3.4.14	Services - water, compressed air, power, gases eg Helium	1 wk	06/07/02	06/13/02	
1.2.3.4.15	Vacuum pumps	1 wk	06/14/02	06/20/02	
1.2.3.4.16	Interlocks/security	1 wk	06/21/02	06/27/02	
1.2.3.5	Costing	2 wks	01/18/02	01/31/02	
1.2.3.6	More project management	1 wk	02/06/02	02/12/02	Preliminary Cost estimate (+/- 20%) Risk Analysis

					Develop Preliminary Acquisition Strategy - Build/Buy/Subcontract Quality management } Communications management } Human Resources management } Preliminary only Contract management }
1.2.3.7	Produce Design Proposal for BIAG	1 wk	02/13/02	02/19/02	
2	Phase 2 - Construction	193.2 wks	02/20/02	11/02/05	
2.1	Detailed design and Procurement	157.2 wks	02/20/02	02/23/05	Costing and ordering of components For each item Design, Procure, Assess, Commission
2.1.1	Sample Environment	3 mons	07/01/03	09/22/03	
2.1.2	Software development	15 mons	01/01/04	02/23/05	Low level Instrument control program Photography level Experiment level Analysis Suite Documentation
2.1.3	Monochromator	18 mons	02/20/02	07/08/03	
2.1.4	Monochromator shielding	18 mons	02/20/02	07/08/03	secondary beam shutter exit tube which is a sub assembly supermirrors on top and bottom faces? Secondary beam shutter and control mechanism inside Collimators, filters, beam monitor inside
2.1.5	Sample tables	40 days	07/01/02	08/23/02	
2.1.6	Analyser and drum	80 days	08/26/02	12/13/02	small ?
2.1.7	Detector and shielding and electronics	40 days	12/16/02	02/07/03	
2.1.8	Dancefloor & Air pads	40 days	02/10/03	04/04/03	
2.1.9	Instrument space shielding & interlocks	60 days	04/07/03	06/27/03	
2.1.10	Motors, angle encoders and controllers	80 days	06/30/03	10/17/03	
2.1.11	Guide fields and flippers	20 days	10/20/03	11/14/03	
2.1.12	Filters	20 days	11/17/03	12/12/03	
2.1.13	Supermirror trumpets	20 days	12/15/03	01/09/04	
2.1.14	Services - water, compressed air, power, gases eg Helium	60 days	01/12/04	04/02/04	
2.1.15	Vacuum pumps	2 wks	04/05/04	04/16/04	
2.1.16	Computers	20 days	04/19/04	05/14/04	Buy as late as possible - use old ones for software development
2.2	Assembly	120 days	02/24/05	08/10/05	
2.3	Off-line Commissioning	60 days	08/11/05	11/02/05	
3	Phase 3 - On-line Commissioning	40 wks	11/03/05	08/09/06	
3.1	In situ testing & adjustments	120 days	11/03/05	04/19/06	Safety features/interlocks Hardware - tolerances Motor controls - Produce a document with standard setting times and accuracy for later reference Counting chain Software testing Data links - Ideally all data links both from the instrument and the control cabin will be wireless
3.2	Calibration	40 days	04/20/06	06/14/06	Main beam; Background ; Resolution ; Tests on standard samples:
3.3	Completion Document	40 days	06/15/06	08/09/06	Deliverable is a detailed description of all instrument components, their function and their inter-relationship Instrument Driving Manual Instrument detailed description manual Data Analysis Manual
3.4	Quality Procedures, ANSTO acceptance	0 wks	01/02/06	01/02/06	start 5 yr upgrade plan

This report edited by Leo Cussen 10/10/2001